



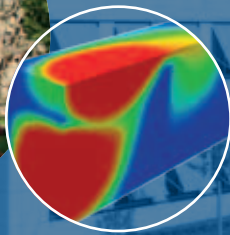
FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

NATURWISSENSCHAFTLICHE
FAKULTÄT

SIAM Conference on

Mathematical and Computational Issues in the Geosciences 2017

September 11–14, 2017 • Erlangen (Germany)



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Department
MATHEMATIK

siam
Society for Applied and Industrial Mathematics

PROGRAM



Margrave Friedrich, the founder of the University (1742)

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IMPORTANT INFORMATION

Media center

The media center is located in room Übung 3. For further information, please see page 11/12.

Poster exhibition

The poster exhibition is located in the area of the Mensa (Cafeteria/Medienraum; please follow the signs).
On Wednesday, September 13, from 18:30–20:30, the poster session with refreshments takes place within this area.
Further information regarding mounting and removal times is available on page 11.

Catering

Lunch is provided within the Mensa. Please use one of the vouchers printed on page 193 for each day and hand it to the staff of the Mensa.

Local transport ticket

Your registration includes free transportation with the local services (VGN) in the city of Erlangen (Zone 400/including Erlangen-Tennenlohe) for the time of the conference. The ticket is directly printed on the back page of your name badge.

ORGANIZATION AND IMPRINT

Venue

Friedrich-Alexander University Erlangen-Nürnberg
Cauerstrasse 11
91058 Erlangen/DE

Dates

September 10, 2017:
17:00–21:00 • Icebreaker at the Orangery Erlangen
September 11–14, 2017:
Scientific program

Conference website

www.siam-gs17.de



Organizing committee co-chairs

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University of Hamburg/DE

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Oak Ridge National Laboratory, Oak Ridge, TN/US

Rainer Helmig
University of Stuttgart/DE

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University of Erlangen-Nürnberg/DE

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Design/layout

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Print	Silber Druck oHG
Circulation	650
Editorial deadline	August 28, 2017

Ranging from science to public policy, there is a growing need for advanced modeling and simulation and their application in various fields of the geosciences. These include renewable energies (e. g. thermal, wind), underground waste disposal and cleanup of hazardous waste, earthquake prediction, weather prediction, and global climate change, along with the well-established fields of petroleum exploration and recovery. In the interdisciplinary enterprise of modeling of such processes, mathematical modeling at appropriate scales is impossible without further developments in mathematical theory, probability and statistics, numerical approximations, and large-scale computational algorithms. The conference has a long tradition in subsurface modeling

as well as atmospheric/ocean/climate and general hydrologic modeling. It aims to facilitate communication between scientists of varying backgrounds facing similar issues in different fields and perspectives and provide a forum in which advances in parts of the larger modeling picture can become known to those working in other parts. In particular, this enables an enhanced exchange between various branches of applied mathematics with the geosciences, ensures the dissemination of appropriate tools and methods, and fosters useful fundamental research in applied mathematics. These kinds of interactions are needed for meaningful progress in understanding and predicting complex physical phenomena in the geosciences.

ENDORSEMENTS

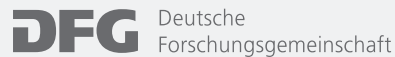
SIAM – Society for Industrial and Applied Mathematics
Philadelphia, PA/US



Springer International Publishing AG
Basel/CH



The conference organizers wish to thank the German Research Foundation (DFG) for the support of the conference.



GENERAL INFORMATION



Conference venue

All scientific sessions and on-site registration will take place on the campus of the Friedrich-Alexander University Erlangen-Nürnberg.

Address: Department of Mathematics
Cauerstrasse 11
91058 Erlangen

The icebreaker and first-day registration will take place at the Orangery in the Schlossgarten at the center of Erlangen:

Address: Orangery
Wasserturmstrasse 3
91054 Erlangen



Check-in

The check-in will be open during the following hours:

At the Orangery:
Sunday, September 10
17:00–21:00

In the foyer of the conference venue:
Monday, September 11
07:30–18:30

Tuesday, September 12
08:00–18:30

Wednesday, September 13
08:00–18:30

Thursday, September 14
08:00–18:00



Registration fees

Early bird (until July 21)

SIAM GS member	320 EUR
SIAM member	330 EUR
Non-member	450 EUR
Non-member/speaker/organizer	390 EUR
Student*	130 EUR

One-day 230 EUR

Late registration (until September 8)

SIAM GS member	400 EUR
SIAM member	410 EUR
Non-member	530 EUR
Non-member/speaker/organizer	470 EUR
Student*	150 EUR

One-day 260 EUR

On-site registration (from September 9)

SIAM GS member	450 EUR
SIAM member	460 EUR
Non-member	580 EUR
Non-member/speaker/organizer	520 EUR
Student*	170 EUR

One-day 300 EUR

* Please provide a confirmation of your status.

The registration fee includes:

- Admission to all scientific sessions and access to the industrial exhibition
- Icebreaker and poster sessions
- Conference materials (conference bag, final program with abstract publication, name badge, etc.)
- Daily coffee breaks
- Daily lunches
- Public transportation ticket



Name badge

Please wear your name badge during all conference events, including the Icebreaker.

Admission to scientific sessions is restricted to participants wearing their badge. Participants will receive their name badge when collecting their conference documents at the check-in.

Please note: Participants who misplace their badge need to pay a fee of 25 EUR for a new one.



Local transportation ticket

Your registration includes free transportation with the local services (VGN) in the city of Erlangen (Zone 400) for the time of the conference.

Note that this includes also Erlangen-Tennenlohe, if your hotel is located there.



General terms and conditions

Please find our general terms and conditions at www.siam-gs17.de.



Corporate members and affiliates

SIAM corporate members provide their employees with knowledge about, access to, and developments in the applied mathematics and computational science community through their membership benefits. Corporate membership is more than just a bundle of tangible products and services; it is an expression of support for SIAM and its programs. SIAM is pleased to acknowledge its corporate members. In recognition of their support, non-member attendees, who are employed by the following organizations are entitled to the SIAM member registration rate.

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 IDA Center for Communications Research, La Jolla
 IDA Center for Communications Research, Princeton
 Institute for Defense Analyses, Center for Computing Sciences
 Lawrence Berkeley National Laboratory
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 Lockheed Martin
 Los Alamos National Laboratory
 Max-Planck-Institute for Dynamics of Complex Technical Systems
 Mentor Graphics
 National Institute of Standards and Technology (NIST)
 National Security Agency (DIRNSA)
 Naval PostGrad
 Oak Ridge National Laboratory, managed by UT-Battelle for the Department of Energy
 Sandia National Laboratories
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 United States Department of Energy
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 US Naval Research Labs

List current August 2017

Leading the applied mathematics community

SIAM members save up to 130 EUR on full registration for the 2017 SIAM Conference on Mathematical and Computational Issues in the Geosciences! Join your peers in supporting the premier professional society for applied mathematicians and computational scientists. SIAM members receive subscriptions to SIAM Review, SIAM News and SIAM Unwrapped, and enjoy substantial discounts on SIAM books, journal subscriptions, and conference registrations. If you are not a SIAM member and paid the non-member or non-member/speaker/organizer rate to attend the conference, you can apply the difference between what you paid and what a member would have paid (130 EUR for a non-member and 60 EUR for a non-member/speaker/organizer) towards a SIAM membership. Contact SIAM Customer Service for details. If you are a SIAM member, it only costs 10 EUR to join the SIAM Activity Group on Geosciences (SIAG/GS). As a SIAG/GS member, you are eligible for an additional 10 EUR discount on this conference, so if you paid the SIAM member rate to attend the conference, you might be eligible for a free SIAG/GS membership. Free student memberships are available to students who attend an institution that is an academic member of SIAM, are members of student chapters of SIAM, or are nominated by a regular member of SIAM.

Go to www.siam.org/joinsiam to join online or download an application form, or contact the SIAM customer service:

Telephone: +1 215 382 9800 (worldwide);
 800 447 7426 (US and Canada only)
 Fax: +1 215 386 7999
 E-mail: membership@siam.org



Margrave Friedrich, the founder of the University (1742)
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GENERAL INFORMATION



Internet access

Wi-Fi is available for free in the conference area. Access is possible with eduroam, or a temporary login which can be provided at the check-in. You also have the possibility to use a desktop computer in PC-Pool 1 (room 00.230, ground floor). Please ask the staff at the check-in for the login data.



Certificate of attendance

Certificates of attendance are available at the check-in.



Evaluation

Please take a few moments to fill out the evaluation form to help us refine and improve our program. You can hand in your evaluation form at the check-in.



Cloakroom

The coat and luggage room (room Übung 1) at the conference is free and not guarded.



SIAG/GS business meeting

The business meeting is held on Thursday, September 14, at 12:00 in room H13. It is open to SIAG/GS members.



Program

For current detailed information regarding the scientific program please have a look at the program planner via programm.conventus.de/siam2017. Compose your individual program and review it at any time on your way.



Publication of abstracts

All abstracts of oral and poster presentations are published within the final program (from p. 66).



Need room for discussions or studies?

If you are looking for rooms for discussions and meetings during SIAM GS 2017, we can offer you several facilities in the Department of Mathematics. You can book those rooms (for up to 20 people) for one or two hours. Please ask at the check-in. Furthermore you have access to the library of mathematics and computer science in Cauerstrasse 11 (ground floor), or to the library of the technical faculty (Erwin-Rommel-Str. 60), in the same complex of buildings.



Social media

SIAM is promoting the use of social media, such as Facebook and Twitter, in order to enhance scientific discussion at its meetings and enable attendees to connect with each other prior to, during and after conferences. If you are tweeting about a conference, please use the designated hashtag to enable other attendees to keep up with the Twitter conversation and to allow better archiving of our conference discussions. The hashtag for this meeting is #SIAMGS17.



View over Erlangen
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We wish you a pleasant journey.

¹ You can buy your ticket by phone: just contact our service number +49 (0)1806 - 31 11 53 and use the keyword "CONVENTUS". Make sure you have your credit card to hand for payment (please note that Deutsche Bahn AG levies a surcharge for all credit card payments in accordance with the conditions of carriage for persons travelling with Deutsche Bahn AG companies ("BB Personenverkehr"). The service hotline is open Mondays to Friday from 8am to 8pm. There is a charge of EUR 0.20 per call from a German landline and a maximum of EUR 0.60 per call from mobile networks.

**Public transportation from the main station to the venue**

From Erlangen main station you can choose the following buses. Your conference badge serves as a bus ticket in Erlangen, furthermore tickets are sold by the bus driver.

Bus 20 or 287: Walk 300 m to Arcaden bus stop (or take one of the many buses in southern direction for one stop). At Arcaden take the bus 20 with destination Nürnberg / Am Wegfeld (9 stops) or the bus 287 with destination Erlangen Sealdussiedlung (12 stops). Leave at bus stop Erlangen Technische Fakultät (see campus map).

Bus 30: At Erlangen Hauptbahnhof take the bus 30 with destination Nürnberg and leave at bus stop Erlangen-Süd (7 stops). From there it is a 10 min. walk to the venue (see campus map), signs will lead you the way.

Note that the icebreaker on Sunday takes place at the Orangery in the Schloßgarten, which is a 5 minutes walk away from the main station.

More information on public transport at Verkehrsverbund Nürnberg-Erlangen: www.vgn.de/en

Public transport

You can also access public transport information using the smartphone application of the VGN <http://www.vgn.de/en/timetable/apps>

**Local transportation ticket**

Your registration includes free transportation with the local services (VGN) in the city of Erlangen (Zone 400) for the time of the conference.

Note that this includes also Erlangen-Tennenlohe, if your hotel is located there.

**Travel by car**

Navigation address:

Friedrich-Alexander-Universität Erlangen-Nürnberg
Cauerstrasse 11
91058 Erlangen, Germany

Erlangen is located at two federal motorways: The A73 from Nürnberg to Erfurt (exit Erlangen-Bruck) and the A3 from Frankfurt to Passau (exit Tennenlohe). The A3 and the A9 Munich to Berlin intersect in southeast Nuremberg.

Both motorways also lead further south to the A6 Stuttgart – Prague.

Simply follow the signs to Erlangen. Take the exit "Universität Südgelände" and turn left to Erlangen or Südgelände (Kurt-Schumacher-Str.). Follow the road until you can turn left into Cauerstrasse. You can see the Felix Klein building to the right.

**Parking**

Free parking is available at a car park at Cauerstrasse, right around the corner of the venue.

TRAVEL INFORMATION



Arrival by plane

Nürnberg Airport (20km) is the best destination to choose if you want to go to Erlangen. From Nürnberg airport you can take the following busses:

- Bus 30: Leave the arrival hall and take the bus 30 with destination Erlangen Arcaden. Leave at bus stop Erlangen/Süd. Use the stairs to reach the small bridge (Preussensteg). Turn right; after a few meters you will arrive at the T-junction Egerlandstrasse/Haberstrasse (see campus map).
- Bus 33: Leave the arrival hall and take the bus 33 with destination Fürth Rathaus (tickets are sold by the bus driver). At the bus stop Am Wegfeld take the following bus line:
- Bus 20: At bus stop Am Wegfeld take the bus 20 with destination Erlangen Arcaden. Leave at bus stop Technische Fakultät. You arrive at the junction Erwin-Rommel Strasse/Egerlandstrasse (see campus map).

Arriving at Frankfurt Airport (250km):

- Intercity bus: You can either choose Frankfurt main station or Frankfurt Airport. Please check this website for a detailed schedule and prices.
- By train: Please refer to our train ticket information above (Train – Conventus event ticket).

Arriving in Munich Airport (180km):

- Intercity bus: Please check the following website for detailed schedules and prices: FlixBus
- By train: Please refer to our train ticket information above (Train – Conventus event ticket).

More information on public transport at Verkehrsverbund Nürnberg-Erlangen: www.vgn.de/en

USEFUL COUNTRY INFORMATION

Citizens of the EU:

EU nationals do not require a visa to enter the Federal Republic of Germany.

Non-EU citizens:

All Non-EU citizens require a visa. However, a visa is not required for visits of up to 90 days in an 180-day period for nationals of those countries for which the European Community has abolished the visa requirement.

You may apply for short stay visas (Schengen Visas) at diplomatic missions of the German Federal Foreign Office.

Please also visit the homepage of "Auswärtiges Amt" to find a detailed table of all countries requiring a visa and also more information about visa regulations, as well as a list of German diplomatic missions around the world.

Weather

Please check www.weather.com for up-to-date weather forecasts in the city that you are travelling to.

Currency

As in most countries of the European Union, the official currency is the Euro (€).

Please note that there are no general bank hours in Germany. Most banks are open in the morning hours and just a few hours in the afternoon or early evening. Major credit cards are accepted at most cash points (ATM machines), stores, restaurants and hotels.

Language

English is spoken by the staff of most hotels, restaurants and shops.

Telephone and internet

Germany's international pre-dial is +49 (0049). Public places like airports, universities, libraries, restaurants and cafés may offer "free"-WiFi Hotspots.

Electricity

The electrical power supply in Germany is 220 V, 50 Hz, AC.

Official plugs in Germany are:

"Schuko-stecker" (round) Type F/ CEE 7/4

"Eurostecker" (flat) Type C/ CEE 7/16

Time

Germany's standard time zone is UTC/GMT +1 hour.

Health

All visitors are advised to have valid international insurance before coming to Germany. Citizens of the EU are insured with their EHIC (European Health Insurance Card).

Standard audio/visual set-up in meeting rooms

The presentation should be prepared as PDF, MS Office PowerPoint for Windows or key for Macintosh DVD in format 4:3.

A presentation notebook with a PDF reader and MS Office PowerPoint 2016 will be provided. The use of personal notebooks is possible upon agreement. However, it may interrupt the flow of the program in the lecture hall. Please provide an adapter for VGA if necessary. To guarantee a smoothly running program please upload your presentation in time – at least 2 hours before your presentation is due to start.

Should you wish to use non-digital equipment, please contact us at siam2017@conventus.de.



Presentation upload

The speakers' preview area for uploading your presentation is located in room Übung 3.

For submission, please use a USB flash drive, CD or DVD disc that is not protected by any software. Professional staff and equipment will be available for you to arrange and preview your presentation.



Time allocation

Please prepare your presentation for the allotted amount of time. Chairs and moderators may interrupt should you overrun your time limit. Allotted time is assigned as follows (speaking + discussion time):

- | | |
|-----------------------|----------------|
| 1. Oral presentations | 15 + 5 minutes |
| 2. Poster quick fire | 3 minutes |



Poster session

The size of your poster has to be in accordance with DIN portrait format A0 (84,1 cm width x 118,9 cm height) and should not be laminated. Mounting materials will be provided at the poster board onsite. All poster boards will be labelled with a poster number. The poster exhibition will be located in the area of the Mensa (please follow the signs). Please note that all posters should be mounted by Monday, September 11 until 18:30 and be removed, at the latest, by Wednesday, September 13 until 21:00. Any poster remaining after the designated removal time will be discarded.



Important notice to poster presenters

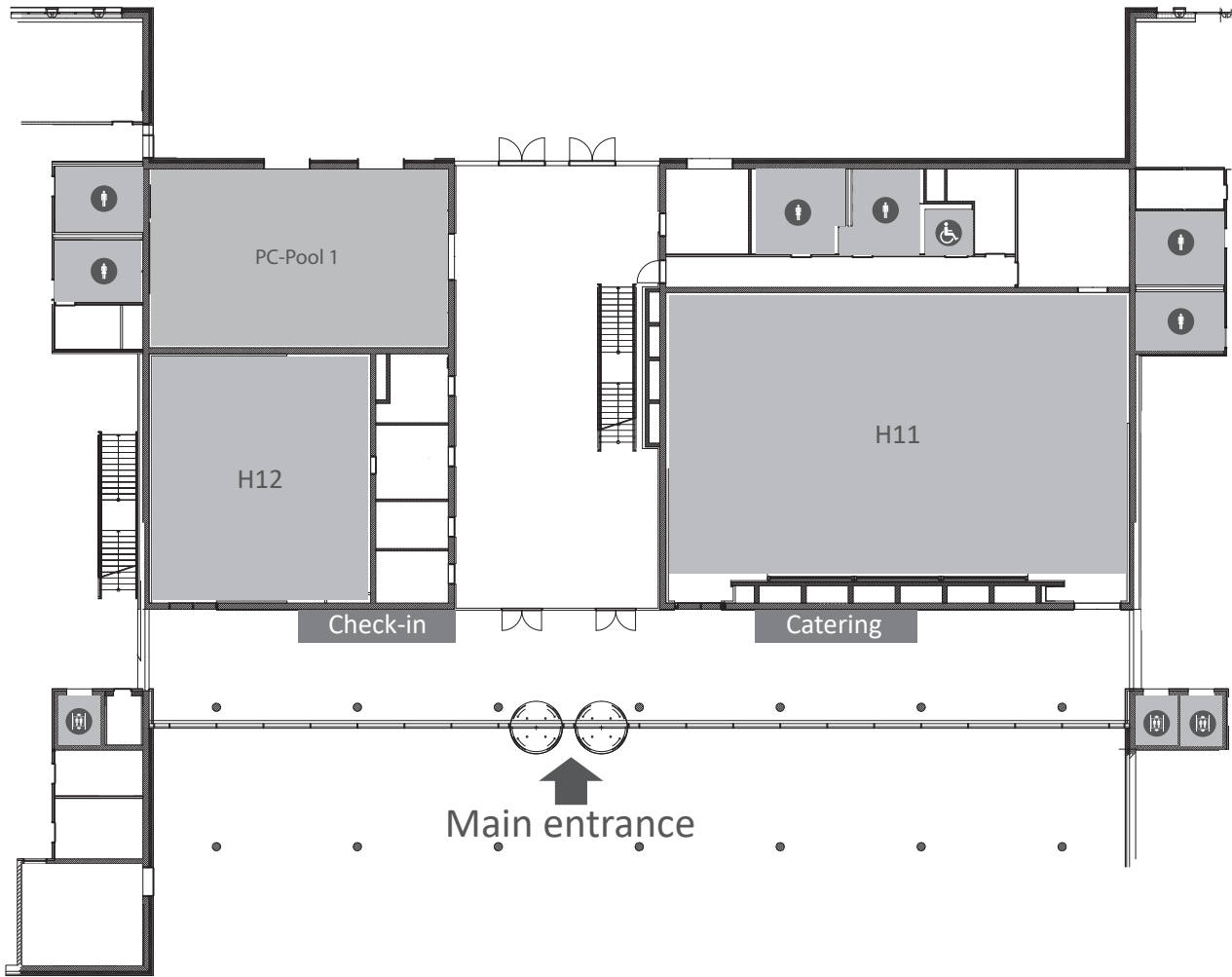
The poster session will take place on Wednesday, September 13, between 18:30–20:30. Poster presenters are required to be present at their poster while this time to present their poster and answer questions. Additionally poster quick fires are planned within minisymposia. Please have at most 3 slides prepared to present your topic within 3 minutes.

Abbreviations

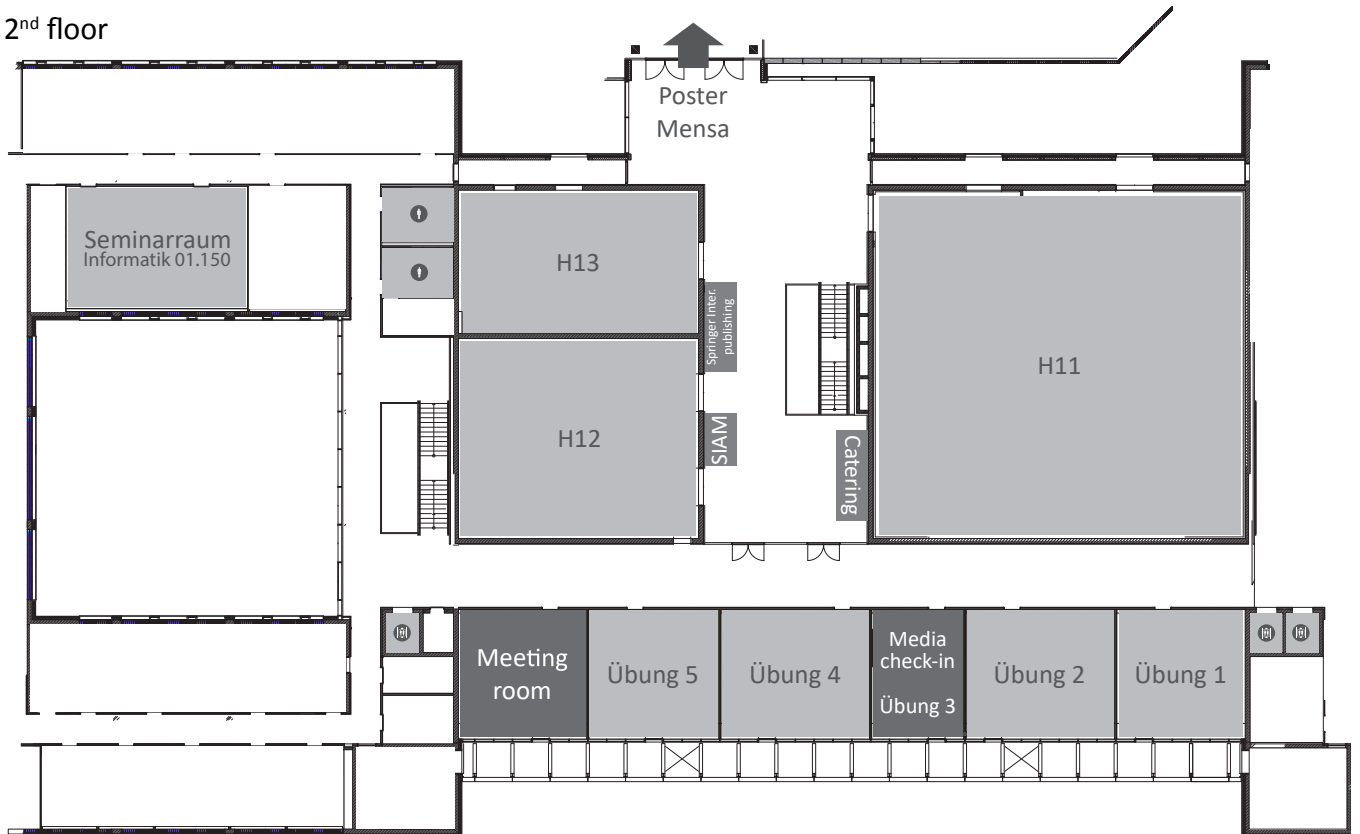
- | | |
|----|---------------------|
| PS | Plenary session |
| MS | Minisymposium |
| QF | Quick fire |
| PL | Prize lecture |
| O | Oral presentation |
| P | Poster presentation |

ROOM OVERVIEW

1st floor



2nd floor



State at printing



Sunday, September 10 • Orangerie Erlangen

Orangerie
17:00–21:00
Icebreaker
p. 6

Monday, September 11 • Department Mathematik

H11	H12	H13	Seminarraum Informatik 01.150	Übung 2	Übung 4	Übung 5
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08:15–08:35
Opening and Welcome
p. 20

08:35–09:35
PS1
Scalable nonlinear and linear solvers for multiphase flow in heterogeneous porous media
p. 20

10:00–12:00	10:00–12:00	10:00–11:20	10:00–12:00	10:00–12:00	10:00–12:00	10:00–12:00
MS1 Direct numerical simulation of pore-scale multiphase flow and transport p. 20	MS2 Development and application of numerical algorithms for lake, coastal, ocean flows p. 21	MS3 Hamiltonian dynamics of climate and forecast p. 21 11:20–12:00 QF1 Poster quick fire session 1 p. 21	MS4 CO ₂ -Hydrocarbon interactions for CO ₂ storagen with EOR/EGR p. 22	MS5 Ensemble-based data assimilation and optimization in geosciences Part 1 p. 22	MS6 Computational methods for density driven flow in heterogeneous and fractured porous media p. 23	MS7 Advanced discretization schemes for subsurface flow and transport p. 23

13:00–14:00
PS2
New frontiers in earth-system modeling p. 24

14:10–15:30	14:10–16:10	14:10–16:10	14:10–15:50	14:10–16:10	14:10–16:50	14:10–16:10
MS8 Multiscale modeling for subsurface processes Part 1 p. 24 15:30–16:10 QF2 Poster quick fire session 2 p. 24	MS9 Mathematical and numerical advances in shallow water modeling Part 1 p. 25	MS10 Advances in numerical methods for weather and climate modeling Part 1 p. 25	MS11 Effective models for porous media containing thin structures p. 26 15:50–16:10 QF3 Poster quick fire session 3 p. 26	MS12 Ensemble-based data assimilation and optimization in geosciences Part 2 p. 26	MS13 The mathematics and computing of seismic, MT and CSEM data inversion p. 27	MS14 Numerical methods for the characterization of geothermal reservoirs Part 1 p. 27

16:30–18:30	16:30–18:30	16:30–17:50	16:30–18:30	16:30–18:30	16:30–18:30	16:30–18:30
MS15 Multiscale modeling for subsurface processes Part 2 p. 28	MS16 Mathematical and numerical advances in shallow water modeling Part 2 p. 28	MS17 Advances in numerical methods for weather and climate modeling Part 2 p. 29 17:50–18:50 MS18 Advances in numerical methods for weather and climate modeling Part 3 p. 29	MS19 Limit processes in porous media p. 29	MS20 Machine learning applications in subsurface reservoir modeling p. 30	MS21 Modeling and simulation of melt in the mantle Part 1 p. 30	MS22 Numerical methods for the characterization of geothermal reservoirs Part 2 p. 31

H11	H12	H13	Seminarraum Informatik 01.150	Übung 2	Übung 4	Übung 5
08:30–09:30						
PS3 Discontinuous skeletal methods for computational geosciences p. 32						
10:00–11:20 MS23 Modeling and simulation of melt in the mantle Part 2 p. 32 11:20–12:00 QF4 Poster quick fire session 4 p. 32	10:00–12:00 MS24 HPC advances and trends in simulation tools for flow and transport in geosciences Part 1 p. 33	10:00–11:20 MS25 Numerical methods towards next generation ice sheet modeling Part 1 p. 33	10:00–12:00 MS26 Recent advances in computational poromechanics p. 34	10:00–12:00 MS27 Ensemble-based data assimilation and optimization in geosciences Part 3 p. 34	10:00–12:00 MS28 Multiscale modeling for subsurface processes Part 3 p. 35	10:00–12:00 MS29 Advanced numerical methods in subsurface flow simulations in discrete fracture networks Part 1 p. 35
13:00–14:00						
PL1 "How warm is it getting?" and other tales in uncertainty p. 36						
14:10–16:10 MS30 Compositional flow modeling and reactive transport in porous media Part 1 p. 36	14:10–16:10 MS31 HPC advances and trends in simulation tools for flow and transport in Geosciences Part 2 p. 37	14:10–16:10 MS32 Numerical methods towards next generation ice sheet modeling Part 2 p. 37	14:10–16:10 MS33 Krylov-based deflation methods in flow for porous media p. 38	14:10–16:10 MS34 Understanding the impact of heterogeneity on CO ₂ plume spreading and immobilisation p. 38	14:10–16:10 MS35 Implementation aspects of reusable and efficient software and algorithms Part 1 p. 39	14:10–16:10 MS36 Advanced numerical methods in subsurface flow simulations in discrete fracture networks Part 2 p. 39
16:30–18:30 MS37 Compositional flow modeling and reactive transport in porous media Part 2 p. 40	16:30–18:30 MS38 Geophysical inversion and imaging p. 40	16:30–18:30 MS39 Dynamics and data in stochastic systems, far from equilibrium p. 41	16:30–18:30 MS40 Uncertainty quantification for nonlinear transport problems in porous media p. 41	16:30–18:30 MS41 Extended image volumes p. 42	16:30–18:30 MS42 Implementation aspects of reusable and efficient software and algorithms Part 2 p. 42	16:30–18:30 MS43 Simulation of complex multiphase flows in porous media with the Lattice Boltzmann method p. 43

- Abbreviations: PS | Plenary session
 MS | Minisymposium
 QF | Quick fire
 PL | Prize lecture
 O | Oral presentation
 P | Poster presentation

PROGRAM OVERVIEW • WEDNESDAY, SEPTEMBER 13

H11	H12	H13	Seminarraum Informatik 01.150	Übung 2	Übung 4	Übung 5
08:30–09:30						
PS4 Methane hydrate modeling, analysis, and simulation: Coupled systems and scales p. 44						
10:00–12:00	10:00–12:00	10:00–11:20	10:00–12:00	10:00–12:00	10:00–12:00	10:00–11:20
MS44 Advances in nonlinear methods for flow and transport modeling p. 44	MS45 Multi-resolution three-dimensional modeling of coastal, regional, and deep ocean p. 45	MS46 Numerical methods towards next generation ice sheet modeling Part 3 p. 45	MS47 Advances in uncertainty quantification methods for hydrological applications Part 1 p. 46	MS48 Flow, reactive transport and deformation in fractured porous media p. 46	MS49 Advances and applications of periodic and stochastic homogenisation Part 1 p. 47	MS50 Modeling approaches for flow and transport in discrete fracture networks p. 47 11:20–12:00 QF5 Poster quick fire session 5 p. 48
13:00–14:00						
PS5 High resolution atmospheric turbulence simulations for applied problems p. 48						
14:10–15:30	14:10–16:10	14:10–16:10	14:10–16:10	14:10–16:10	14:10–16:10	14:10–16:10
MS51 Recent advances in numerical flow and transport in porous media: A mini symposium in honor of the late Jim Douglas, Jr. Part 1 p. 49	MS52 Multi-resolution three-dimensional modeling of coastal, regional, and deep ocean Part 2 p. 49	MS53 Mimetic discretizations in geoscience and advances in geologic carbon sequestration modeling Part 1 p. 50	MS54 Advances in uncertainty quantification methods for hydrological applications Part 2 p. 51	MS55 Data assimilation in terrestrial hydrosystems Part 1 p. 51	MS56 Advances and applications of periodic and stochastic homogenisation Part 2 p. 52	MS57 Modeling approaches for flow and transport in discrete fracture networks Part 2 p. 52
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QF6 Poster quick fire session 6 p. 49	QF7 Poster quick fire session 7 p. 50					
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MS58 Recent advances in numerical flow and transport in porous media: A mini symposium in honor of the late Jim Douglas, Jr. Part 2 p. 52	MS59 Standard and nonstandard models and numerical methods for complex porous media flows with applications p. 53	MS60 Mimetic discretization methods in geoscience and advances in geologic carbon sequestration modeling Part 2 p. 53	MS61 Physics-based rupture and tsunami simulation Part 2 p. 54	MS62 Data assimilation in terrestrial hydrosystems Part 2 p. 54	MS63 Computational methods for flow in subsurface porous media Part 1 p. 55	MS64 Advanced numerical methods in subsurface flow simulations in discrete fracture networks Part 3 p. 55
18:30–20:30						
Poster session Cafeteria/Medienraum please follow the signs						

H11	H12	H13	Seminarraum Informatik 01.150	Übung 2	Übung 4	Übung 5
08:30–09:30						
PS6 Bridging scales in weather and climate models with adaptive mesh refinement techniques p. 56						
10:00–12:00 MS65 Coupled geomechanics and flow systems in porous media Part 1 p. 56	10:00–12:00 MS66 Recent advances on numerical methods for shallow water models Part 1 p. 57	10:00–11:20 MS67 Uncertainty quantification and data assimilation: Computational challenges in large-scale geoscience models Part 1 p. 57	10:00–12:00 MS68 Mathematical and computational advances in geoelectromagnetic forward and inverse modelling p. 58	10:00–12:00 MS69 Advances and applications of periodic and stochastic homogenisation Part 3 p. 58	10:00–12:00 MS70 Computational methods for flow in subsurface porous media Part 2 p. 59	10:00–12:00 MS71 Level-set methods for inverse problems in the geosciences – Seismic inversion p. 59
12:00–12:45 SIAM AG Geosciences business meeting p. 60						
12:45–13:00 Closing remarks p. 60						
13:00–14:00 PL2 Coupled problems in porous media with a focus on Biot p. 60						
14:10–16:10 MS72 Coupled geomechanics and flow systems in porous media Part 2 p. 60	14:10–16:10 MS73 Recent advances on numerical methods for shallow water models Part 2 p. 61	14:10–16:10 MS74 Uncertainty quantification and data assimilation: Computational challenges in large-scale geoscience models Part 2 p. 61	14:10–16:10 MS75 Physics-based rupture and tsunami simulation Part 2 p. 62	14:10–16:10 MS76 Quality assurance and sustainable development of simulation software in the geosciences Part 1 p. 62	14:10–16:10 MS77 Computational methods for flow in subsurface porous media Part 3 p. 63	
16:30–18:30 MS78 Mathematical and computational advances in geoelectromagnetic forward and inverse modelling Part 2 p. 63	16:30–18:30 MS79 Multi-resolution three-dimensional modeling of coastal, regional, and deep ocean Part 3 p. 64	16:30–18:30 MS80 Increasing the physical realism of models and simulations involving fractured rocks p. 64		16:30–18:30 MS81 Quality assurance and sustainable development of simulation software in the geosciences Part 2 p. 65		

- Abbreviations: PS | Plenary session
MS | Minisymposium
QF | Quick fire
PL | Prize lecture
O | Oral presentation
P | Poster presentation

INVITED PLENARY SPEAKERS AND PRIZE PRESENTATIONS

All invited plenary and prize presentations take place in lecture room H11.

Monday, September 11

08:30–09:30

PS1 • Scalable nonlinear and linear solvers for multiphase flow in heterogeneous porous media

Hamdi Tchelepi, Stanford University, USA

13:00–14:00

PS2 • New frontiers in earth-system modeling

Nils Wedi, ECMWF, Great Britain

Tuesday, September 12

08:30–09:30

PS3 • Discontinuous skeletal methods for computational geosciences

Alexandre Ern, ParisTech, France

13:00–14:00

PL1 • “How warm is it getting?” and other tales in uncertainty quantification

Juan M. Restrepo, Oregon State University, USA

Wednesday, September 13

08:30–09:30

PS4 • Methane hydrate modeling, analysis, and simulation: Coupled systems and scales

Malgorzata Peszynska, Oregon State University, USA

13:00–14:00

PS5 • High resolution atmospheric turbulence simulations for applied problems

Siegfried Raasch, University of Hanover, Germany

Thursday, September 14

08:30–09:30

PS6 • Bridging scales in weather and climate models with adaptive mesh refinement techniques

Christiane Jablonowski, University of Michigan, USA

13:00–14:00

PL2 • Coupled problems in porous media with a focus on Biot

Kundan Kumar, University of Bergen, Norway

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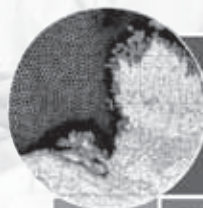
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Opening and welcome

08:15–08:35 • Room: H11

Günter Leugering
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 Erlangen/DE

James Crowley
 Executive director SIAM
 Philadelphia, PA/US

Peter Knabner
 Organizing committee co-chair
 Friedrich-Alexander University of Erlangen-Nürnberg
 Erlangen/DE

PS1 | Invited plenary
Scalable nonlinear and linear solvers for multiphase flow in heterogeneous porous media

08:35–09:35 • Room: H11

Chair: Hector Klie (Houston, TX/US)
Speaker: Hamdi A. Tchelepi (Stanford, CA/US)

Numerical reservoir simulation of flow and transport processes in subsurface formations is an integral part of managing underground hydrocarbon and water resources with application areas that include oil/gas recovery, management of water resources, and subsurface CO₂ sequestration. We discuss the challenges associated with Reservoir Simulation of multiphase flow in large-scale heterogeneous formations. The focus is on developing scalable (i.e., efficient for heterogeneous, large-scale problems) linear and nonlinear solvers. The discussion is split into two parts: (1) Algebraic Multi-Scale (AMS) linear solvers and (2) trust-region nonlinear solvers. AMS linear solvers are designed to deal with the multiscale distributions of the properties of natural geologic formations (e.g., permeability/conductivity). The complex multiscale spatial variations in the permeability field lead to complex multiscale fluid dynamics (e.g., pressure and velocity). A brief description of two-level AMS formulations for the pressure field is given. Then, we discuss the development of massively parallel AMS linear solvers on multi-core and GPU architectures. We demonstrate that significant progress has been made in our collective ability to capture the impact of multiscale spatial variations in formation properties on the pressure and velocity fields in large subsurface systems.

We then discuss the multiscale nature of the time scales associated with the nonlinear fluid transport processes and the strong nonlinear coupling between the governing conservation equations and constitutive relations. Specifically, we describe a nonlinear solver framework based on constructing trust-regions of the fractional-flow (phase flux) function. We demonstrate that the nonlinearity of the transport (saturation) equations can be resolved efficiently through analysis of the discrete/numerical flux functions. The theory is elaborated for immiscible two-phase fluid flow in highly heterogeneous formations. The robustness and computational efficiency of the flux-based trust-region nonlinear solver are demonstrated

using challenging problems in the presence of counter-current flow due to strong buoyancy effects. Combining multiscale linear solvers with trust-region nonlinear solvers has made it possible to simulate multiphase flow and transport processes in problems of growing size (resolution) and complexity. Nevertheless, enormous challenges lie ahead, and we conclude with a perspective on these important and exciting computational geoscience problems.

MS1
Direct numerical simulation of pore-scale multiphase flow and transport

10:00–12:00 • Room: H11

Chairs: Florian Frank, Faruk O. Alpak
 Beatrice Riviere (Houston, TX/US)

This minisymposium addresses recent advances in modeling and direct numerical simulation of pore-scale multiphase flow and transport processes including all aspects of mass, momentum, and energy exchange. Of particular interest are the study of two or more phases and of mixtures with two or more components in compressible/incompressible regimes on spatial scales that resolve or approximate the phase-interfaces. Applications include but are not limited to enhanced oil recovery (EOR), CO₂ sequestration, and groundwater remediation. Talks may cover modeling aspects of multiphase systems including the coupling to further physical models (e.g., geomechanics and chemical reactions), numerical methods, large scale computing, and physical insights gained from laboratory and numerical experiments.

- 10:00 **A DG method for pore scale flows**
 O1 *Beatrice Riviere (Houston, TX/US)*
- 10:20 **Modeling two-phase flow at the pore-level within the volume-of-fluid method framework**
 O2 *Mosayeb Shams, Ali Q. Raeini, Branko Bijeljic, Martin Blunt (London/GB)*
- 10:40 **Micro-continuum approach for pore-scale simulation of subsurface processes**
 O3 *Cyprien Soulaine, Hamdi A. Tchelepi (Stanford, CA/US)*
- 11:00 **Pore-scale characteristics of wetting phase entrapment during drainage/imbibition: SPH-based direct numerical simulations**
 O4 *Holger Steeb, Rakulan Sivanesapillai (Stuttgart/DE)*
- 11:20 **Approaches to modeling flow and transport at porescale in changing geometries**
 O5 *Timothy B. Costa, Malgorzata Peszynska, Joe Umhoefer (Corvallis, OR/US)*
- 11:40 **Modeling and simulation of colloidal-like particles transport in an oil-water flow in porous media**
 O6 *Max Endo Kokubun, Florin A. Radu, Eirik Keilegavlen, Kristine Spildo (Bergen/NO)*

MS2

Development and application of numerical algorithms for lake, coastal, ocean flows

10:00–12:00 • Room: H12

Chairs: *Jose Castillo (San Diego, CA/US)*
Hansong Tang (New York, NY/US)

There is an urgent need to develop new algorithms for simulations of emerging coastal ocean flow problems. These problems are multiscale and multiphysics in general, and their simulations with desired accuracy are beyond the capabilities of existing methods and software packages. This minisymposium reports recent development in numerical of such problems including high-fidelity simulation of multiscale flows, storm surge and floods, water quality, and ... The session welcomes researchers from related areas and will provide a platform for them to exchange ideas and discuss about encountered difficulties, possible approaches, and future directions.

10:00 Validation of the General Curvilinear Coastal
07 Ocean Model (GCCOM) for the case of 3D
non-hydrostatic stratified flow

Mariangel Garcia (San Diego, CA/US)
Paul Choboter, Ryan Walter
(San Luis Obispo, CA/US)
Jose Castillo (San Diego, CA/US)

10:20 Towards high-fidelity simulation of small-scale
08 coastal ocean flows by model coupling
approach

Hansong Tang, Ke Qu
Anil Agrawal (New York, NY/US)

10:40 A new D-Flow FM (Flexible Mesh) type of
09 shallow water model for Lake Marken for
forecasting and impact assessments of
different societal aspects.

Menno Genseberger (Delft/NL)

11:00 The simulation of the hydrodynamics of the
010 Upper Gulf of California

Isabel Ramirez, Rafael Ramirez, Rene Navarro Modesto
Ortiz, Nidia Angulo
Victor Godinez (Ensenada/MX)

11:20 Boundary layers for the 3D primitive equations
011 in a cube

Chang-Yeol Jung (Ulsan/KR)

11:40 Modeling and stochastic parametrization of
012 wave breaking data

Juan Restrepo, Jorge Ramirez, Luc Deike
Ken Melville (Corvallis, OR/US)

MS3

Hamiltonian dynamics of climate and forecast models

10:00–11:20 • Room: H13

Chairs: *Andrew Steyer (Albuquerque, NM/US)*
Werner Bauer (London/GB)

Conservation of energy plays a fundamental role in the dynamics of geophysical models for the Earth's ocean and atmosphere. For many climate and forecast models the energy conservation law is embodied in the symmetries of the Poisson bracket of the Hamiltonian functional and these models can be systematically derived in terms of variational principles. This mini-symposium brings together researchers focused on developing computational methods for preserving Hamiltonian dynamics in climate and forecast models.

10:00 A nonhydrostatic model for atmospheric
013 motion in ACME-HOMME

Andrew Steyer
Mark Taylor (Albuquerque, NM/US)

10:20 Variational integrators in geophysical fluid
014 dynamics

François Gay-Balmaz (Paris/FR)

10:40 Dynamico-FE – A structure-preserving
015 hydrostatic dynamical core based on
Hamiltonian methods

Christopher Eldred, Thomas Dubos
Evangelos Kritsikis (Paris/FR)

11:00 Structure-preserving variational integrators for
016 anelastic, pseudo-incompressible, and
shallow-water flows

Werner Bauer (London/GB)
François Gay-Balmaz (Paris/FR)

QF1

Poster quick fire session 1

11:20–12:00 • Room: H13

Chairs: *Andrew Steyer (Albuquerque, NM/US)*
Werner Bauer (London/GB)

11:20 Detecting break points in the Arctic Sea Ice:
P1 Decline and linked atmospheric moisture
sources

Luis Gimeno-Sotelo, Marta Vázquez
Raquel Nieto (Ourense/ES)

11:24 Probability distributions of summer Arctic Sea
P2 extension variability driven by the atmospheric
circulation and moisture transport

Luis Gimeno-Sotelo, Marta Vázquez, Raquel Nieto
(Ourense/ES), Rosemeri Da Rocha (São Paulo/BR)
Luis Gimeno (Ourense/ES)

11:28 P3	Impact of the North Atlantic oscillation on the synoptic processes in Europe – Continuous wavelets transform approach <i>Valeriy Khokhlov</i> <i>Larisa Nedostrelava (Odessa/UA)</i>	10:00 O17	Stability analysis of non-monotonic density driven convective mixing <i>Maria Elenius, Sarah Gasda (Bergen/NO)</i>
11:32 P4	Assimilation of cloud-affected radiances in deep convection – A case study <i>Josef Schröttle (Munich/DE)</i> <i>Axel Hutt (Offenbach/DE), Leonhard Scheck Martin Weissmann (Munich/DE)</i>	10:20 O18	New thermodynamic models for CO ₂ hydrocarbon mixtures <i>Ivar Aavatsmark (Bergen/NO)</i>
11:36 P5	Large-eddy simulations of a wind turbine wake above a forest <i>Josef Schröttle (Munich/DE)</i> <i>Zbigniew Piotrowski (Warsaw/PL)</i>	10:40 O19	Parametrization in physical space for modeling of challenging CO ₂ -EOR applications <i>Mark Khait, Denis Voskov (Delft/NL)</i>
11:40 P6	Thermoconvective instabilities for the formation and tilt of the eye in a dust devil-like vortex <i>María Cruz Navarro, Damián Castaño</i> <i>Henar Herrero (Ciudad Real/ES)</i>	11:00 O20	Wettability control on multiphase flow in porous media <i>Chris MacMinn (Oxford/GB), Benzhong Zhao</i> <i>Ruben Juanes (Cambridge, MA/US)</i>
11:44 P7	Moment approximations for shallow flow <i>Julia Kowalski, Manuel Torrilhon (Aachen/DE)</i>	11:20 O21	A finite element setting for macroscale simulations of wetting flows in fibrous media <i>Yujie Liu (Guangzhou/CN), Julien Bruchon</i> <i>Nicolas Moulin (Saint-Étienne/FR)</i>
11:48 P8	Numerical and computational strategies for the EULAG conservative dynamical core of COSMO NWP framework <i>Farnoush Ataei, Zbigniew Piotrowski</i> <i>Marcin Polkowski, Adam Ryczkowski (Warsaw/PL)</i>	11:40 O22	Numerical aspects of molecular diffusion calculations during gas injection in fractured reservoirs <i>Marjan Sherafati</i> <i>Kristian Jessen (Los Angeles, CA/US)</i>

MS4

CO₂-Hydrocarbon interactions for CO₂ storage with EOR/EGR

10:00–12:00 • Room: Seminarraum Informatik 01.150

Chairs: Sarah Gasda, Maria Elenius (Bergen/NO)

Storage of carbon dioxide (CO₂) in geological formations is a means to reduce atmospheric emissions of this greenhouse gas. CO₂ storage combined with enhanced oil recovery (EOR) or enhanced gas recovery (EGR) is perceived as the most cost-effective method of disposing captured CO₂ emissions. CO₂-EOR has been performed for many decades with a focus on hydrocarbon recovery. With CCUS, CO₂ storage will be emphasized in order to meet CO₂ emissions targets. Interactions of CO₂ with in-situ fluids and the host rock could fundamentally alter the ability to recover trapped hydrocarbons while simultaneously affecting CO₂ storage potential.

This minisymposium focuses on two relevant processes, convective mixing and wettability alteration, along with their analytical and numerical solution strategies. Density-driven convective mixing of CO₂ in oil increases mixing and alters the oil mobility. Wettability may change dynamically with CO₂ exposure, which impacts the capacity of the rock to trap CO₂. Recent studies have shown compelling results that may have a significant, yet still largely unknown, impact on field-scale fluid flow (recovery) and trapping (storage).

MS5

Ensemble-based data assimilation and optimization in geosciences • Part 1

10:00–12:00 • Room: Übung 2

Part 2 see page 26

Chairs: Xiaodong Luo (Bergen/NO)
Ibrahim Hoteit (Thuwal/SA), Geir Evensen
Geir Nævdal (Bergen/NO)

In the past decade, ensemble-based data assimilation and optimization methods have received great attention from researchers in various disciplines of geosciences, given their reliable performance, reasonable computational costs, the simplicity in implementations and the ability to quantify the uncertainties of the estimates. This minisymposium will bring together researchers in the field to communicate and discuss their recent developments and applications of the ensemble-based data assimilation and optimization methods. We encourage presentations on new methodologies, ideas or perspectives, numerical algorithm implementations, and open problems and challenges in real world applications.

10:00 O23	An efficient state-parameter filtering scheme combining ensemble Kalman and particle filters <i>Boujemaa Ait-El-Fquih, Ibrahim Hoteit (Thuwal/SA)</i>
10:20 O24	Ensemble methods for combined state and parameter estimation <i>Arnold Heemink (Delft/NL)</i>

10:40 O25 **Assimilating all-sky SEVIRI infrared brightness temperatures using the KENDA ensemble data assimilation system**
Axel Hutt, Roland Potthast, Christoph Schraff
Robin Faulwetter, Hendrik Reich
Andreas Rhodin
Christina Köpken-Watts (Offenbach a. M./DE)

11:00 O26 **Use of correlation-based localization for history matching seismic data**
Rolf Lorentzen, Xiaodong Luo, Tuhin Bhakta
Randi Valestrand (Bergen/NO)

11:20 O27 **A spatiotemporal stochastic model for tropical precipitation and water vapor dynamics**
Scott Hottovy (Annapolis, MD/US)
Samuel Stechmann (Madison, WI/US)

MS6
Computational methods for density driven flow in heterogeneous and fractured porous media
 10:00–12:00 • Room: Übung 4

Chairs: Arne Nägel, Andreas Vogel (Frankfurt a. M./DE)
Gabriel Wittum (Thuwal/SA)

This mini-symposium is on recent developments in numerical methods for modeling flow in subsurface porous media. This includes locally conservative finite-volume and finite element methods, multiscale modeling and upscaling. Elliptic and hyperbolic PDE approximation issues are addressed for single and multiphase flow including higher resolution, accuracy and efficiency on structured and unstructured grids, with application to problems that include full tensor permeability fields, faults and fractures.

10:00 O28 **Parallel and adaptive vertex-centered finite volume simulations for density driven flow**
Andreas Vogel (Frankfurt a. M./DE)

10:20 O29 **Modeling thermo-hydraulic flow in fractured rock**
Klaus-Peter Kröhn (Braunschweig/DE)

10:40 O30 **Mesh generation for parallel multigrid based simulations of density driven flow in domains with thin layers**
Sebastian Reiter (Frankfurt a. M./DE)

11:00 O31 **Validity criterion for models of density-driven flows in porous media with low-dimensional representation of fractures**
Dmitry Logashenko (Thuwal/SA)
Alfio Grillo (Turin/IT)
Gabriel Wittum (Thuwal/SA)

11:20 O32 **Modeling variable density flow with heat generation caused by radioactive decay**
Ivan Kapyrin, Fedor Grigoriev
Aleksandr Rastorguev (Moscow/RU)

11:40 O33 **Fractal structures in freezing brine**
Sergey Alyaev, Eirik Keilegavlen (Bergen/NO)
Jan M. Nordbotten (Bergen/NO; Princeton, NJ/US),
I. Sorin Pop (Bergen/NO; Diepenbeek/BE)

MS7
Advanced discretization schemes for subsurface flow and transport
 10:00–12:00 • Room: Übung 5

Chairs: Ahmad Abusahikha (Doha/QA)
Christine Maier (Stanford, CA/US)

This mini-symposium discusses the latest advances in discretization schemes for sub-surface flow and transport. It brings speakers from three different continents (North America, Europe, and Asia) with each presenting the latest technological advances on their discretization scheme: high order finite-element with dual meshes, MPFA for dual-media with fractures, non-linear finite volume and mixed-hybrid finite-element. Monotonicity, convergence and application are to be discussed and presented.

10:00 O34 **An MPFA-based dual continuum – Discrete feature model for simulating flow in fractured reservoirs**
Christine Maier
Mohammad Karimi-Fard (Stanford, CA/US)
Alexandre Lapene (Stanford, Paolo Alto, CA/US)
Louis Durlofsky (Stanford, CA/US)

10:20 O35 **A robust control volume finite element method for highly distorted meshes**
Pablo Salinas, Dimitrios Pavlidis
Carl Jacquemyn (London/GB)
Zhihua Xie (Cardiff/GB), Christopher Pain
Matthew Jackson (London/GB)

10:40 O36 **Investigation of physically based interpolation strategies for a class of monotone nonlinear finite volume methods**
Wenjuan Zhang
Mohammed S. Al Kobaisi (Abu Dhabi/AE)

11:00 O37 **Advanced discretization schemes for general purpose reservoir simulation – Review, analysis and comparison**
Ahmad Abusahikha (Doha/QA)
Kirill Kerekhov (Stanford, CA/US)

11:20 O38 **Adaptive discontinuous Galerkin methods for flow in porous media**
Birane Kane (Stuttgart/DE)
Robert Kloefkorn (Bergen/NO)
Christoph Gersbacher (Freiburg i. Br./DE)

11:40 O39 **A linear domain decomposition method for partially saturated flow in porous media**
David Seus, Koondanibha Mitra (Stuttgart/DE)
I. Sorin Pop (Bergen/NO; Diepenbeek/BE)
Florin A. Radu (Bergen/NO)
Christian Rohde (Stuttgart/DE)

PS2 | Invited plenary
New frontiers in earth-system modeling

13:00–14:00 • Room: H11

Chair: Katherine J. Evans (Oak Ridge, TN/US)

Speaker: Nils P. Wedi (Reading/GB)

The gradual progress in global numerical weather prediction includes a systematic approach to assess and quantify the associated forecast uncertainty by means of high-resolution ensembles of assimilation and forecasts. This involves simulations with billions of gridpoints, the continuous assimilation of billions of observations, rigorous verification, validation and uncertainty quantification, and it involves increasing model complexity through completing the descriptions of the global water and carbon cycles. The research requires a deeper understanding of multi-scale interactions within the atmosphere and oceans, and through interactions at the interfaces of atmosphere, land surface, ocean, lakes, and sea-ice. All this is necessary to increase the fidelity of daily forecasts and of European Copernicus Services, e.g. through the provision of state-of-the-art atmospheric monitoring services, warning systems for flood and fires, and providing reanalyses. A particular challenge arises from ensuring energy efficiency for these extreme-scale applications. This talk will comprehensively describe the steps taken towards preparing complex numerical weather predictions systems for potentially disruptive technology changes. This includes adaptation to heterogeneous architectures, accelerators and special compute units, adaptation to hierarchical memory layouts, increasing flexibility to use different numerical techniques with fundamentally different communication and computational patterns, frontier research on algorithm development for extreme-scale parallelism in time and in space, and minimising both time- and energy-to-solution. For example, a significant step towards further savings both in terms of throughput and speed-up is provided by the impact on simulations if numerical precision is selectively reduced in high resolution simulations.

MS8
Multiscale modeling for subsurface processes
Part 1

14:10–15:30 • Room: H11

Part 2 see page 28

Chairs: Mary F. Wheeler, Benjamin Ganis

Gergina Pencheva

Gurpreet Singh (Austin, TX/US)

This minisymposium seeks to gather the most recent advancements in numerical and analytical techniques for multiscale methods. The high fidelity simulation of subsurface processes involves highly heterogeneous media, multiple spatial and temporal scales, and large domains. Even under basic modeling assumptions, these systems are computationally intensive and require specialized techniques for efficient solution while preserving accuracy. In particular, this session will include topics on homogenization techniques, adaptive mesh refinement, offline/online calculations, and specialized discretizations.

14:10 O40 **Adaptive mesh refinement with a mixed finite element method using a fully-coupled enhanced velocity solver**
Benjamin Ganis (Austin, TX/US)

14:30 O41 **Multiscale methods in fractured media**
Yalchin Efendiev, Maria Vasilyeva
Eric Chung Wing Tat Leung (College Station, TX/US)

14:50 O42 **Multiscale Unstructured Discrete Fracture Model (MS-DFM)**
Sebastian Bosma (Delft/NL; Stanford, CA/US)
Hadi Hajibeygi, Matei Tene (Delft/NL)
Hamdi A. Tchelepi (Stanford, CA/US)

15:10 O43 **A multiphysics/multiscale pore network (MP/MSPN) simulation framework to bridge the gap between pore- and darcy scale**
Karim Khayrat, Robert Epp
Patrick Jenny (Zurich/CH)

QF2
Poster quick fire session 2

15:30–16:10 • Room: H11

Chairs: Mary F. Wheeler, Benjamin Ganis

Gergina Pencheva

Gurpreet Singh (Austin, TX/US)

15:30 P9 **Multiscale reconstruction of compositional transport**
Chandrashekar Ganapathy
Denis Voskov (Delft/NL)

15:34 P10 **Multiscale gradient computation for sequentially coupled flow and transport in heterogeneous porous media**
Rafael Moraes, Hadi Hajibeygi
Jan-Dirk Jansen (Delft/NL)

15:38 Multiscale finite volume method for
P11 sequentially coupled flow-heat system of
equations in fractured porous media:
Application to geothermal systems
Timothy Praditia (Delft/NL)
Rainer Helmig (Stuttgart/DE)
Hadi Hajibeygi (Delft/NL)

15:42 Geoscientific application of the reduced basis
P12 method and high-performance simulations
Denise Degen, Karen Veroy
Florian Wellmann (Aachen/DE)

15:46 Surface-based reservoir modeling using NURBS
P13 surfaces
Carl Jacquemyn, Yulia Melnikova
Margaret P. Rood, Gary J. Hampson
Matthew Jackson (London/GB)

15:50 FESTUNG – The Finite Element Simulation
P14 Toolbox for UNstructured Grids
Balthasar Reuter (Erlangen/DE)
Florian Frank (Houston, TX/US)
Vadym Aizinger (Bremerhaven/DE)

15:54 Numerical computation of effective parameters
P15 in an evolving porous medium
Jens Oberlander, Nadja Ray
Raphael Schulz (Erlangen/DE)
Peter Frolkovič (Bratislava/SK)

MS9 Mathematical and numerical advances in shallow water modeling • Part 1

14:10–16:10 • Room: H12
Part 2 see page 28

Chairs: *Mario Putti (Padua/IT)*
Robert L. Higdon (Corvallis, OR/US)

Shallow water models, and generalizations such as three-dimensional stratified models, are being applied to increasingly complex real world settings, from flow of water and air over complex terrain to simulation of debris flow, snow/avalanche modeling, tsunami modeling and ocean dynamics, and so on. Accurate, almost realtime simulations require advances in both model development and numerical accuracy, efficiency and robustness. This minisymposium aims to address the mathematical and numerical challenges for the simulation of shallow water type phenomena at different scales.

14:10 Solving depth averaged equations using
O44 parallel GeoClaw
Donna Calhoun (Boise, ID/US)
Carsten Burstedde (Bonn/DE), Melody Shih
Kyle Mandli (New York, NY/US)

14:30 2D versus 1D models for shallow water
O45 equations
Pascal Noble (Toulouse/FR)

14:50 A new family of efficient semi-implicit
O46 discontinuous Galerkin finite element schemes
on staggered grids for the shallow water and
the incompressible Navier-Stokes equations
Michael Dumbser (Trento/IT)

15:10 Efficient multi-layer shallow water models
O47
José Garres Díaz
Enrique D. Fernández Nieto (Sevilla/ES)
Luca Bonaventura (Milan/IT)
Gladys Narbona Reina (Sevilla/ES)

15:30 Simulation of shallow-water flows on general
O48 terrain
Elena Bachini (Padua/IT)
Ilaria Fent (Louvain-la-Neuve/BE)
Mario Putti (Padua/IT)

MS10 Advances in numerical methods for weather and climate modeling • Part 1

14:10–16:10 • Room: H13
Part 2 see page 29

Chairs: *Luca Bonaventura (Milan/IT)*
Tommaso Benacchio (Exeter/GB)
Frank Giraldo (Milan/IT)

This is the first part of a three sessions minisymposium that will present an overview of the research on advanced numerical methods for geophysical fluid dynamics applications, with special (but not exclusive) focus on dynamical cores for weather prediction and climate models. Recent developments in the formulation, implementation and application of modern numerical techniques will be reviewed, including high order finite elements, mimetic discretizations and dynamical adaptation techniques. The participants are all active in major research centers, weather prediction services and university departments with significant record of research activity in this field. The minisymposium can be of great interest to all the participants of the SIAM Conference on Mathematical and Computational Issues in the Geosciences by presenting recent research results of major relevance and potential also in other areas of the Geosciences.

14:10 A finite-volume module for cloud-resolving
O49 simulations of global atmospheric flows
Piotr Smolarkiewicz
Christian Kühnlein (Reading/GB)
Wojciech Grabowski (Boulder, CO/US)

14:30 A finite-volume module for all-scale earth
O50 system modeling at ECMWF
Christian Kühnlein, Sylvie Malardel
Piotr Smolarkiewicz (Reading/GB)

14:50 Flexible earth system modeling on multiple
O51 grids
Willem Deconinck
Michail Diamantakis (Reading/GB)
Mike Gillard (Loughborough/GB), Pedro Maciel
Andreas Mueller, Christian Kuehnlein
Nils P. Wedi (Reading/GB)

15:10 GungHo – A mixed finite element-based
O52 dynamical core for next-generation numerical weather prediction
Tommaso Benacchio, Thomas Melvin
The GungHo Team (Exeter/GB)

15:30 Modifications to the Global Environmental
O53 Multiscale (GEM) model dynamical core for improved forecast accuracy
Syed Z. Husain, Claude Girard
André Plante (Dorval/CA)

MS11

Effective models for porous media containing thin structures

14:10–15:50 • Room: Seminarraum Informatik 01.150

Chairs: *Markus Gahn, Maria Neuss-Radu (Erlangen/DE)*

Porous media containing thin structures occur in a wide range of applications in the geosciences like e.g., ground water contamination, but also in other fields like engineering and biology. Flow and reactive transport processes in fractured porous media lead to great mathematical challenges in the numerical treatment of the mathematical models, since the magnitude of the thin fractures is several orders of magnitude smaller than the surrounding media. The aim of this minisymposium is the derivation of reduced effective models for the microscopic problems which can be treated numerically with an reasonable effort and give an approximation of the microscopic model. In the effective models the thin layer reduces to an interface and the influence of the layers arise in these models as effective transmission conditions.

14:10 Analysis and upscaling of a model for reactive
O54 flow in porous media
I. Sorin Pop (Bergen/NO; Diepenbeek/BE)
Florin A. Radu, Kundan Kumar (Bergen/NO)
David Seus (Stuttgart/DE), Koondanibha Mitra
Florian List (Eindhoven/NL)

14:30 Effective pressure boundary condition for the
O55 filtration through porous medium via homogenization
Eduard Marusic-Paloka (Zagreb/HR)
Andro Mikelic (Villeurbanne/FR)
Thomas Carraro (Heidelberg/DE)

14:50 Effective transmission conditions for transport
O56 processes through a thin layer
Markus Gahn, Maria Neuss-Radu
Peter Knabner (Erlangen/DE)

15:10 Homogenization via unfolding in domains
O57 separated by a thin layer of thin beams
Orlik Julia (Kaiserslautern/DE)
Georges Griso (Paris/FR)
Anastasia Migunova (Kaiserslautern/DE)

15:30 Space-time domain decomposition for a
O58 nonlinear parabolic model of two-phase flow with discontinuous capillary pressure
Elyes Ahmed (Marne-la-Vallée, Villetaneuse/FR)
Caroline Japhet (Villetaneuse/FR)
Michel Kern (Paris, Saclay/FR)

QF3

Poster quick fire session 3

15:50–16:10 • Room: Seminarraum Informatik 01.150

Chairs: *Markus Gahn, Maria Neuss-Radu (Erlangen/DE)*

15:50 Effective models including dynamic Wentzell
P16 type transmission conditions for domains separated by a thin heterogeneous layer
Markus Gahn, Maria Neuss-Radu
Peter Knabner (Erlangen/DE)

15:54 An upscaled model for permeable biofilm
P17 formation in a thin strip
David Landa Marban, Florin A. Radu
I. Sorin Pop (Bergen/NO; Diepenbeek/BE)
Kundan Kumar (Bergen/NO)

15:58 Numerical model for phase transitions at pore
P18 scale
Azhar Alhammali
Malgorzata Peszynska (Corvallis, OR/US)

16:02 Microbial metabolic lag in a bio-reactive
P19 transport model for underground hydrogen storage
Birger Hagemann (Clausthal-Zellerfeld/DE)
Mikhail Panfilov (Nancy/FR)
Leonhard Ganzer (Clausthal-Zellerfeld/DE)

16:06 Simulation of microbial growth in complex
P20 geometries
Jan Zawallich (Clausthal-Zellerfeld/DE)
Steffen Schlüter
Hans-Jörg Vogel (Halle a. d. Saale/DE)
Olaf Ippisch (Clausthal-Zellerfeld/DE)

MS12

Ensemble-based data assimilation and optimization in geosciences • Part 2

14:10–16:10 • Room: Übung 2

Part 3 see page 34

Chairs: *Xiaodong Luo (Bergen/NO)*
Ibrahim Hoteit (Thuwal/SA), Geir Evensen
Geir Nævdal (Bergen/NO)

In the past decade, ensemble-based data assimilation and optimization methods have received great attention from researchers in various disciplines of geosciences, given their reliable performance, reasonable computational costs, the simplicity in implementations and the ability to quantify the uncertainties of the estimates. This minisymposium will bring together researchers in the field to communicate and discuss their recent developments and applications of the

ensemble-based data assimilation and optimization methods. We encourage presentations on new methodologies, ideas or perspectives, numerical algorithm implementations, and open problems and challenges in real world applications.

14:10 Ensemble-based reservoir optimization

O59 *Zhenyu Guo, Bailian Chen, Ranran Lu*
Fahim Forouzanfar
Albert Reynolds (Tulsa, OK/US)

14:30 An evaluation of sampling strategies for ensemble-based optimization

O60 *Karthik Ramaswamy (Utrecht, Eindhoven/NL)*
Rahul Fonseca, Paul Egberts
(Utrecht/NL), Paul Van den Hof (Eindhoven/NL)
Olwijn Leeuwenburgh (Utrecht/NL)

14:50 Robustness evaluation of ensemble-based methods for production optimization

O61 *Yuqing Chang, Andreas S. Stordal (Bergen/NO)*

15:10 Geomechanical parameter estimation with a coupled flow-geomechanical model

O62 *Femke Vossepoel, Denis Voskov (Delft/NL)*

15:30 Orthonormal residuals for large-scale geostatistical model validation

O63 *Ole Klein (Heidelberg/DE)*

15:50 Synchronous history matching of multiple SCAL experiments for relative permeability and capillary pressure interpretation

O64 *Roman Manasipov, Bettina Jenei*
Holger Ott (Leoben/AT)

MS13

The mathematics and computing of seismic, MT and CSEM data inversion

14:10–16:50 • Room: Übung 4

Chair: *Eduardo Sanchez (Barcelona/ES)*

Subsurface imaging is a fundamental problem in exploration geophysics. Geological surveys gather diverse geophysical data to increase the accuracy of the imaging process. Specifically, wavelet attributes, magnetotelluric (MT), and controlled-source electromagnetic (CSEM) data are useful for this purpose, although the inversion of these types of data in realistic scenarios is usually a challenge. From the mathematical standpoint, inversion processes seek to solve a non-linear constrained data-fitting problem. This problem is ill-posed and objective functions have multiple local minima, thus the inversion process is inherently ambiguous. From the computational standpoint, the performance of the process is very sensitive to the selection of the non-linear data-fitting method, and to the computation of the forward problem required to fit the observed data. In this symposium, we summarize current efforts in formulating and implementing seismic, MT and CSEM inversion processes. We focus on the mathematical choices pertaining forward modeling and the inversion process, their implementation on HPC architectures, and on successful application cases.

14:10 Modeling seismic wave propagation using staggered-grid mimetic finite differences

O65 *Juan Guevara (Caracas/VE)*

14:30 Retrieving low-frequency model with cross correlation misfit – A realistic synthetic study case

O66 *Jean Kormann (Leoben/AT), Josep De La Puente*
Otilio Rojas, Mauricio Hanzich (Barcelona/ES)

14:50 A review of the numerics in seismic full wave inversion and a robust implementation

O67 *Otilio Rojas (Barcelona/ES)*

15:10 Overview of numerical techniques and applications for CSEM/MT geophysical surveys

O68 *Pilar Queralt, Juanjo Ledo, Alejandro Marcuello*
Eloi Vilamajo, Octavio Castillo
David Modesto (Barcelona/ES)

15:30 Volume source-based extended waveform inversion method for seismic velocity inversion

O69 *Guanghui Huang (Houston, TX/US)*

15:50 The analysis of Earth's global gravitational field by using spherical wavelet transform

O70 *Natalia Matveeva, Edward Utemov*
Danis Nurgaliev (Kazan/RU)

16:10 Love wave frequency under the influence of linearly varying shear moduli, initial stress and density of orthotropic half space

O71 *Sumit Vishwakarma (Hyderabad/IN)*

16:30 Green function approach to study of surface seismic wave propagation

O72 *Santanu Manna (Indore/IN)*

MS14

Numerical methods for the characterization of geothermal reservoirs • Part 1

14:10–16:10 • Room: Übung 5

Part 2 see page 31

Chairs: *Alessio Fumagalli*
Eirik Keilegavlen (Bergen/NO), Anna Scotti
Luca Formaggia (Milan/IT)

An accurate description of geothermal reservoirs is of paramount importance to economically enhance the economic profitability of existing reservoirs and increase the attractiveness and sustainability of this renewable source of energy. The challenges related to the multiscale nature of fluid flow in hot rocks are coupled with complex phenomena like the presence of natural or induced fractures and faults. Issues like flow in fractured media, fracture generation, propagation, and stimulation, chemical reactions, multi-phase flows and data uncertainty have to be investigated with effective numerical tools. In this minisymposium we address new developments in mathematical models and numerical methods to overcome these challenges and make simulations more reliable and effective for the exploitation of geothermal energy.

14:10
O73 Simulation of deformation and flow in fractured poroelastic materials
Katja K. Hanowski, Oliver Sander (Dresden/DE)

14:30
O74 Upscaled models for two-phase flow in fractured rock
*Insa Neuweiler, Jan Tecklenburg (Hanover/DE)
Marco Dentz (Barcelona/ES)*

14:50
O75 Using topology to estimate permeability of fracture networks
Pål Næverlid Sævik, Casey Nixon (Bergen/NO)

15:10
O76 Hydraulic stimulation and friction laws for fracture deformation – A numerical study
*Runar Berge, Inga Berre
Eirik Keilegavlen (Bergen/NO)*

15:30
O77 A space-time adaptive method for reservoir flows
*Savithru Jayasinghe, David Darmofal
Marshall Galbraith, Steven Allmaras
Eric Dow (Cambridge, MA/US)*

15:50
P30 A discrete, conductive fracture model of single phase flow in porous media using non-conforming grids
*Markus Köppel (Stuttgart/DE)
Vincent Martin (Compiègne/FR)
Jean-Elizabeth Roberts (Paris/FR)*

MS15
Multiscale modeling for subsurface processes
Part 2

16:30–18:30 • Room: H11
Part 3 see page 35

*Chairs: Mary F. Wheeler, Benjamin Ganis
Gergina Pencheva
Gurpreet Singh (Austin, TX/US)*

This minisymposium seeks to gather the most recent advancements in numerical and analytical techniques for multiscale methods. The high fidelity simulation of subsurface processes involves highly heterogeneous media, multiple spatial and temporal scales, and large domains. Even under basic modeling assumptions, these systems are computationally intensive and require specialized techniques for efficient solution while preserving accuracy. In particular, this session will include topics on homogenization techniques, adaptive mesh refinement, offline/online calculations, and specialized discretizations.

16:30
O78 Seismic wave propagation simulation in fractured media
Mrinal Sen (Austin, TX/US)

16:50
O79 Generalized multiscale discontinuous Galerkin method for subsurface flow and wave problems
*Wing Tat Leung
Yalchin Efendiev (College Station, TX/US)
Eric Chung (Hong Kong/HK)*

17:10
O80 Multiscale parallel-in-time coupling for wave propagation in heterogeneous media
Yen-Hsi Tsai (Austin, TX/US)

17:30
O81 Modeling multiphase hydraulic fracture propagation
*Andro Mikelic (Villeurbanne/FR)
Sanghyun Lee (Tallahassee, FL/US)
Mary F. Wheeler (Austin, TX/US)
Thomas Wick (Paris/FR)*

17:50
O82 A multiscale hybrid-mixed method for the elastodynamic model in time domain
*Wesley da Silva Pereira
Antônio T. Azevedo Gomes
Frédéric G. C. Valentin (Petrópolis/BR)*

18:10
O83 The 3D elastodynamic wave equation with transparent boundary conditions
Sarah Eberle (Tübingen/DE)

MS16
Mathematical and numerical advances in shallow water modeling • Part 2

16:30–18:30 • Room: H12

*Chairs: Mario Putti (Padua/IT)
Robert L. Higdon (Corvallis, OR/US)*

Shallow water models, and generalizations such as three-dimensional stratified models, are being applied to increasingly complex real world settings, from flow of water and air over complex terrain to simulation of debris flow, snow/avalanche modeling, tsunami modeling and ocean dynamics, and so on. Accurate, almost realtime simulations require advances in both model development and numerical accuracy, efficiency and robustness. This minisymposium aims to address the mathematical and numerical challenges for the simulation of shallow water type phenomena at different scales.

16:30
O84 Accurate and stable time stepping in ice sheet modeling
*Lina von Sydow, Gong Cheng
Per Lötstedt (Uppsala/SE)*

16:50
O85 Modified shallow-water equations for direct bathymetry reconstruction
Hennes Hajduk, Vadym Aizinger (Erlangen/DE)

17:10
O86 Modeling the oscillations of the thermocline in a lake by means of a fully consistent and conservative 3D finite-element model with a vertically adaptive mesh
Vincent Legat (Louvain-La-Neuve/BE)

17:30
O87 Automatic well-balancing in a formulation of pressure forcing for DG modeling of stratified oceanic flows
Robert L. Higdon (Corvallis, OR/US)

MS17**Advances in numerical methods for weather and climate modeling • Part 2**

16:30–17:50 • Room: H13

Chairs: Luca Bonaventura (Milan/IT)
Tommaso Benacchio (Exeter/GB)
Frank Giraldo (Milan/IT)

This is the second part of a three session minisymposium that will present an overview of the research on advanced numerical methods for geophysical fluid dynamics applications, with special (but not exclusive) focus on dynamical cores for weather prediction and climate models. Recent developments in the formulation, implementation and application of modern numerical techniques will be reviewed, including high order finite elements, mimetic discretizations and dynamical adaptation techniques. The participants are all active in major research centers, weather prediction services and university departments with significant record of research activity in this field. The minisymposium can be of great interest to all the participants of the SIAM Conference on Mathematical and Computational Issues in the Geosciences by presenting recent research results of major relevance and potential also in other areas of the Geosciences.

16:30 O88 **Semi-implicit time integration, blended models, and balanced data**
Rupert Klein (Berlin/DE)

16:50 O89 **B-series and order conditions for split-explicit integrators**
Oswald Knöth (Leipzig/DE)

17:10 O90 **Time parallel methods for oscillatory stiffness in atmosphere and ocean modeling – Fast singular limits**
Beth Wingate (Exeter/GB)

17:30 O91 **Direct FEM parallel-in-time computation of turbulent flow**
Johan Jansson (Stockholm/SE)
Tania Bakhos (Bilbao/ES)
Johan Hoffman (Stockholm/SE)

MS18**Advances in numerical methods for weather and climate modeling • Part 3**

17:50–18:50 • Room: H13

Chairs: Luca Bonaventura (Milan/IT)
Tommaso Benacchio (Exeter/GB)
Frank Giraldo (Milan/IT)

This is the third part of a three session minisymposium that will present an overview of the research on advanced numerical methods for geophysical fluid dynamics applications, with special (but not exclusive) focus on dynamical cores for weather prediction and climate models. Recent developments in the formulation, implementation and application of modern numerical techniques will be reviewed, including high

order finite elements, mimetic discretizations and dynamical adaptation techniques. The participants are all active in major research centers, weather prediction services and university departments with significant record of research activity in this field. The minisymposium can be of great interest to all the participants of the SIAM Conference on Mathematical and Computational Issues in the Geosciences by presenting recent research results of major relevance and potential also in other areas of the Geosciences.

17:50 O92 **The Galerkin Numerical Modeling Environment (GNuMe) for geophysical fluids dynamics simulations on next-generation architectures**
Frank Giraldo, Daniel Abdi (Monterey, CA/US)
Michal Kopera (Santa Cruz, CA/US)
Jeremy Kozdon (Monterey, CA/US)

18:10 O93 **Large eddy simulation of gravity currents with a high order DG method**
Caterina Bassi, Antonella Abbà
Luca Bonaventura
Lorenzo Valdetaro (Milan/IT)

18:30 O94 **A parallel library of p-adaptive high order finite elements for geophysical applications**
Luca Bonaventura, Giovanni Tumolo (Milan/IT)

MS19**Limit processes in porous media**

16:30–18:30 • Room: Seminarraum Informatik 01.150

Chair: Kundan Kumar (Bergen/NO)

Management of porous media resources such as hydrocarbons, water resources, and energy storage systems requires understanding of coupled processes that can result in complete alteration of the system dynamics. These altering processes are manifestations of so-called limit phenomena that include clogging, phase change of the fluid, sinkhole formation, and mechanical instability. Despite their evident importance, incorporating the possible limit effects of a system during its evolution remains a scientific challenge. This challenge manifests itself at every stage from the development of appropriate mathematical models to efficient simulation techniques. Accordingly, this MS will discuss mathematical models and numerical algorithms for limit processes in porous media/geosciences. The presentations will focus on the limit processes arising out of reactive and geomechanical phenomena.

16:30 O95 **Clogging in effective equations for non isothermal reactive porous media flow**
Carina Bringedal, Kundan Kumar (Bergen/NO)

16:50 O96 **Numerical methods for a multiscale biofilm model in porous media**
Raphael Schulz (Erlangen/DE)

17:10 O97 **Towards multi-continuum formulations with dynamic fracture permeabilities**
Florian Doster (Edinburgh/GB)

- 17:30 O98 Mixed methods for hierarchical flow models for non-isothermal wells in porous media
Ingeborg Gåseby Gjerde (Bergen/NO)
- 17:50 O99 Advantages of mixed hybrid finite element method in swelling computation
Cong Yu, Kamyar Malakpoor (Eindhoven/NL)
Jacques Huyghe (Eindhoven/NL; Limerick/IE)
- 18:10 O100 Biologically inspired formulation of optimal transportation problems and applications
Enrico Facca, Franco Cardin
Mario Putti (Padua/IT)

MS20
Machine learning applications in subsurface reservoir modeling

16:30–18:30 • Room: Übung 2

Chairs: Ahmed H. Elsheikh (Edinburgh/GB)
Behnam Jafarpour (Los Angeles, CA/US)

Machine learning (ML) have contributed significantly to recent advances in image and signal processing, pattern recognition, recommendation systems, natural language processing and machine translation. Most of these machine learning techniques, could be adapted for a wide range of applications in reservoir modeling. This Mini-symposium covers recent applications of machine learning algorithms for multi-scale modeling, reduced order modeling and uncertainty quantification (UQ) of subsurface reservoirs. Targeted applications includes: (1) Machine Learning assisted Uncertainty Quantification (2) ML accelerated statistical model calibration against multiple data sources (production, seismic, outcrops, experts) (4) Quantitative risk assessment using data-driven approaches. Also of relevance are Bayesian approaches, compressed sensing and sparse reconstruction methods, reduced-order parameterization, physical model cross-validation techniques, and response surface proxies.

- 16:30 O101 A machine learning approach for uncertainty quantification using the Multiscale Finite Volume method
Ahmed H. Elsheikh
Shing C. Chan Chang (Edinburgh/GB)
- 16:50 O102 Efficient big data assimilation through sparse representation
Xiaodong Luo, Tuhin Bhakta, Morten Jakobsen
Geir Nævdal (Bergen/NO)
- 17:10 O103 A data-scalable randomized misfit approach for solving large-scale PDE-constrained inverse problems
Tan Bui (Austin, TX/US)
- 17:30 O104 Parametrization of geological models with generative adversarial networks
Shing C. Chan Chang
Ahmed H. Elsheikh (Edinburgh/GB)

- 17:50 O105 Redistribution of steam injection in heavy oil reservoir management to improve EOR economics, powered by a unique integration of reservoir physics and machine learning
Pallav Sarma (Danville, CA/US)
- 18:10 O106 DR-RNN – A deep residual recurrent neural network for model reduction
Nagoor K. Jabarullah Khan
Ahmed H. Elsheikh (Edinburgh/GB)

MS21
Modeling and simulation of melt in the mantle Part 1

16:50–18:30 • Room: Übung 4

Part 2 see page 32

Chairs: Todd Arbogast, Marc A. Hesse (Austin, TX/US)

The Earth’s mantle is almost entirely solid, but at depths up to about 100 km beneath plate-tectonic boundaries (mid-ocean ridges and subduction zones) and beneath ocean islands, a small fraction of the mantle will melt, forming a porous medium of a few percent porosity. Melted rock will tend to rise to the surface, giving rise to volcanic activity and forming new crust. Magmatism also plays a key role in the chemical evolution and dynamics of the Earth. Developing a fundamental understanding the formation and migration of melt in the mantle presents a formidable scientific and mathematical challenge. This minisymposium will bring together mathematicians and solid Earth scientists to discuss recent developments in modeling and computational simulation of melt migration in the Earth’s mantle.

- 16:50 O107 Equilibrated melt networks
Marc A. Hesse, Soheil Ghanbarzadeh
Masha Prodanovic (Austin, TX/US)
- 17:10 O108 Modeling of magma-mantle dynamics in subduction zones
David Rees Jones, Richard Katz, Dave May
Meng Tian (Oxford/GB)
John Rudge (Cambridge/GB)
- 17:30 O109 Tracer transport in solitary porosity waves
Jacob Jordan, Marc A. Hesse (Austin, TX/US)
- 17:50 O110 Adjoint-based inversion to model the nonlinear rheology of the lithosphere
Lukas Holbach, Martin Hanke, Boris Kaus
Anton Popov (Mainz/DE)

MS22

Numerical methods for the characterization of geothermal reservoirs • Part 2

16:30–18:30 • Room: Übung 5

Chairs: Alessio Fumagalli
 Eirik Keilegavlen (Bergen/NO), Anna Scotti
 Luca Formaggia (Milan/IT)

An accurate description of geothermal reservoirs is of paramount importance to economically enhance the economic profitability of existing reservoirs and increase the attractiveness and sustainability of this renewable source of energy. The challenges related to the multiscale nature of fluid flow in hot rocks are coupled with complex phenomena like the presence of natural or induced fractures and faults. Issues like flow in fractured media, fracture generation, propagation, and stimulation, chemical reactions, multi-phase flows and data uncertainty have to be investigated with effective numerical tools. In this minisymposium we address new developments in mathematical models and numerical methods to overcome these challenges and make simulations more reliable and effective for the exploitation of geothermal energy.

- 16:30 O111 **Efficient solution techniques for the simulation of multi-phase, geothermal reservoirs**
Henrik Büsing, Jan Niederau
Christoph Clauser (Aachen/DE)
- 16:50 O112 **Uncertainty quantification analysis of subsurface flow simulations in poro-fractured media**
Stefano Berrone, Claudio Canuto
Sandra Pieraccini, Stefano Scialò (Turin/IT)
- 17:10 O113 **A new hybrid method for crack propagation in poroelastic media**
Bianca Giovanardi, Anna Scotti
Luca Formaggia (Milan/IT)
- 17:30 O114 **BDDC preconditioner for robust discretization of flow in fractured porous media**
Ana Budisa, Eirik Keilegavlen, Jan M. Nordbotten
Florin A. Radu (Bergen/NO)
- 17:50 O115 **Homogenization and inverse analysis of heterogeneous rock samples**
Radim Blaheta, Michal Beres
Simona Domesova, Tomas Lubor (Ostrava/CZ)
Peng-Zhi Pan (Wuhan/CN)

PS3 | Invited plenary
Discontinuous skeletal methods for computational geosciences

08:30–09:30 • Room: H11

Chair: *Beatrice Riviere (Houston, TX/US)*

Speaker: *Alexandre Ern (Paris/FR)*

Discontinuous Skeletal methods are based on discrete unknowns that are discontinuous polynomials on the mesh skeleton. Such methods offer several attractive features: a dimension-independent construction, and the use of arbitrary polynomial orders combined with general grids, including non-matching interfaces and polyhedral cell shapes. Positioning unknowns at mesh faces is also a natural way to express fundamental continuum properties at the discrete level such as local mass or force balance. One prominent example of Discontinuous Skeletal methods is the Hybridizable Discontinuous Galerkin method. Recently, another method has emerged: the Hybrid High-Order (HHO) method. HHO methods were originally devised to approximate scalar diffusive and linear elasticity problems, and have undergone a substantial development in terms of analysis and applications. The cornerstone of HHO methods are fully local, reconstruction operators, which can offer reduced computational costs by organizing simulations into (fully parallelizable) local solves and a global transmission problem. In this talk, we aim at providing a (gentle) introduction to the devising and analysis of HHO methods and to briefly touch upon some of the more recent developments.

MS23
Modeling and simulation of melt in the mantle Part 2

10:00–11:20 • Room: H11

Chairs: *Todd Arbogast, Marc A. Hesse (Austin, TX/US)*

The Earth's mantle is almost entirely solid, but at depths up to about 100 km beneath plate-tectonic boundaries (mid-ocean ridges and subduction zones) and beneath ocean islands, a small fraction of the mantle will melt, forming a porous medium of a few percent porosity. Melted rock will tend to rise to the surface, giving rise to volcanic activity and forming new crust. Magmatism also plays a key role in the chemical evolution and dynamics of the Earth. Developing a fundamental understanding the formation and migration of melt in the mantle presents a formidable scientific and mathematical challenge. This minisymposium will bring together mathematicians and solid Earth scientists to discuss recent developments in modeling and computational simulation of melt migration in the Earth's mantle.

10:00 **Compressible magma/mantle dynamics:**
 O116 **3D adaptive simulations**

Juliane Dannberg (Fort Collins, CO/US)

Timo Heister, Ryan Grove (Clemson, SC/US)

10:20 **High order discontinuous Galerkin methods**
 O117 **for modeling magma dynamics**

Seshu Tirupathi (Dublin/IE)

Jan Hesthaven (Lausanne/CH; Providence, RI/US)

Yan Liang

Marc Parmentier (Providence, RI/US)

10:40 **Mixed methods for two-phase Darcy-Stokes**
 O118 **mixtures of partially melted materials with regions of zero porosity**

Todd Arbogast, Marc A. Hesse

Abraham Taicher (Austin, TX/US)

11:00 **Preconditioners for models of coupled**
 O119 **magma/mantle dynamics**

Sander Rhebergen (Waterloo/CA)

QF4
Poster quick fire session 4

11:20–12:00 • Room: H11

Chairs: *Todd Arbogast, Marc A. Hesse (Austin, TX/US)*

11:20 **Impact of transport pathways in radionuclide**
 P21 **accumulation under groundwater discharge areas**

Elena Abarca (Barcelona/ES)

Alvaro Sainz-Garcia (Barcelona/ES; Toulouse/FR)

Diego Sampietro, David Garcia

Jorge Molinero (Barcelona/ES)

Ulrik Kautsky (Stockholm/SE)

11:24 **Understanding the physics of the Yellowstone**
 P22 **magmatic system with geodynamic inverse modeling**

Georg Reuber, Boris Kaus (Mainz/DE)

- 11:28 P23 **Determining scaling laws from geodynamic simulations using adjoint gradients**
Boris Kaus, Georg Reuber
Anton Popov (Mainz/DE)
- 11:32 P24 **Uncertainty estimation of onset arrival times using parametric bootstrap of statistical time series models**
Charles Vollmer, David Stracuzzi
Matthew Peterson (Albuquerque, NM/US)
- 11:36 P25 **Image processing for mass transport deposit retrieval in seismic data**
Pauline Le Bouteiller, Florence Delprat-Jannaud
Jean Charléty (Rueil-Malmaison/FR)
Christian Gorini (Paris/FR)
- 11:40 P26 **LaMEM – A massively-parallel code for 3D modeling of visco-elasto-plastic lithosphere**
Anton Popov, Boris Kaus (Mainz/DE)
- 11:44 P27 **H(div) mixed finite elements of minimal dimension on quadrilaterals and hexahedra**
Todd Arbogast, Maicon Correa
Zhen Tao (Austin, TX/US)
- 11:48 P28 **ROFMP – An iterative algorithm for the solution of inverse problems**
Roger Telschow, Christian Gerhards (Vienna/AT)
- 11:52 P29 **Multi-physics inversion through joint sparsity**
Dmitry Molodtsov (Saint Petersburg/RU)

MS24 HPC advances and trends in simulation tools for flow and transport in geosciences • Part 1

10:00–12:00 • Room: H12

Part 2 see page 37

Chairs: Vadym Aizinger, Harald Köstler (Erlangen/DE)
Michael Bader (Garching/DE)

Current hardware and software development trends in the area of high performance computing pose a number of specific near-term challenges for developers of numerical models: Improving parallel scaling for large numbers of processes, adding support for GPUs and hybrid execution modes, increasing energy efficiency of simulation packages, and many more. The goal of our mini-symposium is to present methods and tools for performance analysis, modeling, and engineering of applications in Earth sciences as well as to discuss advances in parallel scaling, hybrid and alternative computer architectures, energy efficiency, and all other issues of interest that may be helpful in making numerical simulation software for flow and transport in geophysical problems fit for the emerging computing architectures.

- 10:00 O120 **sam(oa)² – parallel adaptive mesh refinement for tsunami simulation and porous media flow**
Michael Bader, Chaulio Ferreira
Ao Mo-Hellenbrand, Leonhard Rannabauer
Philipp Samfaß (Garching/DE)

- 10:20 O121 **Exploring low-power embedded processors for ocean simulation**
Dietmar Fey, Sebastian Rachuj
Christian Widerspich (Erlangen/DE)
- 10:40 O122 **Performance analysis of a fully functional unstructured 3D coastal ocean model**
Balthasar Reuter (Erlangen/DE)
- 11:00 O123 **Efficient implementation of higher-order discontinuous Galerkin methods**
Peter Bastian, Steffen Müthing, Dominic Kempf
Marian Piatkowski (Heidelberg/DE)
Eike Mueller (Bath/GB)

MS25 Numerical methods towards next generation ice sheet modeling • Part 1

10:00–12:00 • Room: H13

Part 2 see page 37

Chairs: Irina Tezaur (Livermore, CA/US)
Xylar Asay-Davis (Potsdam/DE)
Stephen Price (Los Alamos, NM/US)
Katherine J. Evans (Oak Ridge, TN/US)

Mass loss from the polar ice sheets is expected to have a significant contribution to future sea-level changes. Scientifically meaningful projections of sea-level change in the 21st century and beyond require accurate and efficient computational modeling of the Greenland and Antarctic ice sheets. This minisymposium will focus on numerical and computational methods for reliable, next-generation stand-alone and ice sheet models (ISMs). A variety of topics in the areas of ice sheet modeling and simulation will be covered, including: improved modeling of critical physical processes, stable and efficient numerical methods for ISMs, performance-portability of ISMs to new and emerging computer architectures, model verification/validation, data assimilation, mesh generation/adaptation, ice sheet initialization, inverse problems arising in ice sheet modeling, uncertainty quantification, and coupling of ISMs to other climate components.

- 10:00 O124 **Marine ice sheet retreat hastened by mechanical weakening of shear margins**
Chris Borstad (Longyearbyen/NO)
Helene Seroussi (Pasadena, CA/US)
Mathieu Morlighem (Irvine, CA/US)
Eric Larour (Pasadena, CA/US)
- 10:20 O125 **Anisotropic mesh adaptation for marine ice sheet modeling**
Fabien Gillet-Chaulet, Laure Tavard
Ignacio Merino, Vincent Peyaud, Julien Brondex
Gael Durand, Olivier Gagliardini (Grenoble/FR)
- 10:40 O126 **Improved discretization of grounding lines and calving fronts using an embedded-boundary approach in BISICLES**
Daniel Martin, Peter Schwartz, Amneet Bhalla
Hans Johansen, Esmond Ng (Berkeley, CA/US)

- 11:00 Ice sheet models – Quo vadis?
O127 *Thomas Kleiner, Martin Rückamp*
Angelika Humbert (Bremerhaven/DE, Bremen/DE)
- 11:20 Efficient numerical ice-sheet simulations over
O128 long time spans
Gong Cheng, Lina von Sydow
Per Lötstedt (Uppsala/SE)
- 11:40 Towards stable ice sheet simulations – Inf-sup
O129 stabilization of the p-Stokes equations on
anisotropic meshes
Josefin Ahlkrone (Kiel/DE)
Christian Helanow (Stockholm/SE)
Malte Braak (Kiel/DE)

MS26

Recent advances in computational poromechanics

10:00–12:00 • Room: Seminarraum Informatik 01.150

Chairs: *Florin A. Radu (Bergen/NO)*
Markus Bause (Hamburg/DE)

The numerical simulation of coupled mechanical deformation and fluid flow in porous media has become of increasing importance in several branches of technology and natural sciences including civil, environmental, mechanical, petroleum and reservoir engineering as well as biomechanics and medicine. The numerical analysis and approximation of the mathematical models that are built upon the work of Biot are subject to various complexities due to the coupling structure of the involved subproblems and inherent mechanisms like nonlinearities and degeneracies. In this minisymposium we discuss recent trends and progress in the development and application of robust and efficient discretization methods and solver techniques. Various types of Galerkin methods, variational and multivariate time discretization as well as splitting and monolithic solver and their application are addressed. Multiphase flow and nonlinear models are also considered.

- 10:00 Dimensional model reduction for flow through
O130 fractures in poroelastic media
Ivan Yotov (Pittsburgh, PA/US)
Martina Bukac (South Bend, IN/US)
Paolo Zunino (Milan/IT)
- 10:20 Scalable preconditioners for multiphase
O131 poromechanics
Nicola Castelletto (Stanford, CA/US)
Joshua A. White (Livermore, CA/US)
Sergey Klevtsov (Stanford, CA/US)
Massimiliano Ferronato (Padua/IT)
Hamdi A. Tchelepi (Stanford, CA/US)
- 10:40 Efficient solver for variational space-time
O132 approximation of poroelasticity
Markus Bause, Uwe Köcher (Hamburg/DE)

- 11:00 Upscaling of coupled geomechanics, flow and
O133 non-reactive transport of a poro-elastic
medium in the quasi-static situation
Mats Brun (Bergen/NO)
- 11:20 Monolithic multigrid methods for coupled
O134 fluid-flow and porous media problems
Francisco Gaspar
Cornelis W. Oosterlee (Amsterdam/NL)
Peiyao Luo (Delft/NL)
Prashant Kumar (Amsterdam/NL)
Carmen Rodrigo (Zaragoza/ES)
- 11:40 Linearization for coupled water flow and
O135 mechanical deformation in unsaturated soil
Jakub W. Both, Kundan Kumar
Jan M. Nordbotten, Florin A. Radu (Bergen/NO)

MS27

Ensemble-based data assimilation and optimization in geosciences • Part 3

10:00–12:00 • Room: Übung 2

Chairs: *Xiaodong Luo (Bergen/NO)*
Ibrahim Hoteit (Thuwal/SA), Geir Evensen
Geir Nævdal (Bergen/NO)

In the past decade, ensemble-based data assimilation and optimization methods have received great attention from researchers in various disciplines of geosciences, given their reliable performance, reasonable computational costs, the simplicity in implementations and the ability to quantify the uncertainties of the estimates. This minisymposium will bring together researchers in the field to communicate and discuss their recent developments and applications of the ensemble-based data assimilation and optimization methods. We encourage presentations on new methodologies, ideas or perspectives, numerical algorithm implementations, and open problems and challenges in real world applications.

- 10:00 Properties of iterative ensemble smoothers
O136 for history matching
Geir Evensen (Bergen/NO)
- 10:20 An efficient robust ensemble smoother with
O137 multiple data assimilations
Albert Reynolds, Javad Rafiee (Tulsa, OK/US)
- 10:40 Damping of resonant wave loads on arrays of
O138 vertical cylinders and a transfer-matrix
approach to array problems
Malte A. Peter (Augsburg/DE)
Luke G. Bennetts (Adelaide/AU)
Fabien M. Montiel (Dunedin/NZ)
- 11:00 An ensemble-based framework for
O139 assimilation of image-type data – Application to
seismic history matching
Yanhui Zhang
Olwijn Leeuwenburgh (Utrecht/NL)

11:20 Uncertainty estimation of onset arrival times
 O140 using parametric bootstrap of statistical time series models
Charles Vollmer (Fort Collins, CO/US)
David Stracuzzi
Matthew Peterson (Albuquerque, NM/US)

MS28 Multiscale modeling for subsurface processes Part 3

10:00–12:00 • Room: Übung 4

Chairs: *Mary F. Wheeler, Benjamin Ganis*
 Gergina Pencheva
 Gurpreet Singh (Austin, TX/US)

This minisymposium seeks to gather the most recent advancements in numerical and analytical techniques for multiscale methods. The high fidelity simulation of subsurface processes involves highly heterogeneous media, multiple spatial and temporal scales, and large domains. Even under basic modeling assumptions, these systems are computationally intensive and require specialized techniques for efficient solution while preserving accuracy. In particular, this session will include topics on homogenization techniques, adaptive mesh refinement, offline/online calculations, and specialized discretizations.

10:00 Comparison of splitting schemes for
 O141 compositional multiscale solvers
Olav Møyner (Oslo/NO)
Hamdi A. Tchelepi (Stanford, CA/US)

10:20 Adaptive Homogenization for Upscaling
 O142 Heterogeneous Porous Media
Gurpreet Singh, Yerlan Amanbek
Mary F. Wheeler (Austin, TX/US)

10:40 Stable sequential fully implicit scheme allowing
 O143 for compositional multiscale simulation
Arthur Moncorge (Aberdeen/GB)
Patrick Jenny (Zurich/CH)
Hamdi A. Tchelepi (Stanford, CA/US)

11:00 Mathematical model of two-phase
 O144 compositional flow in porous media in vapor intrusion problems
Jakub Solovský, Radek Fučík (Prague/CZ)
Tissa H. Illangasekare (Golden, CO/US)

11:20 Development and comparison of efficient
 O145 constraint-handling techniques for well placement optimization
Mathias Bellout (Trondheim/NO)
Oleg Volkov (Stanford, CA/US)

MS29 Advanced numerical methods in subsurface flow simulations in discrete fracture networks Part 1

10:00–12:00 • Room: Übung 5
 Part 2 see page 39

Chairs: *Sandra Pieraccini, Stefano Berrone (Turin/IT)*
 Jeffrey Hyman (Los Alamos, NM/US)

In several applications related to subsurface exploitation (geothermal applications, geological storage, enhanced oil & gas production...), the underground medium is frequently described by the Discrete Fracture Network (DFN) model, in order to properly account for the directionality of the flow in fractured media. Within the DFN model the fractures are explicitly described, and the flow mainly occurs along the fractures and their intersections. Issues in numerical simulations in DFNs are typically related to: the flow model, the coupling with the surrounding rock matrix, the geometrical complexity of the domain, and the uncertainty both in the hydro-geological and in the geometrical parameters describing the fractures. Recent advances in numerical methods related to these issues will be the primary topic of the minisymposium.

10:00 New approaches for the simulation of flows in
 O146 complex poro-fractured domains with non-conforming meshes
Stefano Berrone, Andrea Borio
Sandra Pieraccini, Stefano Scialo`
Fabio Vicini (Turin/IT)

10:20 Control-Volume Distributed Multi-Point Flux
 O147 Approximation (CVD-MPFA), hybrid-upwind convection, unstructured grids, porous and fractured media
Michael Edwards (Swansea/GB)
Raheel Ahmed (Wuhan/CN)
Yawei Xie (Swansea/GB)

10:40 The role of efficient meshing and discretization
 O148 in modeling flow through discrete fracture networks (DFNs")
Mayur Pal (Doha/QA), Sandip Jadhav (Pune/IN)
Brijesh K. Yadav (Roorkee/IN)

11:00 High-resolution simulations of mass or heat
 O149 transfers using conforming meshes of discrete fracture networks
Tri Dat Ngo, André Fournon
Benoit Noetinger (Rueil Malmaison/FR)

PL1 | Prize lecture 1
“How warm is it getting?” and other tales in uncertainty quantification

13:00–14:00 • Room: H11

Chair: Jodi Mead (Boise, ID/US)

Speaker: Juan Restrepo (Corvallis, OR/US)

In the statistics community “Big Data” science is meant to suggest the combining of inferential and computational thinking. We also speak of big data in the geosciences. However, the problems we pursue are often extreme in the number of degrees of freedom, and in many instances, non-stationary in its statistics. This usually means that we are working with sparse observational data sets, even if the number of observations is large. The Bayesian framework is a natural inferential data assimilation strategy in geosciences, to some extent because the degrees of freedom in the problem vastly outnumber observations but more critically, because the models we use to represent nature have considerable predictive power.

Looking toward the future, we expect improvements in computational efficiency and finer resolutions in models, as well as improved field measurements. This will force us to contend with physics and statistics across scales and thus to think of ways to couple multiphysics and computational resolution, as well as to develop efficient methods for adaptive statistics and statistical marginalization.

How this coupling is exploited to improve estimates that combine model outcomes and data will be described in tracking hurricanes and improving the prediction of the time and place of coastal flooding due to ocean swells. Estimating the trend of Earth’s temperature from sparse multi-scale data will be used as an example of adaptivity in time series analysis.

Other open challenges in non-stationary big data problems will be described, where progress could result from “Big Data Geoscience,” the tighter integration of geoscience, computation, and inference.

MS30
Compositional flow modeling and reactive transport in porous media • Part 1

14:10–16:10 • Room: H11

Part 2 see page 40

Chairs: Mary F. Wheeler, Gergina Pencheva

Benjamin Ganis, Gurpreet Singh (Austin, TX/US)

Many solution schemes exist for compositional flow modeling, following the early developments by Watts, Coates, Acs, and others. Additionally, these schemes may use implicit or explicit methods, complementarity conditions, Jacobian approximations, or other methods. Furthermore, both reactive transport and phase behavior models can be used for determining component partitioning. This session seeks to compare and contrast these methods in terms of computational efficiency and solution accuracy.

14:10 O150 **A fully-implicit reactive flow formulation for a low-salinity water flooding process**

Gergina Pencheva, Gurpreet Singh
 Ashwin Venkataraman
 Mary F. Wheeler (Austin, TX/US)

14:30 O151 **Development of advanced compositional models for hysteresis and foam and their application to EOR processes**

Mary F. Wheeler, Gurpreet Singh
 Mohammad Lotfollahi
 Mohammad Beygi (Austin, TX/US)

14:50 O152 **Study of compositional multiphase flow formulation using complementarity conditions**

Ibtihel Ben Gharbia
Eric Flauraud (Rueil malmaison/FR)
 Irene Lusetti (Milan/IT)

15:10 O153 **Utilization of multi-objective optimization for pulse testing dataset from a geological CO₂ sequestration site**

Baehyun Min (Seoul/KR), Mary F. Wheeler
 Alexander Sun (Austin, TX/US)

15:30 O154 **Mathematical and numerical formulations for multiphase reactive transport in porous media**

Anthony Michel, Thibault Faney
 Sylvain Desroziers (Rueil Malmaison/FR)

15:50 O155 **A multigrid reduction preconditioning strategy for multiphase flow with phase transitions**

Quan Bui (College Park, MD/US), Lu Wang
 Daniel Osei-Kuffuor (Livermore, CA/US)

MS31

HPC advances and trends in simulation tools for flow and transport in geosciences • Part 2

14:10–16:10 • Room: H12

Chairs: *Vadym Aizinger, Harald Köstler (Erlangen/DE)*
Michael Bader (Garching/DE)

Current hardware and software development trends in the area of high performance computing pose a number of specific near-term challenges for developers of numerical models: Improving parallel scaling for large numbers of processes, adding support for GPUs and hybrid execution modes, increasing energy efficiency of simulation packages, and many more. The goal of our mini-symposium is to present methods and tools for performance analysis, modeling, and engineering of applications in Earth sciences as well as to discuss advances in parallel scaling, hybrid and alternative computer architectures, energy efficiency, and all other issues of interest that may be helpful in making numerical simulation software for flow and transport in geophysical problems fit for the emerging computing architectures.

14:10 O156 **Firedrake – Composable abstractions for high performance finite element computations**
Lawrence Mitchell, David Ham, Miklós Homolya
Tianjiao Sun, Fabio Luporini (London/GB)
Andrew McRae (Bath/GB)
Paul Kelly (London/GB)

14:30 O157 **Accelerating the weather and climate model COSMO on heterogeneous architectures**
Hannes Vogt (Lugano/CH), Oliver Fuhrer
Xavier Lapillonne, Carlos Osuna (Zurich/CH)
Thomas Schulthess (Lugano/CH)
Pascal Spörri (Zurich/CH)

14:50 O158 **Preparing ExaStencils for applications in geosciences**
Harald Koestler (Erlangen/DE)

15:10 O159 **The ICON ocean model computational performance; optimization techniques for unstructured grids**
Leonidas Linardakis (Hamburg/DE)

15:30 O160 **To reduce numerical precision to achieve higher accuracy in weather and climate modeling**
Peter Dueben (Reading/GB)

15:50 O161 **Scalable subsurface flow simulations with ParFlow**
Jose A. Fonseca, Carsten Burstedde (Bonn/DE)
Stefan J. Kollet (Jülich/DE)

MS32

Numerical methods towards next generation ice sheet modeling • Part 2

14:10–16:10 • Room: H13

Part 3 see page 45

Chairs: *Irina Tezaur (Livermore, CA/US)*
Xylar Asay-Davis (Potsdam/DE)
Stephen Price (Los Alamos, NM/US)
Katherine J. Evans (Oak Ridge, TN/US)

Mass loss from the polar ice sheets is expected to have a significant contribution to future sea-level changes. Scientifically meaningful projections of sea-level change in the 21st century and beyond require accurate and efficient computational modeling of the Greenland and Antarctic ice sheets. This minisymposium will focus on numerical and computational methods for reliable, next-generation stand-alone and ice sheet models (ISMs). A variety of topics in the areas of ice sheet modeling and simulation will be covered, including: improved modeling of critical physical processes, stable and efficient numerical methods for ISMs, performance-portability of ISMs to new and emerging computer architectures, model verification/validation, data assimilation, mesh generation/adaptation, ice sheet initialization, inverse problems arising in ice sheet modeling, uncertainty quantification, and coupling of ISMs to other climate components.

14:10 O162 **Performance and performance portability of the Albany/FELIX finite element land-ice solver**
Irina Tezaur, Jerry Watkins, Ray Tuminaro
Irina Demeshko (Livermore, CA/US)

14:30 O163 **Mechanical error estimators for shallow ice flow models**
Guillaume Jovet (Zurich/CH)

14:50 O164 **Evaluating the performance of ice sheet models using LIVVkit**
Joseph H. Kennedy, Katherine J. Evans
Andrew R. Bennett
Patrick Worley (Oak Ridge, TN/US)
Matthew Hoffman
Stephen Price (Los Alamos, NM/US)

15:10 O165 **Nonlinear solvers for Stokes thermomechanical ice models**
Hongyu Zhu (Austin, TX/US)
Tobin Isaac (Chicago, IL/US)
Georg Stadler (New York, NY/US)
Omar Ghattas (Austin, TX/US)

15:30 O166 **Phase change with natural convection: Simulation and segmentation of water-ice interfaces**
Kai Schüller, Benjamin Berkels
Julia Kowalski (Aachen/DE)

15:50 O167 **Finite element implementation and verification of a monolithic method for phase-change problems with natural and compositional convection**
Alexander G. Zimmerman
Julia Kowalski (Aachen/DE)

MS33
Krylov-based deflation methods in flow for porous media

14:10–16:10 • Room: Seminarraum Informatik 01.150

 Chairs: *Cornelis Vuik, Gabriela B. Diaz Cortez
Jan-Dirk Jansen (Delft/NL)*

Presently, Krylov subspace methods are among the common approaches for solving linear systems of equations arising in flow through large-scale porous media. Intensive research is needed to develop suitable preconditioners that can account for extreme properties of the media. Is the information of related systems useful to solve the current system in a faster way? The increasing complexity of various subsurface problems has motivated the formulation of more robust preconditioning methods. A more recent technique to enhance the convergence further is the reuse of previous solutions or search direction vectors as deflation vectors. However, a good selection of the available vectors is crucial for an efficient method. One way to select and reduce the number of vectors is to combine it with a Proper Orthogonal Decomposition (POD) approach. The objective of this minisymposium is to promote fruitful discussions to identify commonalities and new avenues of research that may lead to the development of improved robust and efficient deflation preconditioners for problems of flow in porous media. We expect that this interaction may also shed light on other more general, unexplored issues that exist between Krylov subspace methods and domain decomposition/multilevel types of solvers.

- 14:10 O168 **POD-deflation method for highly heterogeneous porous media**
*Gabriela B. Diaz Cortez, Cornelis Vuik
Jan-Dirk Jansen (Delft/NL)*
- 14:30 O169 **Krylov methods applied to reactive transport models**
Jocelyne Erhel (Rennes/FR)
- 14:50 O170 **A feature-enriched multiscale solver for complex geomodels**
*Olav Møyner, Knut-Andreas Lie (Oslo/NO)
Øystein Klemetsdal (Trondheim/NO)*
- 15:10 O171 **Combining model order reduction and preconditioned conjugate gradient for the solution of transient diffusion equations**
*Damiano Pasetto (Lausanne/CH), Mario Putti
Massimiliano Ferronato (Padua/IT)*
- 15:30 O172 **Componentwise time-stepping for radially symmetric PDEs**
*James Lambers
Megan Richardson (Hattiesburg, MS/US)*
- 15:50 O173 **Multigrid KSS methods for time-dependent, variable-coefficient partial differential equations**
Haley Dozier, James Lambers (Hattiesburg, MS/US)

MS34
Understanding the impact of heterogeneity on CO₂ plume spreading and immobilisation

14:10–16:10 • Room: Übung 2

 Chairs: *Stephan K. Matthai (Parkville/AU)
Rudolf Hilfer (Stuttgart/DE)*

Predicting CO₂ plumes in saline aquifers is challenging: the displacement front is unstable due to the low viscosity of CO₂. Different types of saturation patterns can evolve dependent on the flow regime in the aquifer: near-well inertia to viscous-force dominated flow is characterised by viscous and heterogeneity-induced fingering; peripheral buoyancy-capillary dominated flow might evolve into non-compact ganglia migration [2]. Flow property and compositional heterogeneity further implies small-scale spatial variations in force balances and wettability. Which instabilities are captured by current simulation approaches? To what degree are predictions of storage capacity and plume extent compromised by sub-seismic heterogeneity influencing sweep, micro-displacement efficiency, and residual trapping? 20-yr injection at Sleipner, create a plume with a mean CO₂ saturation of 5%, why? This minisymposium focuses on numeric methods and simulation approaches that address these challenges and discontinuous material property variations, including modeling of anisotropy and flow-regime dependent saturation functions in particular.

- 14:10 O174 **The impact of sedimentary facies on plume spreading in fluvial sandstone aquifers as investigated by simulations with a hybrid FEM-FVM embedded discontinuity method**
Stephan K. Matthai (Parkville/AU)
- 14:30 O175 **Hysteresis in relative permeabilities suffices for propagation of saturation overshoot**
Rudolf Hilfer (Stuttgart/DE)
- 14:50 O176 **Reservoir-scale modeling of CO₂ injection with impurities and convective dissolution**
Irina Sin (Melbourne/AU)
- 15:10 O177 **3D geophysical data inversion using quasi-Newton methods with multi-grid preconditioning and its application to CO₂ injection monitoring**
*Lutz Gross, Andrea Codd (St. Lucia/AU)
Stephan K. Matthai (Parkville/AU)*
- 15:30 O178 **Vertically integrated approaches for carbon storage modeling in heterogeneous domains**
*Karl Bandilla (Princeton, NJ/US)
Bo Guo (Stanford, CA/US)
Michael Celia (Princeton, NJ/US)*

MS35

Implementation aspects of reusable and efficient software and algorithms • Part 1

14:10–16:10 • Room: Übung 4

Part 2 see page 42

Chairs: Tobias Elbinger, Balthasar Reuter (Erlangen/DE)

The predictive power of simulation techniques has become a valuable contribution to many fields of science – including geosciences – and researchers have designed powerful methods for many kinds of problems in the last decades. Two crucial points can be identified for the implementation of these methods: i) Reuseable implementations are the key factor for decreasing developing times for different scenarios in terms of “time to implementation”. Proper software design techniques have to be applied. ii) Performance is especially important for very complex problems. Software has to be able to use the power of today’s supercomputers without wasting their resources. This requires in-depth knowledge of hardware aspects. The aim of this minisymposium is to give researchers the chance to present their implementation ideas about reusable and high-performance software, algorithms and packages and to create a base for fruitful discussions about future directions.

- 14:10 Richy: A C++ finite element solver
O180 *Tobias Elbinger, Andreas Rupp, Jens Oberlander, Peter Knabner (Erlangen/DE)*
- 14:30 MRST – An open-source framework for rapid prototyping in subsurface modeling
O181 *Knut-Andreas Lie (Oslo/NO)*
- 14:50 Nonlinear solvers in OPM flow
O182 *Atgeirr Flø Rasmussen (Oslo/NO)*
- 15:10 Dumux – Using DUNE and facilitating the addition of new modeling capabilities
O183 *Bernd Flemisch (Stuttgart/DE)*
- 15:30 Parallel preconditioners for iterative solvers within fully implicit blackoil simulators
O184 *Markus Blatt (Heidelberg/DE)*

MS36

Advanced numerical methods in subsurface flow simulations in discrete fracture networks Part 2

14:10–16:10 • Room: Übung 5

Part 3 see page 55

Chairs: Sandra Pieraccini, Stefano Berrone (Turin/IT)
Jeffrey Hyman (Los Alamos, NM/US)

In several applications related to subsurface exploitation (geothermal applications, geological storage, enhanced oil & gas production...), the underground medium is frequently described by the Discrete Fracture Network (DFN) model, in order to properly account for the directionality of the flow in fractured media. Within the DFN model the fractures are explicitly described, and the flow mainly occurs along the fractures and their intersections. Issues in numerical simulations in DFNs are typically related to: the flow model, the coupling with the surrounding rock matrix, the geometrical complexity of the domain, and the uncertainty both in the hydro-geological and in the geometrical parameters describing the fractures. Recent advances in numerical methods related to these issues will be the primary topic of the minisymposium.

- 14:10 Efficient linear solvers for the numerical simulation of fractured media
O185 *Massimiliano Ferronato, Andrea Franceschini, Carlo Janna (Padua/IT), Nicola Castelletto (Stanford, CA/US), Joshua A. White (Livermore, CA/US)*
- 14:30 A grid convergent discrete fracture/extended finite volume method (DF/XFVM) for poroelastic coupling with flow induced shear failure
O186 *Rajdeep Deb, Patrick Jenny (Zurich/CH)*
- 14:50 A hybrid high-order method for Darcy flows in fractured porous media
O187 *Florent Chave (Milan/IT), Daniele A. Di Pietro (Montpellier/FR), Luca Formaggia (Milan/IT)*
- 15:10 An optimization approach for flow simulations in 3D poro-fractured media
O188 *Fabio Vicini, Stefano Scialo', Stefano Berrone (Turin/IT)*
- 15:30 Fully coupled fluid flow and geomechanical model for reservoir fracturing accounting for poroelastic effects
O189 *Emil Gallyamov (Delft/NL), Timur Garipov (Stanford, CA/US), Denis Voskov, Paul Van den Hoek (Delft/NL)*

MS37

Compositional flow modeling and reactive transport in porous media • Part 2

16:30–18:30 • Room: H11

*Chairs: Mary F. Wheeler, Gergina Pencheva
Gurpreet Singh (Austin, TX/US)*

Many solution schemes exist for compositional flow modeling, following the early developments by Watts, Coates, Acs, and others. Additionally, these schemes may use implicit or explicit methods, complementarity conditions, Jacobian approximations, or other methods. Furthermore, both reactive transport and phase behavior models can be used for determining component partitioning. This session seeks to compare and contrast these methods in terms of computational efficiency and solution accuracy.

- 16:30 O190 **Adaptive vertical equilibrium concept for energy storage in subsurface systems**
Rainer Helmig (Stuttgart/DE)
- 16:50 O191 **Modeling multicomponent diffusions and natural convection in fractured media by discontinuous Galerkin and mixed methods**
Hussein Hoteit (Thuwal/SA)
Abbas Firoozabadi (Palo Alto, CA/US)
- 17:10 O192 **Efficient and stable simulation of compositional grading in hydrocarbon reservoirs**
Shuyu Sun (Thuwal/SA)
Jisheng Kou (Xiaogan/CN)
- 17:30 O193 **Upscaling of a reactive transport model in fractured porous media**
Kundan Kumar, I. Sorin Pop (Bergen/NO; Diepenbeek/BE)
Alessio Fumagalli, Martin Dugstad (Bergen/NO)
- 17:50 O194 **Multi-scale reconstruction of compositional transport**
Chandrashekar Ganapathy
Denis Voskov (Delft/NL)
- 18:10 O195 **Various alternative formulations of the flash equilibrium calculation**
Jiří Mikyška, Tomáš Smejkal
Tereza Petříková (Prague/CZ)
Abbas Firoozabadi (Palo Alto, CA/US)

MS38

Geophysical inversion and imaging

16:30–18:30 • Room: H12

Chairs: Jodi Mead (Boise, ID/US)
Rosemary Renaut (Tempe, AZ/US)

Inverse methods enable modelers to convert geophysical measurements into images of the subsurface. They require accurate and efficient forward models for wave propagation that capture the physics of the data collection technique, and can be run multiple times in an inversion. Even with good forward models imaging is challenging because the inverse process inherently produces non-unique results. Recent advances in inverse methods have made geophysical imaging more stable. This includes using multiple types of data to help constrain the inverse problem, whereby an image is created through joint inversion. The range of geophysical methods includes electrical resistivity, ground penetrating radar, and seismic waves.

- 16:30 O196 **Electrical resistivity imaging with subsurface boundary constraints**
Jodi Mead, Hank Hetrick
John Bradford (Boise, ID/US)
- 16:50 O197 **Some fast algorithms for mathematical modeling and inversion in geophysical exploration**
Jianliang Qian (East Lansing, MI/US)
Shingyu Leung, Eric Chung
Chi-Yeung Lam (Hong Kong/HK)
- 17:10 O198 **A look at surface wave dispersion imaging and deblurring**
T. Dylan Mikesell (Boise, ID/US)
- 17:30 O199 **Some higher-order compact finite difference schemes for acoustic wave equation in heterogeneous media**
Wenyuan Liao (Calgary/CA)
- 17:50 O200 **Application of least square support vector machine and multivariate adaptive regression spline in long term prediction modeling of river water**
Kulwinder S. Parmar
Ozgur Kisi (Hoshiarpur/IN)
- 18:10 O201 **Free geodetic network analysis by selective bias control**
Kyle Snow
Burkhard Schaffrin (Columbus, OH/US)

MS39
Dynamics and data in stochastic systems, far from equilibrium

16:30–18:30 • Room: H13

 Chairs: *Juan Restrepo (Corvallis, OR/US)*
Dan Crisan (London/GB)

The challenges in complex systems are familiar: coupling of physics at different scales, high dimensions, model uncertainty, unresolved scales, etc. Further complications arise when equilibrium ideas arising from statistical physics do not apply. The purpose of this mini-symposium is to foster a cross-fertilization of computational, statistical, and theoretical techniques and strategies, applicable to complex systems, far from equilibrium. We will focus on strategies that combine dynamics, stochasticity, and data. The talks will expand on data-driven, computational as well as theoretical approaches.

- 16:30 **Stochastic modeling of transport noise**
 O202 *Dan Crisan (London/GB)*
- 16:50 **A dynamically driven paradigm for data assimilation in geophysical models**
 O203 *Colin Grudzien, Alberto Carrassi (Bergen/NO)*
Marc Bocquet (Paris/FR)
- 17:10 **Assessing the reliability of ensemble forecasting systems**
 O204 *Jochen Broecker (Reading/GB)*
- 17:30 **Iterative updating of model error in Bayesian inversion for efficient posterior sampling**
 O205 *Matthew Dunlop*
Andrew Stuart (Pasadena, CA/US), Erkki Somersalo
Daniela Calvetti (Cleveland, OH/US)
- 17:50 **Tensor product decomposition methods for compact representations of large data sets**
 O206 *Thomas von Larcher, Rupert Klein*
Reinhold Schneider, Sebastian Wolf (Berlin/DE)

MS40
Uncertainty quantification for nonlinear transport problems in porous media

16:30–18:30 • Room: Seminarraum Informatik 01.150

 Chair: *Per Pettersson (Bergen/NO)*

Numerical simulation of transport in subsurface porous media is prone to uncertainty due to lack of reliable data, model error, and infeasibility of exact mathematical representation. This pertains to a range of applications, covering CO₂ storage to reduce greenhouse gas emission, optimization of the production of an oil field, and energy production in geothermal flow. Efficient uncertainty quantification for these transport problems is challenging, and includes handling of multiple sources of uncertainty, efficient representation of uncertainty despite slow decay of the stochastic modes, and treatment of discontinuities in stochastic space. This mini-symposium targets uncertainty quantification of nonlinear multi-phase transport problems with focus on methods to tackle the aforementioned challenges.

- 16:30 **Data-driven uncertainty quantification for transport problems in structured porous media**
 O207 *Per Pettersson, Anna Nissen (Bergen/NO)*
- 16:50 **A stochastic galerkin method for hyperbolic elliptic systems governing two-phase flow in porous media**
 O208 *Markus Köppel, Ilja Kröker*
Christian Rohde (Stuttgart/DE)
- 17:10 **Underpinning modern random walk models for transport UQ in the heterogeneous subsurface with results from classical perturbation theory**
 O209 *Daniel Meyer (Zurich/CH)*
- 17:30 **Stochastic Galerkin methods with hyperspherical transformation for vertical equilibrium CO₂ migration models**
 O210 *Daniel S. Olderkjær, Per Pettersson (Bergen/NO)*
- 17:50 **Time series parameterization of evolution equations for probability density functions of uncertain concentrations transported in groundwater**
 O211 *Nicolae Suci, Calin Vamos*
Maria Craciun (Cluj-Napoca/RO)
Peter Knabner (Erlangen/DE)

MS41

Extended image volumes

16:30–18:30 • Room: Übung 2

Chairs: *Felix Herrmann (Vancouver/CA)*
Tristan van Leeuwen (Utrecht/NL)

In seismic imaging, the goal is to retrieve detailed quantitative images of the subsurface from seismic reflection data. These data are collected at the surface for various source and receiver locations, leading to a $(2n+1)$ -dimensional data-volume. In the traditional approach, the data are back-propagated in a reference model. This process, called reverse-time migration, yields an n -dimensional image, that shows the location of the various rock-layers. Quantitative information cannot be gleaned from such an image. If the reference model is not kinematically correct, the image will also be distorted. Through an extended imaging procedure, we can obtain an $(2n+1)$ -dimensional image volumes that contain all the information that was present in the original data-set. These extended image volumes can yield both quantitative information about the earth-layers and can be used to detect inaccuracies in the reference model. Gleaning information from these high-dimensional image volumes requires physical insight and state-of-the-art numerical techniques in particular in 3D, where these images become prohibitively large. In this mini-symposium, we aim to bring together researchers who have worked on various aspects of these extended images.

16:30 O212 **Enabling target-oriented imaging for large scale seismic data acquisition using probing techniques**
Rajiv Kumar (Vancouver/CA)

16:50 O213 **Target-enclosing extended imaging – The role of image extensions in pushing resolution limits**
Ivan Vasconcelos (Utrecht/NL)
Matteo Ravasi (Bergen/NO)
Joost van der Neut (Delft/NL)

17:10 O214 **Exploring the dynamics of wavefield correlations**
Tristan van Leeuwen (Utrecht/NL)

17:30 O215 **Low-rank compression of subsurface-offset extended image volumes**
Felix Herrmann (Vancouver/CA)

17:50 O216 **Vertical seismic profiling with distributed acoustic sensing**
Heather Hardeman, Matt McDonald
Michael Lamoureaux (Calgary/CA)

MS42

Implementation aspects of reusable and efficient software and algorithms • Part 2

16:30–18:30 • Room: Übung 4

Chairs: *Tobias Elbinger, Balthasar Reuter (Erlangen/DE)*

The predictive power of simulation techniques has become a valuable contribution to many fields of science – including geosciences – and researchers have designed powerful methods for many kinds of problems in the last decades. Two crucial points can be identified for the implementation of these methods: i) Reusable implementations are the key factor for decreasing developing times for different scenarios in terms of “time to implementation”. Proper software design techniques have to be applied. ii) Performance is especially important for very complex problems. Software has to be able to use the power of today’s supercomputers without wasting their resources. This requires in-depth knowledge of hardware aspects. The aim of this minisymposium is to give researchers the chance to present their implementation ideas about reusable and high-performance software, algorithms and packages and to create a base for fruitful discussions about future directions.

16:30 O217 **Inexact hierarchical scale separation: an efficient linear solver for discontinuous Galerkin discretizations**
Florian Frank (Houston, TX/US)

16:50 O218 **The AMR (Exa)HyPE**
Tobias Weinzierl
Dominic E. Charrier (Durham/GB)

17:10 O219 **TerraNeo – mantle convection modeling and the road to Exa-scale**
Hans-Peter Bunge, Marcus Mohr (Munich/DE)
Ulrich Rüde (Erlangen/DE)
Barbara Wohlmuth (Garching/DE)

17:30 O220 **An efficient tool for transport-reaction modeling with its test application**
Jan Šembera (Brno/CZ), Pavel Štrof (Prague/CZ)
Josef Zeman (Brno/CZ)
Nada Rapantová (Ostrava/CZ)

MS43**Simulation of complex multiphase flows in porous media with the Lattice Boltzmann method**

16:30–18:30 • Room: Übung 5

*Chairs: Ernesto Monaco (Erlangen/DE)
 Jens Harting (Nuremberg/DE)
 Peter Knabner (Erlangen/DE)*

The Lattice Boltzmann method (LBM), is becoming a valuable alternative to Navier-Stokes based simulation tools in the field of coupled processes in porous media at pore- and continuum scale. Its kinetic theory based formulation provides a unique framework for simulating complex processes like multi-phase flows, flows through realistic pore geometries, reactive transport processes with evolving media, etc. This minisymposium aims to bring together researchers involved in the field of porous media and LBM. The featured talks will cover issues like (i) New developments in the theory of LBM related to multiscale formulations, coupling with other numerical methods, new boundary conditions, non-Newtonian fluids (ii) Optimization of porous media layouts (iii) Development and application of LBM for multiphase and reactive transport processes in porous media, in comparison with experiments and/or other numerical techniques.

- 16:30 O221 **Modeling complex multiphase flows with the Lattice Boltzmann method – An introduction**
Ernesto Monaco (Erlangen/DE)
- 16:50 O222 **Mesoscopic simulations of electrokinetic phenomena**
Nicolas Rivas, Jens Harting (Nuremberg/DE)
- 17:10 O223 **Thermal lattice Boltzmann method for catalytic flows through porous media**
Daniel Berger, Jens Harting (Nuremberg/DE)
- 17:30 O224 **Computation of wall shear stresses and characterisation of fluid flow domains by a coupled CFD-MRI method in a medical application**
*Fabian Klemens, Mathias Krause, Gudrun Thäter
 Willy Dörfler (Karlsruhe/DE)*

PS4 | Invited plenary 4
Methane hydrate modeling, analysis, and simulation – Coupled systems and scales

08:30–09:30 • Room: H11

Chair: *Mario Putti (Padua/IT)*

Speaker: *Malgorzata Peszynska (Corvallis, OR/US)*

Methane hydrate is an ice-like substance abundantly present in deep ocean sediments and in the Arctic. Geoscientists recognize the tremendous importance of gas hydrate as a crucial element of the global carbon cycle, a contributor to climate change studied in various deep ocean observatories, as well as a possible energy source evaluated in recent pilot engineering projects in the US and Japan. Hydrate evolution however is curiously not very well studied by computational mathematics community.

In the talk we present the challenges of hydrate modeling, which start with the need to respond to the interests of geophysicists to enable lasting collaborations that deliver meaningful results. Next we present a cascade of complex to simplified models. For the latter, some analysis of the underlying well-posedness in a very weak setting can be achieved. For the former, interesting scenarios involving multiple scales, and coupled phenomena of flow, transport, phase transitions, and geomechanics, can be formulated.

I will report on most recent results obtained jointly with the geophysicists Marta Torres (Oregon State), Wei-Li Hong (Arctic University of Norway), mathematicians Ralph Showalter (Oregon State) and F. Patricia Medina (WPI), computational scientist Anna Trykozko (University of Warsaw), as well as many current and former students to be named in the talk.

MS44
Advances in nonlinear methods for flow and transport modeling

10:00–12:00 • Room: H11

Chairs: *Daniil Svyatskiy (Los Alamos, NM/US)*

Yuri Vassilevski (Moscow/RU)

Modeling of flow and transport processes plays an important role in a wide range of multiphysics applications which include subsurface and surface flows, enhanced oil recovery, reactive transport and others. In complex simulations, the computational mesh has to be fitted to surface topography, subsurface geology, and graded towards small engineering and natural subsurface structures. These requirements create significant challenges for accurate discretization schemes and efficient nonlinear solvers. Efficiency and robustness of the existing solvers rely on many factors, including numerical stability of discretization schemes, quality control of intermediate iterates, complexity and efficiency of a customized preconditioner. This mini-symposium encourages submissions on novel nonlinear solvers and discretization methods for multi-component flows and transport modeling.

- 10:00 O225 **Advances in nonlinear solvers for coupled systems in watershed modeling**
Daniil Svyatskiy (Los Alamos, NM/US)
- 10:20 O226 **A finite volume scheme with improved well modeling in subsurface flow simulation**
Kirill Nikitin, Vasilii Kramarenko (Moscow/RU)
- 10:40 O227 **Nonlinear finite-volume scheme for complex flow processes on corner-point grids**
Martin Schneider, Bernd Flemisch
Rainer Helmig (Stuttgart/DE)
- 11:00 O228 **A hybrid finite volume finite element method for transport modeling in fractured media**
Maxim Olshanskii (Houston, TX/US)
Alexey Chernyshenko
Yuri Vassilevski (Moscow/RU)
- 11:20 O229 **Dynamic adaptive simulations of immiscible viscous fingers**
Alexander Adam, Dimitrios Pavlidis
James Percival, Pablo Salinas (London/GB)
Romain de Loubens (Pau/FR), Christopher Pain
Ann Muggeridge, Matthew Jackson (London/GB)
- 11:40 O230 **Compositional modeling of two-phase flow in porous media using VT-Flash**
Ondřej Polívka, Jiří Mikyška (Prague/CZ)
- 12:00 O415 **A nonlinear domain decomposition method to couple non-isothermal compositional gas liquid Darcy and free gas flows**
Nabil Birgale (Nice, Chatenay-Malabry/FR)
Roland Masson (Nice/FR)
Laurent Trenty (Chatenay-Malabry/FR)

MS45

Multi-resolution three-dimensional modeling of coastal, regional and deep ocean

10:00–12:00 • Room: H12

Chairs: *Vadym Aizinger (Erlangen/DE)*
Sergey Danilov (Bremerhaven/DE)

Rapid increase in available computational power, better resolution and coverage of geophysical data, and advances in mathematical modeling and numerical methodology hold potential to conduct ocean simulations with a much higher spatial and temporal resolution of physical processes of interest or parts of the computational domain. However a number of key modeling, numerical, and computational issues connected with producing multi-resolution simulations using either unstructured meshes or nesting techniques are still open. The goal of this mini-symposium is to discuss recent advances in methodology of multi-resolution ocean modeling and propose ways to deal with still unsolved problems arising in such models.

10:00 **An adaptive numerical method for free surface flows passing rigidly mounted obstacles**

O231

*Yuri Vassilevski**Ruslan Yanbarisov (Moscow/RU)**Maxim Olshanskii (Houston, TX/US)*

10:20 **FESOM-coastal – 3D modeling of coastal long wave dynamics on the mixed meshes**

O232

*Alexey Androsov**Vera Fofonova (Bremerhaven/DE)**Ivan Kuznetsov (Geesthacht/DE), Sergey Danilov**Natalja Rakowsky**Karen Wiltsher (Bremerhaven/DE)*

10:40 **On global ocean dynamics on unstructured grids**

O233

Peter Korn (Hamburg/DE)

11:00 **Ice-sheet/ocean interaction model using high order continuous/discontinuous Galerkin methods with a non-conforming adaptive mesh**

O234

*Michal Koperka (Santa Cruz, CA/US)**Wieslaw Maslowski**Frank Giraldo (Monterey, CA/US)*

11:20 **Parameter estimation, uncertainty quantification and optimization of measurement designs for a biogeochemical model**

O235

Joscha Reimer (Kiel/DE)

MS46

Numerical methods towards next generation ice sheet modeling • Part 3

10:00–12:00 • Room: H13

Chairs: *Irina Tezaur (Livermore, CA/US)*
Xylar Asay-Davis (Potsdam/DE)
Stephen Price (Los Alamos, NM/US)
Katherine J. Evans (Oak Ridge, TN/US)

Mass loss from the polar ice sheets is expected to have a significant contribution to future sea-level changes. Scientifically meaningful projections of sea-level change in the 21st century and beyond require accurate and efficient computational modeling of the Greenland and Antarctic ice sheets. This minisymposium will focus on numerical and computational methods for reliable, next-generation stand-alone and ice sheet models (ISMs). A variety of topics in the areas of ice sheet modeling and simulation will be covered, including: improved modeling of critical physical processes, stable and efficient numerical methods for ISMs, performance-portability of ISMs to new and emerging computer architectures, model verification/validation, data assimilation, mesh generation/adaptation, ice sheet initialization, inverse problems arising in ice sheet modeling, uncertainty quantification, and coupling of ISMs to other climate components.

10:00 **Probabilistic sea-level projections from ice sheet and earth system models**

O236

Stephen Price (Los Alamos, NM/US)

10:20 **A robust and extensible toolkit for ice sheet model validation**

O237

*Katherine J. Evans**Joseph H. Kennedy (Oak Ridge, TN/US)**Mary M. Forrester, Dan Lu (Golden CO/US)*

10:40 **Modeling glacier calving using discrete element and full Stokes continuum models**

O238

*Doug Benn (St Andrews/GB)**Jan Åström, Thomas Zwinger (Espoo/FI)**Joe Todd (St Andrews/GB)*

11:00 **Numerical methods for ice sheet–ocean coupling in the POPSICLES model**

O239

*Xylar Asay-Davis (Berlin/DE)**Daniel Martin (Berkeley, CA/US)*

11:20 **Viscoelastic modeling approaches for glaciological applications**

O240

*Julia Christmann**Ralf Müller (Kaiserslautern/DE)**Martin Rückamp**Thomas Kleiner (Bremerhaven/DE)**Timm Schultz (Bremen/DE), Sebastian Beyer**Angelika Humbert (Bremerhaven/DE)*

11:40 O241 **Ice-free topography of the Svalbard archipelago**
Johannes J. Furst (Erlangen/DE)
Francisco Navarro (Madrid/ES), Toby J. Benham
Julian Dowdeswell (Cambridge/GB)
Rickard Petterson (Uppsala/SE), Katrin Lindback
Jack Kohler (Troms/NO)
Thorsten Seehaus (Erlangen/DE)
Xavier Fettweis (Lige/BE)
Fabien Gillet-Chaulet (Grenoble/FR)
Matthias H. Braun (Erlangen/DE)

MS47
Advances in uncertainty quantification methods for hydrological applications • Part 1

10:00–12:00 • Room: Seminarraum Informatik 01.150
 Part 2 see page 51

Chairs: *Steven Mattis (Garching/DE)*
Clint Dawson (Austin, TX/DE)
Barbara Wohlmuth (Garching/DE)

Hydrological problems including groundwater flow and transport, storm surge, and tsunamis are often complicated by inevitable uncertainties in initial conditions, boundary conditions, and parameter fields. Large-scale simulations and ensemble-based methodologies for uncertainty quantification are now widely used in the analysis of such problems. These simulations are often computationally prohibitive due to high-dimensional parameter spaces and expensive forward models. New techniques for quantifying uncertainty in hydrological problems, especially in large-scale problems, are of utmost interest to the community. This minisymposium focuses on recent advances in uncertainty quantification methodologies and applications to problems in hydrology as well as presenting newer problems for which there is a need for practical uncertainty analysis.

10:00 O242 **Ensemble Kalman filter inference of spatially varying Manning’s n coefficients in the coastal ocean**
Adil Siripatana (Thuwal/SA)
Talea Mayo (Orlando, FL/US)
Clint Dawson (Austin, TX/US)
Omar Knio (Thuwal/SA)
Olivier Le Maitre (Paris/FR)
Ibrahim Hoteit (Thuwal/SA)

10:20 O243 **Surrogate accelerated inversion and propagation of tsunamis for the Indian coast**
Devaraj Gopinathan, Serge Guillas (London/GB)
Debasish Roy, Kusala Rajendran (Bangalore/IN)

10:40 O244 **Uncertainty quantification with graph-based flow/transport models**
Daniel O’Malley, Satish Karra, Jeffrey Hyman
Hari Viswanathan
Gowri Srinivasan (Los Alamos, NM/US)

11:00 O245 **A measure-theoretic stochastic inverse method for parameter estimation in subsurface flows**
Clint Dawson, Jiachuan He (Austin, TX/US)
Steven Mattis (Garching/DE)
Troy Butler (Denver, CO/US), Don Estep
Monty Vesselinov (Fort Collins, CO/US)

11:20 O246 **Path Integrals for flow through porous media**
Marise J. E. Westbroek, Peter R. King
Dimitri D. Vvedensky (London/GB)

11:40 O247 **Temporal oscillations in the porous medium equation – Why harmonic averaging itself is not to blame**
Danielle Maddix, Margot Gerritsen
Luiz Sampaio (Stanford, CA/US)
Anna Nissen (Bergen/NO)

MS48
Flow, reactive transport and deformation in fractured porous media

10:00–12:00 • Room: bung 2

Chairs: *I. Sorin Pop (Bergen/NO; Diepenbeek/BE)*
Rainer Helmig (Stuttgart/DE)

Many natural and technological processes are involving flow, reactive transport and deformation in fractured porous media. The corresponding mathematical models are formulated in terms of coupled systems of nonlinear partial and ordinary differential equations, defined in complex domains and involving different scales in time and space. The talks in this minisymposium will address mathematical and numerical questions related to flow, reactive transport and deformation in porous media. Particular attention will be paid to aspects emerging in heterogeneous and fractured media.

10:00 O248 **Event-driven methods for some geochemical problems**
Luca Formaggia, Anna Scotti, Abramo Agosti
Bianca Giovanardi (Milan/IT)

10:20 O249 **Dynamic multilevel multiscale projection based embedded discrete fracture model**
Matteo Cusini, Mousa Hosseinimehr
Hadi Hajibeygi (Delft/NL)

10:40 O250 **A robust, mass conservative scheme for two phase flow in porous media including Hoelder continuous nonlinearities**
Florin A. Radu, I. Sorin Pop (Bergen/NO; Diepenbeek/BE)
Kundan Kumar, Jan M. Nordbotten (Bergen/NO)

11:00 O251 **Modeling flow in complex faulted media**
Marie-Christine Cacas-Stentz
Guillaume Enchery, Isabelle Faille, Pascal Have
Franoise Willien (Rueil Malmaison/FR)

15:50 O252 **Modeling fractured porous media as coupled porous-medium and free-flow systems**
Iryna Rybak (Stuttgart/DE)

MS49
Advances and applications of periodic and stochastic homogenisation • Part 1

10:00–12:00 • Room: Übung 4

Part 2 see page 52

Chairs: *Nadja Ray (Erlangen/DE)*
Matteo Icardi (Warwick/GB)
Andro Mikelic (Villeurbanne/FR)
Florian Theil (Warwick/GB)

Homogenisation theory has been successfully transferred to porous media, fluid dynamics, and material science problems in the last decades. More recently, connections with numerical methods and statistical techniques are emerging. In this mini-symposium, a particular focus will be devoted to: random porous materials and connection with uncertainty quantification- multiscale computational techniques- problems in deformable media or where scales are not fully separable- applications to environmental, engineered, and biological porous media

- 10:00
O253 **Sequential homogenization of reactive transport in polydisperse porous media**
Ilenia Battiatto
Svyatoslav Korneev (Stanford, CA/US)
- 10:20
O254 **Challenges of micro-meso-macro porous media**
Malgorzata Peszynska
Anna Trykozko (Corvallis, OR/US)
- 10:40
O255 **On numerical upscaling of reactive flow in porous media with application to adsorption of MCPA in goethite**
Torben Prill, Oleg Iliev (Kaiserslautern/DE)
Frieder Enzmann, Michael Kersten (Mainz/DE)
- 11:00
O256 **Upscaling reactive ion transport under dominant flow conditions**
Nadja Ray, Raphael Schulz (Erlangen/DE)
Kundan Kumar (Bergen/NO)
- 11:20
O257 **Discrete-continuum multiscale model for transport, biofilm development and solid restructuring in porous media**
Andreas Rupp, Nadja Ray, Alexander Prechtel
Peter Knabner (Erlangen/DE)
- 11:40
O258 **A stochastic approach on aggregate development based on diffusion-limited aggregation**
Thomas Ritschel, Uwe Totsche (Jena/DE)

MS50
Modeling approaches for flow and transport in discrete fracture networks

10:00–11:20 • Room: Übung 5

Chairs: *Stefano Berrone (Turin/IT)*
Jeffrey Hyman (Los Alamos, NM/US)

Discrete Fracture Network (DFN) models explicitly represent interconnected fractures that are the principal pathways for flow and associated transport through low-permeability media. While this increase in detail allows DFN to model a wider range of transport phenomena than traditional continuum methods the inclusion of detailed geometry and hydrological attributes results in higher degrees of uncertainty with respect to these parameters. The focus of this mini-symposium will be on recent advances in modeling techniques using DFN for flow and transport through fracture networks, with a particular focus on model calibration, increased detail and realism, uncertainty quantification, and analytic expressions for transport.

- 10:00
O259 **Accurate and efficient predictions of first passage times in sparse discrete fracture networks using graph-based reductions**
Jeffrey Hyman, Aric Hagberg, Gowri Srinivasan
Jamaludin Mohd-Yusof
Hari Viswanathan (Los Alamos, NM/US)
- 10:20
O260 **Anomalous transport in disordered fracture networks – evolution of the lagrangian velocity distribution and CTRW model for arbitrary injection modes**
Peter K. Kang (Seoul/KR)
Marco Dentz (Barcelona/ES)
Tanguy Le Borgne (Rennes/FR)
Seunghak Lee (Seoul/KR)
Ruben Juanes (Cambridge, MA/US)
- 10:40
O261 **The mechanisms of anomalous transport in heterogeneous media: From medium structure to stochastic particle motion**
Marco Dentz, Alessandro Comolli
Vivien Hakoun (Barcelona/ES)
- 11:00
O262 **An integrated mathematical-geological workflow for fractured geothermal system in metamorphic rocks**
Alessio Fumagalli, Eirik Keilegavlen (Bergen/NO)

QF5

Poster quick fire session 5

11:20–12:00 • Room: Übung 5

Chairs: *Stefano Berrone (Turin/IT)*
Jeffrey Hyman (Los Alamos, NM/US)

11:20 P31 **A topology based simulated annealing framework to generate fracture networks for geothermal systems**

Alessio Fumagalli, Eirik Keilegavlen
Pål Næverlid Sævik (Bergens/NO)

11:24 P32 **Pilot-point ensemble Kalman filter for permeability estimation tested in synthetic tracer-test**

Johannes Keller (Aachen/DE)
Harrie-Jan Hendricks Franssen (Jülich/DE)
Gabriele Marquart (Aachen/DE)
Wolfgang Nowak (Stuttgart/DE)

11:28 P33 **A newly derived one step computational algorithm for the solution of initial value problems**

Bosede Roseline (Ado Ekiti/NG)

11:32 O179 **Propagation of saturation overshoots for two phase flow in porous media**

Tobias Köppl, Martin Schneider
Rainer Helmig (Stuttgart/DE)

11:36 P51 **Space-time domain decomposition methods and a posteriori error estimates for the subsurface**

Elyes Ahmed (Villetaneuse, Paris/FR)
Sarah Ali Hassan (Paris/FR)
Caroline Japhet (Villetaneuse/FR)
Michel Kern, Martin Vohralik (Paris/FR)

PS5 | Invited plenary 5

High resolution atmospheric turbulence simulations for applied problems

13:00–14:00 • Room: H11

Chair: *Jörn Behrens (Hamburg/DE)*
Speaker: *Siegfried Raasch (Hanover/DE)*

Originally applied to study convective atmospheric boundary layers (CBL), large-eddy simulation (LES) is meanwhile used in many fields of science. This is mainly the consequence of a massive increase in available computer resources. State-of-the-art massively parallel computers have opened the field for a wide variety of new applications. On these machines, simulations with extremely large numerical grids of up to 40003 grid points and even more are currently carried out in acceptable time. In Meteorology, beside for the fundamental research of neutral and stable stratified flows, where the typical eddy size is much smaller than for pure convectively driven flows, LES starts to be used also for more applied topics like air pollution modeling, flow around buildings, or wind energy. Moreover, the interaction of turbulence of different scales can be studied for the first time. Lagrangian particle models coupled to LES allow for further interesting applications, e.g. to calculate footprints of turbulence sensors in heterogeneous terrain, or to simulate the effect of turbulence on the growth of cloud droplets. Respective simulations require both, a large model domain size to capture the large scales and a sufficiently fine grid spacing to resolve the interacting smaller scales, creating a very high demand on computational resources.

The talk will start with a short general introduction to LES and will then give an overview of current studies with very high spatial resolution performed at IMUK, like simulations of coherent structures in the convective boundary layer, simulations of the urban environment, and the effect of turbulence on cloud droplet growth or aircraft during takeoff and landing, as well as LES applications for wind energy systems.

MS51
Recent advances in numerical flow and transport in porous media – a mini symposium in honor of the late Jim Douglas, Jr. • Part 1

14:10–15:30 • Room: H11

Part 2 see page 52

Chairs: Todd Arbogast (Austin, TX/US)
 Malgorzata Peszynska (Corvallis, OR/US)
 Son-Young Yi (Austin, TX/US)

In this minisymposium, speakers discuss their recent work in areas pioneered by Jim Douglas, Jr. In particular, discussion will focus on numerical algorithms for the accurate simulation of flow, transport, geochemistry, phase behavior, and geomechanics phenomena in porous materials. Of special interest are applications to petroleum reservoir production and groundwater hydrology.

14:10 The Douglas School of porous media
 O263 Ralph Showalter (Corvallis, OR/US)

14:30 On the extension of the Douglas/Arbogast dual
 O264 positivity models for shale gas reservoirs
 containing natural and hydraulic fractures
 Marcio Murad, Aline Rocha
 Eduardo Garcia (Petrópolis, Rio de Janeiro
 Brasil/BR), Adolfo Puime (macae/BR)

14:50 Elliptic equations in heterogeneous media with
 O265 highly anisotropic fibres
 Li-Ming Yeh (Hsinchu/TW)

15:10 Two modes of locking in poroelasticity – Causes
 O266 and remedies
 Son-Young Yi (El Paso, TX/US)

QF6
Poster quick fire session 6

15:30–16:10 • Room: H11

Chairs: Todd Arbogast (Austin, TX/US)
 Malgorzata Peszynska (Corvallis, OR/US)
 Son-Young Yi (Austin, TX/US)

15:30 Reactive transport simulations with iCP
 P34 (Interface Comsol-Phreeqc) v1.3.1 and iCP Apps
 Alvaro Sainz-Garcia, David Negro
 Diego Sampietro, Emilie Coene, Elena Abarca
 Andres Idiart, Marcelo Laviña, Orlando Silva
 Jorge Molinero (Barcelona/ES)

15:34 Finite volume discretizations for coupled
 P35 thermo-mechanical problems
 Ivar Stefansson, Inga Berre
 Eirik Keilegavlen (Bergen/NO)

15:38 Time adaptive domain decomposition method
 P36 for non-linear reactive transport problems
 Yerlan Amanbek, Gurpreet Singh
 Mary F. Wheeler (Austin, TX/US)

15:42 Mathematical modeling of reactive transport in
 P37 porous media with mineral precipitation-
 dissolution – Uniqueness and nonnegativity of
 solutions
 Serge Krättele, Peter Knabner (Erlangen/DE)
 Joachim Hofmann (Nuremberg/DE)

15:46 StoichPack – A general C++-library for treating
 P38 stoichiometries in multi-species transport
 problems
 Tobias Elbinger, Peter Knabner (Erlangen/DE)

15:50 First steps towards a simulation tool to predict
 P39 the long-time performance of geothermal
 plants – Changes in permeability by dissolution
 and precipitation
 Manfred W. Wuttke, Dennis Hiller (Hanover/DE)

15:54 Numerical model of coupled free gas and
 P40 hydrate
 Choah Shin
 Malgorzata Peszynska (Corvallis, OR/US)

15:58 A pseudo-vertical equilibrium model for slow
 P41 gravity drainage dynamics
 Beatrix Becker (Stuttgart/DE)
 Bo Guo (Stanford, CA/US), Karl Bandilla
 Michael Celia (Princeton, NJ/US), Bernd Flemisch
 Rainer Helmig (Stuttgart/DE)

16:02 The “Open Porous Media Initiative” (OPM)
 P42 software
 Kai Bao (Oslo/NO)
 Markus Blatt (Heidelberg/DE)
 Atgeirr Flø Rasmussen (Oslo/NO)

16:06 Implementation of efficient global optimization
 P43 algorithm for well placement optimization
 Einar Baumann
 Mathias Bellout (Trondheim/NO)

MS52
Multi-resolution three-dimensional modeling of coastal, regional, and deep ocean • Part 2

14:10–15:30 • Room: H12

Part 3 see page 64

Chairs: Vadym Aizinger (Erlangen/DE)
 Sergey Danilov (Bremerhaven/DE)

Rapid increase in available computational power, better resolution and coverage of geophysical data, and advances in mathematical modeling and numerical methodology hold potential to conduct ocean simulations with a much higher spatial and temporal resolution of physical processes of interest or parts of the computational domain. However a number of key modeling, numerical, and computational issues connected with producing multi-resolution simulations using either unstructured meshes or nesting techniques are still open. The goal of this mini-symposium is to discuss recent advances in methodology of multi-resolution ocean modeling and propose ways to deal with still unsolved problems arising in such models.

- 14:10
O267 Non-hydrostatic projection method for dispersive wave modeling with discontinuous Galerkin methods
Jörn Behrens, Anja Jeschke
Stefan Vater (Hamburg/DE)
- 14:30
O268 High-resolution baroclinic modeling using discontinuous Galerkin method
Vadym Aizinger, Balthasar Reuter (Erlangen/DE)
- 14:50
O269 Soret and dufour effects on thermohaline convection in rotating fluids
Thama Duba, Maharaj Marudappa Shekar
Mahesha Narayana, Precious Sibanda (Durban/ZA)
- 15:10
O403 A new coastal ocean modeling framework with applications in renewable energy
Stephan Kramer, Matthew Piggott
Tuomas Kärrnä, Lawrence Mitchell (London/GB)

QF7
Poster quick fire session 7

15:30–16:10 • Room: H12

- Chairs: Vadym Aizinger (Erlangen/DE)*
Sergey Danilov (Bremerhaven/DE)
- 15:30
P44 A shallow water model for roof modeling in free surface flow
Fabien Wahl, Edwige Godlewski, Cindy Guichard
Martin Parisot (Paris/FR), Jacques Sainte-Marie
(Margny-Lès-Compiègne/FR)
- 15:34
P45 Multi-scale numerical simulation of a tsunami using mesh adaptive methods
Joe Wallwork (London/GB)
- 15:38
P46 Dynamical reconstruction of AMOC variability at the mouth of the South Atlantic
Timothy Smith, Patrick Heimbach (Austin, TX/US)
- 15:42
P47 A comparison between intrusive and non-intrusive spectral projection method with implementation on shallow water system
Chen Chen (Austin, TX/US)
- 15:46
P48 A new D-Flow FM (flexible mesh) shallow water model for Lake Marken
Menno Genseberger, Christophe Thiange
Asako Fujisaki, Carlijn Eijsberg-Bak, Jamie Morris
Migena Zagonjulli, Mart Borsboom, Alfons Smale
Pascal Boderie (Delft/NL)
- 15:50
P49 Towards an integrated hydrodynamic, waterquality, and ecological modeling approach for Lake IJssel and Lake Marken
Menno Genseberger (Delft/NL)
- 15:45
P50 Derivation of a bedload transport model with nonlocal effects
Lea Boittin (Paris/FR)
Emmanuel Audusse (Villetaneuse/FR)
Martin Parisot, Jacques Sainte-Marie (Paris/FR)

MS53
Mimetic discretizations in geoscience and advances in geologic carbon sequestration modeling • Part 1

14:10–16:10 • Room: H13

Chairs: Jose Castillo
Christopher Paolini (San Diego, CA/US)

This symposium focuses on research topics related to the numerical simulation of geologic CO₂ sequestration. Presentations will address numerical schemes, algorithms, and data structures suitable for CO₂ storage simulation on high-performance computing infrastructure. Topics will address geochemical, geothermal, and geomechanical effects of high-pressure CO₂ injection in deep saline formations and depleted oil-and-gas reservoirs that typically reside 1000m–4000m below the surface. Specific topics include the thermal effects of solute interaction during carbonation and water-rock reactions, numerical modeling of fracture prediction and characterization, and changes in rock porosity and permeability based on rock stresses and strains induced by injection, modeling reservoir pressure using a diffusive pore pressure approach, and the use of high-order mimetic discretization methods to model solute species mass transport. We will also demonstrate a new, open-source, object-oriented, and distributed-parallel capable software application for modeling CO₂ storage in saline formations that is available to the academic community.

- 14:10
O271 High order compact mimetic methods
Jose Castillo (San Diego, CA/US)
- 14:30
O272 Applications of mimetic methods to geophysical imaging
Josep De La Puente, Miguel Ferrer
Otilio Rojas (Barcelona/ES)
- 14:50
O273 An intragranular microfracture model for geologic sequestration of CO₂
Jonathan Matthews, Christopher Paolini
Jose Castillo (San Diego, CA/US)
- 15:10
O274 Regularization schemes in the CSEM inversion problem
Eduardo Sanchez (Barcelona/ES)

MS54
Advances in uncertainty quantification methods for hydrological applications • Part 2

14:10–16:10 • Room: Seminarraum Informatik 01.150

Chairs: *Steven Mattis (Garching/DE)*
Clint Dawson (Austin, TX/DE)
Barbara Wohlmuth (Garching/DE)

Hydrological problems including groundwater flow and transport, storm surge, and tsunamis are often complicated by inevitable uncertainties in initial conditions, boundary conditions, and parameter fields. Large-scale simulations and ensemble-based methodologies for uncertainty quantification are now widely used in the analysis of such problems. These simulations are often computationally prohibitive due to high-dimensional parameter spaces and expensive forward models. New techniques for quantifying uncertainty in hydrological problems, especially in large-scale problems, are of utmost interest to the community. This minisymposium focuses on recent advances in uncertainty quantification methodologies and applications to problems in hydrology as well as presenting newer problems for which there is a need for practical uncertainty analysis.

 14:10 **Quantification of decision uncertainties**

 O275 *Velimir Vesselinov*
Daniel O'Malley (Los Alamos, NM/US)

 14:30 **Fast and scalable bathymetry inversion in riverine and near-shore environments**

 O276 *Matthew Farthing (Vicksburg, MS/US)*
Jonghyun Lee (Vicksburg, MS/US, Stanford, CA/US)
Hojat Ghorbanidehno (Stanford, CA/US)
Tyler Hesser
Matthew Geheran (Vicksburg, MS/US)
Eric Darve, Peter Kitanidis (Stanford, CA/US)

 14:50 **Goal-oriented adaptive sampling for groundwater problems**

 O277 *Steven Mattis*
Barbara Wohlmuth (Garching/DE)

 15:10 **Do we need to include short length scale variability in reservoir models?**

 O278 *Hossam Osman (London/GB), Gavin Graham*
Arthur Moncorge (Aberdeen/GB)
Matthew Jackson (London/GB)

 15:30 **Characterization of modern river deltas using remote sensing data**

 O279 *Erik Nesvold, Tapan Mukerji (Stanford, CA/US)*
MS55
Data assimilation in terrestrial hydrosystems Part 1

14:10–16:10 • Room: Übung 2

Part 2 see page 54

Chairs: *Insa Neuweiler (Hanover/DE)*
Harrie-Jan Hendricks Franssen (Jülich/DE)
Clemens Simmer (Bonn/DE)

Integrated hydrological models allow for the representation of water and energy fluxes as internal fluxes instead of prescribing them as boundary forcing in compartmental models. Internal flux coupling allows for cross-compartmental influences of assimilated measurements on the system state analysis and may enhance model predictions. As an example, remotely sensed soil moisture data can help to improve the characterization of soil states, the aquifer beneath, vegetation, and the atmospheric boundary layer. In the mini-symposium we will have contributions on data assimilation with terrestrial hydrosystem models from scientists of a variety of fields, ranging from atmospheric science to hydrogeology and petroleum engineering. The presentations address topics such as multi-scale and multi-variate data assimilation methods or discuss the benefits and challenges of cross-compartmental data assimilation. The mini-symposium will provide a platform for scientific exchange among researchers working on data assimilation theory, methods and applications.

 14:10 **Assimilation of satellite humidity information within the ICON EnVar system at the DWD**

 O280 *Stefanie Hollborn (Offenbach/DE)*

 14:30 **Hydrological data assimilation using the Particle Batch Smoother**

 O281 *Susan Steele-Dunne, Jianzhi Dong, Yang Lu*
Nick van de Giesen (Delft/NL)

 14:50 **Effects of subsurface conceptualization on the assimilation of soil moisture data:**

 O282 **An example from the Rur catchment**
Wolfgang Kurtz (Jülich/DE), Mauro Sulis
Prabhakar Shrestha, Stefan J. Kollet (Jülich/DE Bonn/DE), Harry Vereecken
Harrie-Jan Hendricks Franssen (Jülich/DE)

 15:10 **Determination of the relevant spatial scale for reservoir simulation**

 O283 *Stephan de Hoop, Denis Voskov*
Femke Vossepoel (Delft/NL)

MS56

Advances and applications of periodic and stochastic homogenisation • Part 2

14:10–16:10 • Room: Übung 4

Part 3 see page 58

Chairs: Nadja Ray (Erlangen/DE)
Matteo Icardi (Warwick/GB)
Andro Mikelic (Villeurbanne/FR)
Florian Theil (Warwick/GB)

Homogenisation theory has been successfully transferred to porous media, fluid dynamics, and material science problems in the last decades. More recently, connections with numerical methods and statistical techniques are emerging. In this mini-symposium, a particular focus will be devoted to: - random porous materials and connection with uncertainty quantification- multiscale computational techniques- problems in deformable media or where scales are not fully separable- applications to environmental, engineered, and biological porous media

14:10 O284 **An analysis of variance reduction methods in stochastic homogenization**
Julian Fischer (Klosterneuburg/AT)

14:30 O285 **Stochastic homogenization of porous visco plastic materials based on a measure theoretic approach**
Sergiy Nesenenko (Berlin/DE)

14:50 O286 **Stokes flows in rough fractures**
Daniel M Tartakovsky (Stanford, CA/US)

15:10 O287 **Boundary layers in periodic homogenization**
Christophe Prange (Talence/FR)

15:30 O288 **Analysis and simulation of the Newman model**
Florian Theil, Matteo Icardi (Coventry/GB)

15:50 O289 **Homogenisation of thin periodic frameworks with high-contrast inclusions**
Kiril Cherednichenko (Bath/GB)

MS57

Modeling approaches for flow and transport in discrete fracture networks • Part 2

14:10–16:10 • Room: Übung 5

Chairs: Stefano Berrone (Turin/IT)
Jeffrey Hyman (Los Alamos, NM/US)

Discrete Fracture Network (DFN) models explicitly represent interconnected fractures that are the principal pathways for flow and associated transport through low-permeability media. While this increase in detail allows DFN to model a wider range of transport phenomena than traditional continuum methods the inclusion of detailed geometry and hydrological attributes results in higher degrees of uncertainty with respect to these parameters. The focus of this mini-symposium will be on recent advances in modeling techniques using DFN for flow and transport through fracture networks, with a

particular focus on model calibration, increased detail and realism, uncertainty quantification, and analytic expressions for transport.

14:10 O290 **An optimization approach for flow simulations in 3D poro-fractured media**
Stefano Berrone, Sandra Pieraccini, Stefano Scialo' (Turin/IT)

14:30 O291 **Conditioned simulation of discrete fracture networks using structural and hydraulic data from the ONKALO underground research facility, Finland**
Steven Baxter, Lee Hartley, Pete Appleyard, Thomas Williams (Didcot/GB), Lasse Koskinen, Outi Vanhanarkaus (Olkiluoto/FI), Jan-Olof Selroos, Raymond Munier (Stockholm/SE)

14:50 O292 **Flow channelling in discrete fracture networks with connected and disconnected permeability fields**
Andrew Frampton (Stockholm/SE), Jeffrey Hyman (Los Alamos, NM/US)

15:10 O293 **Modeling of fluid flow and solute mixing in 3D rough-walled rock fracture intersections**
Liangchao Zou, Lanru Jing, Vladimir Cvetkovic, Andrew Frampton (Stockholm/SE)

MS58

Recent advances in numerical flow and transport in porous media – A mini symposium in honor of the late Jim Douglas, Jr. • Part 2

16:30–18:30 • Room: H11

Chairs: Todd Arbogast (Austin, TX/US)
Malgorzata Peszynska (Corvallis, OR/US)
Son-Young Yi (Austin, TX/US)

In this minisymposium, speakers discuss their recent work in areas pioneered by Jim Douglas, Jr. In particular, discussion will focus on numerical algorithms for the accurate simulation of flow, transport, geochemistry, phase behavior, and geomechanics phenomena in porous materials. Of special interest are applications to petroleum reservoir production and groundwater hydrology.

16:30 O294 **Virtual Element Methods (VEM) for porous media flow**
Paola Pietra (Pavia/IT)

16:50 O295 **A primal-dual finite element method with application to fluid flow in porous media**
Junping Wang (Arlington/US), Yujie Liu, Qingsong Zou (Guangzhou/CN)

17:10 O296 **A generalized multiscale method with Robin boundary conditions for porous media flows**
Roberto Ausas, Gustavo Buscaglia, Rafael Guiraldello (Sao Carlos/BR), Felipe Pereira, Fabricio S. Sousa (Plano, TX/US)

- 17:30 On implicit finite volume WENO schemes for
O297 convection diffusion equation
Chieh-Sen Huang (Kaohsiung/TW)
Todd Arbogast (Austin, TX/US)
- 17:50 Simulating polymer flooding using implicit
O298 high-resolution methods
Trine S. Mykkeltvedt (Bergen/NO)
Knut-Andreas Lie, Xavier Raynaud (Oslo/NO)
- 18:10 Mathematical and computational efficiency for
O299 the subsurface solute transport under a radial
flow field
Mohammed Abdulhameed (Bauchi/NG)

MS59

Standard and nonstandard models and numerical methods for complex porous media flows with applications

16:30–18:30 • Room: H12

Chairs: Prabir Daripa (College Station, TX/US)
S. Majid Hassanizadeh (Utrecht/NL)

In this minisymposium, the speakers will present standard and non-standard fluid flow models of simple and complex fluids through porous media that arise in displacement processes of many injection policies of oil recovery including chemical enhanced oil recovery. New numerical methods based on new global pressure based formulations modeling multiphase multi-component multi-physics porous media flows in heterogeneous media will be presented. Numerical simulation results for chemical enhanced oil recovery by polymer-surfactant flooding will be presented. Fundamentals of well stimulation of gas wells will be addressed.

- 16:30 Chemical enhanced oil recovery driven models
O300 and methods for multiphase multicomponent
Newtonian and non-Newtonian/viscoelastic
porous media flows
Prabir Daripa (College Station, TX/US)
- 16:50 Nonstandard models for two-phase flow in
O301 porous media
S. Majid Hassanizadeh (Utrecht/NL)
- 17:10 Numerical methods for the Darcy-Brinkman
O302 two phase flow in porous media
Mazen Saad
Houssein Nasser El Dine (Nantes/FR)
- 17:30 Application of water-induced, self-conforming
O303 and multifunctional stimulation of gas wells:
Fundamentals and case histories
Istvan Lakatos (Miskolc/HU)
- 17:50 Enhancing subsurface transport by Lagrangian
O304 chaos
Michel Speetjens, Stephen Varghese
Ruben Trieling (Eindhoven/NL)

- 18:10 Assessment of feasible strategies for seasonal
O305 underground hydrogen storage in a saline
aquifer
Alvaro Sainz-Garcia (Barcelona/ES; Toulouse/FR)
Elena Abarca, Violeta Rubi
Fidel Grandia (Barcelona/ES)

MS60

Mimetic discretization methods in geoscience and advances in geologic carbon sequestration modeling • Part 2

16:30–18:30 • Room: H13

Chairs: Jose Castillo
Christopher Paolini (San Diego, CA/US)

This symposium focuses on research topics related to the numerical simulation of geologic CO₂ sequestration. Presentations will address numerical schemes, algorithms, and data structures suitable for CO₂ storage simulation on high-performance computing infrastructure. Topics will address geochemical, geothermal, and geomechanical effects of high-pressure CO₂ injection in deep saline formations and depleted oil-and-gas reservoirs that typically reside 1000m–4000m below the surface. Specific topics include the thermal effects of solute interaction during carbonation and water-rock reactions, numerical modeling of fracture prediction and characterization, and changes in rock porosity and permeability based on rock stresses and strains induced by injection, modeling reservoir pressure using a diffusive pore pressure approach, and the use of high-order mimetic discretization methods to model solute species mass transport. We will also demonstrate a new, open-source, object-oriented, and distributed-parallel capable software application for modeling CO₂ storage in saline formations that is available to the academic community.

- 16:30 Mimetic discretization methods in geoscience
O306 and advances in geologic carbon sequestration
modeling
Trevor Hawkins (San Diego, CA/US)
- 16:50 Modeling multiphase buoyancy driven plume
O307 migration during geologic CO₂ injection
Kyle Campbell, Christopher Paolini
Jose Castillo (San Diego, CA/US)
- 17:10 Mimetic discretization methods on overlapping
O308 grids
Angel Boada, Jose Castillo (San Diego, CA/US)
- 17:30 Simulation of hydrocarbon pollution removal
O309 from subsoil by bioventing
Filippo Notarnicola (Bari/IT)

MS61

**Physics-based rupture and tsunami simulation
Part 1**

16:30–18:30 • Room: Seminarraum Informatik 01.150

Part 2 see page 62

Chairs: *Stefan Vater (Hamburg/DE)*
Michael Bader (Garching/DE)
Alice-Agnes Gabriel (Munich/DE)

Despite active research, the source mechanisms leading to recent tsunamogenic earthquakes and resulting devastating inundation events still raise a lot of questions. Effects of complex rupture mechanics on displacement of the ocean floor, or of hydrodynamic wave behavior during generation and propagation of tsunami remain challenges for physics-based earthquake and tsunami simulation. This minisymposium strives to review current development in this field – and brings together complex source modeling and coupled tsunami modeling. Algorithmic approaches and discretization methods for the complex multi-scale problems will be discussed, as well as results of large-scale simulations of earthquakes and tsunamis.

- 16:30 O310 **Large-scale multi-physics simulation of the 2004 Sumatra-Andaman earthquake**
Elizabeth H. Madden, Thomas Ulrich
Alice-Agnes Gabriel (Munich/DE)
- 16:50 O311 **Physics-based numerical simulations of earthquake ground motion in the Beijing area**
Ilario Mazzieri, Chiara Smerzini
Paola F. Antonietti, Roberto Paolucci (Milan/IT)
Alfio Quarteroni (Milan/IT; Lausanne/CH)
Marco Stupazzini (Munich/DE)
- 17:10 O312 **Modeling rupture of Dip-Slip Faults with variable Dip and heterogeneous stress fields: Implications for corresponding tsunamis**
Kenny Ryan, Eric Geist (Menlo Park, CA/US)
David Oglesby (Riverside, CA/US)
- 17:30 O313 **Large scale dynamic rupture simulations of the 2004 Sumatra earthquake**
Carsten Uphoff, Michael Bader (Garching/DE)
Alice-Agnes Gabriel (Munich/DE)
- 17:50 O314 **A well-balanced meshless tsunami propagation and inundation model**
Rüdiger Brecht (St. John's/CA)

MS62

**Data assimilation in terrestrial hydrosystems
Part 2**

16:30–18:30 • Room: Übung 2

Chairs: *Insa Neuweiler (Hanover/DE)*
Harrie-Jan Hendricks Franssen (Jülich/DE)
Clemens Simmer (Bonn/DE)

Integrated hydrological models allow for the representation of water and energy fluxes as internal fluxes instead of prescribing them as boundary forcing in compartmental models. Internal flux coupling allows for cross-compartmental influences of assimilated measurements on the system state analysis and may enhance model predictions. As an example, remotely sensed soil moisture data can help to improve the characterization of soil states, the aquifer beneath, vegetation, and the atmospheric boundary layer. In the mini-symposium we will have contributions on data assimilation with terrestrial hydrosystem models from scientists of a variety of fields, ranging from atmospheric science to hydrogeology and petroleum engineering. The presentations address topics such as multi-scale and multi-variate data assimilation methods or discuss the benefits and challenges of cross-compartmental data assimilation.

The mini-symposium will provide a platform for scientific exchange among researchers working on data assimilation theory, methods and applications.

- 16:30 O315 **Challenges and issues of data assimilation for Richards equation-based integrated hydrological models**
Matteo Camporese, Anna Botto (Padua/IT)
- 16:50 O316 **Data assimilation in integrated groundwater: Surface water hydrological modeling**
Henrik Madsen, Marc Ridler (Horsholm/DK)
- 17:10 O317 **Simplified subsurface modeling – Data assimilation and violated model assumptions**
Daniel Erdal (Tübingen/DE), Natascha Lange
Insa Neuweiler (Hanover/DE)
Olaf A. Cirpka (Tübingen/DE)
- 17:30 O318 **Generic approaches to reducing data assimilation Monte-Carlo error for subsurface applications**
Kristian Fossum, Trond Mannseth
Andreas S. Stordal (Bergen/NO)
- 17:50 O319 **The transversal method of lines for the numerical solution of 1D Richards' equation**
Marco Berardi (Bari/IT)
Fabio Difonzo (Santeramo/IT), Michele Vurro
Luciano Lopez (Bari/IT)

MS63

Computational methods for flow in subsurface porous media • Part 1

16:30–18:30 • Room: Übung 4

Part 2 see page 59

Chairs: Michael Edwards (Swansea/GB)
Hadi Hajibeygi (Delft/NL)

This mini-symposium is on recent developments in numerical methods for modeling flow in subsurface porous media. This includes locally conservative finite-volume and finite element methods, multiscale modeling and upscaling. Elliptic and hyperbolic PDE approximation issues are addressed for single and multiphase flow including higher resolution, accuracy and efficiency on structured and unstructured grids, with application to problems that include full tensor permeability fields, faults and fractures.

- 16:30 **Upscaling for flow in porous media**
O320 *Peter R. King (London/GB)*
- 16:50 **A robust implicit scheme for two-phase flow in porous media**
O320 *Anna Kvashchuk (Bergen/NO)*
Robert Klöfkorner (Stavanger, Bergen/NO)
Florin A. Radu (Bergen/NO)
- 17:10 **Hybrid discretization of multi-phase flow in porous media in the presence of viscous, gravitational and capillary forces**
O322 *Seong Lee (Houston, TX/US)*
Yalchin Efendiev (College Station, TX/US)
- 17:30 **Consistent non-local flow formulation and stochastic transport**
O323 *Patrick Jenny, Daniel Meyer (Zurich/CH)*
- 17:50 **Upscaling of finite volume discretizations using graph-based spectral multigrid algorithms**
O324 *Andrew Barker, Chak Shing Lee*
Panayot Vassilevski (Livermore, CA/US)

MS64

Advanced numerical methods in subsurface flow simulations in discrete fracture networks Part 3

16:30–18:30 • Room: Übung 5

Chairs: Sandra Pieraccini, Stefano Berrone (Turin/IT)
Jeffrey Hyman (Los Alamos, NM/US)

In several applications related to subsurface exploitation (geothermal applications, geological storage, enhanced oil & gas production...), the underground medium is frequently described by the Discrete Fracture Network (DFN) model, in order to properly account for the directionality of the flow in fractured media. Within the DFN model the fractures are explicitly described, and the flow mainly occurs along the fractures and their intersections. Issues in numerical simulations in DFNs are typically related to: the flow model, the coupling with the surrounding rock matrix, the geometrical

complexity of the domain, and the uncertainty both in the hydro-geological and in the geometrical parameters describing the fractures. Recent advances in numerical methods related to these issues will be the primary topic of the minisymposium.

- 16:30 **Multiscale simulation of flow through fractured porous media under elastic deformation**
O325 *Matei Tene (Delft/NL)*
Mohammed S. Al Kobaisi (Abu Dhabi/AE)
Hadi Hajibeygi (Delft/NL)
- 16:50 **Coupled thermo-mechanical-numerical framework for highly fractured formations**
O326 *Timur Garipov*
Hamdi A. Tchelepi (Stanford, CA/US)
- 17:10 **Mixed-dimensional approach to flows in fractured, deformable media**
O327 *Wietse Boon, Jan M. Nordbotten (Bergen/NO)*
- 17:30 **A general framework for DFN flow simulations with the virtual element method**
O328 *Andrea Borio, Stefano Berrone*
Stefano Scialo' (Turin/IT)
- 17:50 **Fundamental frequency of laminated composite thick spherical shells**
O329 *Mohammad Zannon (Tafila/JO)*

Poster session with refreshments

18:30–20:30 • Room: Cafeteria/Medienraum (follow the signs)

P1–P51

Abstracts: see page 166–178

PS6 | Invited plenary 6
Bridging scales in weather and climate models with adaptive mesh refinement techniques

08:30–09:30 • Room: H11

Chair: *Irina Tezaur (Livermore, CA/US)*
 Speaker: *Christiane Jablonowski (Ann Arbor, MI/US)*

Extreme atmospheric events such as tropical cyclones are inherently complex multi-scale phenomena. Such extremes are a challenge to simulate in conventional atmosphere models which typically use rather coarse uniform-grid resolutions. Adaptive Mesh Refinement (AMR) techniques seek to mitigate these challenges. They dynamically place high-resolution grid patches over user-defined features of interest, thus providing sufficient local resolution over e.g. a developing cyclone while limiting the total computational burden. Studying such techniques in idealized simulations enables the assessment of the AMR approach in a controlled environment and can assist in identifying the effective refinement choices for more complex, realistic simulations.

The talk reviews a newly-developed, non-hydrostatic, finite-volume dynamical core for future-generation weather and climate models. It implements refinement in both space and time on a cubed-sphere grid and is based on the AMR library Chombo, developed by the Lawrence Berkeley National Laboratory. Idealized 2D shallow-water and 3D test cases are discussed including interacting vortices, flows over topography, and a tropical cyclone simulation with simplified moisture processes. These simulations test the effectiveness of both static and dynamic grid refinements as well as the sensitivity of the model results to various adaptation criteria and forcing mechanisms. The AMR results will furthermore be compared to more traditional variable-resolution techniques, such as the use of a statically-nested mesh in NCAR's Community Atmosphere Model CAM with its Spectral Element (SE) dynamical core. This sheds light on the pros and cons of both approaches.

MS65
Coupled geomechanics and flow systems in porous media • Part 1

10:00–12:00 • Room: H11

Part 2 see page 60

Chairs: *Sanghyun Lee (Tallahassee, FL/US)*
Benjamin Ganis, Mary F. Wheeler (Austin, TX/US)

Numerical models for coupled PDEs involving mechanics and flow in porous media can be challenging to solve, and have many applications including groundwater, petroleum, environmental, and biomedical. This minisymposium aims at highlighting the current research status, model capabilities, and numerical methods for solving the coupled geomechanical fluid-rock interactions. Considered processes may also include flow and deformation of fractured geological formations and geochemical effects, which are relevant in applications such as subsurface CO₂ storage.

10:00 O330 **Phase-Field modeling for fracture propagation in porous media**

Sanghyun Lee (Tallahassee, FL/US)
Andro Mikelic (Villeurbanne/FR)
Mary F. Wheeler (Austin, TX/US)
Thomas Wick (Paris/FR)

10:20 O331 **A macroscopic modeling of hydraulic fracturing in fully-saturated porous materials**

Yousef Heider, Bernd Markert (Aachen/DE)

10:40 O332 **Iterative schemes for non-linear poromechanics**

Manuel Borregales, Florin A. Radu
Kundan Kumar, Jan M. Nordbotten (Bergen/NO)

11:00 O333 **On some algorithms for the coupling of flow with geomechanics in a poroelastic medium**

Tameem Almani (Dhahran/SA)
Kundan Kumar (Bergen/NO)
Mary F. Wheeler (Austin, TX/US)

11:20 O334 **An ALE approach to mechano-chemical processes in fluid-structure interactions**

Yifan Yang (Heidelberg/DE)
Thomas Richter (Magdeburg/DE)
Willi Jäger (Heidelberg/DE)
Maria Neuss-Radu (Erlangen/DE)

11:40 O335 **A fully coupled XFEM-EDFM with dual porosity simulator for the fractured reservoir**

Guotong Ren (Tulsa, OK/US)

MS66

Recent advances on numerical methods for shallow water models • Part 1

10:00–12:00 • Room: H12

Part 2 see page 61

Chairs: *Alina Chertock (Raleigh, NC/US)*
Alexander Kurganov
(Shenzhen, Guangdong/CN; New Orleans, MS/US)

This minisymposium focuses on numerical methods for hyperbolic systems of conservation and balance laws used to model shallow water and related geophysical flows. Specific numerical difficulties different shallow water models have in common are due to the presence of (possibly singular) geometric source terms and/or nonconservative exchange terms. These may lead to the loss of hyperbolicity, nonlinear resonance, very complicated wave structures and, as a result, to appearance of spurious oscillations and slow convergence of numerical methods. Therefore development of highly accurate and efficient numerical methods for these systems is a very important and challenging task.

10:00 **Well-balanced central-upwind schemes**
 O336 *Alexander Kurganov (Shenzhen, Guangdong/CN)*
New Orleans, LA/US)

10:20 **Well-balanced methods for the Shallow Water equations in spherical coordinates – application to tsunami modeling**
 O337 *Sergio Ortega Acosta, Manuel J. Castro Díaz*
Carlos Parés Madroñal (Málaga/ES)

10:40 **Numerical simulations for erosion processes**
 O338 *Emmanuel Audusse (Villetaneuse/FR)*
Philippe Ung (Chatou/FR)
Christophe Chalons (Versailles/FR)
Nicole Goutal (Chatou/FR)

11:00 **A class of staggered schemes for the shallow water equations**
 O339 *Nicolas Therme (Nantes/FR)*

11:20 **Shallow water solvers and the wet-dry front**
 O340 *Sebastian Noelle (Aachen/DE)*

MS67

Uncertainty quantification and data assimilation – computational challenges in large-scale geoscience models • Part 1

10:00–12:00 • Room: H13

Part 2 see page 61

Chairs: *Massimiliano Ferronato (Padua/IT)*
Luisa D'Amore (Naples/IT)

Assessing and reducing the uncertainty of large-scale simulations in the geosciences have become fundamental to increase the reliability of model forecasts. One of the major challenges arises when the description of model uncertainty and the availability of field observations are not straightforward. Especially in these cases, it is necessary to develop robust assimilation approaches combined with computationally efficient procedures. For instance, the use of appropriate surrogate models and the implementation on emerging computing architectures can help reduce the computational burden, provided that the most significant non-linearities of the physical system are preserved. This mini-symposium aims to discuss recent advances in geoscience applications where parameter and state estimation problems are tackled. Contributions dealing with novel algorithmic approaches and efficient computational procedures used in challenging applications are welcome.

10:00 **Challenges for enhanced solutions in large scale data assimilation**
 O341 *Luisa D'Amore (Naples/IT)*

10:20 **Rapid deployment of adjoint-based data assimilation for large scale problems**
 O342 *Emil Constantinescu*
Hong Zhang (Lemont, IL/US)

10:40 **Ensemble Kalman filter on a reduced model of the North Brazil Current**
 O343 *César Quilodrán, Nathan Sparks*
Ralf Toumi (London/GB)

11:00 **Developing efficient surrogates of coupled flow and geomechanical deformation models for data assimilation applications**
 O344 *Domenico Bau (Sheffield/GB)*

11:20 **Wavelet-based priors for subsurface parameter inference**
 O345 *Philipp Wacker (Erlangen/DE)*

MS68

Mathematical and computational advances in geoelectromagnetic forward and inverse modeling

10:00–12:00 • Room: Seminarraum Informatik 01.150

Chairs: Mikhail Kruglyakov (Zurich/CH),
Vladimir Puzyrev (Perth/AU)
Giuseppe Rodriguez (Cagliari/IT)

Electromagnetic methods are widely used in geophysics to study the subsurface electrical conductivity distribution. Conductivity is affected by the rock type and composition, temperature, and fluid/melt content and thus plays an important role in various engineering and industrial problems, such as hydrocarbon and mineral exploration, CO₂ storage monitoring, geothermal reservoir simulation, and many others. Numerical modeling of the electromagnetic fields in complex geological structures with a high level of accuracy requires a large number of model unknowns and is computationally challenging. Topography and bathymetry, complex reservoir geometries, anisotropy and large material contrasts pose serious challenges to existing modeling algorithms. At the same time, typical inversion procedure invoke thousands of forward modeling problems. All of these challenges should be addressed by new approximation algorithms and computational methods to harness the power of modern high-performance computing systems. The speakers will discuss theoretical and computational mathematical issues concerning geoelectromagnetic modeling.

10:00 Novel integral equation solver for the large
O346 scale 3D geoelectromagnetic modeling based on polynomials
Mikhail Kruglyakov (Zurich/CH)

10:20 Advances in the numerical solution of the time
O347 domain EM inverse problem
Ralph-Uwe Börner, Felix Eckhofer
Mario Helm (Freiberg/DE)

10:40 Electromagnetic modeling of geology cluttered
O348 with infrastructure and other thin conductors: A finite element method for hierarchical model parameters on volumes, faces and edges of an unstructured grid
Chester Weiss (Albuquerque NM/US)

11:00 Efficient and accurate ways of modeling the
O349 electromagnetic response of metallic pipelines and well casings
Rita Streich (Rijswijk/NL)
Colton Kohnke (Golden, CO/US)
Lifei Liu (Houston, TX/US)
Andrei Swidinsky (Golden, CO/US)

11:20 Integral equations method for electrical
O350 tomography sounding above ground surface relief
Tolkyn Mirgalikzy
Balgaisha Mukanova (Astana/KZ)
Kseniya Baranchuk, Igor Modin (Moscow/RU)

11:40 Imaging by joint inversion of electromagnetic
O351 waves and DC currents
Diego Domenzain, John Bradford
Jodi Mead (Boise, ID/US)

MS69

Advances and applications of periodic and stochastic homogenisation • Part 3

10:00–12:00 • Room: Übung 2

Chairs: Matteo Icardi (Warwick/GB)
Nadja Ray (Erlangen/DE)

Homogenisation theory has been successfully transferred to porous media, fluid dynamics, and material science problems in the last decades. More recently, connections with numerical methods and statistical techniques are emerging. In this mini-symposium, a particular focus will be devoted to: - random porous materials and connection with uncertainty quantification- multiscale computational techniques- problems in deformable media or where scales are not fully separable- applications to environmental, engineered, and biological porous media

10:00 Upscaling reactive transport in porous media:
O352 homogenisation and computational approaches in periodic and random media
Matteo Icardi (Coventry/GB)

10:20 Homogenization of the Stokes problem with
O353 application to particle flow
Matthieu Hillairet (Montpellier/FR)

10:40 A mixed stochastic–deterministic approach to
O354 particles interacting in a flow
Clemens Bartsch, Robert I. A. Patterson
Volker John (Berlin/DE)

11:00 Homogenization of nonlinear transmission
O355 conditions in porous media
Maria Neuss-Radu, Markus Gahn
Peter Knabner (Erlangen/DE)

MS70

Computational methods for flow in subsurface porous media • Part 2

10:00–12:00 • Room: Übung 4

Part 3 see page 63

Chairs: Michael Edwards (Swansea/GB)
Hadi Hajibeygi (Delft/NL)

This mini-symposium is on recent developments in numerical methods for modeling flow in subsurface porous media. This includes locally conservative finite-volume and finite element methods, multiscale modeling and upscaling. Elliptic and hyperbolic PDE approximation issues are addressed for single and multiphase flow including higher resolution, accuracy and efficiency on structured and unstructured grids, with application to problems that include full tensor permeability fields, faults and fractures.

- 10:00 Trends and Challenges in Computational
O356 Modeling of Giant Hydrocarbon Reservoirs
Ali Dogru (Dhahran/SA)
- 10:20 An implicit SPH multiscale method for porous
O357 media flow
*Cornelis Vuik, Owen Clark
Alex Lukyanov (Delft/NL)*
- 10:40 CVD-MPFA with full pressure support for
O358 computation of flow in fractured porous media
on unstructured grids
*Raheel Ahmed (Wuhan/CN)
Michael Edwards (Swansea/GB)*
- 11:00 Localized computation of Newton updates in
O359 the implicit time-stepping of Advection
Diffusion-Reaction approximations
Rami Younis (Tulsa, OK/US)
- 11:20 Semi-implicit methods for advection
O360 dominated problems
Peter Frolkovič (Bratislava/SK)
- 11:40 A lightweight numerical model of the
O361 generation and expulsion of hydrocarbon in the
source rock
*Daniele Rossi, Anna Scotti
Ludovica Delpopolo Carciopolo
Luca Bonaventura (Milan/IT)*

MS71

Level-set methods for inverse problems in the geosciences – seismic inversion

10:00–12:00 • Room: Übung 5

Chair: Tristan van Leeuwen (Utrecht/NL)

Detailed characterizations of the subsurface can be obtained from geophysical measurements by solving an inverse problem. As with many inverse problems, regularization is required to render the problem well-posed. Because subsurface medium-properties can vary discontinuously on various scales, standard Tikhonov regularization is often not appropriate. More advanced regularization terms such as (generalized) Total Variation address this issue to some extent, but may fail to capture certain types of prior information. For instance, in the presence of subsurface salt bodies, the medium can be split into two distinct parts; the salt body and the surrounding sediment. The medium parameters inside the salt body are (almost) constant, while those in the surrounding sediment can vary over a large range. Such structure can be captured by means of a level-set function. In this mini-symposium, we intend to bring together experts on level-set methods for inverse problems and geophysical inversion to discuss the state-of-the-art in methods and theoretical results. Part I of the symposium focuses on seismic imaging in the presence of salt bodies, while part II focuses on multi-physics inversion.

- 10:00 Salt reconstruction with full waveform
O362 inversion and a parametric level-set method
*Ajinkya Kadam, Tristan van Leeuwen (Utrecht/NL)
Wim Mulder (Delft/NL)*
- 10:20 Using second order information for updating
O363 salt body boundaries with level sets
Taylor Dahlke (Stanford, CA/US)
- 10:40 A level set method for seismic full waveform
O364 inversion in 2D
Oliver Dorn, Yifan Wu (Manchester/GB)
- 11:00 A level set ensemble Kalman filter method for
O365 history matching of production data
incorporating electromagnetics
*Clement Etienam, Rossmary Villegas
Oliver Dorn (Manchester/GB)*
- 11:20 Joint inversion of gravity and traveltime data
O366 using a level-set based structural
parametrization
Wenbin Li (East Lansing, MI/US)
- 11:40 Fractional differential operators to detect
O367 multi-scale geophysical features
*Bart van Bloemen Waanders
(Albuquerque, NM/US)
Harbir Antil (Fairfax, VA/US), Denis Ridzal
Chester Weiss (Albuquerque, NM/US)*

SIAM AG Geosciences business meeting

12:00–12:45 • Room: H13

Closing remarks

12:45–13:00 • Room: H11

PL2 | Prize lecture 2

Coupled problems in porous media with a focus on Biot

13:00–14:00 • Room: H11

Chair: Sorin Pop (Diepenbeek/BE; Bergen/NO)

Speaker: Kundan Kumar (Bergen/NO)

The key challenge in the successful utilisation of subsurface resources is the coupling of different physical processes involved. The model equations for the coupled behaviour of thermal, hydro, mechanical and chemical effects lead to a system of nonlinear, coupled, possibly degenerate PDEs.

We consider a system of coupled PDEs that incorporates the evolution in the pore-scale geometry. Starting from a reactive flow transport model describing the precipitation-dissolution processes, we visit the recent works that take into account the variation in the pore-scale geometry. Next, we consider the coupled flow and geomechanics model (Biot model) that takes into account the deformations due to the mechanical effects. Specifically, we show the iterative schemes for solving the Biot equation and the different extensions including non-linearities and further physics.

MS72

Coupled geomechanics and flow systems in porous media • Part 2

14:10–16:10 • Room: H11

Chairs: Sanghyun Lee (Tallahassee, FL/US)

Benjamin Ganis, Mary F. Wheeler (Austin, TX/US)

Numerical models for coupled PDEs involving mechanics and flow in porous media can be challenging to solve, and have many applications including groundwater, petroleum, environmental, and biomedical. This minisymposium aims at highlighting the current research status, model capabilities, and numerical methods for solving the coupled geomechanical fluid-rock interactions. Considered processes may also include flow and deformation of fractured geological formations and geochemical effects, which are relevant in applications such as subsurface CO₂ storage.

14:10 O368 **Linearly implicit extrapolation methods for density driven flow problems**

Arne Nägel (Frankfurt a. M./DE)

Peter Deuflhard (Beijing/CN)

Gabriel Wittum (Frankfurt a. M./DE)

14:30 O369 **Strain localization in a solid-water-air system with random heterogeneity via stabilized mixed finite elements.**

Xiaoyu Song, Kaiqi Wang

Yichi Du (Gainesville, FL/US)

14:50 O370 **Modeling multiscale behavior of hydraulic fractures via analytical and numerical approaches**

Egor Dontsov (Houston, TX/US)

15:10 O371 **Coupled hydromechanical numerical simulations of the production of tight reservoirs in complex discrete and deformable fracture networks**

Olivier Ricois

Jean Marc Gratien (Rueil-Malmaison/FR)

15:30 O372 **A non-local integral Ehlert plastic-damage model for shales**

Francesco Parisio, Dmitri Naumov

Xing-Yuan Miao (Leipzig/DE)

Olaf Kolditz (Dresden/DE)

Thomas Nagel (Leipzig/DE)

MS73
Recent advances on numerical methods for shallow water models • Part 2

14:10–16:10 • Room: H12

Chairs: *Alina Chertock (Raleigh, NC/US)*
Alexander Kurganov (Shenzhen, Guangdong/CN;
New Orleans, LA/US)

This minisymposium focuses on numerical methods for hyperbolic systems of conservation and balance laws used to model shallow water and related geophysical flows. Specific numerical difficulties different shallow water models have in common are due to the presence of (possibly singular) geometric source terms and/or nonconservative exchange terms. These may lead to the loss of hyperbolicity, nonlinear resonance, very complicated wave structures and, as a result, to appearance of spurious oscillations and slow convergence of numerical methods. Therefore development of highly accurate and efficient numerical methods for these systems is a very important and challenging task.

- 14:10
O373 **Hybrid finite-volume/ finite-element simulations of fully-nonlinear/ weakly dispersive wave propagation, breaking, and runup on unstructured grids**
Andrea G. Filippini, Maria Kazolea
Mario Ricchiuto (Talence cedex/FR)
- 14:30
O374 **Numerical simulation of shallow water flows with sediment transport and variable density**
Majid Mohammadian (Ottawa/CA)
- 14:50
O375 **An all-flow confluence condition for 1-dimensional river systems**
Karlan Wolfkill, Alina Chertock (Raleigh, NC/US)
Alexander Kurganov (Shenzhen, Guangdong/CN;
New Orleans, LA/US)
- 15:10
O376 **Dynamically adaptive data-driven simulation of extreme hydrological flows**
Pushkar Kumar Jain (Austin, TX/US)
Kyle Mandli (New York, NY/US), Ibrahim Hoteit
Omar Knio (Thuwal/SA)
Clint Dawson (Austin, TX/US)
- 15:30
O377 **Modeling shallow water flows through solid obstacles with Windows**
Alina Chertock (Raleigh, NC/US)

MS74
Uncertainty quantification and data assimilation – computational challenges in large-scale geoscience models • Part 2

14:10–16:10 • Room: H13

Chairs: *Massimiliano Ferronato (Padua/IT)*
Luisa D'Amore (Naples/IT)

Assessing and reducing the uncertainty of large-scale simulations in the geosciences have become fundamental to increase the reliability of model forecasts. One of the major challenges arises when the description of model uncertainty and the availability of field observations are not straightforward. Especially in these cases, it is necessary to develop robust assimilation approaches combined with computationally efficient procedures. For instance, the use of appropriate surrogate models and the implementation on emerging computing architectures can help reduce the computational burden, provided that the most significant non-linearities of the physical system are preserved. This mini-symposium aims to discuss recent advances in geoscience applications where parameter and state estimation problems are tackled. Contributions dealing with novel algorithmic approaches and efficient computational procedures used in challenging applications are welcome.

- 14:10
O378 **Preliminary results on seismic data assimilation in geomechanical modeling**
Claudia Zoccarato, Massimiliano Ferronato
Andrea Franceschini, Pietro Teatini (Padua/IT)
- 14:30
O379 **Parameter estimation in subsurface flow using ensemble data assimilation techniques**
Sangeetika Ruchi (Amsterdam/NL)
- 14:50
O380 **Multi-level ensemble data assimilation**
Andreas S. Stordal, Kristian Fossum
Trond Mannseth (Bergen/NO)
- 15:10
O381 **Domain decomposition approaches for data assimilation in large scale models**
Rossella Arcucci (Naples/IT)
- 15:30
O382 **A computational framework for uncertainty quantification in CSEM with stochastic conductivity models**
Dimitris Kamilis
Nick Polydorides (Edinburgh/GB)

MS75
Physics-based rupture and tsunami simulation
Part 2

14:10–16:10 • Room: Seminarraum Informatik 01.150

Chairs: *Stefan Vater (Hamburg/DE)*
Michael Bader (Garching/DE)
Alice-Agnes Gabriel (Munich/DE)

Despite active research, the source mechanisms leading to recent tsunamogenic earthquakes and resulting devastating inundation events still raise a lot of questions. Effects of complex rupture mechanics on displacement of the ocean floor, or of hydrodynamic wave behavior during generation and propagation of tsunami remain challenges for physics-based earthquake and tsunami simulation. This minisymposium strives to review current development in this field – and brings together complex source modeling and coupled tsunami modeling. Algorithmic approaches and discretization methods for the complex multi-scale problems will be discussed, as well as results of large-scale simulations of earthquakes and tsunamis.

14:10 O383 **Numerical approximation of single faults with rate-and-state dependent friction**

Joscha Podlesny, Elias Pipping
Ralf Kornhuber (Berlin/DE), Matthias Rosenau
Onno Oncken (Potsdam/DE)

14:30 O384 **A new discontinuous Galerkin spectral element method for elastic waves with physically motivated numerical fluxes**

Kenneth C. Duru, Alice-Agnes Gabriel
Heiner Igel (Munich/DE)

14:50 O385 **Adaptive simulation of the tsunami resulting from the 2004 Sumatra-Andaman earthquake: dynamic rupture vs. seismic inversion source model**

Stefan Vater, Jörn Behrens (Hamburg/DE)

15:10 O386 **Robust adaptive simulations for the 2011 Tohoku tsunami**

Luca Arpaia, Mario Ricchiuto (TalenceFR)

15:30 O387 **Hydrostatic vs non-hydrostatic NLSW tsunami modeling. Some comments to the light of the numerical results**

Jorge Macias, Manuel J. Castro Díaz
Cipriano Escalante (Málaga/ES)

15:50 O388 **The impact of numerical schemes on time to solution in adaptive shallow water equations**

Leonhard Rannabauer
Michael Bader (Garching/DE)

MS76
Quality assurance and sustainable development of simulation software in the geosciences
Part 1

14:10–16:10 • Room: Übung 2

Part 2 see page 65

Chairs: *Peter Bastian (Heidelberg/DE)*
Bernd Flemisch (Stuttgart/DE)
Dominic Kempf (Heidelberg/DE)
Timo Koch (Stuttgart/DE)

Developing research software for computational modeling in the geosciences faces many challenges due to the ever-growing complexity of mathematical models, software dependencies and computer architectures. The fundamental challenge of assuring the quality of the developed software can be tackled by establishing a sustainable development process that emphasizes quality measures such as reliability, accuracy and reusability.

This minisymposium will address the scientific as well as the practical questions arising from this endeavor. Several small to medium-size projects will present their approaches, experiences and recommendations for developing simulation software in the geosciences. The main aspects to be discussed are automated testing, open-source development, software design, usability, archiving and reproducibility.

14:10 O389 **Quality assurance in scientific software frameworks and automated system testing in DUNE**

Dominic Kempf (Heidelberg/DE), Timo Koch
Bernd Flemisch (Stuttgart/DE)
Peter Bastian (Heidelberg/DE)

14:30 O390 **Code-driven automated test environments and workflows**

Lars Bilke (Leipzig/DE)

14:50 O391 **Maintaining quality assurance within software evolution – Lessons learned with PFLOTRAN**

Jennifer Frederick
Glenn Hammond (Albuquerque, NM/US)

15:10 O392 **OPM – Open source software for reservoir simulation and visualization**

Tor Harald Sandve (Bergen/NO)
Atgeirr Flø Rasmussen (Oslo/NO)

15:30 O393 **Development of an open-source, community hydrology model – Discussion of best software practices**

Reed Maxwell (Golden, CO/US)
Stefan J. Kollet (Jülich, Bonn/DE)
James Beisman (Golden, CO/US)
Laura Condon (Syracuse, NY/US)
Klaus Goergen (Jülich/DE)
Daniel Osei-Kuffuor (Livermore, CA/US)
Wendy Sharples (Jülich/DE), Steven Smith
Carol Woodward (Livermore, CA/US)

MS77

Computational methods for flow in subsurface porous media • Part 3

14:10–16:10 • Room Übung 4

Chairs: Michael Edwards (Swansea/GB)
Hadi Hajibeygi (Delft/NL)

This mini-symposium is on recent developments in numerical methods for modeling flow in subsurface porous media. This includes locally conservative finite-volume and finite element methods, multiscale modeling and upscaling. Elliptic and hyperbolic PDE approximation issues are addressed for single and multiphase flow including higher resolution, accuracy and efficiency on structured and unstructured grids, with application to problems that include full tensor permeability fields, faults and fractures.

14:10 O394 Comparison of linear reconstructions for second order finite volume schemes on polyhedral grids

Robert Klöfkorn (Bergen/NO)
Anna Kvashchuk (Stavanger/NO)
Martin Nolte (Freiburg i. Br./DE)

14:30 O395 Optimal reconstruction of constitutive relations for porous media flows

Vladislav Bukshynov (Melbourne, FL/US)

14:50 O396 Improvement of numerical approximation of coupled two-phase multicomponent flow with reactive geochemical transport in porous media

Etienne Ahusborde, Brahim Amaziane (Pau/FR)
Mustapha El Ossmani (Meknes/MA)

15:10 O397 Application of the multirate TR-BDF2 method to the time discretization of non-linear conservation laws.

Ludovica Delpopolo Carciopolo
Luca Bonaventura, Luca Formaggia
Anna Scotti (Milan/IT)

MS78

Mathematical and computational advances in geoelectromagnetic forward and inverse modeling • Part 2

16:30–18:30 • Room: H11

Chairs: Mikhail Kruglyakov (Zurich/CH)
Vladimir Puzyrev (Perth/AU)
Giuseppe Rodriguez (Cagliari/IT)

Electromagnetic methods are widely used in geophysics to study the subsurface electrical conductivity distribution. Conductivity is affected by the rock type and composition, temperature, and fluid/melt content and thus plays an important role in various engineering and industrial problems, such as hydrocarbon and mineral exploration, CO₂ storage monitoring, geothermal reservoir simulation, and many others. Numerical modeling of the electromagnetic fields in complex geological structures with a high level of accuracy requires a large number of model unknowns and is computationally challenging. Topography and bathymetry, complex reservoir geometries, anisotropy and large material contrasts pose serious challenges to existing modeling algorithms. At the same time, typical inversion procedure invoke thousands of forward modeling problems. All of these challenges should be addressed by new approximation algorithms and computational methods to harness the power of modern high-performance computing systems. The speakers will discuss theoretical and computational mathematical issues concerning geoelectromagnetic modeling.

16:30 O398 A relaxed Gauss-Newton algorithm for low frequency EM data inversion with applications in geophysics

Giuseppe Rodriguez, Gian P. Deidda
Patricia Diaz De Alba, Giulio Vignoli (Cagliari/IT)

16:50 O399 Large-scale 3D controlled-source EM modeling with a block low-rank multifrontal direct solver

Daniil Shantsev, Piyosh Jaysaval
Sébastien de la Kethulle de Ryhove (Oslo/NO)
Patrick Amestoy, Alfredo Buttari (Toulouse/FR)
Jean-Yves L'Excellent (Lyon/FR)
Theo Mary (Toulouse/FR)

17:10 O400 Adaptive regularization in variable exponent Lebesgue spaces for microwave subsurface prospecting

Claudio Estatico, Fabio Di Benedetto
Alessandro Fedeli, Matteo Pastorino
Andrea Randazzo (Genoa/IT)

17:30 O401 Analysis of a statistical descriptor for classification of seismic scatterers

Susanne Maciel (Brasilia/BR)
Ricardo Biloti (Campinas/BR)

MS79

Multi-resolution three-dimensional modeling of coastal, regional, and deep ocean • Part 3

16:30–18:30 • Room: H12

*Chairs: Vadym Aizinger (Erlangen/DE)
Sergey Danilov (Bremerhaven/DE)*

Rapid increase in available computational power, better resolution and coverage of geophysical data, and advances in mathematical modeling and numerical methodology hold potential to conduct ocean simulations with a much higher spatial and temporal resolution of physical processes of interest or parts of the computational domain. However a number of key modeling, numerical, and computational issues connected with producing multi-resolution simulations using either unstructured meshes or nesting techniques are still open. The goal of this mini-symposium is to discuss recent advances in methodology of multi-resolution ocean modeling and propose ways to deal with still unsolved problems arising in such models.

16:30 O402 **The analysis and implementation of a vorticity divergence-based numerical scheme for the shallow water equations**
Qingshan Chen (Clemson, SC/US)

16:50 O270 **Simulating mesoscale eddies on unstructured meshes**
*Sergey Danilov, Qiang Wang, Dmitry Sein
Dmitry Sidorenko (Bremerhaven/DE)*

17:10 O404 **Modeling of random ocean waves in an irregular shaped harbor with variable bathymetry by using 3D boundary element method**
Prashant Kumar, Gulshan (Delhi/IN)

17:30 O405 **DG-based simulation of coupled surface subsurface flow**
*Dmitry Mazilkin (Clausthal-Zellerfeld/DE)
Peter Bastian, Steffen Müthing (Heidelberg/DE)
Olaf Ippisch (Clausthal-Zellerfeld/DE)*

17:50 O406 **A new scheme for water flow-driven stratigraphic forward modeling**
*Clément Cancès (Lille/FR), Didier Granjeon
Nicolas Peton, Quang H. Tran
Sylvie Wolf (Rueil-Malmaison/FR)*

MS80

Increasing the physical realism of models and simulations involving fractured rocks

16:30–18:30 • Room: H13

*Chairs: Stephan K. Matthai (Parkville/AU)
Anna Scotti (Milan/IT)*

The shallow subsurface is fractured, and such displacement discontinuities can have a critical impact on the engineering of water resources, tunnels and mines, underground gas storage, CO₂ geo-sequestration, geothermal systems and hydrocarbon reservoirs. Understanding how rock fractures affect related activities in this now heavily explored environment is very important. Arguably, realistic modeling and simulation of processes involving rock fractures, exemplifies the complexity of industrial applications of mathematics. It necessitates multi-process multi-scale models of often formidable geometric complexity. These are difficult to impossible to verify and validate. Here we invite novel contributions to this cross-disciplinary subject: forward modeling of reactive (multiphase) flow processes, geomechanics, effective media property determination, model construction, benchmarking and validation. This mini symposium will explore how we can improve the physical realism of fracture modeling and simulation with the goal of better prediction, improved design of, and early anticipation of risks and side effects of engineering measures.

16:30 O407 **Modeling and simulation of fracture aperture**
*Stephan K. Matthai, Caroline Milliottte
Hossein Agheshlui (Parkville/AU)*

16:50 O408 **Prediction of fracture aperture in fragmented rocks**
*Hossein Agheshlui
Stephan K. Matthai (Parkville/AU)*

17:10 O409 **Impact of natural fracture reactivation on gas production from shale gas plays**
*Jun Wang, Stephan K. Matthai (Parkville/AU)
He Ping Xie (Chengdu/CN)*

17:30 O410 **Flow and tracer transport in coupled fracture and porous block – code comparison and singularity study**
*Milan Hokr, Aleš Balvín (Liberec/CZ)
Hua Shao (Hanover/DE)
William P. Gardner (Missoula, MT/US)
Herbert Kunz (Hanover/DE)
Yifeng Wang (Albuquerque, NM/US)
Marek Venc (Prague/CZ)*

MS81

Quality assurance and sustainable development
of simulation software in the geosciences

Part 2

16:30–18:30 • Room: Übung 2

Chairs: *Peter Bastian (Heidelberg/DE)*
Bernd Flemisch (Stuttgart/DE)
Dominic Kempf (Heidelberg/DE)
Timo Koch (Stuttgart/DE)

Developing research software for computational modeling in the geosciences faces many challenges due to the ever-growing complexity of mathematical models, software dependencies and computer architectures. The fundamental challenge of assuring the quality of the developed software can be tackled by establishing a sustainable development process that emphasizes quality measures such as reliability, accuracy and reusability. This minisymposium will address the scientific as well as the practical questions arising from this endeavor. Several small to medium-size projects will present their approaches, experiences and recommendations for developing simulation software in the geosciences. The main aspects to be discussed are automated testing, open-source development, software design, usability, archiving and reproducibility.

16:30 **GeoClaw software development and testing**O411 *Randall LeVeque (Seattle, WA/US)**Donna Calhoun (Boise, ID/US)**Kyle Mandli (New York, NY/US)*16:50 **Reaktoro – an overview of its software design
and algorithms for geochemical and reactive
transport modeling**

O412

*Allan Leal, Martin Saar (Zurich/CH)*17:10 **Dumux-Pub – enhancing the transparency of
simulation results**

O413

*Bernd Flemisch, Timo Koch (Stuttgart/DE)*17:30 **Multi-physical process modeling and
validation for the deep geological disposal of
nuclear waste in the DECOVALEX project**

O414

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O1

A DG method for pore scale flows

Thermodynamically based diffuse-interface methods are promising methods for direct pore-scale numerical simulations of multiphase multicomponent flows. The Cahn-Hilliard equations for a two-component flow are obtained after minimization of the total Helmholtz free energy. In this talk, we present a discontinuous Galerkin discretization of the coupled Cahn-Hilliard equations with the Navier-Stokes equations. Wettability on rock-fluid interfaces is accounted for via an energy-penalty based wetting (contact-angle) boundary condition. The method is numerically verified by obtaining optimal convergence rates. Several physical validation tests show the robustness and accuracy of the proposed algorithm.

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O2

Modeling two-phase flow at the pore-level within the volume-of-fluid method framework

A numerical method has been developed to perform multiphase direct numerical simulations at sub-pore resolution. The volume-of-fluid method is employed to capture the interface while its dynamics is explicitly described based on finite volume discretization of the Navier-Stokes equations. We employ a simple yet efficient method to calculate the interfacial tension force based on an interface reconstructed via gridblock faces that are shared between cells with different fluids. The stability and accuracy of the implemented scheme is validated on several test cases. We also discuss the potential of the method to study multiphase flow in images of reservoir rocks.

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O3

Micro-continuum approach for pore-scale simulation of subsurface processes

Advances in imaging technologies and high-performance computing are making it possible to perform Direct Numerical Simulation (DNS) of flow processes at the pore scale; nevertheless, the restrictions on the physical size of the sample (porous rock) that can be fully resolved using Navier-Stokes-based DNS are quite severe. Even for samples on the order of a cm³, the complexity of the spatial heterogeneity of the pore space precludes Navier-Stokes-based DNS. To deal with this challenge of having a wide range of length scales – even for “small” systems, we describe a micro-continuum formalism, whereby locally averaged equations and associated coefficients can be used to model the effects of scales that are below instrument resolution and/or DNS capability. A hybrid modeling framework based on the Darcy-Brinkman-Stokes (DBS) equation is employed. The effectiveness of the approach is demonstrated for highly nonlinear multiscale dissolution processes. An additional focus area is on multiphase reactive transport. We discuss two specific applications: dissolution associated with fractures in CO₂-brine systems, and dissolution instabilities (worm-holing phenomena) associated with acidization treatment of carbonate formations.

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O4

Pore-scale characteristics of wetting phase entrapment during drainage/imbibition – SPH-based direct numerical simulations

Classical macroscale approaches to modeling two-phase flow of immiscible fluids through porous media are based on phenomenological extensions of Darcy’s law and additional closing equations relating macroscopic capillary pressure, the difference in mean phase pressures, to saturation. Hysteretic effects and non-equilibrium contributions are typically lumped into an algebraic capillary pressure-saturation relationship wherefore corresponding fitting coefficients lack general validity. Pore-scale direct numerical simulations are becoming a valuable complementary tool for such problems. Our approach to pore-scale resolved multiphase flow simulation is a weakly compressible Smoothed Particle Hydrodynamics (SPH) scheme which incorporates the Navier-Stokes equations together with a diffuse-interface continuum surface force model to account for the interfacial momentum balances. The aim of our contribution is to discuss the influence of microstructure and fluid properties on dynamic capillary pressure and non-equilibrium processes characteristic of non-Darcian flow at low capillary numbers.

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O5

Approaches to modeling flow and transport at porescale in changing geometries

Modeling porescale processes is important for understanding the large scale flow and transport models in subsurface. In particular, when the porescale geometry changes due to reactive transport or phase transitions, the crucial parameters such as porosity and permeability change as well. A porescale flow model should be flexible in accounting for geometry changes, and in modeling the coupling to the (transport or phase change) processes changing the pore geometry. In the presentation we discuss several approaches to the modeling of flow at porescale, and in particular we discuss HybGe-Flow3D, a library designed for the solution of fluid flow problems in complex, uncertain and evolving geometries in 2D and 3D. We compare the use of HybGe-Flow3D to other Stokes solvers available in the public domain.

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O6

Modeling and simulation of colloidal-like particles transport in an oil-water flow in porous media

We analyze a simple heuristic, experimentally based, mathematical model for the transport of colloidal-like particles in a porous medium. The particles are sufficiently small such that one single particle cannot block a pore throat. Nevertheless, under certain conditions they can clog a pore through a log-jamming effect (accumulation of a sufficient number of particles at the pore throat entrance). This leads to a microscopic diversion of the flow, causing a redistribution of the local pressure and which can mobilize initially trapped oil, thus enhancing recovery. We perform numerical simulations of the proposed heuristic model and compare the results with experimental data obtained at the laboratory scale. Simulation results show that the log-jamming effect plays an important role in the recovery of initially trapped oil and that the proposed model is able to reproduce, qualitatively, the results obtained in laboratory.

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O7

Validation of the General Curvilinear Coastal Ocean Model (GCCOM) for the case of 3D non-hydrostatic stratified flow

The GCCOM model solves the 3D Navier-Stokes equations using the Boussinesq approximation and is capable of simulating non-hydrostatic flow, built to work on high-resolution problems (tens of meters). It uses the Large Eddy Simulation (LES) and sub-grid scale (SGS) models. One of the most important features of this model is its use of general curvilinear coordinates in all three dimensions (requiring no vertical averaging), this feature allows the model to efficiently adapt to a very steep slope, feature mainly need it to study the propagation and breaking of internal waves in nearshore events. It also gives more flexibility to distribute the grid nodes along the vertical line to reduce the grid-induced errors. The model was previously validated for an idealized homogeneous environment and showcased the 3D curvilinear features of the model. To continue the validation of the model, in this work non-stratified test cases are presented: the classical lock release gravity currents and the internal seiche in a flat bottom tank. Comparison of the front speeds and wave speeds of the model with reference data from the literature are in good agreement.

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O8

Towards high-fidelity simulation of small-scale coastal ocean flows by model coupling approach

A modeling system as hybrid of a fully 3D fluid dynamics model and a geophysical fluid dynamics model is presented to simulate multiscale coastal ocean flows. The former is the solver for incompressible flow on unstructured mesh (SIFUM) that we developed to resolve local flows of interest, and the latter is the finite volume method for coastal ocean flows (FVCOM), which models background estuary flows. The SIFUM-FVCOM system is the first of its kind and able to simulate various flow phenomena at spatial scales $O(1)$ m -- $O(10,000)$ km, especially those complicated, fully 3D flows at small scales in high-fidelity. The SIFUM-FVCOM system is an extension of the SIFOM-FVCOM system we developed previously, and it captures free surfaces at local flows with a VOF method. This presentation outlines the methodology of the SIFUM-FVCOM system and presents its validations and tests, together with a modeling example in which tsunami-like waves propagate all the way from a deep ocean to seashore and then impinge a coastal structure. Difficulties and further development will be also discussed.

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O9

A new D-Flow FM (Flexible Mesh) type of shallow water model for Lake Marken for forecasting and impact assessments of different societal aspects

Forecasting of flooding, morphology and water quality in coastal areas, rivers, and lakes is of great importance for society. To tackle this, the modeling suite Delft3D, was developed by Deltares. Delft3D is open source and used worldwide. For Lake Marken in the Netherlands important societal aspects are:

- safety assessments of dikes,
- operational forecasting of flooding,
- improving water quality and ecology,
- maintenance of navigation channels.

In forecasting and impact assessments of these aspects, modeling water levels, currents, and water balances is essential. Currently there is a transition to the shallow water solver D-Flow FM (Flexible Mesh) for unstructured computational meshes in the Delft3D Flexible Mesh Suite. A new model with D-Flow FM is being developed for the Lake Marken area. We aim for an integrated approach in which the new model can be used for the different societal aspects. Key idea is to have the unstructured computational mesh optimized for required local resolution and computational time. In this presentation we will illustrate the different modeling stages (a.o. grid generation, calibration, and validation).

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O10

The simulation of the hydrodynamics of the Upper Gulf of California

Due to the ecological importance in nursing important endemic species, the Upper Gulf of California (UGC) as part of the Colorado river delta was designed as a UNESCO Biosphere reserve since 1993. This increased the importance on knowing the hydrodynamics of the area as well as predicting the response of the ocean circulation to extreme events.

Based on this, we have continued studies of the Upper Gulf of California using numerical modeling. To do this, we implemented the hydrodynamic model ELCOM from UWA, to solve the hydrodynamics forced by tides and meteorological events. The model was implemented with a dx equals to 600 meters, a dt of 40 seconds, and a vertical resolution of 5m.

A field campaign from July 2016 was used as a baseline to initiate the simulation. The sea level and the data from the meteorological station from San Felipe were used to force the simulation at the open boundaries. The main results of the simulation shows that the UGC are responding well to the sea level forcing producing currents about .1 m/s on the deeper parts of the bathymetry and about .6 cm/s on the shallows areas. Temperature results are also consistent with the radiation provided at the open boundaries.

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O11

Boundary layers for the 3D primitive equations in a cube

We study the boundary layers for the viscous Linearized Primitive Equations (LPEs) when the viscosity is small. The LPEs are considered here in a cube. Besides the usual boundary layers that we analyze here too, corner layers due to the interaction between the different boundary layers are also studied. The boundary layers are essential features which cause some numerical difficulties as they require highly refined meshes near the domain boundaries. This talk can give some insights on analyzing various types of boundary layers as well as meshing the computational domains.

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O12

Modeling and stochastic parametrization of wave breaking data

Using a Lagrangian approach, data from laboratory and computational experiments of wave breaking of water waves are analyzed, with the aim of understanding the underlying kinematics of the process. A model for the wave breaking is formulated that relies on separating the probabilistic dynamics of the ensemble into a recurring and a non-recurring, non-equilibrium portion. A model of this sort is useful in formulating the large scale momentum exchanges between waves and currents as well as in estimating the wave generated dissipation and its effect on large scale, mean-flow, ocean dynamics. Comparisons between synthetic and laboratory data and models suggest confidence in the use of the computational tools we use to capture and understand the laboratory data. The stochastic parametrization captures the kinematics of the wave breaking process and the dependence of wave breaking energetics and wave slope. The transition between the Lagrangian and Eulerian frame reveals the inter-dependence of mass and momentum exchanges between waves and currents.

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O13

A nonhydrostatic model for atmospheric motion in ACME-HOMME

Traditional atmospheric models for climate make the assumption that the Earth's atmosphere is in hydrostatic balance. While the hydrostatic approximation is justified down to grid scales of about 10 kilometers, grids of this scale and smaller are used for local refinement, where a higher resolution mesh is used in certain regions of interest, and are feasible at global scales on future exascale computing systems. In this talk we discuss a new formulation and implementation of the primitive equations for nonhydrostatic atmospheric motion. We show that the removal of the hydrostatic assumption gives rise to a larger system of PDEs with a natural Hamiltonian structure. While being more physically realistic at small grid scales, the nonhydrostatic equations support vertically propagating acoustic waves that are unimportant for forecast and climate predictions. This work is joint with Mark Taylor and Oksana Guba as part of the ACME project.

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O14

Variational integrators in geophysical fluid dynamics

We present a unified approach for the derivation of structure preserving numerical schemes in geophysical fluid dynamics. The numerical schemes are based on a finite dimensional approximation of the group of volume preserving diffeomor-

phisms and on its recent extensions to the compressible case. The schemes are derived from a discretization of the Euler-Poincaré variational formulation of fluid dynamics. The resulting variational integrators allow for a discrete version of Kelvin circulation theorem, are applicable to irregular meshes and exhibit excellent long term energy behavior. Applications to the Boussinesq, anelastic, and shallow water equations will be presented.

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O15
Dynamico-FE – A structure-preserving hydrostatic dynamical core based on Hamiltonian methods

The equations of inviscid, adiabatic fluid dynamics are Hamiltonian; and this structure underlies many of the most basic principles we know about them (such as conservation laws). Guided by the philosophy that we are not discretizing arbitrary PDEs, but building a model of a physical system, it is desirable to mimic this structure in a discrete model. Doing so, it is possible to simultaneously obtain many useful properties such as energy conservation, curl-free pressure gradients and the absence of spurious computational modes. A very general approach to the design of such models is outlined: the combination of a Hamiltonian formulation for the continuous equations with a mimetic discretization (Galerkin in our case). This talk will present a concrete realization of this philosophy: Dynamico-FE, a high-order, structure-preserving hydrostatic dynamical core targeting moderate-resolution (~25km) climate applications. It will also discuss development efforts towards future sound-proof and non-hydrostatic dynamical cores targeting high resolution, global convection permitting climate and weather forecasting, built on the same principles.

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O16
Structure-preserving variational integrators for anelastic, pseudo-incompressible, and shallow-water flows

Structure-preserving discretizations of the equations of geophysical fluid dynamics can be derived in terms of variational principles. The discretization approach relies on a finite dimensional approximation of the (Lie) group of diffeomorphisms that describe the configuration of the fluid. The corresponding Lie algebra permits to define discrete Lagrangian. Variations of the latter results in the discrete model equations. In this talk, we numerically investigate variational discretizations for the Boussinesq, anelastic, pseudo-incompressible, and shallow-water equations that are derived according to such variational

principles. In particular, we verify the structure-preserving nature of these schemes for several test cases on both regular and irregular computational meshes. We show, for instance, that these schemes perfectly reflect the models' dispersion relations and that they present very well the dynamics, in both divergence- and advection-dominated scenarios. In all cases studied, the schemes conserve mass up to machine precision and show excellent long term energy behavior.

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O17
Stability analysis of non-monotonic density-driven convective mixing

Density-driven convective mixing of CO₂ in oil increases mixing and alters the oil mobility. We study the stability of this system with linear stability analysis and direct numerical simulations. When CO₂ contacts the oil from below, as a result of injection in an underlying aquifer, the system is very unstable because of the significantly lower density of CO₂ relative to oil. However, as the components mix, the fluid becomes denser than pure CO₂, which changes the dynamics.

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O18
New thermodynamic models for CO₂-hydrocarbon mixtures

Traditional formulations of cubic equations of state show convergence problems and unphysical densities for binary mixtures of carbon dioxide and heavy alkanes. These difficulties appear for high mole fractions of carbon dioxide at low temperatures. Procedures for expanding the domain of validity of cubic equations of state for such mixtures are presented. The validation is performed with respect to phase boundary location and density. These properties have large impact on density-driven convective mixing.

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O19
Parametrization in physical space for modeling of challenging CO₂-EOR applications

The nonlinear nature of flow and transport in porous media requires a linearization of governing equations for numerical solution. In this work, we utilize the operator-based linearization approach for the solution of complex physical problems related to CO₂ Enhanced Oil Recovery. The key idea of the approach is a transformation of discretised mass- and energy-conservation equations to an operator form with separate space-dependent and state-dependent operators. This transformation provides an opportunity for an approximate representation of the exact

physics of a problem through an interpolation in physical-parameter space. We apply an adaptive coarsening to identify major nonlinearities in physical descriptions and control the approximation error. The advanced nonlinear solver based on the global-inflection-point correction was designed for the proposed linearization approach. The new simulation framework was applied to several challenging problems related to CO₂-EOR with various physical kernels. In all cases studied, the proposed strategy improves the robustness and efficiency of the nonlinear solution in comparison to conventional simulation approaches.

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O20

Wettability control on multiphase flow in porous media

When two fluids coexist in a porous medium, the solid will prefer to be coated by one of the fluids rather than the other. This preference is known as wettability. It has been known for decades that wettability can have a profound impact on flows in porous media because of the very large area of contact between the fluids and the solid. Wettability is particularly important when one fluid invades a porous medium by displacing a different fluid, such as when CO₂ is stored in deep saline aquifers by displacing brine or injected into petroleum reservoirs to displace oil, but the microscale physics and macroscopic consequences remain poorly understood. Here, we study the impact of wettability in detail by systematically varying the wetting properties of a microfluidic porous medium. Our high-resolution images reveal the fundamental control that wettability can exert on multiphase flow, highlight the inherently 3D nature of pore-scale displacement mechanisms, and help explain the striking macroscopic displacement patterns that emerge.

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O21

A finite element setting for macroscale simulations of wetting flows in fibrous media

A new variational formulation of the triple junction equilibrium has been proposed for the dynamic wetting flow simulations in fibrous media. The main idea of the approach is to consider the Laplace's law not only over the liquid - gas interface, but also over the liquid - solid and gas - solid interfaces. Hence, when the substrate is planar, the triple line motion is not driven by the solid curvature, but by the jump of the surface tension parameter. The Laplace's law is expressed in a weak form to take into account this discontinuity, which appears as a Neumann boundary condition in the model. Both liquid and gas are as-

sumed to be incompressible Newtonian fluids with different viscosities. The resulting Stokes's equations are solved by using finite elements, linear both in velocity and pressure, stabilised by a variational multiscale method. The moving interface is captured by a Level-Set methodology, combined with a mesh adaptation technique. In the elements crossed by the interface, the discrete pressure field is enriched in order to describe the pressure discontinuity. This framework is assessed with 2D-simulations of a droplet spreading. 3D-simulations of classic wetting problems are also investigated. Expected numerical results are obtained.

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O22

Numerical aspects of molecular diffusion calculations during gas injection in fractured reservoirs

Molecular diffusion plays a significant role in oil recovery during gas injection in fractured reservoirs, especially when matrix permeability is low and fracture intensity is high. Diffusion of gas components from a fracture into a matrix extracts oil components from matrix and delays the gas breakthrough, increasing sweep and displacement efficiencies.

In most reservoir simulation tools, diffusion is modeled using classical Fick's law approach with constant coefficients. In this approach, the dragging effects are neglected and the gas-oil diffusion at the interface is modeled by assuming an average composition at the interface which does not have a sound physical basis.

In this work, we analyze the numerical aspects of implementation of sophisticated models such as generalized Fick's law in a dual-porosity simulator to arrive at robust and efficient algorithms for molecular diffusion that can be used in simulation of gas injection in fractured reservoirs. We discuss in detail the accuracy and computational speed of various models for diffusion and present field-scale examples to demonstrate the importance of correct implementation of diffusion models.

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O23

An efficient state-parameter filtering scheme combining ensemble Kalman and particle filters

We consider the state-parameter filtering problem for systems with large-dimensional state and small number of parameters. We propose to exploit the strengths of the particle filter (PF) and the ensemble Kalman filter (EnKF) to derive a Bayesian filter that combines them. At each filtering cycle of the proposed EnKF-PF, the PF is first used to sample the particles, followed by the EnKF to compute the state ensemble conditional on

the resulting parameters ensemble. The proposed scheme should be more robust than the traditional state augmentation techniques, which suffer from the curse of dimensionality and inconsistency when the state and the parameters are nonlinearly correlated. The EnKF and PF interact based on the ensembles members in contrast with the recently introduced two-stage EnKF-PF (TS-EnKF-PF), which exchanges point estimates between EnKF and PF while requiring almost twice the computational load. Numerical experiments are conducted with the Lorenz-96 model to evaluate the behavior the EnKF-PF performance against the joint PF, joint EnKF and TS-EnKF-PF. The EnKF-PF provides the best results and is found more robust in all tested scenarios.

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O24
Ensemble methods for combined state and parameter estimation

Schemes based on the well-known Ensemble Kalman filtering are often used for state estimation problems. By augmenting the state with the uncertain parameters this algorithm can also be used for joint state and parameter estimation. This is a very attractive approach because is it very easy to implement. However, a problem with the use of the (Ensemble) Kalman filter is filter divergence. This problem is even more pronounced if the filter is used for parameter estimation problems. Variational data assimilation schemes can also be used for joint state and parameter estimation problems. These schemes require the implementation of the adjoint model. Even with the use of the adjoint compilers that have become available this is a tremendous programming effort, that hampers new applications of the method. Therefore recently new ensemble approaches to variational data assimilation have been proposed that does not require the implementation of the adjoint of (the tangent linear approximation of) the original model. In the presentation some ensemble approaches for solving joint state and parameter estimation problems will be summarized. The characteristics and performance of these methods will be illustrated with a number of applications.

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O25
Assimilating all-sky SEVIRI infrared brightness temperatures using the KENDA ensemble data assimilation system

Infrared brightness temperatures (BTs) from geostationary satellites provide detailed information about the cloud distributions. More effective use of this information in modern data assimilation systems has the potential to greatly improve the forecast accuracy for high impact weather events. Specifically water vapor tends to be one of the least accurate variables in initialization datasets due to a lack of in situ observations. In this presentation, we discuss results from ongoing efforts

to assimilate clear and cloudy sky water vapour channel BTs from the SEVIRI sensor in the Kilometer Scale Ensemble Data Assimilation (KENDA) system. The spatial domain of the COSMO model considered in this study covers most of central Europe with 2.8 km resolution, with observations assimilated once per hour. Efforts are underway to develop correction methods of the bias and the variance of first-guess departures that can effectively remove the bias from both clear and cloudy sky observations. We present first guess departure statistics of BTs classified corresponding to a recently developed cloud impact measure. In addition, we show the impact of SEVIRI water vapour channel BT on temperature, wind and relative humidity during a cycled 4-week data assimilation experiment in summer 2014.

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O26
Use of correlation-based localization for history matching seismic data

The number of data values after seismic inversion of acoustic traces are large, compared to the amount of production data. When using ensemble based data assimilation techniques, number of data values exceeding the ensemble size may lead to underestimated uncertainty, and prevents the filter to further update the reservoir parameters (ensemble collapse). In this talk we present a novel approach for reducing the number of data values. First, the seismic information is transformed using discrete wavelets, and the (possibly colored) noise in the wavelet coefficients is estimated. Based on the noise level, small wavelet coefficients are truncated, and the amount of data is reduced to only the leading coefficients. Second, localization is applied. Traditional distance based localization schemes are not applicable, as the coefficients are not associated with a location in the reservoir. Instead, we compute the correlation between the coefficients and the reservoir parameters. For each parameter that is updated, only coefficients that are correlated above a given threshold are used.

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O27
A spatiotemporal stochastic model for tropical precipitation and water vapor dynamics

A linear stochastic model is presented for the dynamics of water vapor and tropical convection. Despite its linear formulation, the model reproduces a wide variety of observational statistics from disparate perspectives, including (i) a cloud cluster area distribution with an approximate power law; (ii) a power spectrum of spatiotemporal red noise, as in the “background spectrum” of tropical convection; and (iii) a

suite of statistics that resemble the statistical physics concepts of critical phenomena and phase transitions. The physical processes of the model are precipitation, evaporation, and turbulent advection–diffusion of water vapor, and they are represented in idealized form as eddy diffusion, damping, and stochastic forcing. Consequently, the form of the model is a damped version of the two-dimensional stochastic heat equation. Exact analytical solutions are available for many statistics, and numerical realizations can be generated for minimal computational cost and for any desired time step. Potential applications of the model include several situations where realistic cloud fields must be generated for minimal cost, such as cloud parameterizations for climate models or radiative transfer models.

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O28
Parallel and adaptive vertex-centered finite volume simulations for density driven flow

Density driven flow in porous media can be discretized by vertex-centered finite volume methods. With the availability of supercomputers and their growing computational resources, the efficient parallelization of these schemes becomes more and more important. In addition, adaptive approaches are desirable in order to refine only those grid regions where the accuracy is required while saving computational costs in less resolved areas. We present our strategies for parallelization and adaptivity for such problem settings and show their applicability in empirical studies.

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O29
Modeling thermo-hydraulic flow in fractured rock

A model for thermo-hydraulic flow in the vicinity of the Prototype Repository (PR) at the Hard Rock Laboratory at Äspö in Sweden was developed. It comprised not only the PR but also three adjacent tunnels as well as two major and six minor fractures influencing flow at the PR. From outflow measurements into the PR-tunnel a third major fracture was assumed where it could have been missed by the extensive hydrogeological investigations. The model required calibrating the isothermal flow system as most data about the flow field concerned the pre-installation phase. For the thermo-hydraulic model the heater power representing the heat production of waste canisters was translated into temperature boundary conditions at the borehole walls with the help of a pure heat conduction model. Coupling heat transport with groundwater flow in the code d3f++ allowed then to have a direct comparison of the isothermal and the non-isothermal flow field.

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O30
Mesh generation for parallel multigrid based simulations of density driven flow in domains with thin layers

The generation of detailed three dimensional meshes for the simulation of groundwater flow in thin layered domains is crucial to capture important properties of the underlying domains and to reach a satisfying accuracy. At the same time this level of detail poses high demands both on suitable hardware and numerical solver efficiency. Parallel multigrid methods have been shown to exhibit near optimal weak scalability for massively parallel computations of density driven flow. A fully automated parameterized algorithm for prism based meshing of coarse grids from height data of individual layers is presented. Special structures like pinch outs of individual layers are preserved. The resulting grid is used as a starting point for parallel mesh and hierarchy creation through interleaved projected refinement and redistribution. Efficiency and applicability of the proposed approach are demonstrated for a parallel multigrid based simulation of a realistic sample problem.

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O31
Validity criterion for models of density-driven flows in porous media with low-dimensional representation of fractures

In simulations of potential flows in fractured porous media, the fractures are often considered as low-dimensional manifolds. This allows to avoid difficulties with numerical methods but obtain sufficiently accurate solutions. However, this reduction of the dimensionality can result in neglecting important phenomena in the density-driven case. This leads sometimes to computation of wrong flow fields, but the error cannot be easily recognized in the context of the simplified model itself. In the talk, we investigate the restrictions of the validity of the models of the density-driven flows in porous media with the low-dimensional representation of the fractures. For this, we propose a criterion for the validity and verify it by numerical tests. Furthermore, we construct and test a dimensionality-adaptive technique for the simulations of this type of the flows.

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O32

Modeling variable density flow with heat generation caused by radioactive decay

A model of density and temperature driven flow and transport in porous media coupled with radioactive decay and the corresponding heat generation is presented. Two aspects of this model implemented in the GeRa numerical code are discussed. First, the treatment of dissolution boundaries in density-driven flow models is investigated. Besides the known effect of pressure drop in case of inconsistent dissolution boundary condition formulation we study its influence on the salt dissolution speed. Second, we provide verification results for a model with coupled volumetric heat production and temperature driven convection.

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O33

Fractal structures in freezing brine

The process of initial ice formation in brine is a highly complex problem. In this paper, we propose a mathematical model that captures the dynamics of nucleation and development of ice inclusions in brine. The model focuses on the interaction between ice growth and salt diffusion on the smallest continuous scale, subject to external forcing provided by temperature. Within this setting, two freezing regimes are identified: a slow freezing regime where a continuous ice domain is formed, and a fast freezing regime where recurrent nucleation appears within the fluid domain. The second regime is of primary interest, as it leads to fractal-like ice structures. We analyse the critical threshold between the slow and fast regimes, by identifying the explicit rates of external temperature control that lead to self-similar salt concentration profiles in the fluid domains in 1D. Subsequent heuristic analysis provides estimates of the structural properties of formed ice depending on the time-variation of the temperature. The analysis is confirmed by numerical simulations.

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O34

An MPFA-based dual continuum – discrete feature model for simulating flow in fractured reservoirs

Discrete feature models (DFMs) are applicable for complex geological systems containing fractures and faults. DFMs explicitly resolve these features, and as a result the complexity of the simulation model increases substantially when a large number of features is included. This has motivated the development of a Dual Continuum–Discrete Feature Model (DC-DFM) that accounts for the permeability effects of subgrid fractures as well as the dual-continuum nature of matrix–subgrid fracture interactions. To account for the full-tensor character of the effective matrix and fracture permeability, the MPFA-O discretization scheme is applied to each continuum. Mass transfer between the two continua is modeled using a transfer function. Numerical results for single-phase gas and two-phase oil-water systems are presented to demonstrate the performance of the methodology.

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O35

A robust control volume finite element method for highly distorted meshes

It can be challenging to produce good quality meshes for models of heterogeneous porous media as domains can have very large aspect ratio and/or complex geometry. Here, a novel control volume finite element method (CVFEM) for simulating multi-phase flow in heterogeneous porous media with highly distorted meshes is presented. In this new formulation, velocity and saturation are discretised as in the classical CVFE method, whereas the pressure is discretised using finite volumes. The use of finite volumes to discretise

the pressure creates a pressure matrix that converges very efficiently even when large angle elements are present in the mesh. Heterogeneous geologic features are represented as volumes bounded by surfaces. Our approach conserves mass and the use of implicit time integration allows the method to efficiently converge using highly anisotropic meshes without reducing the time-step. Results are presented showing the robustness of the presented method under a set of highly heterogeneous and complex geometries, showing very high aspect ratio elements, and using the black-box iterative solvers provided in the PETSc library.

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O36

Investigation of physically based interpolation strategies for a class of monotone nonlinear finite volume methods

In this presentation we investigate various interpolation strategies used in a class of cell-centered nonlinear finite volume methods. We apply the principles of several Multi Point Flux Approximation (MPFA) methods to design the node-based interpolation algorithms that interpolate unknowns at grid vertices using primary unknowns at cell centers. Face-based interpolation methods associate one point with each face of the grid. The first face-based interpolating method uses the harmonic averaging point proposed in the literature. However, a problem with harmonic averaging point is that it may lie anywhere on the hyperplane containing the grid face when the permeability tensor is highly heterogeneous and anisotropic, which can be quite problematic for the subsequent nonlinear solver. To have some control over the location of the interpolating point, we propose a directional-permeability averaging point that is well defined on the grid face. The weighing coefficients are then derived using the concept of directional permeability. Extensive numerical experiments are conducted to test the accuracy of the above interpolating strategies.

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O37

Advanced discretization schemes for general purpose reservoir simulation – review, analysis and comparison

Subsurface reservoirs are generally highly heterogeneous and geometrically complex. Therefore, modeling their fluid flow requires robust and accurate discretization schemes for the

governing equations. In this talk, we focus on the latest advances on the flux approximation schemes for general purpose reservoir simulation; MPFA, non-linear FV, mixed hybrid finite-element, and memetic finite-difference. We review the theoretical basis for each scheme, perform numerical analyses, and compare the methods' computational accuracy for all the main physics that dictate the fluid flow at the subsurface level.

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O38

Adaptive discontinuous Galerkin methods for flow in porous media

We present an adaptive Discontinuous Galerkin discretization for the solution of porous media flow problems. We implement and evaluate numerically interior penalty DG methods for 2D and 3D incompressible, immiscible, two-phase flow. We consider a strongly heterogeneous porous medium and discontinuous capillary pressure functions. First and second order Adam-Moulton time discretization are combined with various interior penalty DG discretizations in space. This implicit space time discretization leads to a fully coupled nonlinear system. The adaptive approach implemented allows for refinement/coarsening in both the element size, the polynomial degree and the time step size. To our knowledge, this is the first time the concept of local hp-adaptivity is incorporated in the study of 2D and 3D incompressible, immiscible, two-phase flow problems. The implementation is based on the Open-Source PDE software framework DUNE.

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O39

A linear domain decomposition method for partially saturated flow in porous media

Soil remediation, CO₂ storage and harvesting of geothermal energy are notable examples of multiphase flow processes through porous media. Modeling these processes leads to coupled nonlinear partial differential equations that change type and involve largely varying physical properties of the soil, like porosity and permeability and make the design of robust discretisation methods a non-trivial task. We combine a globally convergent L-scheme with a non-overlapping do-

main decomposition of the Richards equation making use of a linearised Robin type interface conditions to decouple both problems and obtain a globally convergent scheme which is robust, compares well even against a Newton iteration, and allows to account for very heterogeneous soil properties (different permeabilities, discontinuous over the interface). We present an analytical convergence result and discuss in detail numerical experiments and comparisons to different schemes (modified Picard, Newton, non-DD FV scheme). This is joint work with Koondanibha Mitra (TU/e), Florin Radu (UIB), I. Sorin Pop (Hasselt University) and Christian Rohde (Univ. of Stuttgart).

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O40

Adaptive mesh refinement with a mixed finite element method using a fully-coupled enhanced velocity solver

This work describes novel approach for performing adaptive mesh refinement using mixed finite elements. It uses the enhanced velocity (EV) method to directly construct a strongly flux-continuous velocity approximation between non-matching subdomain grids. The EV method was recently generalized to allow subdomain interfaces on the interiors of subdomains adjacent to inactive cells. Subdomains with different spatial resolutions are stacked on top of each other, producing a very general semi-structured grid. The decomposition is still non-overlapping, but now the subdomains can have holes, ragged edges, and be nested. Several examples with runtime adaptive mesh refinement are demonstrated. A fully-coupled solver was also implemented in this work, which shows a dramatic reduction in the number of Newton iterations versus the previously implemented nonlinear block Jacobi solver, when systems have a strong elliptic component.

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O41

Multiscale methods in fractured media

In this talk, we will discuss multiscale finite element methods for flows in fractured media. A systematic multiscale approach will be presented and its extension to various problems will be discussed. We will also discuss the relation between multiscale approaches and multi-continuum methods.

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O42

Multiscale unstructured discrete fracture model (MS-DFM)

A novel multiscale method for discrete fracture modeling on unstructured grids (MS-DFM) is developed. The fine-scale DFM system is constructed using unstructured conforming matrix cells with lower-dimensional fracture elements placed at their interfaces. On this fine grid, MS-DFM imposes independent coarse grids for the fracture and matrix domains. While the conservative coarse-scale system is solved on these coarse cells, a dual-grid is also formed to provide local supports for the multiscale basis functions. To maintain computational efficiency, fracture-matrix coupling is only considered in the matrix domain. This results in enriching fracture basis functions in the matrix. Furthermore, to enable error reduction to any desired level, a convergent iterative strategy is developed, where MS-DFM is employed along with a fine-scale smoother to resolve low- and high-frequency modes in the error. The performance of MS-DFM is assessed for several 2D and 3D test cases. Notably, the method proves accurate for many cases without any iterations. As such, MS-DFM provides a promising efficient framework for real-field application of unstructured DFM.

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O43

A multiphysics/multiscale pore network (MP/MSPN) simulation framework to bridge the gap between pore- and darcy scale

Algorithms for solving multiphase flow in networks are used to study various phenomena such as viscous fingering, reactive transport and dispersion. However, in various algorithms a pressure equation is solved at each time step. This limits the domain size to below that of a representative elementary volume. We present a multiphysics/multiscale simulation framework to overcome this limitation. In this framework an approximate pressure solution is computed such that the fluxes across pre-defined subnetwork boundaries are conservative. Second, these fluxes are used as boundary conditions to solve decoupled subproblems. The local subproblems can be solved with different algorithms, depending on the local flow conditions. Third, once the subproblems are solved, the coefficients in the global pressure problem can be updated. The simulation framework is amenable to parallel processing, and potentially capable of simulating flows in pore-network domains of sizes comparable to that of core samples. This is important in extracting meaningful macroscopic quantities.

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O44

Solving depth averaged equations using parallel GeoClaw

We demonstrate our success in incorporating GeoClaw (LeVeque, George, Berger, Mandli), a widely used code for simulation tsunamis, debris flow, flooding, storm surges and so on, into ForestClaw, an adaptive quadtree code based on the highly scalable library p4est (C. Burstedde). This new adaptive mesh framework allows us to run GeoClaw simulations on large scale parallel computing environments, and achieve resolutions not available on a desktop computers. We will demonstrate results by simulating the 1976 Teton Dam failure in eastern idaho, USA, and show that we get good agreement with historical data know about the resulting flood.

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O45

2D versus 1D models for shallow water equations

We present a general framework to construct 1D width averaged models when the flow is constrained -e.g. by topography- to be almost 1D. We start from two dimensional shallow

water equations, perform an asymptotic expansion of the fluid elevation and velocity field in the spirit of wave diusive equations and establish a set of 1D equations made of a mass, momentum and energy equations which are close to the one usually used in hydraulic engineering. We show that in some special cases, like the U-shaped river bed, that our set of equations reduces to the classical 1d shallow water equations. Out of these configurations, there is an $O(1)$ deviation of our model from the classical one.

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O46

A new family of efficient semi-implicit discontinuous Galerkin finite element schemes on staggered grids for the shallow water and the incompressible Navier-Stokes equations

We propose a novel family of semi-implicit discontinuous Galerkin methods for the shallow water and the incompressible Navier-Stokes equations on staggered unstructured meshes. While staggered meshes are state of the art in classical finite difference schemes, their use in high order DG schemes still quite rare. Here, the discrete pressure is defined on a primary grid, while the discrete velocity is defined on staggered dual control volumes. Substitution of the discrete momentum equation on the dual grid into the discrete continuity equation on the primary grid yields a very sparse block system for the scalar pressure that can be efficiently solved with matrix-free iterative solvers. From numerical experiments we find that the linear system is well conditioned, since all simulations shown here can be run without the use of any preconditioner. For a piecewise constant polynomial approximation in time, the resulting system is symmetric and positive definite. This is the first time that a semi-implicit discontinuous Galerkin finite element method on staggered unstructured meshes is presented for the shallow water and the incompressible Navier-Stokes equations. The method is verified on a series of typical 2D and 3D benchmark problems.

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O47

Efficient multi-layer shallow water models

Multilayer shallow models were introduced as an alternative to depth-averaged models in order to recover the vertical structure of the fluid. On the other hand, these models used to be discretized by explicit schemes, for which a CFL condition must be assumed. This condition depends on the velocity (U) and the thickness (H) of the fluid. In 1992, a semi-implicit finite difference method for the time discretization was introduced for shallow water systems in order to get a less restrictive CFL condition, which only depends on the velocity. This method importantly reduces the computational cost when we deal with subcritical flows. We present a semi-implicit method for multilayer system, based on the previous method proposed by Casulli et al.. Nevertheless, there are several important differences. Mainly the fact that the vertical mesh moves with the

flow, i.e., it is not fixed. We also consider a variable number of layer and include an IMEX-ARK second order scheme for the time discretization. Finally, we present some numerical tests showing that the computational cost of simulate large geophysical flows is improved without losing accuracy.

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O48

Simulation of shallow-water flows on general terrain

The typical derivation of the SW equations is based on the integration of the Navier-Stokes equations over the fluid depth in combination with an asymptotic analysis enforcing the SW assumptions. For almost flat bottom topographies, fluid depth is evaluated along the direction normal to the bottom surface. An integration path that better adapts to the shallow water hypothesis follows the “cross-flow” path, i.e., a path that is normal to the velocity field at any point of the domain. We approximate the “cross-flow” path by performing depth integration along a local direction normal to the terrain. The resulting equations are characterized by non-autonomous flux functions and source terms containing surface metric coefficients and related derivatives. The proposed model is numerically discretized with a first order upwind Godunov Finite Volume scheme associated with an approximated Riemann solver. The results show that it is important to take into full consideration the bottom geometry and slope even for relatively mild and slowly varying curvatures.

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O49

A finite-volume module for cloud-resolving simulations of global atmospheric flows

We extend to moist-precipitating dynamics a recently documented high-performance finite-volume module (FVM) for simulating global all-scale atmospheric flows [Smolarkiewicz et al., J. Comput. Phys. (2016)]. The thrust of this development is a seamless coupling of the conservation laws for moist variables engendered by cloud physics with the semi-implicit,

non-oscillatory forward-in-time integrators proven for dry dynamics of FVM. The adopted representation of water substance assumes a canonical “warm-rain” bulk microphysics parametrisation, recognised for its minimal physical intricacy while accounting for the essential mathematical complexity of cloud-resolving models. A key feature of the presented numerical approach is global conservation of the water substance to machine precision---implied by the local conservativeness and positivity preservation of the numerics---for all water species. The moist formulation assumes the compressible Euler equations as default, but includes reduced anelastic equations as an option. Theoretical considerations are illustrated with a benchmark simulation of a tornadic thunderstorm on a reduced size planet.

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O50

A finite-volume module for all-scale earth-system modeling at ECMWF

We highlight recent advancements in the development of the finite-volume module (FVM) for the Integrated Forecasting System (IFS) at ECMWF. FVM represents an alternative dynamical core that complements the operational spectral dynamical core of the IFS with new capabilities. Most notably, these include a compact-stencil finite-volume discretisation, flexible meshes, conservative non-oscillatory transport and all-scale governing equations. As a default, FVM solves the compressible Euler equations in a geospherical framework. A hybrid computational mesh, fully unstructured in the horizontal and structured in the vertical, enables efficient global atmospheric modeling. Moreover, a centred two-time-level semi-implicit integration scheme is employed with 3D implicit treatment of acoustic, buoyant, and rotational modes. The integration employs the finite-volume MPDATA advection scheme that is bespoke for the compressible dynamics on the hybrid mesh. The recent progress of FVM is illustrated with results of benchmark simulations of intermediate complexity, and comparison to the operational spectral dynamical core of the IFS.

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O51

Flexible earth system modeling on multiple grids

The algorithms underlying numerical weather prediction (NWP) and climate models that have been developed in the past few decades face an increasing challenge to adapt to paradigm shifts imposed by new hardware developments. The emerging diverse and complex hardware solutions have a large impact on the programming models traditionally used in NWP software, triggering a rethink of design choices for future software

frameworks. On the other hand, there is a drive to increase the model complexity to include ever more processes of the whole Earth system. Some of these processes may require computations on grids of different type or resolution than the atmospheric grid. Multiple grid structures may be required as part of the numerical filtering strategy for atmospheric wave motions or to simply save computational cost of selected physical processes. These different grids may have different domain decompositions for parallel computations, and different parallelisation strategies. Moreover the internal memory layout for a field that is optimal for one numerical algorithm may not be optimal for another. These complexities will inevitably break NWP modeling infrastructures that did not take these aspects into consideration 30+ years ago. To address the above mentioned challenges, the European Centre for Medium Range Weather Forecasts (ECMWF) is developing Atlas, a new modern software framework that is designed to take into account these new developments. Atlas helps to accommodate flexibility in hardware and software choices as well as increasing model complexity. Atlas is not a new model but rather forms a foundation layer that new models can be built with, or for existing models to be complemented or redesigned with.

In this talk, we demonstrate how Atlas is used to complement ECMWF's Integrated Forecasting System (IFS) model to enable a number of physical processes to be implemented on multiple grids.

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O52
GungHo – A mixed finite element-based dynamical core for next-generation numerical weather prediction

Current efforts in numerical weather prediction with prospective resolutions approaching the sub-kilometre scale are aiming at scalability as the primary target for next-generation dynamical cores on massively parallel computing architectures. Following the GungHo project, work at the Met Office is focusing on the implementation of a three-dimensional nonhydrostatic dynamical core based on a cubed-sphere grid arrangement with a mixed finite element scheme. The adoption of a more homogeneous grid together with the mimetic properties of the spatial discretization aim to tackle the scalability and conservation issues of the currently operational ENDGame model whilst retaining its accuracy properties. For advection the target method is a direction-split COSMIC scheme, with a finite volume method of lines option also available. Code paralleliza-

tion and flexibility to the underlying computing architecture are afforded by a Python engine featuring auto-generation of the parallel layer. Numerical results to date confirm expected behaviour on two- and three-dimensional tests of nonhydrostatic flows on Cartesian and spherical domains.

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O53
Modifications to the Global Environmental Multiscale (GEM) model dynamical core for improved forecast accuracy

The Global Environmental Multiscale (GEM) model is used operationally to forecast weather by Environment and Climate Change Canada. Several modifications have recently been implemented within the model to achieve more consistent and accurate numerical discretization across the different components of the dynamical core. A major change in this regard is related to the definition of the model vertical coordinate. The existing terrain-following log-hydrostatic pressure-type vertical coordinate in GEM has been modified to adopt a smooth level vertical (SLEVE) coordinate structure. The introduction of a SLEVE-type coordinate leads to better control of noise due to the presence of complex orography, particularly at the upper troposphere and stratosphere. Other changes to the dynamical core include more consistent numerical approach for the semi-Lagrangian trajectory calculations, implementation of differential off-centering for averaging the source terms in the dynamical equations and replacement of purely numerical hyper-diffusion schemes by a more physically-based Smagorinsky-type second-order diffusion scheme. All these modifications are found to result in considerable improvements in forecast accuracy.

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O54
Analysis and upscaling of a model for reactive flow in porous media

We consider a reactive flow model in a fractured porous medium. The particularity appears in the conditions imposed at the interface separating the block and the fracture, which involves a nonlinear transmission condition. Depending on the ratio between the fracture thickness and the medium thickness we discuss different regimes and study the existence of a weak solution. Next assuming that the ratio approaches 0, we study the convergence towards a reduced model with the fracture model component becoming a boundary condition.

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O55

Effective pressure boundary condition for the filtration through porous medium via homogenization

We present homogenization of the viscous incompressible porous media flows under the stress boundary conditions at the outer boundary. In addition to Darcy's law describing filtration in the interior of the porous medium, we derive rigorously the effective pressure boundary condition at the outer boundary. Intuitively, it is expected that the homogenized pressure will take the prescribed value at the boundary equal to the outside pressure. It turns out that the prescribed value is not just the outside pressure but a linear combination of the outside pressure and the applied shear stress. We use the two-scale convergence in the sense of boundary layers, introduced by Allaire and Conca to study the effects of the thin boundary layer next to the outer boundary. The approach allows establishing the strong convergence of the velocity corrector and identification of the effective boundary velocity slip jump. The theoretical results are confirmed through numerical experiments.

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O56

Effective transmission conditions for transport processes through a thin layer

In this talk we consider reaction-transport processes in two bulk domains separated by a thin layer with thickness of order ϵ .

The equations in the thin domain depend on the parameter ϵ and on an additional parameter $\gamma \in [-1, 1]$, where γ is a measure for the strength of the diffusion within the thin layer. The numerical treatment of such kind of microscopic problems leads to high computational costs. Therefore, for $\epsilon \rightarrow 0$, when the thin layer reduces to an lower dimensional interface Σ , we derive macroscopic models with effective transmission conditions across the interface Σ . The solution of this macroscopic problem approximates the solution of the microscopic one. The effective model depends on the different choices of the parameter γ . For the limit process we use the method of two-scale convergence and unfolding, where the crucial part is to go to the limit in the nonlinear reaction terms. For that we derive strong convergence results in a suitable sense in the thin layer.

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O57

Homogenization via unfolding in domains separated by a thin layer of thin beams

We consider a thin heterogeneous periodic layer consisted of thin beams and we study the limit behaviour of this problem as the periodicity, the thickness and the radius of the beams tend to zero. A decomposition of the displacement field in the beams is used, which allows to obtain a priori estimates. Two types of an unfolding operators are introduced to deal with the different parts of the decomposition. In conclusion we obtain the limit problem together with the transmission conditions across the interface.

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O58

Space-time domain decomposition for a nonlinear parabolic model of two-phase flow with discontinuous capillary pressure

We consider two-phase flow in a porous medium composed of different rock types, so that the capillary pressure field is discontinuous at the interface between the rocks and creates a capillary trap for oil or gas. This is a nonlinear and degenerate parabolic problem with nonlinear and discontinuous transmission conditions on the interface.

We describe a space-time domain decomposition method based on the Optimized Schwarz Waveform Relaxation algorithm (OSWR) with Robin or Ventcell transmission conditions. Space-time subdomain problems across the time interval are

solved at each OSWR iteration, and the exchange between the subdomains uses time-dependent and higher order transmission operators. Full numerical approximation is achieved by a finite volume scheme, using the Matlab Reservoir Simulation Toolbox.

By introducing Robin to Robin (or Ventcell to Ventcell) operators in each subdomain, the problem can be formulated as a (space-time) interface problem of fixed point type, with one unknown on each side of the interface. This allows the use of methods with better efficiency than simple fixed point, such as Newton-Krylov or Anderson acceleration.

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O59

Ensemble-based reservoir optimization

We apply a flexible, computationally-efficient ensemble-based stochastic optimization algorithm (StoSAG) to a variety of reservoir optimization problems including water flooding and water-alternating-gas WAG optimization where the objective (cost) function is the net present value of life-cycle production and the design (optimization) variables may include well pressures and rates as a function of time, WAG half-cycle lengths and parameters defining well locations and trajectories. In all cases, robust optimization is applied in order to account for geological uncertainty.

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O60

An evaluation of sampling strategies for ensemble-based optimization

Determining the optimal exploitation and management of subsurface resources or storage sites typically requires evaluation of alternative operational strategies within a context of potentially conflicting objectives, complex constraints and large uncertainties. Different strategies are normally evaluated with the help of numerical simulation models whose

inputs represent the strategy and whose outputs represent objective functions or constraints. Given the large dimensions of the input space efficient exploration of the input space is crucial for a successful identification of suitable strategies. We consider ensemble methods for gradient-based optimization as a framework for such exploration. Current implementations of ensemble optimization methods tend to rely on a finite-size set of random samples. Here we explore different approaches to define criteria for improved static and adaptive sample designs and evaluate the computational cost and added value of different design concepts. We consider different test cases based on synthetic reservoir models and oil recovery strategies.

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O61

Robustness evaluation of ensemble-based methods for production optimization

The ensemble-based optimization (EnOpt) attracts wide interests with its advantages of easy implementation, high compatibility with various simulation tools and capability of gradient approximation. Despite of various highlights of EnOpt, the robustness of this method need to be evaluated and improved when considering geological uncertainty. Instead of sampling from the same Gaussian distribution, we propose the use of Gaussian Mixture optimization (GMOpt) to enable the application of EnOpt with multiple starting points sampled from different Gaussian distributions. In addition, smart ensemble components are designed such that certain components can be selected or discarded accordingly. In the presence of geological uncertainty, this work also investigates the impact of different geological representations on objective function evaluations and optimal solutions. We perform various experiments on a synthetic study case. Results show significant variations of net present value (NPV) resulted from multiple factors such as stochastic perturbation of ensembles and uncertainty of geo-models.

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O62

Geomechanical parameter estimation with a coupled flow-geomechanical model

By applying ensemble-based methods, governing parameters of a coupled flow-geomechanical model are estimated by assimilating observations of surface deformation such as leveling, GPS and/or InSAR. With this approach, we study the influence of heterogeneous geology to the compaction of hydrocarbon producing reservoirs. Particular interest is paid on how heterogeneities and the presence of faults affect the observed deformation.

Starting from a simplified configuration, the complexity of the model is increased in a number of synthetic data assimilation experiments. The unstructured discretization of the model allows for local refinements in those areas where parameters are expected to vary at a small scale. Given the non-linearity of fault behaviour, the use of ensemble-based particle methods is especially attractive.

The resulting data assimilation system can be used to assess the value of various sources of information and help to effectively balance the various uncertain parameters in the subsurface to obtain the most likely description of the compaction-related phenomena.

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O63

Orthonormal residuals for large-scale geostatistical model validation

Geostatistical methods are widely used to estimate spatial model parameter functions, like hydraulic conductivity, based on measurements of dependent quantities, like hydraulic heads or solute arrival times. In this framework, the unknown parameter values are treated as random variables that have to be conditioned on given state observations. In recent years, highly efficient methods for large-scale problems of this type have been developed, allowing the simultaneous estimation of millions of parameters based on thousands of measurements. However, the applicability of the parameterized model depends on the involved modeling errors and stochastic approximation error, which makes validation a necessity. We present a novel approach for the validation of large-scale geostatistical models: orthonormal residuals generated through randomized decomposition of the covariance matrix of measurement residuals. In contrast to studentized residuals, these orthonormal residuals take the high amount of correlation between individual measurement residuals into account. We discuss strategies for efficient computation and present examples of application.

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O64

Synchronous history matching of multiple SCAL experiments for relative permeability and capillary pressure interpretation

Conventional approaches of SCAL data interpretation are suffering from significant diminishing of important effects such as capillary and viscous force interaction, capillary end effect and space variation of centrifuge acceleration in case of centrifuge experiment. But any small error obtained on this stage of interpretation can cause a much bigger one on a field scale. On another hand the numerical simulations of SCAL experiments can be used in solving corresponding inverse problem.

In the present work the history matching algorithm was developed in open source MATLAB tool namely MRST. To take into account the interaction of capillary and viscous forces in full perspective the history matching process was done simultaneously for different type of experiments such as steady state and centrifuge, which were performed on several similar samples of Barea sandstone. For relative permeability and capillary pressure representation a generalized piecewise linear approximation is used and each discrete point on the curve is considered as a parameter. To cover such wide range of model parameters the optimization algorithm was implemented with adjoint formulation in the scope of L-BFGS-B approach, which showed a high convergence rate and accuracy.

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O65

Modeling seismic wave propagation using staggered-grid mimetic finite differences

Mimetic finite difference (MFD) approximations of continuous gradient and divergence operators satisfy a discrete version of the Gauss-Divergence theorem on staggered grids. On the mimetic approximation of this integral conservation principle, a unique boundary flux operator is introduced that also intervenes on the discretization of a given boundary value problem (BVP). In this work, we present a second-order MFD scheme for seismic wave propagation on staggered grids that discretize free surface and absorbing boundary conditions (ABC) with same accuracy order. This scheme is time explicit after coupling a central three-level finite difference (FD) stencil for numerical integration. Here, we briefly discuss the convergence properties of this scheme and show its higher accuracy on a challenging test when compared to a traditional FD method. Preliminary applications to 2D seismic scenarios are also presented and show the potential of the MFD method.

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O66

Retrieving low-frequency model with cross-correlation misfit – A realistic synthetic study case

Full Waveform Inversion (FWI) in seismic scenarios continues to be a complex procedure for subsurface imaging that might require extensive human interaction, in terms of model setup, constraints and data preconditioning. Especially, extracting low-frequency model content from noisy dataset still remains very challenging. On the other hand, inversion of the high frequency content of the dataset is more prone to cycle skipping if starting models are not good enough. This is why most of the research effort in the last decade has been focus on developing efficient misfit functional that mitigate cycle-skipping effects. The well-known Cross-Correlation misfit will be used here as a robust low frequency model builder for FWI, even though the data are strongly cycle-skipped. Then the highest frequencies will be reconstructed with the classical L2 norm.

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O67

A review of the numerics in seismic full wave inversion and a robust implementation

Full Waveform Inversion (FWI) represents a seismic imaging method able to improve Earth structural models up to spatial resolutions beyond the limits of standard travel time tomography, that only inverts the time residuals of (mostly) P-wave phases picked on the recorded field traces. Conversely, FWI processes the whole waveforms achieving a finer resolution. On this process, FWI convergence to the true model is compromised by noise effects on seismic data, initial models with poor low frequency content, and limitations on surface-to-surface acquisitions. Suitable data processing strategies combined to alternative misfits functionals can make of multiscale FWI a reliable optimization procedure of model reconstruction. On this talk, we review a general mathematical formulation of FWI, necessary tunings on numerical algorithms underneath its implementation, and key data processing devices to gain robustnesses. In addition, we present some applications to challenging synthetic datasets is cases of acoustic and elastic media.

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O68

Overview of numerical techniques and applications for CSEM/MT geophysical surveys

We will present an overview of methodologies that can be used in the field of EM geophysical modeling, in particular applied to CSEM and MT. We will cover some numerical approximations both in 2D and 3D as well as their application to modeling and inversion for both synthetic and real scenarios.

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O69

Volume source-based extended waveform inversion method for seismic velocity inversion

In this talk, I will introduce a volume source-based extended waveform inversion method called Matched Source Waveform Inversion (MSWI), which allows additional, non-physical sources acting at shotting time. The extra sources permit the data to be fit well, even when velocity is kinematically inconsistent with data. A distance-weighted penalty on source energy is minimized when the data is fit. Good data fit throughout the inversion process produces a considerably more convex objective function than does the standard data-domain FWI formulation. A good theoretical foundation for this approach exists for pure transmission problems, while numerical examples suggest that in fact it may be a feasible approach to reflection and transmission inversion when the low frequency components of data is missing.

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O70

The analysis of earth’s global gravitational field by using spherical wavelet transform

Gravimetric (potential) methods are widely used in geophysics for study the Earth’s structure. The main goal of these methods is the determination of the causal sources of potential anomalies measured on the surface.

We present a novel method for analyzing the geopotential data obtained on the surface of a sphere. This method is based on the continuous wavelet transform with so called “native” basis and allows to obtain the large class of the equivalent solutions by changing scale parameter of the wavelet. Moreover, computational experiments show that location and depth of synthetic causative sources are uniquely determined by the proposed method.

Comparison of the results of presented method with ones obtained by seismic methods demonstrates a good agreement. The real examples show that this analyzes is allowed to study global geological structures of the spherical objects such as Earth, Moon, Mars and Venus.

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O71

Love wave frequency under the influence of linearly varying shear moduli, initial stress and density of orthotropic half space

The present work deals with the Love wave propagation in an inhomogeneous anisotropic layer resting over an inhomogeneous half space under the influence of rigid boundary plane. The layer has inhomogeneity which varies quadratically with depth whereas the inhomogeneous orthotropic half space exhibits inhomogeneity in the shear moduli, density and initial stress which varies exponential downward. The frequency equation is deduced in a closed form by the help of displacements and the suitable boundary conditions. For a layer over a homogeneous half space, the dispersion equation agrees with the equation of the standard classical result. It is observed that the inhomogeneity parameter has a prominent and significant effect on the phase velocity of Love wave. Graphical interpretation for each parameter has been presented and the results are discussed in detail.

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O72

Green function approach to study of surface seismic wave propagation

Aim of the abstract is to study the effect of point source, initial stress and various aspects of non-homogeneity parameters on the propagation of surface seismic wave in the Earth layered media. We considered a two layers geometric model of the problem: (1) finite thickness transversely isotropic medium and (2) semi-infinite medium with different rigidity and density in the directions of transversal and longitude. The rigidities, densities and internal friction are varying as the functions of depth. The mathematical analysis of the problem has deal with Fourier transform and Green's function's techniques. The frequency equation of the phase velocity has been obtained and investigated for different cases. As special case when the upper layer and lower half-space are free from initial stress and heterogeneity parameters, then dispersion equation coincides with the standard result of Love wave (A.E.H. Love, 1911). Phase velocity has been calculated numerically and shown graphically using MATLAB coding. It is observed that, the velocity of surface wave is influenced by initial stress, internal friction, rigidity, and density and heterogeneity parameters.

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O73

Simulation of deformation and flow in fractured poroelastic materials

Coupled fluid–solid interaction processes in fractured porous media play an important role in engineering applications such as the design and construction of geothermal power plants, and the risk assessment of waste deposits. Numerical simulation of these processes remains challenging due to the number of physical processes involved, the nonlinear coupling, the complex geometries, and the heterogeneous nature of

fractured porous rock.

In this work we focus on the coupling between hydrology and mechanics in fracture networks. The fluid flow in the fracture network is modeled by a lower-dimensional equation, which interacts with surrounding rock matrix and the fluid it contains. Special coupling conditions modeling the interaction of the fluid flow and the deformation in fracture joints are introduced.

For numerical simulations, we combine a XFEM discretization for the rock matrix deformation and pore pressure problem with a standard finite element method on a lower-dimensional grid for the fracture flow problem. The resulting coupled discrete problem consists of linear subdomain problems coupled by nonlinear coupling conditions. We solve the coupled system using a substructuring solver. The properties of this approach is illustrated by numerical examples.

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O74

Upscaled models for two-phase flow in fractured rock

Double continua models are quite established for two-phase flow problems, where the fracture network is described as a mobile domain and the rock matrix as an immobile domain. The flow is modeled in the mobile domain and the fluid exchange between mobile and immobile domain is described as a source or sink term. We present such a model, where the source / sink term is non-local in time. The influence of the network structure is reflected in the integral kernel (the memory function).

The presentation will demonstrate two such models, one where matrix flow is dominated by capillary counter-current flow and one where it is dominated by gravity co-current flow. It will be demonstrated how the parameters, in particular the memory function, of the upscaled model could be estimated in advance if structure properties of the fracture network are known and how it could be simplified to be used in standard two-phase flow simulators. We will discuss the method to estimate parameters with numerical simulations of flow processes in 2D fracture networks, using detailed models where the fractures are resolved and with upscaled models with pre-estimated model parameters.

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O75

Using topology to estimate permeability of fracture networks

Existing methods for analytical upscaling of fracture network permeability assume that fractures are idealized geometrical objects, scattered randomly in space. In this work, we investigate if these methods can be improved by incorporating topological measurements.

The number of fracture intersections, abutments and tips within a fracture outcrop map is used to characterize the topology of the network. We devise five different ways of incorporating this information into standard methods, and test which approach gives the most predictive permeability estimates.

For the testing, we use both randomly distributed fractures, structured networks and natural networks. In each case, we perform numerical permeability upscaling, and compare the result with analytical upscaling.

Two of the proposed methods did a poor job of predicting permeability of networks with abutments. The three other methods were able to predict the correct permeability across a wide range of topological and geometrical network properties. For the best-fitting method, we devised a single functional relationship between connectivity and permeability, based on the data.

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O76

Hydraulic stimulation and friction laws for fracture deformation – A numerical study

Injection of fluids related to geothermal energy extraction, CO-storage, enhanced oil recovery and energy storage can activate natural fractures due to hydraulic stimulation. For crystalline rock, fractures will dominate subsurface flow patterns as well as rock mechanical deformation, and shear displacement of a fracture can increase its permeability by orders of magnitude.

Elevated pressures perturbs the effective stress and reduce the resistance of a fracture to sliding. Focusing on the choice of friction model for deformation of explicitly represented fractures, we present a model for coupled flow, fracture deformation and rock matrix deformation. A finite-volume discretization is used for both mechanics and flow, based on a discrete fracture-matrix model, where fractures are explicitly discretized in a conforming grid. We investigate several test cases, from a simple case to a case motivated by a real fracture network in 3D.

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O77

A space-time adaptive method for reservoir flows

This work presents a space-time adaptive framework for solving porous media flow problems, with specific application to reservoir simulation. A fully unstructured mesh discretization of space and time is used instead of a conventional time-marching approach. A space-time discontinuous Galerkin finite element method is employed to achieve a high-order discretization on the anisotropic, unstructured meshes. Anisotropic mesh adaptation is performed to reduce the error of a specified output of interest, by using a posteriori error estimates from the dual weighted residual method to drive a metric-based mesh optimization algorithm. The space-time adaptive method is demonstrated on two-phase flow problems in 1D and 2D spatial domains, and compared with a conventional first-order time-marching finite volume method for efficiency.

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O78

Seismic wave propagation simulation in fractured media

Fractures play an important role in subsurface hydrocarbon exploration and production. Although they are observed in sparse outcrops and limited well logs, and their effect is observed in fluid production rates, three dimensional description of subsurface fractures is only possible by making use of seismic data. Unfortunately, the effect of fractures on seismic wave propagation in multiple scales has not been investigated systematically. It is generally believed that at low frequencies, fractures can be replaced by an effective anisotropic medium and large fractures are clearly visible in seismic sections as discontinuities or faults. The effects of more common fracture swarms have not been investigated in detail. We have developed discontinuous Galerkin (DG) and integral based methods for wave propagation modeling in media in which we model the fractures as non-welded contacts. The contacts are characterized by discontinuity in displacement and modeled conveniently with the linear slip model. Our results clearly demonstrate that in low frequency limit, the effective media models are clearly valid. However, at intermediate scales, the fractures show characteristic scattering patterns that can be related to different fracture properties.

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O79

Generalized multiscale discontinuous Galerkin method for subsurface flow and wave problems

Numerical modeling of subsurface flow and wave propagation is important in many applications that include geophysics. For example, subsurface flow and wave propagation simulations

play an important role in determining subsurface properties. Because of multiple scales and high contrast in subsurface model, model reduction techniques are often required. In this talk, we introduce a generalized multiscale discontinuous Galerkin method (GMSDGM) for subsurface flow and wave problems. This method is constructed following the general framework on generalized multiscale finite element method (GMSFEM). While GMSFEM uses continuous Galerkin methods as coarse grid solvers, the GMSDGM considered in this paper is based on the interior penalty discontinuous Galerkin method as the coarse grid solver. The IPDG formulation can handle complex geometries with a block diagonal mass matrix. We present a-priori error estimate and some numerical examples which show the GMSDGM is an efficient coarse grid solver for flow and wave problems.

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O80

Multiscale parallel-in-time coupling for wave propagation in heterogeneous media

We present a new multiscale algorithm that couples localized direct numerical simulations (DNS) of the wave equations with the Gaussian beam (GB) methods in the high frequency regime. The algorithm is based on a stabilized “parareal” method and allows for parallel-in-time computation of the coupled system. The aim is to use the DNS to resolve locally the deficiencies of the GB method, and use GB to propagate the localized DNS solutions.

We will demonstrate some numerical results computed by the proposed algorithm for high frequency wave propagating in a piecewise smooth medium.

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O81

Modeling multiphase hydraulic fracture propagation

In this talk we present a phase field model for a multifluid-driven fracture in a poroelastic medium. We consider a fully coupled system where the pressure field is determined simultaneously with the displacement and the phase field. The mathematical model consists of a linear elasticity system with fading elastic moduli as the crack grows, which is coupled with an elliptic variational inequality for the phase field variable and with the pressure and the saturation equations containing the phase field variable in its coefficients. We establish existence of a solution to the incremental problem through convergence of a finite dimensional approximation. Furthermore, we construct the corresponding Lyapunov functional that is linked to the free energy. Computational results are provided that demonstrate the effectiveness of this approach in treating multifluid-driven fracture propagation.

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O82

A multiscale hybrid-mixed method for the elastodynamic model in time domain

This work proposes a Multiscale Hybrid-Mixed (MHM) method for the second order elastodynamic equation in time domain with highly heterogeneous coefficients. The family of MHM methods naturally incorporates multiple scales in the numerical solution while providing solutions with high-order precision. It is a consequence of a hybridization procedure, in which the computation of local problems is embedded in the upscaling procedure. As such, the local problems are independent to one another, and thus, they can be naturally obtained using parallel computation.

The contribution of this work is two-fold. First, we propose a new theoretical framework in which the MHM method for the elastodynamic model is built. Preliminary theoretical results are addressed. Secondly, several numerical validations verified the error optimality of MHM method and its capacity to deal with multiscale media on non-aligned coarse meshes. Moreover, we show the MHM method is naturally shaped to be used in parallel computing environments.

So, the MHM method turns out to be a highly competitive option to handle realistic three-dimensional wave propagation phenomena in multiscale media.

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O83

The 3D elastodynamic wave equation with transparent boundary conditions

The elastic wave equation is a partial differential equation required in a number of geoscientific problems, e.g., the propagation of seismic waves. We discuss coupled interior-exterior problems of the elastodynamic wave equation in three-dimensions. The equation is solved numerically for non-convex domains with transparent boundary conditions, which means that the wave can re-enter the domain. In addition,

we analyse the stability and convergence of the numerical methods. Finally, we present numerical examples which are implemented by using boundary element methods (BEM) and the convolution quadrature method (CQ).

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O84

Accurate and stable time stepping in ice sheet modeling

We introduce adaptive time step control for simulation of evolution of ice sheets. The discretization error in the approximations is estimated using “Milne’s device” by comparing the result from two different methods in a predictor-corrector pair. The time step is changed in an efficient way that the velocity field equation is only solved once per time step. The stability of the numerical solution is maintained and the accuracy is controlled by keeping the local error below a given threshold using PI-control. Our method takes a shorter time step than an implicit method but with less work in each time step and the solver is simpler. The method is analyzed theoretically with respect to stability and applied to the simulation of a 2D ice slab and a 3D circular ice sheet. The stability bounds in the experiments are explained by and agree well with the theoretical results.

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O85

Modified shallow-water equations for direct bathymetry reconstruction

Improved capabilities of remote sensing and sea surface elevation data availability allow to obtain high-resolution elevation maps for rivers, estuaries, coastal seas, etc. However, the availability of bathymetry information is much more scarce in many locations of interest, and data collection methods for large area coverages are either inaccurate or expensive. To address this problem, a modified shallow water system is proposed that uses bathymetry as the primary unknown, whereas the free surface elevation field enters the system as a prescribed quantity. In addition to formulating and discretizing this modified system, our talk demonstrates first numerical results.

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O86

Modeling the oscillations of the thermocline in a lake by means of a fully consistent and conservative 3D finite-element model with a vertically adaptive mesh

Vertical discretisation is crucial in the modeling of lake thermocline oscillations. For finite element methods, a simple way to increase the resolution close to the oscillating thermocline is to use vertical adaptive coordinates. With an Arbitrary Lagrangian-Eulerian (ALE) formulation, the mesh can be adapted to increase the resolution in regions with strong shear or stratification.

In such an application, consistency and conservativity must be strictly enforced.

SLIM 3D, a discontinuous-Galerkin finite element model for shallow-water flows (www.climate.be/slim, e.g. Kärnä et al., 2013, Delandmeter et al., 2015), was designed to be strictly consistent and conservative in its discrete formulation. In this context, special care must be paid to the coupling of the external and internal modes of the model and the moving mesh algorithm. In this framework, the mesh can be adapted arbitrarily in the vertical direction. Two moving mesh algorithms were implemented. The criteria used to define the optimal mesh and the diffusion function are related to a suitable measure of shear and stratification.

We will present in detail the design of the model and how the consistency and conservativity is obtained.

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O87

Automatic well-balancing in a formulation of pressure forcing for DG modeling of stratified oceanic flows

In the usual formulation of the shallow water equations for a homogeneous fluid, the lateral pressure forcing within the fluid is expressed in terms of the gradient of the free-surface elevation. When this elevation is expressed in terms of the layer thickness, the pressure forcing then includes the gradient of the bottom topography. That gradient is a static forcing term that must be implemented carefully in order to avoid spurious forcing. With an alternative described here for discontinuous Galerkin spatial discretizations, the lateral pressure forcing within the fluid is not represented in terms of the free-surface elevation. Instead, this alternative proceeds directly to a weak form by multiplying by a test function and integrating over the water column that lies on a given horizontal grid element. This formulation is automatically well-balanced, assuming that the method used to compute pressure at element edges reproduces the continuous values in the special case where the DG solution is continuous across element edges. This result generalizes to the case of a stratified fluid with a generalized vertical coordinate.

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O88

Semi-implicit time integration, blended models, and balanced data

The construction of a semi-implicit time integration scheme for the compressible Euler equations is discussed that is to combine the following features: It is in conservation form for mass, momentum, and the potential temperature density, it avoids subtraction of a mean background state in formulating the implicit fast wave discretization, it allows for arbitrary time steps with respect to acoustic and internal waves, and it blends into a pseudo-incompressible solver when a model parameter akin to the Mach number vanishes. The blending property is of interest for a fair comparison of the compressible and pseudo-incompressible models, for the efficient approximate balancing of pressure and potential temperature fields in data assimilation schemes, and for the design of a scale-dependent time integration approach that employs a symplectic integrator for time resolved modes while utilizing A- or L-stable schemes for underresolved ones. The talk will summarize an existing scheme of this type that is implicit only with respect to the acoustic modes, and then focus on current efforts at extending it to include implicit gravity as well.

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O89

B-series and order conditions for split-explicit integrators

Split-explicit methods are common time integration methods in numerical weather forecasting, where part of the right hand side is computed on a smaller time step and the other part is frozen. For an additive splitting Wensch et al. derive order conditions up to order three for a generalized formulation. Here we show that these methods can be interpreted as generalized exponential integrator provided the right hand side depends nonlinearly two times from the integration variable. To derive order conditions we shall use a generalisation of Butcher series based on the use of rooted trees. A novelty of the approach is the integration of equations with B-series as right hand sides. The generalized B-series calculus is implemented in Fortran and can deliver the defect of the order conditions for any given set of coefficients of the integration method. An optimization procedure is outlined to find new methods. Numerical examples will illustrate old and new integration methods.

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O90

Time parallel methods for oscillatory stiffness in atmosphere and ocean modeling – fast singular limits

In this talk I discuss the role of oscillatory stiffness in time-parallel algorithms for atmosphere and ocean modeling. I will discuss exponential integrators and the relationship between fast singular limits and the convergence of the parareal algorithm.

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O91

Direct FEM parallel-in-time computation of turbulent flow

Turbulent flow computation at high Reynolds number is of key importance for wind energy. In this seminar we will present an overview of the Direct FEM methodology for turbulent flow and recent new developments toward parallel-in-time simulation, a key step for effectively taking advantage of supercomputers, and with the potential of enabling fast simulation. Our methodology is based on a piecewise linear approximation in space and time and with a numerical stabilization in the form of a weighted least squares method based on the residual, which acts as a parameter-free implicit model of the unresolved subscales. Goal-oriented error estimates based on an adjoint solution automatically optimize the mesh. We investigate the potential for parallel-in-time methods by analyzing the stability of the adjoint, which we use as an indicator of inter-dependence of partitions of the time-interval.

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O92

The Galerkin Numerical Modeling Environment (GNuMe) for geophysical fluids dynamics simulations on next-generation architectures

In this talk, we shall describe the GNumE framework for solving geophysical fluid dynamics problems on next-generation computers. GNumE is a Galerkin-based (continuous and discontinuous Galerkin) modeling environment for solving systems of nonlinear equations including: the compressible Navier-Stokes equations, incompressible Navier-Stokes, and the shallow water equations. GNumE can solve all of these components in 2D and 3D and uses dynamically adaptive mesh refinement in parallel (thanks to the p4est library) and can run simulations on next-generation computer architectures (thank to the OCCA library). We will present results for atmospheric, ocean, and shallow water simulations with wetting and drying on massively parallel computers.

For my information on GNumE please visit: frankgiraldo.wix-site.com/mysite/gnume

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O93

Large Eddy Simulation of gravity currents with a high order DG method

This work deals with Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) of a turbulent gravity current in a gas, performed by means of a Discontinuous Galerkin (DG) Finite Elements method employing, in the LES case, LES-DG turbulence models introduced in [1]. Numerical simulations of non-Boussinesq lock-exchange benchmark problems show that, in the DNS case, the proposed method allows to correctly reproduce relevant features of variable density gas flows with gravity. Moreover, the LES results highlight, in the gravity current context, the excessively high dissipation of the Smagorinsky model with respect to the Germano dynamic procedure.

Results obtained with more advanced models, like the anisotropic dynamic model (see [2]) and the new proposals in [4], will also be presented.

[1] Abbà A. et al. 2015 Dynamic Models for Large Eddy Simulation of compressible flows with a high order DG method. *Computers and Fluids* 122, 209–222.

[2] Abba A. et al. 2003 Analysis of Subgrid Scale Models. *Computer and Mathematics with Applications* 46, 521–535.

[4] Germano M. et al. 2014 On the extension of the eddy viscosity model to compressible flows. *Physics of Fluids* 26, 041702; doi:10.1063/1.4871292.

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O94

A parallel library of p-adaptive high order finite elements for geophysical applications

High order DG methods pose stringent stability restrictions on explicit time discretization methods. In recent work by the authors, a strategy for the reduction of the computational cost of DG methods has been proposed

A semi-implicit, semi-Lagrangian time discretization is employed, that allows the use of much longer time steps than explicit schemes. Furthermore, a dynamically adaptive choice of the

polynomial degree employed in each element. This adaptive strategy allows to reduce the number of degrees of freedom by a factor of up to 50%. In this work, we will outline the ongoing development of a parallel library that will allow to implement these adaptive techniques by taking full advantage of degree adaptivity in each coordinate direction of generic hexahedral elements. The key ingredients of the parallelization strategy will be presented along with preliminary numerical results in three dimensions. The preliminary results achieved are promising and hint that the proposed approach is useful to achieve the maximum possible flexibility in the application of high order discontinuous finite element methods to environmental flows.

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O95

Clogging in effective equations for non-isothermal reactive porous media flow

Geochemistry has a substantial impact on exploiting geothermal systems due to porosity changes induced by chemical reactions in the pores. Properties such as permeability and effective heat conductivity in the porous medium will then vary with time, affecting the temperature and flow profiles. We study Darcy scale transports using upscaled effective equations for non-isothermal reactive porous media flow where the variability of the effective properties is handled through solutions of cell problems arising from pore scale formulations. This approach can give a more accurate description of how the effective properties develop as the porosity changes. The upscaled effective problem is formulated using a two-dimensional periodic porous medium for the evolving pore structure. Assuming the grains to be either circular or elliptical results in one-parameter cell problems giving numerically efficient solutions for the Darcy scale transports. The models are used for investigating the effective behavior of the permeability and effective heat conductivity, and more specifically studying the behavior when the porous medium is close to clogging.

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O96

Numerical methods for a multiscale biofilm model in porous media

The talk concerns with the growth of biofilms made by bacteria within a saturated porous media. The increase of a biomass on the surface of the solid matrix changes the porosity and impede the flow through the pores. An effective model describes the process via Darcy's law and upscaled transport equations with effective coefficients given by the evolving microstructure at the pore-scale. Furthermore, we apply a mixed finite element scheme to solve this model numerically. In order to compute the effective coefficients, elliptic cell problems have to be solved in each element as well as at each time step. Hence in general such an approach is rather expensive. Investigating

the cell problems in more detail leads to useful estimates for the corresponding effective coefficients and yields finally a more efficient numerical method.

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O97

Towards multi-continuum formulations with dynamic fracture permeabilities

Fractures are ubiquitous in geological porous materials. Naturally fractured reservoirs store a large percentage of the remaining hydrocarbon reserves while operationally induced or reactivated fractures are paramount for hydrocarbons from shales and geothermal energy or pose leakage risks for CO₂ storage formations. In the last decade, substantial progress has been achieved in explicitly representing fractures in numerical simulations. Even the simulation of opening and closing of fractures due to chemical reaction or effective stress alterations start to become feasible. However, for large scale simulations and industrial applications, representative multi-continuum formulations remain the standard. Here, we present first steps to account for dynamic fracture permeabilities in multi-continuum formulations. We discuss implications for the appropriate representation of the different continua as well as dynamic transfer concepts.

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O98

Mixed methods for hierarchical flow models for non-isothermal wells in porous media

Due to the large difference in the spatial scales of a well and the surrounding aquifer, wells are commonly modelled using a lower-dimensional source term. This gives rise to an elliptic problem with a Dirac delta right-hand side in cases where the dimensional gap is larger than one. The solution to this problem does not lie in H¹, leading to suboptimal convergence rates for finite element solutions. In this work we propose a mixed formulation for the problem in a non-isothermal setting, resulting in a system of coupled elliptic and parabolic equations. We perform numerical analysis for the problem and simulate the scenario of heated water being injected into an aquifer.

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O99

Advantages of mixed hybrid finite element method in swelling computation

Swelling is a common phenomenon in geoscience. Some of the clay minerals are able to expand 20 times its own volume after adsorption of water. It is important to study such a phenomena, as swelling of clay can cause serious damage (formation damage problems) in civil engineering and oil/gas industry. Besides clay minerals, other materials that have

wide applications in agriculture, such as, hydrogel, living cells and organ cells experience large degree of swelling during functioning as well. Therefore, a robust numerical model to capture the swelling behavior especially in the large deformation regime is desirable. In this work, we focus on the category of clay that swells due to osmosis. A full three dimensional mixed hybrid finite element model is developed, in which the Raviart-Thomas element is used to approximate the flux field directly. We investigate the influence of the mixed formulation on the calculation results in terms of accuracy, implementation difficulty and computational efficiency.

We demonstrate the advantages of the mixed hybrid model over the conventional finite element model by means of numerical examples.

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O100

Biologically inspired formulation of optimal transportation problems and applications

We have recently developed an approach, based on an extension of a model proposed by Tero et al (2007), for the simulation of the dynamics of a slime mold (*Physarum Polycephalum*). Our model couples an ODE describing transient dynamics for a diffusion coefficient, with an elliptic PDE. We conjecture that the long-time solution of the coupled system approaches the solution of the PDE based Monge-Kantorovich Optimal Transport equations. Analytical and numerical experiments suggest that indeed the conjecture is true. One of the most important advantages of the proposed formulation is that its numerical solution is very efficient and well-defined using simple discretization schemes. Moreover simple modifications of the proposed model yield dynamic versions of the congested and branched transport problems, that finds applications in the description of the formation of river basins and transport networks.

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O101

A machine learning approach for uncertainty quantification using the Multiscale Finite Volume method

Several multiscale methods account for sub-grid scale features using coarse scale basis functions. For example, in the Multiscale Finite Volume method the coarse scale basis functions are obtained by solving a set of local problems over dual-grid cells. We introduce a data-driven approach for the estimation of these coarse scale basis functions. Specifically, we employ a neural network predictor fitted using a set of solution samples from which it learns to generate subsequent basis functions at a lower computational cost than solving the local problems.

The computational advantage of this approach is realized for uncertainty quantification tasks where a large number of realizations has to be evaluated. We attribute the ability to learn these basis functions to the modularity of the local problems and the redundancy of the permeability patches between the different permeability realization. The proposed method is evaluated on several multiphase flow problems yielding very promising results.

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O102

Efficient big data assimilation through sparse representation

The advance of modern technologies leads to a massive growth of high-resolution observational data in geosciences. In the data assimilation community, ensemble-based methods are among the state-of-art assimilation algorithms. When applying ensemble-based methods to assimilate big geophysical data, substantial computational resources are needed. In addition, uncertainty quantification of observational data (UQOD) also becomes computationally challenging, if not impossible.

To tackle the aforementioned challenges in the presence of big data, we propose a sparse data representation procedure. The main idea is to apply a certain transform to the data in a way such that the data can be efficiently represented by a small subset of coefficients in the transform domain. These coefficients are then used as the observations in data assimilation, and UQOD is conducted in the transform domain accordingly. We use a 3D seismic history matching problem to illustrate that, integrating ensemble-based data assimilation algorithms with the sparse representation procedure provides an efficient way to address big geophysical data assimilation problems.

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O103

A data-scalable randomized misfit approach for solving large-scale PDE-constrained inverse problems

A randomized misfit approach is presented for the efficient solution of large-scale PDE-constrained inverse problems with high-dimensional data. A stochastic approximation to the misfit is analyzed using random projection theory. By expanding beyond mean estimator convergence, a practical characterization of randomized misfit convergence can be achieved. The class of feasible distributions is broad yet simple to characterize compared to previous stochastic misfit

methods. This class includes very sparse random projections which provide additional computational benefit. A 5-minute Matlab demonstration will be given.

The main contribution is a theoretical result showing the method guarantees a valid solution for small reduced misfit dimensions. The computational cost savings for large-scale PDE-constrained problems with high-dimensional data will be discussed. Results with different random projections will be presented to demonstrate the viability and accuracy of the proposed approach on single-phase subsurface flow problems.

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O104

Parametrization of geological models with generative adversarial networks

One of the main challenges in the parametrization of geological models is the ability to capture complex geological structures often encountered in real subsurface fields. In recent years, a revolutionary parametrization method has been developed in the machine learning community called Generative Adversarial Networks (GAN) showing state-of-the-art performances in challenging computer vision tasks, such as reproducing natural images (handwritten digits, human faces, etc.). In this work, we study the application of Wasserstein GAN (a variant of GAN) for the parametrization of geological models. The method is assessed on two types of permeability fields exhibiting channelized patterns. It is further assessed for uncertainty propagation in subsurface flow problems. The obtained results empirically show that GANs generate far better sample quality than traditional principal component analysis parametrization, visually and quantitatively.

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O105

Redistribution of steam injection in heavy oil reservoir management to improve EOR economics, powered by a unique integration of reservoir physics and machine learning

The application of a novel modeling and optimization approach is presented, demonstrating the impact of quantitatively optimized steam redistribution in mature heavy oil fields. Results are presented for a steamflood in the San Joaquin Basin in California, demonstrating significant savings of steam and operational costs and significant production increase, ultimately increasing net present value (NPV) by at least 10%.

The new approach, termed Data Physics, is based on a novel combination of state-of-the-art machine learning methods with the partial differential equations of reservoir fluid flow, as present in reservoir simulators. Combined with an advanced data assimilation algorithm that merges a modified ensemble Kalman filter with quadratic programming, this approach allows rapid and simultaneous integration of production, injection, temperature, completion, maintenance and log data for

large fields with thousands of wells. Next, the fitted models are combined with advanced multi-objective optimization algorithms and cloud computing to consider thousands of scenarios to optimize steam redistribution.

Results demonstrate that steam redistribution can be quantitatively optimized rapidly to maximize short and long-term EOR economics.

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O106

DR-RNN – a deep residual recurrent neural network for model reduction

This paper proposes a new deep learning technique to construct reduced order models for nonlinear dynamical systems. Specifically, we introduce a deep residual recurrent neural network (DR-RNN) that emulate the dynamics of physical phenomena to obtain an efficient model reduction of the nonlinear system. The developed DR-RNN is inspired by the iterative steps of line search methods in finding the residual minimiser of the numerically discretized differential equation. We formulate this iterative scheme as stacked recurrent neural network (RNN) embedded with the dynamical structure of the emulated differential equations. Numerical examples demonstrate that DR-RNN can effectively emulate the physical system with a significantly lower number of parameters in comparison to the standard RNN architectures. Further, we combined DR-RNN with Proper Orthogonal Decomposition (POD) for model reduction of time dependent partial differential equations. The presented numerical results show the stability of proposed DR-RNN as an explicit reduced order method. We also show significant gains in accuracy by increasing the depth of DR-RNN similar to other recent applications of deep learning.

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O107

Equilibrated melt networks

We present level-set simulation of texturally equilibrated melt networks in realistic poly-crystalline rocks. The geometry of these melt networks is determined by the porosity/melt fraction and the dihedral angle at the triple line between two solid grains and a melt pocket. If the dihedral angle is below 60 degrees, the melt wets the grain boundaries and forms a percolating melt network. If the dihedral angle is above 60 degrees, the melt does not wet the grain boundaries and collects in isolated pockets until the percolation threshold is overcome. We use our simulations to map the percolation threshold in both idealized and real geometries, that latter have been obtained by microtomography. The percolation threshold in real media is significantly higher than idealized geometries. Simulations also show hysteresis in melt network connectivity.

Once a high-dihedral angle melt has connected above the percolation threshold, the network remain connected even if the porosity drops below the percolation threshold subsequently.

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O108

Modeling of magma-mantle dynamics in subduction zones

Question: Previous geodynamic modeling of subduction zones has largely decoupled the solid velocity and thermal calculations from the liquid velocity calculations. We ask: how does coupled thermochemical magma-mantle dynamics impact the flow and transport in subduction zones?

Methods: We are developing new software in which the equations governing conservation of mass, momentum, energy and chemical species are solved in a coupled fashion, leveraging the PETSc library to deliver high performance, scalable solutions. Results: We demonstrate the significance of solving the conservation equations in a coupled fashion by considering the impact of magmatism on the thermal structure of subduction zones. We show that magmatic transport locally alters the thermal structure of canonical models by ~200–300 K, consistent with evidence from petrological and heat flow observations. Conclusions: The thermal structure of the wedge is likely to rheologically influence the transport of melts through in the wedge. Thus we suggest that magmatism could significantly affect the location, extent and chemical composition of arc volcanism.

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O109

Tracer transport in solitary porosity waves

The isotopic diversity of oceanic basalts requires partial melting of a lithologically heterogeneous mantle source beneath mid-ocean ridges and hot-spots. The importance of heterogeneities for modulating melt supply and rock composition is increasingly recognized. To take advantage of the geochemical observations from oceanic basalts, they have to be linked to heterogeneities that produced them. Partial melting of fertile heterogeneities produces local increases in melt with distinct geochemical signatures. Until recently it was not clear how the geochemical signatures generated by the partial melting could possibly remain intact during transport to the surface. The molten region may evolve into a solitary wave that migrates upward at constant velocity that is larger than the background melt velocity. Melt in the center of the solitary wave recirculates and is transported to the surface without mixing with the ambient background melt. This allows the melt that originated from the fertile heterogeneity to retain its distinct geochemical signature as it rises through the mantle. This process provides a link between mantle heterogeneities and the diversity of trace element compositions observed at oceanic basalts.

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O110

Adjoint-based inversion to model the nonlinear rheology of the lithosphere

We develop an adjoint method to infer rheological parameters of the lithosphere from available observations such as surface velocities or near surface stresses. Modeling lithospheric flow with nonlinear instantaneous Stokes equations based on realistic temperature- and strain rate-dependent viscosities, the inverse problem is formulated as an infinite-dimensional nonlinear least squares optimization problem. Our approach involves a gradient method that requires the action of the adjoint of the derivative of the parameter-to-observable map which is efficiently computed without explicitly implementing the derivative itself. We present preliminary results applying this method to a simple setup of a salt dome under a sedimentary overburden. One spatially varying parameter field, such as rock density or strain rate exponent, can easily be recovered in this way. These simulations appear promising for realistic lithospheric scale models with a more complex geometry.

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O111

Efficient solution techniques for the simulation of multi-phase, geothermal reservoirs

Prediction of temperature at depth is crucial for the evaluation of the possible energy production of geothermal reservoirs. We present a pressure-enthalpy formulation for the simulation of supercritical, geothermal water/steam reservoirs, consisting of one mass balance and one energy balance equation. After discretization in space and time, this equation system is solved by a fully implicit Newton method. For the solution of the arising linear systems, we compare a constrained pressure residual (CPR-AMG) and a Schur complement reduction (SCR-AMG) method, both making use of algebraic multigrid (AMG). We show that both methods allow for an efficient and scalable solution of the corresponding equation systems on parallel high performance computers. In addition, we present simulation results for a geothermal reservoir located in Tuscany, Italy.

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O112

Uncertainty quantification analysis of subsurface flow simulations in poro-fractured media

In the framework of subsurface flow simulations in fractured media, we consider the issue of the non-deterministic description of the medium, focusing on discrete fracture network (DFN) models. Within these models, simulations are indeed usually performed on domains in which fractures are generated starting from probabilistic distributions for both hydro-geological properties (e.g. fracture transmissivity) and geometrical features (e.g. orientation in the 3D space, position, size...). Suitable uncertainty quantification (UQ) strategies should be therefore adopted for quantifying the influence of these stochastic parameters on some quantity of interest in the DFN. The talk, focusing on the challenging case of stochastic geometry of the network, will address the issue of the application of effective, modern UQ strategies, such as the Multi Level Monte Carlo method, for accurately computing suitable statistics of the quantity of interest with a moderate number of calls to the solver.

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O113

A new hybrid method for crack propagation in poroelastic media

We propose a novel method, called Xfield, to simulate crack propagation in a brittle elastic/poroelastic material. The aim is reducing the computational cost by combining a sharp representation of the crack (by means of the XFEM) with a phase field model. This latter is used as a sound energy-based criterion for crack propagation. Since the XFEM allows for the efficient computation of the displacement when the fracture geometry is given, it is used to compute the displacement at the large scale while propagation is governed by the solution of a local phase field problem at the tip scale where we employ a very fine, but small, local mesh (whose radius depends to the characteristic length of the phase field). The method thus inherits some aspects both from phase field models and from the extended finite elements discretization of the elasticity equation. The capabilities of the new method are demonstrated on some test cases. Moreover, we present a first attempt at the application of Xfield to hydraulic fracturing.

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O114

BDDC preconditioner for robust discretization of flow in fractured porous media

Fractured porous media arise in many different applications, such as enhanced geothermal systems, energy storage, and shale gas/oil production. The role of fractures is critical for understanding system behavior, as they may provide both high-conducting pathways or barriers to flow. Therefore, it

is important to integrate the specific properties of fractured porous media into numerical methods. In this presentation, we set to efficiently solve the flow problem by taking into account the multi-dimensional hierarchy formed by fractures and fracture intersections. We propose a domain decomposition type preconditioner that exploits fractures as a natural interface between subdomains. A special focus is set on tailoring the coarse geometry for fracture networks and using constraints on subdomain interfaces to affect the rate of convergence. This method is verified on several examples of fracture networks to showcase the performance of our solver.

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O115
Homogenization and inverse analysis of heterogeneous rock samples

The contribution concerns analysis of heterogeneous rock samples, when geometry of the microstructure is provided by CT scans or alternatively by a stochastic microstructure generation. The physical processes within the samples as heat transfer, porous media flow and mechanical deformations (THM processes) are investigated. In the case of linear THM models, the computation of homogenized, effective properties is straightforward in the case of available local material properties. But the local material properties can be given with some level of uncertainty which motivates sensitivity analysis to different parameters and/or solution of inverse problems for identification of the local properties by output least squares method based on measurements of response or multiresponse of the whole sample. The related problem of finding stochastic description of local material properties and deriving stochastic description for the homogenized material is also discussed.

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O116
Compressible magma/mantle dynamics – 3D, adaptive simulations

Melt generation and migration are an important link between surface processes and the thermal and chemical evolution of the Earth's interior. However, due to the vastly different time and length scales of the motion of solid and molten rock, it

is difficult to study these processes in a unified framework, especially in three-dimensional, global models. Here, we present the open source finite element code ASPECT, which simulates coupled magma/mantle dynamics using adaptively refined meshes. Applying adaptive mesh refinement to this type of problems is particularly advantageous, as the resolution can be increased in areas where melt is present and viscosity gradients are high, whereas a lower resolution is sufficient in regions without melt. Together with a high-performance, massively parallel implementation, this allows for high resolution, 3D, compressible, global mantle convection simulations coupled with melt migration.

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O117
High order discontinuous Galerkin methods for modeling magma dynamics

Generation and segregation of magma in the Earth and the interior of large planets has been a subject of intensive study in the earth science community. In particular, a fundamental understanding of melt migration beneath the mid-ocean ridge is necessary to explain the field observations on sections of the earth's mantle that has been uplifted to the surface. The physical model to describe this process is an advection-reaction type system consisting of two hyperbolic equations to evolve porosity and soluble mineral abundance at local chemical equilibrium and one elliptic equation to recover global pressure. In this talk, the numerical discretization of the physical system using Discontinuous Galerkin methods and matrix-free finite elements is presented. In addition, a projective and adaptively applied pressure estimation is employed to significantly reduce the computational wall time without impacting the overall physical reliability in the modeling of important features of melt segregation, such as melt channel bifurcation in 2D and 3D time dependent simulations. The talk will concentrate on the numerical algorithm as well as the geological implications of the results obtained through the simulations.

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O118

Mixed methods for two-phase Darcy-Stokes mixtures of partially melted materials with regions of zero porosity

The Earth's mantle, or an ice sheet, involves a deformable solid matrix phase within which a second phase, a fluid, may form due to melting processes. The mechanics of this system is modeled as a dual-continuum, with at each point of space the solid matrix being governed by a Stokes system and the fluid melt, if it exists, being governed by a Darcy law. This system is mathematically degenerate when the porosity (volume fraction of fluid) vanishes. We develop the variational framework needed for accurate approximation of this Darcy-Stokes system, even when there are regions of positive measure where only one phase exists. We then develop an accurate mixed finite element method for solving the system and show some numerical results.

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O119

Preconditioners for models of coupled magma/mantle dynamics

In this talk we discuss numerical methods (in particular block preconditioners) to efficiently solve linear systems arising from the discretization of models of coupled magma/mantle dynamics. These models describe the creeping flow of high-viscosity mantle matrix and the porous flow of magma. The model we consider is based on a system of partial differential equations derived by McKenzie [1], which describes mass and momentum conservation of the mantle and magma phases (a coupling of Stokes equations with Darcy's law). Different reduced forms of this two-phase flow model exist, for example, it is possible to eliminate the magma velocity and the solids pressure, resulting in a model for only the mantle velocity and fluids pressure. Although these reduced forms may seem appealing (there are less unknowns to solve for), we will show in this talk, that from an iterative solver point of view, it may be worth solving the full space model instead of these reduced models.

[1] D. McKenzie, The generation and compaction of partially molten rock, *J. Petrol.* (1984) 25:713--765.

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O120

sam(oa)² – parallel adaptive mesh refinement for tsunami simulation and other applications

sam(oa)² is a framework to implement parallel solvers for PDE systems on dynamically adaptive tree-structured triangular meshes. It provides hybrid MPI+OpenMP parallelisation using dynamic load balancing based on the Sierpinski space-filling curve. In this talk, we will give an overview on recent optimisation efforts in sam(oa)², which include introduction of regular patches, vectorisation of Riemann solvers, load balancing on heterogeneous Xeon Phi platforms, as well as computing on a varying number of nodes using an extension of MPI that

allows elastic applications. The simulation scenarios will stem from tsunami simulation and porous media flow.

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O121

Exploring low-power embedded processors for ocean simulation

Performing a tsunami or storm surge simulation is a highly challenging research topic that calls for collaboration between mathematicians and computer scientists. One must combine mathematical models with numerical methods and map them onto appropriate parallel computer architectures. For flood warning systems installed in regions with weak or unreliable power and computing infrastructure, this would significantly decrease the risk of failure at the most critical moments. The main goal is to be able – if necessary – to perform simulations in-situ and battery-powered. This presented work describes a concept how to develop suitable low power hardware architectures for ocean simulations based on cooperative software and hardware simulation. Results are shown how algorithms on such architectures are scaling and performing

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O122

Performance analysis of a fully functional unstructured 3D coastal ocean model

Our 3D coastal ocean model, UTBEST3D, is based on a discontinuous Galerkin discretization on unstructured prismatic meshes to produce a highly scalable, flexible, and adaptive simulation package. It provides a full set of features and parametrizations required for solving the 3D shallow water equations, supports wetting/drying algorithms, and vertical eddy viscosity closures up to the second order. UTBEST3D is implemented in C++ and parallelized using OpenMP and MPI, and demonstrates excellent scaling on a broad range of computing architectures. The large computational domains and long simulation times typical for coastal ocean models put high demands on computational resources, both performance- and energy-wise. While investigating hardware architectures in terms of energy-to-solution and time-to-solution, our experiments comparing UTBEST3D on the Intel Haswell and ARM Cortex-A15 micro architectures showed that using processors from the field of embedded/mobile computing can increase energy efficiency by up to 50%. Moreover, combining multiple Cortex-A15 nodes might allow to match the time-to-solution of the Haswell CPU while resulting in an energy advantage for the ARM architecture.

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O123

Efficient implementation of higher-order discontinuous Galerkin methods

Unleashing the high-performance advertised by current supercomputers provides quite a challenge for finite element methods. The traditional approach of setting up a stiffness matrix in a sparse matrix format and solving it by some preconditioned Krylov space method performs typically only at a few percent of theoretical peak due to memory bandwidth limitations. Matrix-free implementation of high-order methods offers the possibility bypassing the memory bottleneck while at the same time reducing the number of operations substantially. In this talk we present the sum factorization method applied to discontinuous Galerkin discretizations, present performance results for a convection-diffusion operator including a mostly matrix-free algebraic multigrid preconditioner, show applications to the incompressible Navier-Stokes equations and present first results of a code generation framework. The results presented in this talk are joint work with Steffen Müthing, Dominic Kempf, Marian Piatkowski and Eike Mueller.

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O124

Marine ice sheet retreat hastened by mechanical weakening of shear margins

Marine based sectors of Antarctica are at risk of retreat as buttressing ice shelves are thinned by warming ocean currents. To date, modeling studies of the marine ice sheet instability have neglected processes of fracturing and weakening of shear margins. Here, we apply a continuum damage mechanics model to explore the influence of marginal weakening on marine ice sheet retreat. A viscous damage model, developed based on observations of progressive weakening of the remnant Larsen B ice shelf on the Antarctic Peninsula, is applied to the idealized configuration of the 3rd Marine Ice Sheet Model Intercomparison Project (MISMIP+). The damage model, implemented in the Ice Sheet System Model, allows for the evolution and subsequent advection of weakened ice with lower effective viscosity. The standard MISMIP+ experiments are compared to experiments that allow the ice to damage. We demonstrate that damage shear margins are just as important for perturbing the grounding line as ice shelf thinning. Model projections that do not account for marginal weakening are therefore likely to underestimate both the rate of grounding line retreat and subsequent sea level rise.

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O125

Anisotropic mesh adaptation for marine ice-sheet modeling

Improving forecasts of ice-sheets contribution to sea-level rise requires, amongst others, to correctly model the dynamics of the grounding line (GL). Grid refinement in the GL vicinity is a key component to obtain reliable results. Improving model accuracy while maintaining the computational cost affordable has then been an important target for the development of marine ice-sheet models. Adaptive mesh refinement is a method where the accuracy of the solution is controlled by spatially adapting the mesh size. The main difficulty is to find reliable estimators of the numerical error. Here, we use the estimator proposed by Frey and Alauzet (2015). Routines to compute the anisotropic metric defining the mesh size have been implemented in the finite element ice flow model Elmer/Ice where the mesh adaptation is performed using the freely available library MMG. Using a setup based on the inter-comparison exercise MISMIP+, we study the accuracy of the solution when the mesh is adapted using various variables (ice thickness, velocity, basal drag, ...). We show that combining these variables allows to reduce the number of mesh nodes by more than one order of magnitude, for the same numerical accuracy, when compared to uniform mesh refinement.

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O126

Improved discretization of grounding lines and calving fronts using an embedded-boundary approach in BISICLES

Correctly representing grounding line and calving-front dynamics is of fundamental importance in modeling marine ice sheets, since the configuration of these interfaces exerts a controlling influence on the dynamics of the ice sheet. We have developed a front-tracking discretization for grounding lines and calving fronts based on the Chombo embedded-boundary cut-cell framework. This promises better representation of these interfaces vs. a traditional stair-step discretization on Cartesian meshes like those currently used in the block-structured AMR BISICLES code. The dynamic adaptivity of the BISICLES model complements the subgrid-scale discretizations of this scheme, pro-

ducing a robust approach for tracking the evolution of these interfaces. Also, the fundamental discontinuous nature of flow across grounding lines is respected by treating it as a material phase change. We present examples of this approach to demonstrate its effectiveness.

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O127

Ice sheet models – Quo vadis?

In the past decade more and more ice sheets models (ISMs) developed the ability to solve the 3D nonlinear Stokes system. This opened new possibilities, but yet projections for future contributions of ice sheets to sea level rise are not commonly based on Stokes models. Here we give an overview on the current limitations of Stokes model applications with a focus on the requirements on constitutive relations, initial and boundary conditions.

We start with presenting Stokes and higher-order applications using three different ISMs (TIMFD3, COMice and ISSM) discretised on structured or unstructured grids and discuss the advantages and disadvantages. As the viscosity of ice strongly depends on water content and temperature we also provide details on our solution method for the enthalpy equation within those models.

In the second half of the presentation we discuss the effect of the viscoelastic properties on grounding line migration and the challenges of implementing this into ISMs, as well as aspects of a new flow law. Furthermore, we aim to highlight the limitations and uncertainty driven by input parameters like geothermal flux and other basal properties. All these aspects are summarised to draw conclusions on future next generation ice sheet models.

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O128

Efficient numerical ice-sheet simulations over long time spans

The full-Stokes models to palaeo-ice sheet simulations have previously been highly impractical due to the requirement on the mesh resolution close to the grounding-line. We propose and implement a new sub-grid method for grounding-line migration in full Stokes equations with equidistant mesh. The beauty of this work is to avoid remeshing when the grounding-line moves from one steady state to another over long time simulations. A new slip boundary condition is introduced to accommodate the discontinuity at the grounding-line in the

physical and numerical model. The method is implemented in Elmer/ICE that solves the full Stokes equation with the finite element method. The convergence of the sub-grid method is examined as the mesh is refining and the results are compared with the MISMIP benchmark.

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O129

Towards stable ice sheet simulations – Inf-sup stabilization of the p-Stokes equations on anisotropic meshes

Simulations of ice sheets, such as the Greenland Ice Sheet or Antarctic Ice Sheet, are often aimed at predicting future ice volume, or equivalently, ice surface position. A popular method for discretization of the equations governing ice flow (the p-Stokes equations) is equal order bi-linear finite elements formulations. Unfortunately, the ice surface position is susceptible to errors that stem from sub-optimal inf-sup stabilization of such discretizations [1]. We investigate the accuracy and robustness of a stabilization technique commonly used in glaciology – Galerkin Least Squares (GLS) stabilization – and compare it to other techniques such as the classical Local Projection Stabilization (LPS) [2]. Since ice sheets are much wider than they are thick and thus are discretized using highly anisotropic meshes, we especially focus our attention on the effect of anisotropy. Our studies indicate that the classical LPS stabilization is favourable. A specialized LPS stabilization for the p-Stokes equations was developed in [3] on isotropic meshes. We extend it to anisotropic, quadrilateral meshes and compute a-priori estimates which are compared to numerical results.

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O130

Dimensional model reduction for flow through fractures in poroelastic media

We study the interaction between a poroelastic medium and a fracture filled with fluid. The flow in the fracture is described by the Brinkman equations for an incompressible fluid and the poroelastic medium by the quasi-static Biot model. The two models are fully coupled via the kinematic and dynamic conditions. The Brinkman equations are then averaged over the cross-sections, giving rise to a reduced flow model on the fracture midline. We derive suitable interface and closure

conditions between the Biot system and the dimensionally reduced Brinkman model that guarantee solvability of the resulting coupled problem. We design and analyze a numerical discretization scheme based on finite elements in space and the Backward Euler in time, and perform numerical experiments to compare the behavior of the reduced model to the full-dimensional formulation and study the response of the model with respect to its parameters.

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O131

Scalable preconditioners for multiphase poromechanics

In this talk we focus on porous media systems that exhibit strong coupling between multiphase fluid flow and mechanical deformation. In such systems, a fully-implicit solution strategy is often a necessary requirement to obtain reliable model predictions. We propose a multilevel block preconditioner for accelerating the iterative solution of the algebraic systems arising from mixed finite element/finite volume discretizations and linearization of the governing balance equations. The methodology is based on the Constrained Pressure Residual (CPR) approach, which is widely used in reservoir simulation. We combine a local preconditioner and a global preconditioner in a multiplicative fashion. Specifically, in the global stage a Fixed-Stress strategy is used to precondition a reduced system that involves unknowns characterized by near-elliptic behavior with long-range error components, i.e. displacement and pressure. Numerical results are presented to illustrate the performance and robustness of the proposed preconditioning approach on a variety of challenging test problems.

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O132

Efficient solver for variational space-time approximation of poroelasticity

Space-time finite element methods are getting of increasing importance for the accurate numerical approximation of solutions to coupled systems of partial differential equations with complex behavior in space and time. We study families of space-time finite element methods for the discretization of the Biot system of flow in deformable porous media and demonstrate how these methods can be used for the construction of an efficient preconditioning technique within a monolithic approach. At first, an optimized artificial fixed-stress iterative coupling scheme for the space-time finite element approximation of the Biot system is presented. Continuous and discontinuous time discretizations and a mixed finite element approximation of the flow subproblem are used. A proof of its convergence is given. Its numerical performance properties are studied. Then, a monolithic solver that is based on applying the iterative coupling scheme with computationally less expensive lower order space-time approximations as a preconditioner is introduced. Its numerical performance properties are illustrated. Extensions to the dynamic Biot-Allard model are addressed.

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O133

Upscaling of coupled geomechanics, flow and non-reactive transport of a poro-elastic medium in the quasi-static situation

We undertake the formal derivation of Biots law for a poro-elastic medium completely saturated by a fluid, coupled with a convection-diffusion law for non-reactive ions within the fluid phase. We assume small displacements of the solid structure (i.e. linear strain), a fully connected void and grain space, that the fluid flow is incompressible, and that the fluid/solid interface coupling conditions may be linearized. We also assume the force balance at the interface is affected by the presence of a chemical substance (ions) within the fluid. We start with the microscale model, and apply the technique of homogenization in order to derive the upscaled model in the case of periodically distributed pores. Assuming the homogenization ansatz holds true, we obtain a fully coupled system of equations on the macro-scale accounting for the effects of geomechanics, non-reactive transport, and fluid flow within a porous material. The present work relies heavily on previous work done by (Bringedal et al. [6]) and (Mikelic and Wheeler [14]).

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O134

Monolithic multigrid methods for coupled fluid-flow and porous media problems

The multigrid solution of coupled porous media and Stokes flow problems is considered. The equations governing saturated porous media are coupled to the Stokes equations by means of appropriate interface conditions. The finite volume method on a staggered grid is considered as the discretization scheme for this type of problems, giving rise to saddle point linear systems. Special treatment is required regarding the discretization at the interface. We focus on an efficient monolithic multigrid solution technique for the coupled problem, in which we do not distinguish the subproblems and the internal interface. Highly satisfactory multigrid convergence is reported, and, moreover, the algorithm performs well for small values of the hydraulic conductivity and fluid viscosity, that are relevant for applications.

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O135

Linearization for coupled water flow and mechanical deformation in unsaturated soil

The coupling of fluid flow and mechanical deformation in porous media is of emerging interest and relevant for many challenging applications ranging from modeling CO₂ storage to understanding the swelling of cement-based materials. In our application, we consider soils, partially saturated by water, under mechanical loads. We model flow and deformation by a nonlinear extension of the quasi-static Biot equations. Due to the problem's nonlinear and coupled character, several numerical challenges arise, in particular the choice of a suitable linearization scheme. In this work, we propose a new, robust linearization technique, which combines the widely used Fixed Stress Splitting method and the L-Scheme. Both schemes are established techniques for linear Biot's equations and nonlinear flow, respectively. We demonstrate numerically the efficiency and robustness of the proposed iterative scheme.

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O136

Properties of iterative ensemble smoothers for history matching

Properties of Ensemble Smoother (ES), Multiple Data Assimilation Smoother (MDA-ES), and Iterative Ensemble Smoother (IES) are examined for a scalar case. Focus is on the limiting behaviour with large ensembles and nonlinear dynamics. The similarity for linear models is shown and the differences between the steps in MDA-ES and the iterations in IES are discussed. It is explained why iterations helps improve the solution for nonlinear problems. The results from MDA-ES and IES are compared and the convergence properties of MDA-ES with number of steps are examined. A conclusion is that both MDA-ES and IES provides a significant improvement compared to ES, but is not clear which of the iterative methods will generally give the best results. Furthermore, MDA-ES may require many more steps than IES to converge, but since the methods are solving different problems, they will not converge to the same solution.

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O137

An efficient robust ensemble smoother with multiple data assimilations

The ensemble smoother with multiple data assimilations (ES-MDA) was designed in order to avoid large model changes over each iteration (data assimilation step) by inflating the measurement error covariance matrix at each iteration with the inflation factors chosen to guarantee that ES-MDA provides a correct sampling of the posterior probability density function as the ensemble size goes to infinity. However, no best practice for choosing the inflation factors a priori is known and methods to choose them adaptively often result in excessive iterations or even convergence failure. Here, we provide a practical way to choose the inflation factors at each iteration for any pre-specified number of iterations.

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O138

Damping of resonant wave loads on arrays of vertical cylinders and a transfer-matrix approach to array problems

In ocean-wave-structure interactions, it is well-known that bodies in finite line arrays such as columns supporting offshore structures can experience exceptionally high wave loads for certain combinations of incident wave field and (constant) body spacing. This phenomenon is related to array trapped modes and has been intensively investigated for the case of plane linear water waves incident on rigid bottom-mounted cylinders using methods based on local expansions of the solution (e.g. interaction theories). We consider a different approach based on transfer matrices, which gives new insights and, in particular, allows for the straightforward investigation of the stability of the resonant loads with respect to positional disorder, which we relate to localisation of associated Rayleigh–Bloch waves.

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O139

An ensemble-based framework for assimilation of image-type data – Application to seismic history matching

A distance parameterization of flood fronts derived from time-lapse seismic anomalies was recently developed to facilitate incorporation of time-lapse seismic data into history matching workflows based on ensemble methods. In order to evaluate the performance of the proposed workflow for seismic history matching, we first applied the history-matching workflow to the Norne field where synthetic seismic data were used. The objective is to validate the proposed schemes of distance parameterization that give better performance when reservoir condition and well configuration are complex. Then a field case evaluation of the workflow was implemented using real seismic data from Norne field. The observations of front positions were acquired from an inversion of the Norne AVO seismic data set. Stronger signals were observed from the inverted saturation changes of G segment. Well production data were also used to evaluate the potential benefits added by utilizing the front information of 4D seismic data. The results show that additional benefits are received by matching to both production and 4D seismic data which contributes a better understanding of the reservoir and some new insights are gained regarding the performance of the proposed method.

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O140

Uncertainty estimation of onset arrival times using parametric bootstrap of statistical time series models

The time, geolocation, type, and size of a measured seismic event all come from the processing of the raw seismic waveforms that record ground motion at various sensor locations. Many types of measurements are made on the waveforms, but perhaps the most fundamental are the estimated arrival times of the various seismic phases. While considerable effort has been placed into the research of accurately estimating arrival times, relatively little has been done to quantify the uncertainty of these estimates. We extend the state-of-the-art auto-regressive time series methods of phase onset estimation to include a full estimation of the probabilistic uncertainty of the onset estimate. We propose a parametric bootstrap methodology to obtain a full posterior probability distribution to describe the signal onset detection estimates. We demonstrate our approach on both synthetic and real ground motion data, and discuss the substantial implications that a full uncertainty description affords the subsequent stages of downstream analyses.

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O141

Comparison of splitting schemes for compositional multiscale solvers

We present a multiscale solver for compositional three-phase flow problems in which the behavior of the liquid and vapor phases are described by generalized cubic equations of state. The multiscale solver is based on a finite-volume type framework with basis functions computed algebraically using restricted smoothing. These basis functions are computed directly from the system matrix with minimal assumptions on features of the underlying grid, allowing accurate computation of approximate pressures of high contrast porous media discretized on unstructured and stratigraphic grids.

In this work, we compare different approaches for splitting the compositional model equations into a pressure and a transport part and the subsequent multiscale approximation of this scheme. We consider both schemes based on volume-balance and total mass-balance and discuss some advantages and disadvantages between the two schemes. The numerical examples consider different types of gas injection discretized on both structured, unstructured and stratigraphic grids with significant structural and geological complexity.

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O142

Adaptive homogenization for upscaling heterogeneous porous media

The major objective in the development of upscaling approaches is to reduce the computational costs associated with solving fine scale flow and transport problems in heterogeneous porous media. This is due to the availability of reservoir rock property data at fine spatial scales from facies distributions obtained from geological models and field data from well logs. The data sets from each of these sources are themselves at different spatial scales, which further adds to the computational challenge. The upscaling approach must not only accommodate these disparate data sets but also capture the flow physics accurately while maintaining computational efficiency. We present a novel upscaling approach which draws upon previous developments of two-scale homogenization to obtain coarse scale property data in addition to dynamic spatial adaptivity using an enhanced velocity mixed finite element method (EVFEM).

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O143

Stable sequential fully implicit scheme allowing for compositional multiscale simulation

Multi-Scale Finite-Volume (MSFV) methods rely on the decoupling of flow (pressure- and velocity fields) and transport (saturation- and/or composition fields). They have been proven efficient for problems without mass exchange or when the mass exchange terms are direct functions of pressure (e.g. black-oil formulations). For problems with complex coupled nonlinear interactions between flow and transport in multiphase, multi-component systems, MSFV methods may require many more Newton iterations, and/or smaller time steps compared with methods employed by general-purpose reservoir simulations. We extended our previous work on modified sequential fully implicit schemes and combined our coupling approach with a MSFV method. For realistic 2D and 3D models with mass-exchange and gravity it is demonstrated that the resulting MSFV method for compositional formulations has comparable stability properties as established general-purpose reservoir simulators.

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O144

Mathematical model of two-phase compositional flow in porous media in vapor intrusion problems

This work deals with two phase compositional flow in porous media with kinetic mass transfer. We propose a numerical method based on the mixed hybrid finite element method with several linear solvers (direct and iterative) and parallel implementation using MPI. First, the method is verified on problems with known solutions. Numerical experiments show that the errors are similar for all variations of the method and the experimentally estimated order of convergence is slightly less than one. However, there are significant differences in the computational performance. Then, we use the numerical scheme to investigate non-equilibrium mass transfer in unsaturated porous media using experimental laboratory data and hypothetical field-scale scenarios of vapor intrusion problems. The experiment was focused on evaporation of dissolved TCE in laboratory scale. In the field scale, we examine effects of water table drop or rainfall events on the dynamics of the vapor intrusion into building basements.

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O145

Development and comparison of efficient constraint-handling techniques for well placement optimization

Optimal well placement is a critical task within subsurface engineering disciplines such as groundwater resource management and petroleum field development. Well placement problem formulations typically involve nonconvex solution spaces resulting from realistic geological and engineering nonlinear constraints. Commonly, optimization procedures rely on time-consuming subsurface fluid flow simulations for objective function calculation. Complex nonconvex solution spaces coupled with computationally expensive cost function evaluations require efficient constraint-handling approaches to retain search efficiency and avoid poor solution sampling. Two approaches are implemented: the first is based on an alternating projections method that solves the geometric problem of well trajectories across nonconvex feasible sets defined by well length, inter-well distance and reservoir boundary constraints. In the second approach, we reformulate the constraints by means of non-linear functionals. A feasible solution is then determined while combining adjoint-gradient linearization with quadratic programming. These approaches are tested for different constraint configurations using both derivative-free and gradient-based methods.

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O146

New approaches for the simulation of flows in complex poro-fractured domains with non-conforming meshes

Underground fluid flow in fractured media is a heterogeneous multi-scale phenomenon involving complex geological configurations; a possible approach for modeling the phenomenon is given by Discrete Fracture Networks (DFNs), which are complex sets of intersecting fractures modeled as polygons, stochastically generated starting from statistical distributions for orientation, density, size, aspect ratio and hydro-geological properties. Among the several difficulties encountered in flow simulations in poro fractured media, geometrical complexity plays a key role. In order to obtain numerical methods that are sufficiently robust to deal with all the possible intricate geometries that can be produced by a stochastic generation, two main approaches have been proposed: a PDE constrained optimization approach, that independently solve the flow problem in each fracture and then imposes matching

conditions through the minimization of a quadratic functional; a variational method based on the newly conceived Virtual Element Method, that allows for a space discretization based on very general polygonal/polyhedral meshes.

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O147

Control-Volume Distributed Multi-Point Flux Approximation (CVD-MPFA), hybrid-upwind convection, unstructured grids, porous and fractured media

Flux-continuous finite-volume schemes are presented for flow in porous media including fractures. The schemes have control-volume distributed (CVD) flow variables and rock properties, per standard reservoir simulation. The schemes are comprised of families of multipoint flux approximations (CVD-MPFA), providing consistent flux approximations that extend to media with general tensors on structured and unstructured grids. The methods are coupled with convective approximations including the hybrid method upwind method. The schemes are applied to flow problems including anisotropic and fractured media. Comparisons of scheme approximation and method performance are presented.

Y Xie, MG Edwards "Cell-centred Higher Resolution Finite-volume Total Velocity V_t and V_a Formulations on Structured and Unstructured grids" Proc. ECMOR XIV-15th European Conference on the Mathematics of Oil Recovery 29th Aug-1st Sept 2016
 R. Ahmed, M.G. Edwards, S. Lamine, B.A.H. Huisman and M. Pal "Three-dimensional Control Volume Distributed Multi-Point Flux Approximation coupled with a lower-dimensional surface fracture model" J. Comput. Phys vol 303 pp 470–497 Dec 2015

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O148

The role of efficient meshing and discretization in modeling flow through discrete fracture networks (DFNs)

Often modeling of fluid flow through geologically heterogeneous and complex fractured network system is required to model multi-physics processes like, e.g., environmental flow, CO₂ sequestration, nuclear waste disposal, and hydrocarbon flows. Numerical modeling of such a complex system is challenging, both, from gridding and numerical discretization point of view.

In last decade alone modeling of flow through discrete fracture systems has attracted attention from a number of researchers. As a result few new gridding and discretization techniques have been proposed to model flow through discrete fracture network systems (DFNs). In this paper we will present an in-house tool, which has been developed with advance gridding techniques to mesh complex discrete fracture network at small and very large length scales. Tool is also planned to include advance numerical discretization, and upscaling capabilities. The tool will enable modeling of geologically complex discrete fracture networks as lower dimensional objects. We will also try to demonstrate the use of the tool for modeling problems related to flow of hydrocarbons in the fractured reservoirs.

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O149

High-resolution simulations of mass or heat transfers using conforming meshes of discrete fracture networks

Modeling of mass and heat transfers in fractured media has recently received a great attention from the geoscience community, due to its importance for hydrology, geothermal and oil & gas applications. Simplified models involving geometric or hydrodynamic assumptions have been commonly used to reduce effort in mesh generation due to the complex geometry of discrete fracture networks (DFNs). Direct simulations are therefore required for the validation of such models. For this purpose, we first proposed a new conformal meshing approach FraC (Fracture Cut Method for Meshing) that is able to deal with networks containing up to 104 fractures. Then, a tracer transport model implemented in the open-source code DuMux (University of Stuttgart) is used for modeling advection-dispersion equation. We adopt a vertex-centered finite volume scheme that ensures the concentration continuity and mass conservation at intersections between fractures. Numerical results on simple networks (for validation purposes) and on complex realistic DFNs are presented. Other techniques to reduce computational cost while conserving a good mesh quality are also discussed.

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O150

A fully-implicit reactive flow formulation for a low-salinity water flooding process

Low salinity waterflooding process is used to increase oil recovery by exploiting the solid-liquid surface interactions between species in the injected and in situ fluids. One of the hypothesis suggested for observed higher recoveries are the changes occurring at the solid surface due to precipitation/dissolution reactions. This change in surface composition results in wettability alteration leading to higher oil recoveries. We present a coupled reactive transport and flow model formulation assuming slightly compressible flowing phases (oil and water). Further, the reactive term occurring in the species conservation equation is evaluated implicitly without reducing the system of coupled, non-linear partial differential and algebraic equations representing the model. An approximate Jacobian approach is used during Newton linearization of the resulting system where the residuals are constructed exactly. Thus the system always converges to its true solution as the residuals diminish. The implicit approach is particularly important considering the non-linearity of the coupled problem.

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O151

Development of advanced compositional models for hysteresis and foam and their application to EOR processes

CO₂ EOR projects often suffer from poor volumetric sweep efficiency due to adverse mobility ratios between injected and insitu fluids. CO₂ either enters high permeability channels leaving behind low permeability sections or moves along the top of the formation due to gravity rapidly reaching production well resulting in early breakthrough times and low recovery efficiencies. We present a novel CO₂ surfactant foam model which accounts for hysteretic viscosity behavior using a non-Newtonian constitutive law. A number of numerical experiments are presented to validate this model against experimental studies carried out earlier at the University of Texas at Austin. We will also discuss a number of other modeling enhancements as well as its numerical implementation in our in-house reservoir simulator IPARS for incorporating three-phase relative permeability and capillary pressure hysteresis when coupled to this foam model.

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O152

Study of compositional multiphase flow formulation using complementarity conditions

Simulation of oil recovery with miscibility processes requires the resolution of a compositional multiphase flow model coupled with thermodynamic equilibrium constraints. Traditionally, the reservoir simulation industry relies on the formulation introduced by Coats based on natural variables

and flash calculations to detect phase appearance. This formulation is stable with respect to phase transitions but it adds complexity to manage the set of present phases and the associated unknowns and equations at each point of the domain. Recently, unified formulations with nonlinear complementarity conditions have been put forward for systems which have to switch continuously between different states. They provide an elegant formulation for intractable problems and lead to efficient numerical methods.

In this talk, we will discuss how these approaches can be used to solve a compositional multiphase flow problem with Peng and Robinson EoS. Then, we will study results of several cases to compare their numerical behavior and to focus on the challenges posed by nonlinear phenomena, including the phase transitions and crossing into and out of the critical region.

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O153

Utilization of multi-objective optimization for pulse testing dataset from a geological CO₂ sequestration site

This study presents compositional simulation results of pulse testing carried out at a geological carbon sequestration site in Mississippi, USA. We investigate the potential of pulse testing as a monitoring tool to detect CO₂ leakage pathways such as abandoned wells. Experiments performed with one source well injecting CO₂ periodically and two monitoring wells are considered baselines for subsequent experiments that convert one monitoring well into a production well as an artificial CO₂ leakage pathway. The difference between the pressure anomalies obtained from the baseline and leak experiments are considered as a signal of CO₂ leakage detection. Fourier transform is adopted to the pressure anomalies into frequencies. The transformed parameters are employed as target parameters of history matching using a multi-objective optimization algorithm. A trade-off relationship between the matching qualities at the monitoring wells is revealed more clearly by invoking multi-objective optimization than global-objective optimization, indicating diversity-preservation in the model set is advantageous to reducing bias in uncertainty quantification.

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O154

Mathematical and numerical formulations for multiphase reactive transport in porous media

Today, a large number of simulators can be used to simulate flow and transport in porous media. All these tools share a common set of modeling concepts : mass and energy balance, multiphase flow with Darcy law, heat conduction, species diffusion and dispersion and local mass transfer based on thermodynamics and kinetic laws.

We have designed a generic global formulation for multiphase reactive transport in porous media by extending these concepts to any number of phases, species and reactions. This formulation has inspired a new fully implicit method based on variable switching that we name the Reactive Coats formulation. At the same time, we have also explored semi-smooth Newton approaches to deal with phase stability complementary conditions. These methods were proposed separately by Krautle, Knabner and Hoffman for reactive transport problems and by Lauser et al for multiphase flow problems.

In this talk we present an overview of the lessons learned from the study of these formulations and their practical implementation. We will focus on the remaining issues that need to be solved to design a generic fully implicit solver. The results will be illustrated by academic test cases solved with our reactive transport simulators Arxim and Geoxim, respectively for 0D and 3D problems.

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O155

A multigrid reduction preconditioning strategy for multiphase flow with phase transitions

Numerical simulation of multiphase flow in porous media requires solving of a large, sparse linear system resulting from the discretization of the PDEs modeling the flow. In the case of multiphase, multicomponent flow with miscibility and phase transition effects, this is a very challenging task. A new approach to handle phase transitions is to formulate the system as a nonlinear complementarity problem. The use of a fixed set of primary variables in this approach opens up the possibility of using multigrid methods for the linear solve. However, the problem is that when a phase disappears, the linear system has the structure of a saddle point problem and becomes indefinite, and current algebraic multigrid algorithms cannot be applied directly. In this study, we explore the effectiveness of a new multilevel strategy, based on the multigrid reduction technique, to deal with problems of this type. We demonstrate that the new method is efficient and scales optimally with problem size through numerical results for a case of two-phase, two-component flow with phase disappearance. We also present how the algorithm can be extended to the case of multiphase, multicomponent flow with phase transitions.

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O156

Firedrake – composable abstractions for high performance finite element computations

The development of complex numerical models requires a variety of skills. Including, but not limited to, problem-specific knowledge, numerical methods, software engineering, and parallel computing. Polymaths that tick all of these boxes are rare. To combat this complexity, traditional model design employs a separation of concerns using software libraries. This separation is horizontal, and works best when the granularity of the API is large, and one-way. Finite element computations, that contain user-specific variability in the inner loop, seem to preclude such an approach.

In this talk, I will describe how, by teaching computers to manipulate mathematical descriptions of PDE problems, we address this problem, providing high performance finite element computations without requiring that the model developer be an expert low-level code optimisation.

With an efficient model, we also need efficient solvers, and I will also discuss recent work in Firedrake to simplify the development of runtime-configurable block preconditioners using PETSc.

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O157

Accelerating the weather and climate model COSMO on heterogeneous architectures

To benefit from current and emerging computer architectures, a GPU-enabled version of COSMO – a widely used regional weather and climate model – has been developed. The use of GPUs significantly reduces the required time and energy to solution. This allowed MeteoSwiss to run a new high-resolution setup, as well as a 21 member ensemble.

We present an overview of the approach used to refactor the monolithic FORTRAN code of COSMO. A mixed approach using OpenACC compiler directives and rewriting time-critical parts using a domain-specific language (DSL) was employed. While the former offers good performance for column-based algorithms and is less intrusive, the DSL allows aggressive optimizations for the more complex, performance-critical stencils

of the dynamics. The DSL supports backends for CPUs and for CUDA-enabled GPUs, which allows the user to retain a single architecture-independent source code.

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O158

Preparing ExaStencils for applications in GeoSciences

Recent advances in computer hardware technology make more and more realistic simulations possible; however, this progress has a price. On the one hand, the growing complexity of the physical and mathematical models requires the development of new and efficient numerical methods. On the other hand, the trend towards heterogeneous and highly parallel architectures increases the programming effort necessary to implement, develop, and maintain these models.

ExaStencils addresses these issues by providing a multi-layered domain specific language that enables the users to formulate their problems on different levels of abstraction. From these formulations efficient implementations can be generated and optimized automatically since the data layout is restricted to regular grids. This approach both to significantly improve the computational performance of the discontinuous Galerkin finite element method and, at the same time, to decrease the effort to implement new methods and applications.

Experiments show that it is possible to generate scalable and efficient code also for non-trivial applications.

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O159

The ICON ocean model computational performance; optimization techniques for unstructured grids

The ICON project is a collaboration between the German Weather Service (DWD) and the Max Planck Institute for Meteorology aiming to develop a new coupled atmosphere ocean general circulation model that can be used both for climate research and numerical weather forecast. The ICON Ocean model uses a mimetic or "structure-preserving" discretization method of the partial differential equations of ocean dynamics on unstructured C-grids. The model infrastructure for unstructured grids provides the ability to utilize a number of different grids: icosahedron-based, R-refined, Rossby-type, and idealized domains like a channel or a torus. In this presentation I will describe the ICON Ocean computational performance characteristics, and the parallelization and optimizations we

have applied, with a focus on the unstructured-grid aspect of performance. I will also give an introduction to the ICONFOR domain specific language, a language designed for expressing operators on unstructured grids, and discuss the perspectives of such an approach for the computational performance and the model development.

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O160

To reduce numerical precision to achieve higher accuracy in weather and climate modeling

Resolution and model complexity of weather and climate models are limited by performance of today's supercomputers. If numerical precision can be reduced, we can reduce power consumption and increase performance. However, it is difficult to identify the optimal level of precision that should be used in weather and climate models that show non-linear dynamics. We investigate a reduction of numerical precision in a range of models (from Lorenz'95 to IFS) and study approaches to reduce numerical precision to a level that can be justified by information content (e.g. a reduction in precision with spatial scale or forecast lead time). We find that numerical precision can indeed be reduced significantly in many components of weather and climate models and identify savings that are possible if precision is reduced. We could show that a 40% increase in performance is possible when using single precision in the IFS weather forecast model and that power consumption can be reduced by a factor of three when running a spectral dynamical core with only 22 bit floating point numbers. The investigation of numerical precision and information compression is part of the ESIWACE project.

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O161

Scalable subsurface flow simulations with ParFlow

Regional hydrology studies are often supported by high resolution simulations of subsurface flow that require expensive and extensive computations. Efficient usage of the latest high performance parallel computing systems becomes a necessity for models targeting realistic physical scenarios.

The simulation software ParFlow has been shown to have excellent solver scalability for up to 16,384 processes. To scale to the full size of current petascale systems, we propose a reorganization of ParFlow's mesh subsystem: We modified it to use state of the art mesh refinement and partition algorithms provided by the parallel software library p4est, and we removed several overly strict assumptions on the parallel mesh layout in the process.

Evaluating the scalability and performance of the modified version of ParFlow, we demonstrate weak and strong scaling to over 458.000 processes of the Jukeen supercomputer at the Forschungszentrum Juelich.

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O162

Performance and performance portability of the Albany/FELIX finite element land-ice solver

As HPC architectures become more heterogeneous, climate codes must adapt to take advantage of potential performance capabilities. This talk will focus on performance and performance-portability of the Sandia Albany/FELIX finite element land-ice solver. The computational time for an ice sheet simulation in FELIX is divided into 2 pieces, each comprising ~50% of the total run time: finite element assembly (FEA), and linear solves. We will discuss our efforts in transitioning the FEA in FELIX from an MPI-only to an MPI+X programming model via the Kokkos library and programming model. In this model, MPI is used for internode parallelism and X denotes a shared-memory programming model for intranode parallelism (e.g., X=OpenMP, CUDA). With Kokkos data layout abstractions, the same code can run correctly and efficiently on current and future HPC hardware with different memory models. Also described in this talk will be our scalable and robust algebraic multigrid-based iterative linear solver, developed specifically for large-scale ice sheet problems. Perspectives for integrating Kokkos into this solver, towards making it performance-portable, will be given.

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O163

Mechanical error estimators for shallow ice flow models

We develop a posteriori mechanical error estimators that are able to evaluate the solution discrepancy between two ice flow models. We first reformulate the classical shallow ice flow models by applying simplifications to the weak formulation of the Glen-Stokes model. This approach leads to a unified hierarchical formulation which relates the Glen-Stokes model, the Blatter model, the shallow ice approximation, and the shallow shelf approximation. Based on this formulation and on residual techniques commonly used to estimate numerical errors, we derive three a posteriori estimators, each of which compares a pair of models using measures of the velocity field from the simpler (shallower) model. Numerical experiments confirm that these estimators can be used to assess the validity of the shallow ice models that are commonly used in glacier and ice sheet modeling.

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O164

Evaluating the performance of ice sheet models using LIVVkit

Significant development of dynamical ice sheet models is underway to both better understand ice sheet dynamics within the Earth system and take advantage of emerging computer architectures. In order to develop performant models, it is essential to understand current model performance (in various configurations), and to track performance changes over time and across architectures. This process, formally considered software validation, when coordinated with (software and numerical) verification and physical validation, can also evaluate the impact performance decisions on model solutions. We present a series of performance evaluations of the Community Ice Sheet Model and MPAS land-ice in both stand alone mode and coupled to an Earth system model. These evaluations have been built into LIVVkit, the land ice verification and validation toolkit. They are coordinated with other V&V analyses and help build confidence in model developments. Additionally, LIVVkit's output is a portable HTML and Javascript website that can be easily shared or hosted, allowing LIVVkit's evaluations to be transparent, easily reproducible, and discoverable, which is essential for the credibility of ice sheet models.

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O165

Nonlinear solvers for Stokes thermomechanical ice models

The Ymir ice sheet model for modeling and solving the instantaneous nonlinear Stokes equations of ice dynamics has been used in large-scale simulations of the Antarctic ice sheet, as well as highly scalable deterministic and statistical inversion for unknown parameters such as basal sliding conditions. The authors have recently published work on inverting for geothermal heat flux in a thermomechanical model of ice sheet dynamics. We will present work on developing nonlinear solvers for this coupled multiphysics system within the Ymir model.

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O166
Phase change with natural convection – simulation and segmentation of water-ice interfaces

Water-ice systems undergoing melting and re-freezing cycles develop complex spatio-temporal interface dynamics and a non-trivial temperature field. In this contribution, we present computational aspects of a recently conducted validation study that aims at investigating the role of natural convection for cryo-interface dynamics. We will start by introducing the relevant physical regime and the governing equations, as well as by describing the enthalpy-porosity method (EPM), a fixed grid approach to simulate convection-coupled phase change processes. It is based upon introducing a phase field and employing mixture theory. The EPM is solved numerically by means of a finite volume discretization. The second part of this talk is devoted to experiments conducted to validate our model and our approach to segmenting the experimental data. Here, we use a Mumford Shah model to get a piece-wise constant approximation of the experimental image data, whose jump set is the reconstruction of the measured water-ice interface. Our combined simulation and segmentation effort finally enables us to compare modelled and measured interfaces.

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O167
Finite element implementation and verification of a monolithic method for phase-change problems with natural and compositional convection

Accurately resolving the phase-change interface during water-ice melting and freezing processes requires modeling the liquid convection. This involves coupling the energy equation to the unsteady incompressible Navier-Stokes-Boussinesq equations. While existing methods consider natural convection (i.e. from temperature gradients), we must also consider compositional convection (e.g. from salinity gradients). Out of many approaches from the literature, we adopt an enthalpy-based, single domain phase-field, variable viscosity approach, with monolithic system coupling and global Newton linearization. Prior to this work, the method's convergence orders had not been verified, and solution of the linear system relied on direct solvers. We present 1. our implementation with the open-source finite element library deal.II, including verification of empirical convergence orders, 2. validation against classical benchmarks and a compositional convection example, and 3. analysis of the sparse linear system resulting from global Newton linearization, motivated by the goal of applying efficient iterative solution methods.

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O168
POD-deflation method for highly heterogeneous porous media

We propose the use of preconditioning and deflation techniques combined with CG as fast and robust iterative solvers. These techniques are studied for large systems of linear equations resulting from simulation of flow through strongly heterogeneous porous media. For the deflation method, we reuse information obtained from the system to reduce the time spent in the solution of the linear system. An important question when using deflation techniques is how to find good deflation vectors, which lead to a decrease in the number of iterations and a small increase in the required computing time per iteration. We propose the use of deflation vectors based on snapshots and a POD-reduced set of snapshots.

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O169
Krylov methods applied to reactive transport models

Reactive transport models couple advection dispersion equations with chemistry equations. If the reactions are at thermodynamic equilibrium, then the system is a set of partial differential and algebraic equations. After space and implicit time discretizations, a nonlinear system of equations must be solved at each time step. The Jacobian matrix of the nonlinear system can be written with a Kronecker product coupling transport and chemistry. Krylov methods are well-suited to solve such linear systems because the matrix vector product can be done efficiently. The main challenge is to design a preconditioning matrix. We propose here to use the special structure of the matrix. Preliminary experiments show that Krylov methods are much more efficient than a direct method which does not use the coupled structure.

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O170
A feature-enriched multiscale solver for complex geomodels

We present an adaptive and flexible framework for combining multiple multiscale operators that each targets a specific feature of the geomodel (fractures, faults, flow units, facies, etc). Each multiscale operator consists of a prolongation operator P and a restriction operator R , which must satisfy three requirements: 1) P and R are constructed by use of a non-overlapping partition of the fine grid. 2) P is composed of

a set of basis functions, each having compact support within a support region containing a coarse grid block. 3) The basis functions form a partition of unity. The final solver combines different multiscale operators with a second-stage smoother in an additive or multiplicative preconditioner for a Krylov solver. Numerical examples include both synthetic and real reservoir models with complex geological features and large permeability contrasts. We discuss preconditioning for elliptic pressure systems and fully-implicit compositional problems.

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O171

Combining model order reduction and preconditioned conjugate gradient for the solution of transient diffusion equations

The basis functions used in projection-based model order reduction techniques are typically obtained from the solution of the original high-dimensional system, compromising the computational advantages of these surrogate models in many practical applications.

Here, we explore the effectiveness of these basis functions in accelerating the convergence of the preconditioned conjugate gradient (PCG) through two possible approaches: (i) the residual associated with the PCG iterations is projected onto the space spanned by the reduced bases, similarly to the two-grid correction step of the Algebraic Multigrid method, and (ii) the reduced-model basis is used as projection space for the deflated PCG.

The application to a high-dimensional and ill-conditioned groundwater flow problem shows that the two approaches have similar properties. For both methodologies the number of PCG iterations decreases when the number of basis functions increases. However, the cost of the application of the PCG linearly increases with the size of the projection basis, and a trade-off must be found to effectively reduce the PCG computational cost.

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O172

Componentwise time-stepping for radially symmetric PDEs

Time-dependent PDEs with radially symmetric solutions are of particular interest in reservoir simulation, where the center of the domain represents a well. This talk presents a new approach to such PDEs, in which stiffness is overcome through

individualized approximation of each component of the solution, in a basis of orthogonal polynomials. The proposed method represents an extension of Krylov subspace spectral (KSS) methods, which overcome stiffness for PDEs on rectangular domains, to circular domains.

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O173

Multigrid KSS methods for time-dependent, variable-coefficient partial differential equations

Krylov Subspace Spectral (KSS) methods are traditionally used to solve time-dependent, variable-coefficient partial differential equations. Lambers, Cibotarca, and Palchak improved the efficiency of KSS methods by optimizing the computation of high-frequency components. This talk will demonstrate how one can make KSS methods even more efficient by using a multigrid-like approach for low-frequency components. The essential ingredients of multigrid, such as restriction, residual correction, and prolongation, are adapted to the time-dependent case. Numerical experiments demonstrate the effectiveness of this approach.

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O174

The impact of sedimentary facies on plume spreading in fluvial sandstone aquifers as investigated by simulations with a hybrid FEM-FVM embedded discontinuity method

While recent research on CO₂ plume spreading / geo-sequestration has demonstrated the importance of pore-scale or reservoir-scale heterogeneities, these just are end-members of a wide spectrum of geologic features that have the potential to influence plume migration and residual trapping: mm-scale grain-size variations, cm-scale laminations, cross-bedding, m-scale foresets and sedimentary layering all influence sweep in saline aquifers, i.e. where the plume will pass. These features will also impact the maximum CO₂ saturations reached behind the displacement front and residual trapping.

Here we present hybrid FEM-FVM flow-simulations performed on digital outcrop models of highly permeable siliciclastic fluvial rock sequences. The goal of these experiments is to reveal intermediate-scale plume morphology. Our results show that the geologic features diminish sweep, promoting flow localization. At the same time, they act as capillary barriers, increasing capillary hold-up. Thus, intermediate-scale geo-heterogeneity is as important as pore-scale heterogeneity. It cross-links scales, complicating multiphase flow upscaling.

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O175

Hysteresis in relative permeabilities suffices for propagation of saturation overshoot

Quantitative and reliable prediction of gravity driven flows is of paramount importance for CO₂ plumes.

Gravity driven flows exhibit instabilities and saturation overshoot. Traditional Darcy theory for two-phase flow in porous media is shown to predict the propagation of non-monotone saturation profiles, also known as saturation overshoot. The phenomenon depends sensitively on the constitutive parameters, on initial conditions and on boundary conditions. Hysteresis in relative permeabilities is needed to observe the effect. Two hysteresis models are discussed and compared. The shape of overshoot solutions can change as a function of time, or remain fixed and time-independent. Travelling-wave-like overshoot profiles of fixed width exist in experimentally accessible regions of parameter space. They are compared quantitatively against experiment. [1] R. Hilfer and R. Steinle, *The European Physical Journal ST*, vol 223, p. 2323 (2014) [2] R. Steinle and R. Hilfer, *Transport in Porous Media*, vol 111, p. 369 (2016)

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O176

Reservoir-scale modeling of CO₂ injection with impurities and convective dissolution

Dissolution CO₂ in water increases its density, creating gravitational instabilities and giving rise to convective flow. This process enhances CO₂ dissolution trapping. While this convective mixing phenomenon has been studied experimentally, analytically and numerically at the laboratory scale, modeling the fate of the CO₂ plume and density-driven motion at the reservoir scale is still challenging. The onset and transfer flux of convection are strongly dependent on grid resolution. During the capture process, the injection stream can contain small amounts of impurities such as N₂, O₂, Ar, SO₂, CH₄ and H₂S, evolving into highly coupled hydrodynamic and chemical processes.

We present large-scale numerical simulations of pure and impure CO₂ injection and compare these numerical results with a semi-analytical solution predicting the plume extent including convective dissolution. All scenarios demonstrated instabilities in both aqueous and gas phases. The impurities in the injection stream affect plume density and the thermodynamic properties of the whole system that modifies plume extent and structure.

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O177

3D geophysical data inversion using quasi-Newton methods with multi-grid preconditioning and its application to CO₂ injection monitoring.

Geophysical data inversion is an optimization problem where the cost function is comprised of the data misfit and a regularization term. The inversion is constrained by partial differential

equations (PDEs). As a solver, we present the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method in an appropriate function space. Spatial discretization, via finite elements, is left to the last possible moment of each BFGS step, just prior to the solution of the PDE constraints and their corresponding adjoint problems. BFGS is self-preconditioning, but using algebraic multigrid (AMG) dramatically accelerates convergence. This is key to achieving weak scalability with increasing spatial mesh size when solving 3D problems on parallel computers. We demonstrate the use of our approach for monitoring of CO₂ injection using Electrical Resistivity Tomography (ERT). Synthetic data generated from a multiphase, multicomponent CO₂ simulator provides predictions on the evolution of saturation, which is the target of the inversion. Electric conductivity and saturation are linked via a generalized Archie's law.

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O178

Vertically integrated approaches for carbon storage modeling in heterogeneous domains

Numerical modeling is an essential tool for studying the impacts of carbon dioxide (CO₂) injection into deep saline aquifers. The migration of CO₂ and resident brine can be described by a set of three-dimensional (3D) multi-phase flow equations. Vertical integration of the 3D governing equations leads to so-called vertically-integrated (VI) models. While VI models often give results of comparable quality as 3D reservoir simulators when applied to realistic CO₂ injection sites, they usually rely on homogeneous properties over the thickness of a geologic layer. Here, we investigate VI models for geological formations with heterogeneity in intrinsic permeability, relative permeability functions, and capillary pressure functions. We consider formations involving complex fluvial deposition environments and compare the performance of VI models to 3D models for a set of hypothetical test cases consisting of high permeability channels (streams) embedded in a low permeability background (floodplains). Analysis of the computational results allows us to identify the limits of applicability of VI models for CO₂ sequestration.

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O179

Propagation of saturation overshoots for two-phase flow in porous media

Flow and transport processes in porous media play an important role in various application areas like geological CO₂ and energy storage. In order to get a better understanding of two-phase flow in porous media, several water infiltration experiments have been performed. Thereby, it has been revealed that the water saturation exhibits a non-monotone and fluctuating profile with an overshoot region.

In this presentation, we outline how this phenomenon can be modeled by enhancing the standard two-phase flow equations. Since the resulting model is given by a non-linear PDE system, robust numerical solution techniques for this model are presented. In particular, it is of interest how the non-linear systems of equations arising in this context, can be solved. Finally, we discuss how this model can be applied to CO₂- and energy storage problems.

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O180

Richy – A C++ finite element solver

The software package Richy is a C++ finite element solver for reactive multi-component transport. It supports distributed memory parallelization using MPI and a wide range of problems in the field of subsurface flow (and other fields) have been successfully implemented and solved within its framework. Richy offers special support for preprocessing schemes that reduce the number of unknowns in the resulting nonlinear equations as well as the choice between several spatial discretizations. Selected underlying data structures will be presented and investigated in terms of reuseability and performance.

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O181

MRST – An open-source framework for rapid prototyping in subsurface modeling

The Matlab Reservoir Simulation Toolbox (MRST) combines three key features: (i) a highly vectorized scripting language that enables users to work with high-level mathematical objects and continue to develop a program while it runs; (ii) a flexible grid structure that enables simple construction of discrete differential operators; and (iii) automatic differentiation that ensures that no analytical derivatives have to be programmed explicitly as long as the discrete flow equations and constitutive relationships are implemented as a sequence of algebraic operations. We have developed a modular, efficient framework for implementing and comparing different physical models, discretizations, and solution strategies by combining imperative

and object-oriented paradigms with functional programming. MRST also offers extensive support for industry-standard reservoir models.

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O182

Nonlinear solvers in OPM flow

Flow is an open-source reservoir simulator developed within the Open Porous Media (OPM) framework to simulate models of real petroleum assets. Flow offers fully-implicit discretizations of black-oil type models and supports industry-standard input and output formats. It is implemented using automatic differentiation (AD) to avoid error-prone implementation of Jacobians, also making it easier to extend the simulator with new features, for example for Enhanced Oil Recovery (EOR). We describe our approach to solving the nonlinear equations, and investigate how a sequential solution approach combined with a nonlinear Gauss-Seidel algorithm can be used to accelerate the solution process, or be used as a preconditioner for a fully-implicit solution. We discuss how different approaches to automatic differentiation affect performance, flexibility and ease of implementation.

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O183

Dumux – using DUNE and facilitating the addition of new modeling capabilities

Dumux is a simulator mainly for flow and transport processes in porous media. It is based on the PDE software framework DUNE. In this talk, the two projects are introduced briefly. Then, it is illustrated where and how Dumux employs DUNE components and the advantages and possible drawbacks of building up on such a framework are evaluated. After that, it is shown how to add new modeling capabilities to Dumux and the strengths and weaknesses of Dumux concerning this task are presented.

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O184

Parallel preconditioners for iterative solvers within fully implicit blackoil simulators

In this talk we will describe some of the implementational details of the available parallel preconditioners for iterative solvers used in the “Open Porous Media Initiative” (OPM, <http://opm-project.org>) for solving the black-oil equation: hybrid block-ILU0, restricted additive Schwarz with block-ILU0 as inexact subdomain solver, parallel ILU0, and constrained pressure residual (CPR) with non-smoothed AMG or/and ILU0. We will present results for runs on several SPE benchmarks cases as well as on the real-world Norne reservoir. All models are available as open data from OPM and the software is available as open source.

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O185
Efficient linear solvers for the numerical simulation of fractured media

The simulation of the mechanics of fractured media is of paramount importance in several applications, such as ensuring the safety of the underground storage of wastes and hydrocarbons or predicting the possible seismicity triggered by the production and injection of subsurface fluids. A robust numerical method for the prediction of fracture sliding and/or opening is based on the use of Lagrange multipliers to prescribe the constraints on the contact surfaces. A variational formulation, properly modified to take into account the frictional work along the activated contact portion, is advanced. The resulting discrete system of non-linear equations is solved by a Newton method, where the Jacobian matrix has a generalized saddle-point structure. The development of efficient linear solvers for the solution of such problem is discussed. The linearized system is solved iteratively making use of block preconditioners based on approximate commutators for projecting the displacement variables on the space of the Lagrange multipliers, i.e., the contact strengths, and solving the coarse problem. Some test cases are presented to investigate the computational performance of the proposed approach.

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O186
A grid convergent discrete fracture/extended finite volume method (DF/XFVM) for poroelastic coupling with flow induced shear failure

A numerical modeling framework to simulate shear failure in fractured reservoirs has been developed using an extended finite volume method (XFVM). A hierarchical fracture representation is employed to solve for fluid flow and shear failure in the fractured reservoir, and thanks to the new XFVM no grid refinement around the fractures is required. The Coulomb friction law is applied to describe the failure criterion. Grid and time step size independent solutions for failure propagation and slip can be obtained with a time step size scaling with the fracture segment size. The method is further extended for shear failure simulation in three dimensional fractured domains, where additional numerical issues related to the XFVM had to be resolved. One such issue is the replacement of analytical integration of basis functions on the fracture

segments by suitable numerical integration. The method has also been employed for poroelastic simulations relying on the fixed stress approach. The corresponding effect on the time step size restriction has been studied for fluid injection into the poroelastic domain, and grid and time step size convergent results for slip and seismicity have been obtained.

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O187
A hybrid high-order method for Darcy flows in fractured porous media

We develop a novel Hybrid High-Order method for the simulation of Darcy flows in fractured porous media. The discretization hinges on a mixed formulation in the bulk region and on a primal formulation inside the fracture. Salient features of the method include a seamless treatment of nonconforming discretizations of the fracture, as well as the support of arbitrary approximation orders on fairly general meshes. For the version of the method corresponding to a polynomial degree k (including the case $k=0$), we prove convergence in order $(k+1)$ of the discretization error measured in an energy-like norm. In the error estimate, we explicitly track the dependence of the constants on the problem data, showing that the method is fully robust with respect to the heterogeneity of the permeability coefficients, and it exhibits only a mild dependence on the square root of the local anisotropy of the bulk permeability. The numerical validation on a comprehensive set of test cases confirms the theoretical results.

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O188
An optimization approach for flow simulations in 3D poro-fractured media

Flow simulations in Discrete Fracture Networks lead to face a computational domain that might count up to thousands of fractures, such that an efficient implementation is mandatory. We propose an optimization based approach in which the discrete problem, modeled by the Darcy law, can be reformulated as a quadratic problem with linear constraints. The problem is iteratively solved by a gradient based approach. At each iteration only small independent local problems on the fractures have to be solved, requiring only data on the segments of the intersecting fractures. This allows a natural parallel implementation of the method. The implementation is written in C++ language, using the MPI protocol for the communication among processes.

The network connectivity is computed with a parallel algorithm, in which the total number of operations is balanced among the processes. The connected graph is then split using the METIS routine, minimizing the number of arc-cuts and balancing the estimated number of degrees of freedom among the sub-graphs.

We implement a Master Slave parallel structure for the computations, to reduce the communication bottleneck for large networks.

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O189

Fully coupled fluid flow and geomechanical model for reservoir fracturing accounting for poroelastic effects

In our study we develop a fracture propagation model for poroelastic medium. The proposed approach combines the Discrete Fracture Model, contact-plane mechanics model, and fracturing criterion. The flow equations are approximated by FV method and the mechanics equations are discretized by means of Galerkin FE approach. The mechanical behaviour of fractures is modelled as a contact problem between two interfaces. The model captures elastic interaction between fracture and surrounding rock, fluid seepage between fracture and rock and associated poroelastic effects. Two dimensional surfaces between three dimensional finite elements are considered as possible fracture surfaces. Thus most of these surfaces are inactive from the beginning and are being activated throughout the simulation. The fracture propagation criterion is verified on yet inactive segments connected to the active ones. When criterion is satisfied, additional contact elements are added into FEM and DFM formulations respectively. We use criterion based on pressure and fracture opening of active segments as well as stress values in surrounding unfractured media. The proposed approach allows to model open mode, natural pre-existing, and closed fractures within one framework.

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O190

Adaptive vertical equilibrium concept for energy storage in subsurface systems

Simulating large scale underground energy storage for risk assessment and planning purpose requires simulations for multi-phase flow and hysteresis on a large domain over the whole time of plant operation and beyond, including local features such as fault zones and a representation of the transient saline front. Key to an efficient model is to apply only the degree of complexity that is required to accurately describe the physical process but not more. We will present a new conventional full-dimensional model in regions of higher complexity and areas where the vertical equilibrium assumption does not hold and a vertical equilibrium model in the rest of the domain. This model allows for an accurate solution within a short computational time.

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O191

Modeling multicomponent diffusions and natural convection in fractured media by discontinuous Galerkin and mixed methods

Computation of the distribution of species in hydrocarbon reservoirs from diffusions (thermal, molecular, and pressure) and natural convection is an important step in reservoir initialization. Current methods are mainly based on the conventional finite difference approach. Such methods may not be numerically efficient in fractured and other media with complex heterogeneities. In this work, the discontinuous Galerkin (DG) method combined with the mixed finite element (MFE) method is used for the calculation of compositional variation in fractured hydrocarbon reservoirs. The use of unstructured gridding allows efficient computations for disconnected fractured media when the crossflow equilibrium concept is invoked. The DG method has less numerical dispersion than the upwind finite difference (FD) methods. The MFE method ensures continuity of fluxes at the interface of the grid elements. We also used local discontinuous Galerkin (LDG) method instead of the MFE to calculate the diffusion fluxes. Result from several numerical examples are presented to demonstrate the efficiency, robustness, and accuracy of the model. Various features of convection and diffusion in homogeneous, layered, and fractured media are also discussed.

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O192

Efficient and stable simulation of compositional grading in hydrocarbon reservoirs

Compositional grading in hydrocarbon reservoirs significantly affects the design of production and development strategies. Compositional grading is complex subsurface phenomenon linked to phase behavior of multicomponent mixture, the gravity force, the capillary pressure, and others. In this work, we propose a novel mathematical modeling for compositional grading that is consistent with the laws of thermodynamics. A key feature of the model is that it satisfies the energy dissipation property; in addition, the model is formulated for the two scales of free spaces without solids (laboratory scale) and within porous media (geophysical scale). For the numerical simulation, we propose a physically convex-concave splitting of the Helmholtz energy density, which leads to an energy-stable numerical method for compositional grading. Using the proposed methods, we simulate binary and ternary mixtures in the free spaces and porous media, and demonstrate that compared with the laboratory scale, the simulation at large geophysical scales has more advantages in simulating the features of compositional grading.

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O193

Upscaling of a reactive transport model in fractured porous media

We consider a coupled flow and reactive transport model in a fractured domain of thickness ϵ . The permeability tensor inside the fracture is assumed to be diagonal but anisotropic and scales with different powers α, β of ϵ in the vertical and horizontal directions respectively. The reduced model is derived as a limit case of ϵ tending to zero and is defined on an interface (the reduced fracture) and acting as a boundary condition for the equations in the block. We investigate the effect of variation of α, β on the reduced model through analytical and numerical approaches.

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O194

Multi-scale Reconstruction of Compositional Transport

A compositional formulation is a reliable option to understand complex subsurface processes but it is computationally challenging.

A space parameterization method was proposed to speed up the process by parameterizing the problem based on two key tie-lines thereby replacing the flash calculations. Also the phase changes predominantly depends on these tie-lines passing through initial and injection compositions, hence it is convenient to parameterize based on the same.

In the first stage, modified conservation equations are used for reconstruction of leading & trailing shock position in space. This can be performed on a coarse-scale mesh since the structure of the transport solution outside the two-phase region is relatively simple. Next, the structure of the entire solution for N_c components is reconstructed between these two shocks by solving only two equations. Using this approach, simulation time is appreciably reduced ensuring conservation and without significant loss in accuracy.

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O195

Various alternative formulations of the flash equilibrium calculation

Calculation of the phase equilibrium is a common problem arising in compositional simulation, which is essential for simulations of processes related to enhanced oil recovery or CO₂ sequestration. When a gas is injected into a reservoir, the mixture of the gas and the reservoir fluid can remain in a single phase or split into two (or more) phases. The task is to detect which of these two cases occurs (phase stability testing) and, in the multi-phase case, to determine the amount, densities, and chemical composition of the equilibrium phases (phase equilibrium calculation).

In this talk, we will mention the standard formulation using pressure, temperature, and mole numbers (variables PTN) and introduce alternative formulations of the phase stability testing and flash equilibrium problems using total volume, temperature, and moles (variables VTN) or internal energy, volume, and mole numbers (variables UVN) as specification variables. We will present a unified formulation of the phase equilibrium problem that can include all these formulations and show its utility in compositional simulation.

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O196

Electrical resistivity imaging with subsurface boundary constraints

We address the inverse problem to recover earth parameters from Electrical Resistivity (ER) and Ground Penetrating Radar (GPR) data measured at the surface of the earth. Robust least squares inverse methods are commonly used in practice. However, they result in smooth parameter estimates, which is not desirable in many geological and hydrogeological applications because it is common to encounter sharp boundaries in the subsurface.

It has been shown that when a least squares smoothness constraint is relaxed at a known boundary, sharp discontinuities can be recovered. Here we use GPR data to constrain the boundary in least squares inversion of ER data. We also develop a methodology to determine when a boundary estimate is a good choice relative to other boundary estimates. Results from both synthetic and field data from the Boise Hydrogeological Research site will be shown.

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O197

Some fast algorithms for mathematical modeling and inversion in geophysical exploration

Geophysical exploration delineates the depth and structures of natural-resources related geological formations by collecting and analyzing the Earth echoes from passive and active sources. Mathematical geophysics utilizes a variety of modeling and inversion tools to reveal subsurface structure quantitatively from these response data. Since a typical 3D seismic survey yields several terabytes (TBs) data, fast algorithms are essential for processing these data. Over the years we have developed a range of fast algorithms aimed at mathematical problems arising from geophysical exploration.

I will put these algorithms into both mathematical and geophysical perspectives by demonstrating various examples.

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O198

A look at surface wave dispersion imaging and deblurring

The dispersive properties of surface waves in the presence of vertical velocity gradients enables one to invert the dispersion information for layered Earth structure. Accurate estimation of the dispersion data plays a key role in the accuracy of the

inverted velocity model. To measure the dispersion of phase velocity, one can use linear arrays of sensors to monitor the surface-wave propagation. The linear-Radon transform can be applied to the array data to separate frequencies/wavenumbers traveling at different velocities. This transform can be viewed as a low-resolution data estimation method. We present an alternative data estimation method, whereby we 'deblur' the dispersion image using sparsity promoting algorithms. We demonstrate the method with synthetic and field data examples.

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O199

Some higher-order compact finite difference schemes for acoustic wave equation in heterogeneous media

Efficient and higher-order numerical methods for seismic wave equation have been extensively used in various applications in Geophysics. One specific example is the seismic full waveform inversion problem, in which the acoustic wave equation is numerically solved for a large number of times during the iteration process. Despite the tremendous efforts that has been devoted, it still remains a challenging task in the development of efficient and accurate finite difference method with low numerical dispersion for multi-dimensional acoustic wave equation, especially for variable velocity case. In this work, we extended the Padé approximation based Alternative Directional Implicit (ADI) method, to develop a fourth-order compact finite difference scheme to solve three-dimensional acoustic wave equation with variable velocity. The key feature of the new method is to approximate the velocity function as the product of three functions of x , y and z , respectively, so the finite difference operators are commutative. Numerical results are solved to show that the numerical method is accurate, efficient and stable.

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O200

Application of least square support vector machine and multivariate adaptive regression spline in long term prediction modeling of river water

This study investigates the accuracy of least square support vector machine (LSSVM), multivariate adaptive regression splines (MARS) and M5 Model Tree (M5Tree) in modeling river water pollution. Various combinations of water quality parameters, Free Ammonia (AMM), Total Kjeldahl Nitrogen (TKN), Water Temperature (WT), Total Coliform (TC), Fecal Coliform (FC) and Potential of Hydrogen (pH) monitored at Nizamuddin, Delhi Yamuna River in India were used as inputs to the applied models. Results indicated that the LSSVM and MARS models had almost same accuracy and they performed better than the M5Tree model in modeling monthly chemical oxygen demand (COD). The average root mean square error (RMSE) of the LSSVM and M5Tree models was decreased 1.47% and 19.1% using MARS model, respectively. Adding TC input to the models did not increase their accuracy in modeling COD while adding FC and pH inputs to the models generally

decreased the accuracy. The overall results indicated that the MARS and LSSVM models could be successfully used in estimating monthly river water pollution level by using AMM, TKN and WT parameters as inputs.

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O201

Free geodetic network analysis by selective bias control

The analysis of free geodetic networks is oftentimes based on sophisticated least-squares methods such as the Minimum Norm Least-Squares Solution (MINOLESS), which is known to be the Best Least-Squares Solution (BLESS) as well as the Best Linear Uniformly Minimum Biased Estimate (BLUMBE). Less known is that the MINOLESS is the only Least-Squares Solution (LESS) that minimizes the bias uniformly. Here, a selection matrix $S_k = \text{Diag}(1, \dots, 1, 0, \dots, 0)$ is employed for partial bias control in k out of m unknown parameters/coordinates of which $m - d$ are estimateable. The resulting Best Linear Minimum Partial Biased Estimate (BLIMPBE) will be a LESS if and only if $\text{rk}(S_k N) = \text{rk}(N) = m - d$, implying that $k \geq m - d$. Here, $N \in \mathbb{R}^{m \times m}$ is a symmetric, positive-semidefinite matrix typical of that belonging to a system of least-squares normal equations, and d is the nullity of N .

For $d \leq k < m - d$ the BLIMPBE will be unique, but not a LESS. In contrast, if $k < d$ the BLIMPBE is not well defined. We are particularly interested in studying these transition zones, using an example from geodesy.

Keywords: free geodetic network adjustment, least-squares estimation, minimum bias

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O202

Stochastic modeling of transport noise

I will present a new approach of introducing stochasticity in a large class of models for fluid dynamical systems that preserve some of the natural conservation laws satisfied by the deterministic models. I will discuss the statistical calibration of the stochastic noise and the immediate applications to the uncertainly quantification of the models. I will show how one can apply the approach to the 2d Euler equations and to 2d multilayer quasi-geostrophic equation. This is joint work with Colin Cotter, Darryl Holm, Wei Pan and Igor Shevchenko.

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O203

A dynamically driven paradigm for data assimilation in geophysical models

In nonlinear chaotic dynamics, assimilation in the unstable subspace (AUS) of Trevisan et. al. offers an efficient way to operate the assimilation of observations by using only the unstable and neutral Lyapunov subspace to describe the uncertainty in state estimation. AUS methodology is based on two key properties of deterministic, dissipative, chaotic systems: (i) perturbations tend to project on the unstable manifold of the dynamics, and (ii) the dimension of the unstable manifold is typically much smaller than the full phase-space dimension. Applications to atmospheric, oceanic, and traffic models showed that even in high-dimensional systems, an efficient error control is achieved by monitoring only the unstable directions. In perfect linear models we have proven the collapse of the uncertainty to the time varying unstable-neutral subspace. Current work extends AUS to systems with model error. We demonstrate that under generic assumptions the forecast error in the stable, backwards Lyapunov vectors is uniformly bounded independently of filtering. The dynamic evolution of model error is, however, strongly influenced by the local Lyapunov exponents and we connect the variability of this forcing to filter design.

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O204

Assessing the reliability of ensemble forecasting systems

Forecast reliability is an important notion in the context of ensemble forecasts. Definitions of reliability state, roughly speaking, that the verification should be “statistically indistinguishable” from the ensemble members.

The main deficit though with operational definitions of reliability is that they usually do not make statements about the joint distribution of a series of verification--ensemble pairs. Rather, it is often assumed (explicitly or implicitly) that verification--ensemble pairs for different time instances are

independent, while in fact there can be very complicated dependence between them. This precludes a precise analysis of reliability tests (both existing and to be devised).

In this talk, we discuss what form of (in)dependence between verification--ensemble pairs is needed in order to render classical reliability tests applicable. Further, a new notion of reliability, called strong reliability, will be presented. Strong reliability is a natural extension of existing notions of reliability yet it provides a basis for rigorous treatment of reliability tests. Finally, we discuss to what extent strong reliability can be expected to hold in idealised forecasting systems.

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O205

Iterative updating of model error in Bayesian inversion for efficient posterior sampling

In the Bayesian approach to inverse problems it is often of interest to calculate quantities of interest by integrating them against the posterior measure. Monte Carlo methods are typically used for this integration, making use of samples from the posterior. However, sampling the posterior, particularly with MCMC methods, often involves a large number of forward model evaluations. Such evaluations may be prohibitively expensive to perform a large number of times, and so it can be preferable to use a cheaper approximate model instead. The use of an approximate model introduces an error into the posterior, termed the model error, which should be accounted for. In the Bayesian paradigm we treat the model error as a random variable whose distribution is to be jointly inferred along with that of the unknown state in the inverse problem. We introduce an algorithm to estimate and iteratively update the distribution of this model error, leading to a sequence of posterior distributions that more accurately approximate the true posterior, requiring only limited full model evaluations.

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O206

Tensor product decomposition methods for compact representations of large data sets

Low-rank approximation methods are an important tool in numerical analysis and in scientific computing. Those methods are often suited to attack high-dimensional problems successfully and allow very compact representations of large data sets. Specifically, hierarchical tensor product decomposition methods emerge as a promising approach for application to data that are concerned with cascade-of-scales problems as, e.g., in turbulent fluid dynamics. Here, we focus on two particular objectives, that is representing turbulent data in an appropriate compact form and, secondly and as a long-term goal, finding self-similar vortex structures in multiscale prob-

lems. The question here is whether the new tensor product methods can support the development of improved understanding of the multiscale behavior and whether they are an improved starting point in the development of compact storage schemes for solutions of such problems relative to linear ansatz spaces.

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O207

Data-driven uncertainty quantification for transport problems in structured porous media

Stochastic methods for flow and transport simulations of channelized reservoirs must be able to represent both non-smooth material properties and connected structures, such as sharp permeability transitions between channels and surrounding matrix. Traditional two-point statistics methods perform poorly in representing these features, but multiple-point statistics methods can be used to represent channels within a stochastic framework. In this work we use a kernel transformation to create an efficient stochastic parameterization of heterogeneous permeability fields. We then perform uncertainty quantification for transport problems using polynomial chaos and stochastic collocation based on data, combined with stochastic model reduction using analysis of variance (ANOVA) decomposition.

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O208

A stochastic galerkin method for hyperbolic-elliptic systems governing two-phase flow in porous media

The talk is concerned with the dynamics of two-phase flow and random locations of spatial heterogeneity interfaces in porous media. In the deterministic case discontinuities of the flux function occur due to the change of the material parameters. Based on the capillarity-free fractional flow formulation we quantify uncertainties arising from the randomized interfaces by means of the hybrid Stochastic Galerkin (HSG) method. The method extends the concept of the generalized polynomial chaos (PC) expansion for a multi-element decomposition of the multidimensional stochastic space. This results in a deterministic system for the coefficients of the PC expansion of the primary unknowns saturation, total velocity and global pressure. We then use the sequential implicit pressure explicit saturation (IMPES) approach to model the hyperbolic-elliptic system discretized with a central-upwind finite volume scheme for the hyperbolic along with a mixed finite element method for the elliptic part. The overall method permits the consideration of various complex flow problems and is well-suited for parallel computations.

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O209

Underpinning modern random walk models for transport UQ in the heterogeneous subsurface with results from classical perturbation theory

Heterogeneous hydraulic conductivity fields are a key source of uncertainty of flow and transport in subsurface formations. Over the past years sophisticated Lagrangian random-walk models have been developed that enable the quantification of these uncertainties at small computational costs. In spite of recent successful applications in challenging spatially non-stationary settings, these models are typically formulated based on Abstracts empirical data from idealized Monte Carlo simulations.

In this work, we analytically derive and verify the characteristics of the random processes that are at the heart of some of these models.

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O210

Stochastic Galerkin methods with hyperspherical transformation for vertical equilibrium CO₂ migration models

Accurate and efficient uncertainty quantification methods are essential for realizing large scale CO₂ storage in saline aquifers. We propose a stochastic Galerkin (SG) formulation using generalized Polynomial Chaos expansion as a alternative for costly sampling based methods. The SG method is applied to a reduced-physics nonlinear CO₂ migration model taking into account residual

and dissolution trapping. The challenge concerning discontinuities in stochastic space arising from the assumption of sharp interfaces between CO₂ and brine are handled using a hyperspherical sparse approximation technique. Numerical results are presented, and efficiency and accuracy are evaluated through comparison against a classical Monte Carlo approach and a semi-analytic solution respectively.

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O211

Time series parameterization of evolution equations for probability density functions of uncertain concentrations transported in groundwater

Assessments of ecological and human health risks due to chemical contamination in hydro-geological systems use thresh-

old exceedance probabilities determined by the probability density function (PDF) of the uncertain solute concentration. Solutions to PDF evolution equations are not explicitly related to an observation scale. A more flexible approach is that of uncertainty characterization by the filtered density function (FDF). The FDF is the PDF of the sub-grid scale in numerical modeling, and can be associated to the support volume of the measurements in field experiments and hydrological observations. The convergence with increasing filter width of the FDF to the PDF solution proves the consistency of the FDF approach. The PDF/FDF transport in concentration spaces is parameterized by a new mixing model consisting of a process that generates time series of concentration with a prescribed statistics. The PDF/FDF approach and the time series parameterization are appropriate for physical systems modelled as diffusion processes in random velocity fields and, as such, they apply as well to transport in the atmosphere or to turbulent reacting flows.

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O212

Enabling target-oriented imaging for large-scale seismic data acquisition using probing techniques

Imaging in geological challenging environments have led to new developments, including the idea of generating Green's function at a given target datum in the subsurface, where target datum lies beneath the complex overburden, by means of interferometric redatuming. One way to perform the redatuming is via conventional model-based wave-equation techniques, which can be computationally expensive for large-scale seismic data acquisition since one has to solve wave-equation for all the source and receiver locations involved in seismic data acquisition. In this work, we present an alternative approach to redatum both source and receivers at depth, under the framework of reflectivity-based extended images with two-way wave propagation in the background medium. We use a matrix probing scheme that takes advantage of the algebraic structure of the extended imaging system to overcome the computational cost and memory usage associated with the number of wave-equation solutions and explicit storage employed by conventional migration methods. Experimental results on complex geological models demonstrate the efficacy of proposed methodology and enable practical reflectivity-based extended imaging for large-scale 5D seismic data.

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O213

Target-enclosing extended imaging – The role of image extensions in pushing resolution limits

Travelling wide-bandwidth seismic waves have long been used as a primary tool in exploration seismology because they can probe the subsurface over large distances, while retaining relatively high spatial resolution. The well-known Born resolution limit often seems to be the lower bound on spatial imaging resolution in real life examples. In practice, data acquisition cost, time constraints and other factors can worsen the resolution achieved by wavefield imaging. In this talk, we will cover aspects of linear and nonlinear seismic imaging to in the context of “super-resolved” seismic images. New techniques, such as the Marchenko method, enable the retrieval of subsurface fields that include multiple scattering interactions, while requiring relatively little knowledge of model parameters. With the new concept of Target-Enclosing Extended Images, these methods enable new targeted imaging frameworks: these may help in increasing the resolving power of seismic imaging, and in pushing the limits on parameter estimation. We will illustrate this using a field data example. Finally, we will draw connections between seismic and other imaging modalities, and discuss how this framework could be put to use in other applications.

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O214

Exploring the dynamics of wavefield correlations

In traditional reverse-time imaging in inverse scattering, a zero-lag correlation of the forward and reverse-time wavefields yields an image. Extending such correlations to non-zero lag gives additional information about the consistency of the model and the observed data. In this talk, I give an overview of the role of various correlations in wavefield imaging and explore the dynamics of such correlations. Like the forward and reverse-time wavefields themselves, their correlations obey a partial differential equation. Understanding the dynamics of these correlations gives further insight in the information contained in these correlations and their efficient computation.

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O215

Low-rank compression of subsurface-offset extended image volumes

Extended subsurface-offset image volumes play a key role in seismic imaging and inversion. Because they contain information on both the kinematics and dynamics, they are used to drive migration-velocity analyses, target-oriented

imaging, and rock-property characterizations. While clearly useful, these extended imaging volumes are computationally expensive because they involve loops over sources – each involving multiple forward and adjoint wave-equation solves – and explicit cross-correlation calculations. To overcome these challenges, we present a low-rank technique that compresses full omni-directional subsurface-offset image volumes, which are exceedingly large because they are quadratic in the number of model parameters. Aside from making these ominous imaging volumes computationally and storage-wise tractable, our compression method also leverages a recently introduced (randomized) probing technique, which avoids the loop over sources and explicit cross-correlation computations.

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O216

Vertical seismic profiling with distributed acoustic sensing

Question:

We introduce a new sensing technology for use in seismic applications.

Methods:

Seismic vibrations in the earth are monitored by means of a fibre optic cable buried within the subsurface. Optical backscatter from a laser beam directed down the fibre is converted to a strain measurement distributed in time and space along the fibre.

Results:

This distributed acoustic sensing method may be applied to the acquisition of vertical seismic profile data from measurement taken down a well borehole.

Conclusions:

We demonstrate that this fibre data may be effectively used as input to industry standard data processing techniques for seismic imaging in oil and gas exploration.

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O217

Inexact hierarchical scale separation – An efficient linear solver for discontinuous Galerkin discretizations

Hierarchical scale separation (HSS) is a two-scale approximation method for large sparse linear systems arising from discontinuous Galerkin (DG) discretizations. HSS splits the system into a coarse-scale system of reduced size corresponding to the local mean values of the solution and a set of decoupled local fine-scale systems corresponding to the higher order solution components. This reduces the communication overhead, e.g., within sparse matrix-vector multiplications of classical itera-

tive solvers and allows for an~optimal parallelization of the fine-scale solves. We propose a modified algorithm (“inexact HSS”) that shifts the workload to the parallel fine-scale solver to reduce global synchronization, resulting in a significant speedup. We investigate its applicability to systems stemming from the nonsymmetric interior penalty DG discretization of the Cahn-Hilliard equation, discuss its parallel implementation for large-scale simulations, and investigate its performance.

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O218

The AMR (Exa)HyPE

ExaHyPE is a H2020 project where an international consortium writes a simulation engine for hyperbolic equation system solvers based upon ADER-DG. It is used to simulate earthquakes. The talk is a tour de force through ExaHyPE. We start with a brief sketch of ADER-DG. From hereon, we dive into the AMR framework Peano which serves as AMR base. Our talk focuses on three research questions:

How does Peano’s automaton-based grid traversal impact ExaHyPE’s programming workflow? How does Peano decompose ExaHyPE’s algorithmic steps into tasks without explicit task graph assembly? How does Peano decompose the underlying spacetrees representing adaptive Cartesian grids in a distributed memory environment?

Our scalability results suggest that, while we support arbitrary dynamic adaptivity, it makes sense performance-wisely to restrict the adaptivity, i.e. to impose some regularity on the grid structure. It is “regular” dynamic mesh refinement that seems to pave the path to exascale.

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O219

TerraNeo – Mantle convection modeling and the road to Exa-scale

This talk provides an overview on the TerraNeo project which, as part of the SPPEXA priority programme by the German Research Foundation (DFG), develops a software framework and algorithms for next generation mantle convection models. It focuses on high computational efficiency, resilience and fitness for future HPC infrastructures. We present software that can resolve the Earth’s mantle with up to 1012 grid points and scales efficiently to massively parallel hardware having more than 50,000 processors.

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O220

An efficient tool for transport-reaction modeling with its test application

The contribution deals with presentation of two ideas applied in the Communicator component allowing efficient transport-reaction computations. The component was implemented as an interface between the groundwater flow and solute transport modeling software FEFLOW and geochemical process modeling software React (included into The Geochemist’s Workbench package) or PhreeqC. The first idea is utilisation of database of executed geochemical model computations and its fast search. The other idea is use of High Performance Computing in combination with the first idea. There will be presented the real-world problem – transport of solutes in the closed flooded mine with geochemical processes – and the use of the presented software for its solution. The ideas on the next progress in such a modeling will be appended.

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O221

Modeling complex multiphase flows with the Lattice Boltzmann method – An introduction

The Lattice Boltzmann method (LBM), is becoming a valuable alternative to Navier-Stokes based simulation tools in the field of incompressible fluid flows in complex geometries. Its kinetic theory based formulation provides a unique framework for simulating processes like multi-phase flows, flows through realistic pore geometries, reactive transport processes with evolving media, etc. This talk will introduce the LBM and describe its main features, with particular emphasis on the boundary conditions and on the different multiphase models currently available.

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O222

Mesoscopic simulations of electrokinetic phenomena.

Electrokinetic effects play a crucial role in many natural and technological systems, from the biological to nano-fluidics. Numerical simulations of conducting fluids presents a significant challenge mainly due to the variety of length-scales involved, and the presence of two long-range interactions: hydrodynamic and electrostatic. We show an electrohydrodynamic mesoscopic model, discuss its validity, and present results on the dynamics of colloids at fluid/fluid interfaces. The hydrodynamics of two fluids is solved using the lattice-Boltzmann method. Ions present in the solvents are considered at the level of the Nernst-Planck equation, which is solved via a finite-volume, finite-difference discretization, following the link-flux method. Furthermore, colloids can be added provided that a novel discretization scheme is used to avoid large velocity fluctuations. We show that the simulation scheme is robust and remains valid in a wide range of parameters. This allows us to characterize the interaction of two colloids at the interface of an electrolyte and an apolar fluid, and study the collective behaviour of charged colloidal suspensions in flat and curved surfaces.

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O223

Thermal lattice Boltzmann method for catalytic flows through porous media

Many catalyst devices employ porous or foam-like structures to optimize the surface to volume ratio in order to maximize the catalytic efficiency. The porous structure leads to a complex macroscopic mass and heat transport. Local heat accumulation changes the local reaction conditions, which in turn affects the catalytic turn over rate and eventually compromises the stability of the catalytic device. We present a thermal multi-component model based on the entropic lattice Boltzmann method [1] to simulate catalytic reactions through porous media. This method reproduces the Navier-Stokes equations and allows the tracking of temperature dynamics. The viscosity, diffusivity, and heat capacities are calculated from the Lennard-Jones parameters of the gases, while the chemical surface reactions are incorporated in a very flexible fashion through the flux boundary conditions at the walls. To show the strength and flexibility of this model and our implementation, we will report the catalytic turn-over for a wide range of porosities and reaction conditions.

[1] J. Kang et al., Phys. Rev. B 89, 063310, 2014.

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O224

Computation of wall shear stresses and characterisation of fluid flow domains by a coupled CFD-MRI method in a medical application

In this talk, the coupling of magnetic resonance imaging (MRI) measurements and computational fluid dynamics (CFD) for the computation of wall shear stresses and fluid domain identification problems in a medical application is presented.

Thereby, the MRI measurement of blood flow in a human aorta is considered. The novel CFD-MRI method uses the insight of a fluid flow problem to reduce the noise of the measurements and to identify the finer structures of the underlying domain, without a priori knowledge of the geometry.

The problem is formulated as a distributed control problem which minimises the distance of measured and simulated flow field. Thereby, the simulated flow field is the solution of a parameterised porous media BGK-Boltzmann equation. The parameters represent the porosity distributed in the domain which yields a domain and a flow fluid that fits best to the measured data. To calculate the wall shear stress an adapted momentum exchange algorithm (MEA) is proposed.

The problem is solved by using the adjoint lattice Boltzmann method (ALBM) [1,2,3], using the open source software OpenLB (www.openlb.net)

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O225

Advances in nonlinear solvers for coupled systems in subsurface modeling

Unstructured polytopal meshes capture critical variability of topography and stratigraphy in terrestrial applications. The growing complexity of geometric models for simulation of surface and subsurface flows leads to the necessity of using unstructured meshes and advanced discretization methods. Advanced spatial discretizations, such as the Mimetic Finite Difference (MFD) and Nonlinear Finite Volume (NLFV) methods, are required to maintain accuracy and provide oscillation-free numerical solution. Although, the complexity of these discretization methods is manageable, it is problematic for the direct analytic differentiation of the nonlinear discrete system, as it is costly or overly complex to evaluate and the resulting Jacobian matrix may be singular. We develop a new Jacobian-Free nonlinear solver by discretizing the analytic Jacobian to control properties of arising matrices. The efficacy of this approach is demonstrated for coupled systems of thermal hydrology in permafrost environment.

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O226

A finite volume scheme with improved well modeling in subsurface flow simulation

We present the nonlinear correction finite volume scheme (NCFV) for improved modeling of well-driven flows in the near-well regions. The NCFV method takes into account the nonlinear (e.g. logarithmic) singularity of the pressure in the near-well region and introduces the nonlinear correction to improve accuracy of the pressure and the flux calculation. The new method is generalized for anisotropic media, polyhedral grids and nontrivial cases of wells such as slanted, partially perforated or shifted from the cell center. Outside of the near-well region the NCFV method is combined with the nonlinear monotone two-point flux approximation scheme. Numerical experiments show noticeable reduction of numerical errors compared to the original nonlinear monotone scheme with the conventional Peaceman well model or with the given analytical well rate.

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O227

Nonlinear finite-volume scheme for complex flow processes on corner-point grids

The numerical simulation of subsurface processes requires efficient and robust methods due to the large scales and the complex geometries involved. To resolve such complex geometries, corner-point grids are the industry standard to spatially discretize geological formations. Such grids include non-planar, non-matching and degenerated faces. The standard scheme used in industrial codes is the cell-centered finite-volume scheme with two-point flux (TPFA) approximation, an efficient scheme that produces unconditionally monotone solutions. However, large errors in face fluxes are introduced on unstructured grids. The authors present a nonlinear finite-volume scheme applicable to corner-point grids, which maintains the monotonicity property, but has superior qualities with respect to face-flux accuracy. The scheme is compared to linear ones for non-isothermal two-phase two-component flow simulations in realistic geological formations.

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O228

A hybrid finite volume – finite element method for transport modeling in fractured media

This work develops a hybrid method for solving a system of advection-diffusion equations in a bulk domain coupled to advection-diffusion equations on an embedded surface. We use a monotone nonlinear finite volume method for equations posed in the bulk and a trace finite element method for equations posed on the surface. The surface is not fitted by the mesh and can cut through the background mesh in an arbitrary way. Moreover, the surface is not triangulated in the common sense. The background mesh is an octree grid

with cubic cells. The mesh can be easily refined or coarsened locally based on different adaptivity criteria. As an example of an application, we consider the modeling of contaminant transport in fractured porous media. A series of numerical experiments with both steady and unsteady problems and different embedded geometries illustrate the numerical properties of the hybrid approach. The method demonstrates great exibility in handling curvilinear or branching lower dimensional embedded structures.

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O229

Dynamic adaptive simulations of immiscible viscous fingers

The unstable displacement of fluids due to viscosity contrast plays a crucial role in applied physics. Controlled by a balance of viscous and diffusive forces, simulation is challenging as one must ensure physical diffusion dominates numerical diffusion to see convergence, requiring high mesh resolution/higher order numerics. This leads to overly expensive simulations. We demonstrate the use of a novel control volume finite element (CVFE) method with dynamic unstructured mesh adaptivity to simulate viscous fingering. The saturation is defined control-volume wise to enforce mass conservation. We show complex examples of 2D and 3D fingering in high aspect ratio domains and geometries that are challenging to simulate using traditional methods. The growth rate of fingers is compared to analytical results at early-times before exploring the non-linear late-time regime. We are able to simulate immiscible fingers with higher accuracy and lower cost than conventional methods. Mesh adaptivity allows resolution to be focussed on the fingers with lower resolution elsewhere, whilst higher order interpolation minimises damage to the solution after adapts.

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O230

Compositional modeling of two-phase flow in porous media using VT-Flash

We deal with the numerical modeling of compressible multicomponent two-phase flow in porous media with species transfer between the phases. The mathematical model is formulated by means of the extended Darcy's laws for all phases, components continuity equations, constitutive relations, and appropriate initial and boundary conditions. The splitting of components among the phases is described using a formulation of the local thermodynamic equilibrium which uses volume, temperature, and moles as specification variables. The problem is solved numerically using a combination of the mixed-hybrid finite element method for the total flux discretization and the finite volume method for the discretization of continuity equations. These methods ensure the local mass balance. The resulting system of nonlinear algebraic equations is solved by the Newton-Raphson iterative method. We describe the numerical model and show several 2D simulations of homogeneous and heterogeneous subsurface reservoirs.

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O231

An adaptive numerical method for free surface flows passing rigidly mounted obstacles

The paper develops a method for the numerical simulation of a free-surface flow of incompressible viscous fluid around a streamlined body. The body is a rigid stationary construction partially submerged in the fluid. The application we are interested in the paper is a flow around a surface mounted offshore oil platform. The numerical method builds on a hybrid finite volume/finite difference discretization using adaptive octree cubic meshes. The mesh is dynamically refined towards the free surface and the construction. Special care is taken to devise a discretization for the case of curvilinear boundaries and interfaces immersed in the octree Cartesian background computational mesh. To demonstrate the accuracy of the method, we show the results for two benchmark problems: the sloshing 3D container and the channel laminar flow passing the 3D cylinder of circular cross-section. Further, we simulate numerically a flow with surface waves around an offshore oil platform for the realistic set of geophysical data.

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O232

FESOM-coastal – 3D modeling of coastal long-wave dynamics on the mixed meshes

Numerical modeling of coastal zone dynamics provides basis for solving a wide range of hydrogeological, engineering and ecological problems. A novel three-dimensional unstructured-mesh model (FESOM-coastal) is applied to simulate the dynamics of the density field and turbulence characteristics. The model is based on a finite-volume discretization and works on mixed unstructured meshes composed of triangles and quads. Although triangular meshes are most flexible geometrically, quads are more efficient numerically and do not support spurious inertial modes of triangular cell-vertex discretization. Mixed meshes composed of triangles and quads combine benefits of both. In particular, triangular transitional zones can be used to join quadrilateral meshes of differing resolution. The results of several simulations showing the performance of the model with respect to modeling wetting and drying, internal waves, and tidal dynamics are presented.

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O233

On global ocean dynamics on unstructured grids

We describe the ocean model ICON-O, the ocean component of Max-Planck Institute for Meteorology's newly developed Earth System Model MPI-ESM-2 and the ocean model of the ICON modeling system. ICON-O is a global general circulation model, formulated on an icosahedral grid with triangular cells and an Arakawa C-staggering. The models dynamical core as well as its oceanic parametrizations use a coherent structure-preserving discretization that incorporates ideas from finite-element, finite volume and mimetic discretization methods. We present numerical and experimental analysis of global ocean simulation to demonstrate the physical quality of the model solution and the computational efficiency of the model towards the goal of establishing unstructured grid models as a viable and attractive alternative to established structured grid models.

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O234

Ice-sheet/ocean interaction model using high-order continuous/discontinuous Galerkin methods with a non-conforming adaptive mesh.

Ice-sheet/ocean interaction in Greenland is one of the key outstanding challenges in climate modeling, yet present-day climate models are not able to resolve fine-scale processes in the fjords. This is due to orders of magnitude difference in spatial scales between the open ocean (~1000km) and fjord (<1km) as well as complex bathymetry and coastline. I will be presenting the progress of the NUMO project, which goal is to develop a non-hydrostatic ocean model able to resolve ice-sheet / ocean interactions, circulation within the fjord and exchanges with the ocean. As a proof of-concept, we focus on Sermilik Fjord and Helheim glacier system. An unstructured mesh is used to realistically represent the geometry of the fjord, while in the areas of particular importance (i.e. glacier front) the resolution is increased by non-conforming mesh refinement. NUMO models the ocean using the incompressible Navier-Stokes equation discretized with unified continuous/discontinuous Galerkin method. The long-term goal is to simulate all Greenland's fjords and adjacent coastal ocean and couple this simulation to regional or global Earth System Models.

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O235

Parameter estimation, uncertainty quantification and optimization of measurement designs for a biogeochemical model

When estimating model parameters using measurement data, several questions arise: How should the misfit between data and model output be quantified and optimal model parameters be calculated? What is the resulting uncertainty in the model parameters and the model output? How to design new measurements in order to reduce this uncertainty? These questions were studied regarding a three-dimensional, biogeochemical model describing the phosphorus cycle in the global ocean. Therefore statistical models for measurements of different tracers were developed including varying variances and correlations. Different estimators for the model parameters, resulting in different cost functions, were used and their results compared. The uncertainty in the model output arising from the uncertainty in the measurements was estimated. Designs for new measurements, including time, location and tracer, were optimized such that the information gain is maximized. With the used methods, we were able to determine considerably better model parameters. We would like to present these methods, which are not restricted to this model, together with the obtained results.

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O236

Probabilistic sea-level projections from ice sheet and earth system models

Polar ice sheets present the largest potential for future sea-level rise (SLR) and confidence in future SLR projections requires accurate simulations using ice sheet models (ISMs) coupled to Earth System Models (ESMs). We discuss current and planned U.S. Department of Energy (DOE) efforts to remedy existing model deficiencies that prohibit accurate, probabilistic SLR projections. These efforts build on previous DOE ISMs and ESMs and include: (1) new physically-based models for subglacial hydrology, damage mechanics, fracture, iceberg calving, and solid-earth dynamics beneath and proximal to ice sheets; (2) new ocean model physics and advanced coupling required for including ISMs in ESMs; (3) improved optimization methods that minimize non-physical ISM transients and assign uncertainty to model parameters; (4) "end-to-end" frameworks allowing model uncertainties to be forward propagated to output quantities of interest. Computational costs also require efficient and robust ISMs and workflows, which in turn require new methods for stable, accurate, and efficient time stepping and performance portability on next-generation HPC architectures.

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O237

A robust and extensible toolkit for ice sheet model validation

We present a collection of scientific analyses, metrics, and visualization for robust validation ice sheet models, targeting both stand alone and fully active Earth system models designed to run at scale on high-performance computing platforms. Automated postprocessing of simulation data is included, which enables faster and fully reproducible workflows that can handle observational and model derived datasets. Results are produced in a shareable format that can easily be distributed to users and developers for evaluation. We demonstrate the validation process as applied to three models: two versions of the Community Earth System Model with an active ice sheet, CESM1.0 with the Community Ice sheet model (CISM) version 1.0 and a pre-release version of CESM1.3 with CISM2, and a stand-alone ice sheet model, CISM-Albany. configured with 1~km resolution. We compare model results to in-situ and remotely sensed data as well as a recent RACMO2.3 regional model simulation, where appropriate.

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O238

Modeling glacier calving using discrete element and full Stokes continuum models

The simple calving laws currently used in ice sheet models do not adequately reflect the complexity and diversity of calving processes. To be effective, calving laws must be grounded in a sound understanding of how calving actually works. We have developed a new approach to formulating calving laws, using a) the Helsinki Discrete Element Model (HiDEM) to explicitly model fracture and calving processes, and b) the full-Stokes continuum model Elmer/Ice to identify critical stress states associated with HiDEM calving events. A range of observed calving processes emerges spontaneously from HiDEM in response to variations in ice-front buoyancy and the size of subaqueous undercuts, and we show that HiDEM calving events are associated with characteristic stress patterns simulated in Elmer/Ice. Our results open the way to developing calving laws that properly reflect the diversity of calving processes, and provide a framework for a unified theory of the calving process continuum.

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O239

Numerical methods for ice sheet–ocean coupling in the POPSICLES model

We present numerical methods from POPSICLES, a python package for coupled ice sheet–ocean simulations using the Parallel Ocean Program (POP) and the BISICLES ice sheet model. POPSICLES runs these two components synchronously and performs offline coupling between them by modifying monthly restart files, updating heat and freshwater fluxes and extrapolating ocean tracer and velocity fields to accounting for the evolution of ice and bedrock topography. We present the results of both idealized experiments encompassing a single ice shelf and full pan-Antarctic simulations, demonstrating physical phenomena unique to the coupled system such as sub-ice-shelf melt channels. We explore the consequences of various algorithms for representing narrow sub-ice-shelf channels in the ocean component. We also comment on the importance of physically consistent bedrock topography below both the ice-sheet and ocean components.

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O240

Viscoelastic modeling approaches for glaciological applications

While in the past ice dynamics was modeled using constitutive relations of a viscous material due to the time scale under investigation. In the recent past it became obvious, that the short time response of ice sheets cannot be neglected if dealing with calving, with bending in the hinge zone of ice shelves or with the development of subglacial melt channels. GPS observations have shown the phase shift between forcing and response and hence proven that ice in glaciers obeys a viscoelastic material behavior. Viscoelastic modeling of the ice deformation comes along with some challenges: equations need to be solved for strain which does not remain small and hence non-linear continuum mechanics needs to be applied. We present here the modeling concept using finite elements and a Maxwell rheology and three different types of applications of viscoelastic modeling, namely calving, grounding line migration and melt channel evolution. Furthermore, we will elaborate on the need of viscoelastic modeling versus medium complexity models for Earth System Modeling.

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O241

Ice-free topography of the Svalbard archipelago

For the large majority of the many glaciers and ice caps around the globe, there is no information on how thick the ice cover is. The poor knowledge of the bed topography precludes reliably ice-flow model predictions of glacier demise under climatic warming. Thus, the contribution to future sea-level rise from glaciers and ice-caps remains not well constrained. As it is impractical to measure ice thicknesses in many places, reconstruction approaches have been forwarded that can infer thickness fields from available surface information. Here, we apply a mass-conserving reconstruction approach to infer an archipelago-wide ice-thickness map for Svalbard. The abundant record of available thickness measurements was assimilated. An associated error estimate map serves to discern between areas where the reconstruction is more or less reliable. Keywords: Svalbard, Spitsbergen, glacier thickness, reconstruction, data assimilation, mass conservation

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O242

Ensemble Kalman filter inference of spatially-varying Manning's n coefficients in the coastal ocean

In this contribution, we implement and assess the efficiency of the Joint-EnKF for estimating spatially-varying Manning's n coefficients used to define the bottom roughness of a coastal ocean model. Observation System Simulation Experiments (OSSEs) are conducted using the ADvanced CIRCulation (ADCIRC) model. The Singular Evolutive Interpolate Kalman (SEIK) filter is used to directly estimate a full vector of defined Manning's n coefficients at the nodal points by assimilating synthetic water elevation data. To reduce the spurious correlations between distant points, a local analysis (LA) is implemented. We reduced the dimension of the parameter search space through Karhunen-Loeve (KL) expansion of the Manning's n field. We have also iterated on the filter update step to better deal with the nonlinearity of the parameter estimation problem. We study the sensitivity of the system to the ensemble size, localization scale, number of retained KL modes, and number of iterations. The results of this study suggest that a well-tuned Joint-EnKF may perform exceptionally well at estimating spatially varying parameters in the context of coastal ocean modeling.

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O243

Surrogate accelerated inversion and propagation of tsunamis for the Indian coast.

Following the 2004 Sumatra-Andaman (S-A) tsunami, it is highly relevant to understand the tsunami source and hazard on the Indian coast. The computationally expensive composite forward model for the generation of seabed uplift and consequent propagation of tsunami is a detriment towards such an endeavour. We replace the computer model by a

fast statistical surrogate. A sequential design of computer experiment is undertaken. We simulate tsunami scenarios selecting a set of rupture parameters that reflect the variations across the possible rupture events. The inputs are the finite fault geometry and accompanying slips on the subfaults. The outputs are wave heights on satellite tracks reported for the 2004 S-A event as well as tide gauges at key coastal locations. We compare these observations to the modelled solution and infer the inputs via stochastic optimization and Bayesian routes. The surrogate highly accelerates the inversion. The resulting distributions are propagated to quantify the uncertain hazard at the Indian coast. We find good fit between the observations and computed waveforms accompanied by large uncertainties in the rupture parameters.

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O244

Uncertainty quantification with graph-based flow/transport models

Simulating flow and transport in fractured porous media frequently involves solving numerical discretizations of partial differential equations (PDEs) with a large number of degrees of freedom. Uncertainty in the properties of the medium that control flow and transport often mean that a large number of solutions of the PDE are needed to statistically describe quantities of interest. However, the computational cost of solving a single realization of the high-dimensional numerically discretized PDEs combined with the large number of realizations needed, quickly make this problem computationally intractable. We pursue inexpensive graph-based models of flow and transport in fractured porous media as an alternative to highly-discretized PDEs. These graph-based models capture the essential physics and, when combined with machine learning and multi fidelity Monte Carlo methods, enable efficient uncertainty quantification.

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O245

A measure-theoretic stochastic inverse method for parameter estimation in subsurface flows

Question:

Effective modeling of complex physical systems arising in the geosciences is dependent on knowing parameters which are often difficult or impossible to measure in situ. In this talk we focus on estimating parameters for groundwater flow and transport.

Methods:

The approach we will describe is based on a novel stochastic inversion technique based on measure theory. In this approach, given a probability space on certain observable quantities of interest, one searches for the sets of highest probability in parameter space which give rise to these observables. When viewed as mappings between sets, the stochastic inversion problem is well-posed in certain settings, but there are computational challenges related to the set construction.

Results: We will focus the talk on estimating scalar parameters and fields in a contaminant transport setting. The results of the methodology are probabilities of events; i.e. determining the likelihood of parameters given data. The choice of data is also important to the process, and we will discuss how data skewness can impact the inversion process.

Conclusions: The talk will present novel results on a measure theoretic approach for stochastic inversion.

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O246

Path Integrals for flow through porous media

We use simulations of flow in porous media to generate statistics of pressure from the statistics of the permeability, which can be found from outcrops.

We use a stochastic model to represent the permeability, which relates the local flow rate to the local pressure gradient. Conventional calculations of pressure statistics rely on a considerable number of independent realisations of the inverse transmissibility matrix, which results in heavy computational requirements.

We propose the path integral method as a computationally lighter alternative. The path integral is an explicit formula for the probability amplitude associated with each pressure realisation. The method does not depend on the inversion of explicit permeability realisations. Rather, one works with the stochastic model for the inverse permeability. The pressure statistics resulting from the path integral approach are in very good agreement with those obtained through stochastic techniques.

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O247

Temporal oscillations in the porous medium equation: why harmonic averaging itself is not to blame

Harmonic averaging of the coefficient, $k(p) = pm$, $m \geq 1$, has been blamed for nonphysical locking and lagging of pressure solutions of the Porous Medium Equation, $p_t - \nabla \cdot (k(p)\nabla p) = 0$, that occur for small p . This degenerate parabolic equation has applications to plasma heat transfer, gas and ground-water flow. The numerical issues also manifest themselves in spurious temporal oscillations, even with none in space. Arithmetic averaging has been suggested as an alternative. We show that harmonic averaging is not solely to blame and that an improved choice of temporal and spatial discretizations can avoid these issues. The harmonic problems can be traced for standard numerical schemes to a local anti-diffusive term in the modified equation and so can be compensated for. A similar approach works for superslow diffusion, where $k(p) = \exp(-1/p)$.

A more extreme case, arising in foam models, is where $k(p)$ is a step function, e.g. $k(p) = 1$ if $p \geq 0.5$ and 0 otherwise. For this model, both harmonic and arithmetic averaging result in artificial temporal oscillations. To resolve this, we propose a new type of averaging, incorporating the shock position that can be estimated effectively.

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O248

Event-driven methods for some geochemical problems

In many relevant applications concerning subsurface porous media flow, such as geothermal reservoirs, oil formation or CO₂ storage, chemical reactions can be the cause of porosity changes. Indeed minerals can dissolve and precipitate changing the microscopic structure of the rock and, as a consequence, its permeability. At the same time, flow can influence this process advecting the reactants. The geochemical reactions of dissolution/precipitation can also influence the aperture of fractures affecting the overall permeability of reservoirs. In this work we focus on the treatment of the reaction term that can present a discontinuity that depends on the solution: we employ a discretization strategy based on event driven techniques to avoid loss of accuracy, negative concentrations and oscillations in the solution.

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O249

Dynamic multilevel multiscale projection-based embedded discrete fracture model

A dynamic multilevel multiscale method for simulations of flow in fractured porous media is proposed. Fractures are modeled according to the Projection-based Embedded Discrete Fracture Model (p-EDFM) of Tene et al. (2016). A fine-scale grid and sets of nested multilevel coarse grids of different resolutions are considered, independently, for each of the two media (matrix and fractures). At each time-step, independent multilevel grids are formed for both the fractures and the matrix on the basis of a front-tracking criterion so as to minimize the accuracy-efficiency trade-off. The fully-implicit fine-scale Jacobian is then mapped to these dynamically defined grids, by employing sequences of restriction and prolongation operators for all unknowns (both of flow and transport). In particular, finite-volume restriction operators are considered to ensure mass conservation, while multiscale prolongation operators are used for pressure. Numerical results are presented showing the accuracy of the method by comparison against fine-scale simulations.

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O250

A robust, mass conservative scheme for two-phase flow in porous media including Hoelder continuous nonlinearities

We present a mass conservative numerical scheme for two-phase flow in porous media. The model for flow consists on two fully coupled, non-linear equations: a degenerate parabolic equation and an elliptic one. The proposed numerical scheme is based on backward Euler for the temporal discretization and mixed finite element method (MFEM) for the spatial one. A priori stability and error estimates are presented to prove the convergence of the scheme. A monotone increasing, Hoelder continuous saturation is considered. The convergence of the scheme is naturally depending on the Hoelder exponent.

The non-linear systems within each time step are solved by a robust linearization method, called the L-method. This iterative method does not involve any regularization step. The convergence of the L-scheme is rigorously proved under the assumption of a Lipschitz continuous saturation. For the Hoelder continuous case, a numerical convergence is established. Numerical results are presented to sustain the theoretical findings.

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O251

Modeling flow in complex faulted media

Basin modeling is a tool used in petroleum system assessment that simulates the evolution of a sedimentary basin through geological time in order to obtain qualitative and quantitative descriptions of the fluids that fill the sedimentary rocks at present time. In structurally complex settings, accounting for faults as a key controlling factor on fluid flow through time is of primary importance. We present an approach based on an unstructured grid where slip along fault surfaces through geological time is modeled by allowing the mesh associated with one side of a fault to move relative to the mesh associated with the other side. When modeling heat and fluid flow, faults can then be considered as simple contact surfaces or as volumetric zones along which fluid flow occurs. In this talk, we will discuss the HMM (Hybrid Mixed Mimetic) Finite Volume discretization that has been developed and show results on academic and real test cases.

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O252

Modeling fractured porous media as coupled porous-medium and free-flow systems

Fractured porous media are typically modelled as two different flow systems where two porous-medium models are coupled at the fracture-matrix interface. Usually, the flow in the fracture and in the matrix is described by the same model, which is Darcy's law. When the flow rate in the fracture is large enough, the Forchheimer extension of Darcy's law is applied in the fracture, while Darcy's law is used in the matrix. Recently, for modeling fractures and open channels, a Brinkman-Darcy model was also proposed. In this presentation, we consider fractures that act as channels, where most of the fluid is stored and transported, and model fractured porous media as coupled free-flow and porous-medium systems. The fractures are treated as the free-flow region described by the Stokes equations and the solid matrix represents the porous-medium system described by Darcy's law. The model formulation including appropriate coupling conditions at the fracture-matrix interface and efficient numerical methods based on partitioned multiple-time-step schemes will be presented.

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O253

Sequential homogenization of reactive transport in polydisperse porous media

Direct numerical simulations of flow and transport in porous media are computationally prohibitive due to the disparity between the typical scale at which processes are well understood (e.g., the pore-scale) and the scale of interest (the system- or field-scale). Homogenization approaches overcome some of the difficulties of full pore-scale simulations by providing an upscaled representation of fine-scale processes. Real porous systems, e.g., rocks, pose additional challenges since they usually exhibit multimodal distributions in physical and chemical properties. Perforated domains, i.e., domains with impermeable inclusions embedded in a porous matrix, represent one such example. These hierarchical media cannot be approached by a single continuum formulation. Sequential homogenization techniques build a hierarchy of effective equations that sequentially carry the smallest scale information through the intermediate scales up to the macroscale. We show that the accuracy of multiscale methods based on sequential upscaling is strongly influenced by a combination of geometric and dynamical scale separation conditions.

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O254

Challenges of micro-meso-macro porous media

The challenge of pore2core simulations and upscaling addressed in this paper is the multi-level character of pore geometries found in many soils and rocks such as mixtures of sand and clay. The micro-CT geometries are provided as binary data, a collection of voxels assigned either to the rock (impermeable) phase, or to the void phase (fluid in the pores). A typical REV over which we compute and upscale corresponds to $O(10M-50M)$ cells, which is challenging enough. However, after closer inspection, many rock parts are also (weakly) permeable, and this feature is practically impossible to handle with the same micro-CT resolution. The realistic micro-pore matrix permeability is evaluated based on analysis of Scanning Electron Microscopy images, however, it is difficult to handle the flow simultaneously in the micropores and in the macropores. The models in literature use (i) the Stokes in macropores and Darcy in micropore domain coupled by complex interface conditions (Arbogast et al), or (ii) Brinkman flow equation [Popov et al]. In the talk we present another approach in which we systematically study the flow in the combined micro-and macro-pore domains with the same solver.

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O255

On numerical upscaling of reactive flow in porous media with application to adsorption of MCPA in geothite

We discuss upscaling of pore scale reactive flow in case of surface and volumetric reactions for geometries arising from 3D micro-CT images. Homogenization results are recalled, and a software tool, PoreChem, capable of solving cell problems defined in homogenization algorithms, is presented. Solutions of 3D pore-scale problems and respective macroscale models are compared to validate the software.

As a geophysical application we consider adsorption of 2-methyl-4-chlorophenoxyacetic acid (MCPA) in Geothite. The starting point for the study are a 3D μ CT-Image of a soil sample, containing reactive and non reactive surfaces, as well as parameters for the nonlinear reactions. Parametric studies are carried out, and local results (velocity, pressure, concentration, deposited mass) are shown together with integral characteristics (break through curves). Upscaling for this problem is discussed, as well as comparison with some measurement results.

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O256

Upscaling reactive ion transport under dominant flow conditions

We consider a pore-scale model for reactive flow and transport of potentially charged species in a thin 2D strip. Reactions leading to a non-negligible deposited layer on at the lateral boundaries of the strip lead to a free boundary value problem in which the moving interface between the fluid and the deposited (solid) layer is explicitly taken into account. Using asymptotic expansion methods, we derive an upscaled, one-dimensional model by averaging in the transversal direction. In doing so we focus on the cases, where the convective and/or electroosmotic transport dominate the diffusivetransport. The results are consistent with models known in the literature for a constant geometry and models in which either convection or electroosmotic effects dominate diffusion. Finally, numerical computations are complementing the theoretical results.

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O257

Discrete-continuum multiscale model for transport, biofilm development and solid restructuring in porous media

Soil microaggregates have sizes in the range of 20–250 microns and are considered to be the fundamental building blocks for aggregate structure in almost all soils.

Our goal is to gain insight in process mechanisms and derive new mechanistic models on the basis of new experimental techniques. Therefore we establish deterministic partial differential equation models operating on a micro and a macroscale. Thus we can take various small scale soil processes into account as, e.g., molecular diffusion, drift emerging from electric forces, general multicomponent reactions of chemical species, growth and decay of biomass, or interactions between different phases. At the pore scale, the local discontinuous Galerkin method is used to solve differential equations. Likewise, mechanisms tightening together solid or bio cells are considered. This is combined with a cellular automaton method capturing structural changes of the underlying computational domain stemming from biomass development and solid restructuring.

Findings from standard homogenization theory are applied to determine the medium's characteristic time- and space-dependent properties.

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O258

A stochastic approach on aggregate development based on diffusion-limited aggregation

Soil functions are intrinsically related to the amount and structure of soil aggregates, which are stable associations of minerals and soil organic matter with an internal pore structure. However, the physical mechanisms and rates of initial aggregate development are poorly understood by now. We present a stochastic approach to describe aggregate formation from aggregate forming materials. It is based on diffusion-limited aggregation, which we combined with the DLVO theory to describe interaction energies between particles. Furthermore, basic particle shape classes were used to resemble the general shape of mineral particles. In this way, our approach provides a simple method to produce complex structural features with a minimal number of parameters. We systematically tested the influence of particle density, shape and interaction energies. First results revealed the strong impact of interaction energies on the porosity and pore connectivity of formed model aggregates.

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O259

Accurate and efficient predictions of first passage times in sparse discrete fracture networks using graph-based reductions

We present a graph-based methodology to reduce the computational cost of obtaining first passage times through sparse fracture networks. We derive graph representations of generic three-dimensional discrete fracture networks (DFN) using the DFN topology and flow boundary conditions. Subgraphs corresponding to the k shortest loopless paths between the inflow to outflow boundaries are identified and transport on their equivalent subnetworks is compared to transport through the full network. The number of paths included the subgraphs is based on the scaling behavior of the number of edges in the graph with the number of shortest paths. First passage times through the subnetworks are in good agreement with those obtained in the full network, both for individual realizations and in distribution. Accurate estimates of first passage times are obtained with an order of magnitude reduction of CPU time and mesh size using the proposed method.

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O260

Anomalous transport in disordered fracture networks: evolution of the lagrangian velocity distribution and CTRW model for arbitrary injection modes

We investigate tracer transport on random discrete fracture networks that are characterized by the statistics of the fracture geometry and hydraulic conductivity. While it is well known that tracer transport through fractured media can be anomalous and particle injection modes can have major impact on dispersion, the incorporation of injection modes into effective transport modeling has remained to be an open issue. The fundamental reason behind this challenge is that the Lagrangian velocity distribution experienced by tracer particles evolves with time from its initial distribution which is dictated by the injection mode to a stationary velocity distribution. We develop an effective stochastic model that incorporates the initial velocity distribution and quantifies the interplay between Lagrangian velocity distribution and velocity correlation. We demonstrate that the proposed model can successfully predict anomalous transport through discrete fracture networks with different levels of heterogeneity and arbitrary tracer injection modes.

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O261

The mechanisms of anomalous transport in heterogeneous media: From medium structure to stochastic particle motion

Numerical and experimental data for particle motion in heterogeneous porous and fractured media show intermittent patterns in Lagrangian velocities and accelerations, which manifest in long time intervals of low and short durations of high velocities. This phenomenon can be related to the spatial persistence of particle velocities on characteristic heterogeneity length scales. In order to extract the stochastic dynamics of particle motion, we focus on the analysis of Lagrangian velocities sampled equidistantly along trajectories. This method removes the intermittency observed under isochrone sampling. The space-Lagrangian velocity series can be quantified by a Markov process that is continuous in distance along streamline. It is fully parameterized in terms of the flux-weighted Eulerian velocity PDF and the characteristic pore-length. The resulting stochastic particle motion describes a time domain or continuous time random walk. This approach provides a framework for the characterization and upscaling of particle transport and dispersion from the pore to the Darcy scale and Darcy to regional scale based on the medium geometry and Eulerian flow attributes.

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O262

An integrated mathematical-geological workflow for fractured geothermal system in metamorphic rocks

The presence of a well connected network of fracture is of paramount importance in the exploitation of geothermal energy in deep reservoirs. Fractures may behave as open channels dramatically increasing the efficiency of the system. Moreover, fractures boost the heat exchange between the rock matrix and the fluid injected. The development of accurate mathematical models and robust numerical schemes are thus a key ingredient to successfully exploit at best geothermal system. In this work we consider a hierarchy of models, for fluid and heat flow, to employ a discrete fracture matrix model, including matrix, fracture planes, and intersections. Fractures may impose constraints to the gridding, resulting in high number of cells. We consider a coarsening based on ideas from the algebraic multigrid literature, obtaining cells of arbitrary shapes. On this grid, we discretize the equations using the mixed virtual element method, which is ideally suited to handle the grids produced.

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O263

The Douglas School of porous media

Modern numerical analysis and scientific computing developed quickly and on many fronts beginning early 1950's. It was characterized by the synergy of the electronic computer, classical and modern mathematical analysis, and the need to solve large and complex problems in applications. From this beginning, Jim Douglas was a major contributor to the development of numerical methods for differential and integral equations, methods of approximation of solutions, and the impact of these developments on science and technology, especially to those involving the flow of fluids through porous media. His legacy goes beyond his scientific and mathematical achievements and includes the training of generations of Ph.D students and colleagues as postdoctoral advisees or coauthors.

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O264

On the extension of the Douglas/Arbogast dual porosity models for shale gas reservoirs containing natural and hydraulic fractures

We construct a new coupled Dual Porosity/Discrete Fracture Model to describe single phase flow in a shale gas reservoir including networks of hydraulic and natural fractures. Flow in the shale matrix, including the dense network of natural fractures, is captured by the microstructural models of dual porosity type developed by Douglas and Arbogast. In addition to flow, the adsorption isotherms of the gas in the kerogen are rigorously constructed within the framework of the Density Functional Theory based on the Thermodynamics of Confined Fluids. In addition, reduced dimension models are applied to describe the hydrodynamics in the discrete network of hydraulic fractures. Application of these techniques gives to a coupled system on nonlinear parabolic equations posed in multiple domains occupied by the different geological objects. Numerical simulations of a well test are presented to validate the proposed multiscale model.

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O265

Elliptic equations in heterogeneous media with highly anisotropic fibres

The heterogeneous media considered consist of a periodic set of highly anisotropic fibres, included in a connected matrix with high conductivity. The conductivity in the anisotropic fibres is high in the longitudinal direction and low in the transverse directions. The diffusion coefficients of the elliptic equations considered depend on the conductivity.

The problem has applications in oil recovering industry, transport in superconducting multifilamentary composites, the stress in composite materials, and so on. One of the examples is "immiscible displacement in vertically fractured reservoirs" by Douglas, Arbogast, Paes-Leme, Hensley, Nunes in 1993. By the analysis of the transmission problems as well as the

three-step compactness argument, it is shown that the H^2 -order and the gradient L^p norms of the elliptic solutions in the connected matrix are bounded uniformly in the ratios of the conductivity in the media. But, in the anisotropic fibres, the two norms may not be bounded uniformly in the ratios of the conductivity. Also the elliptic solutions in the anisotropic fibres are always smoother along the fibres than in the transverse directions.

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O266

Two modes of locking in poroelasticity – causes and remedies

In this talk, I will consider two modes of locking phenomena in poroelasticity: Poisson locking and pressure oscillations. I will first present the result of the regularity study for the solution of the Biot model to gain some insight into the cause of Poisson locking and show that the displacement gets into a divergence-free state as the Lamé constant $\lambda \rightarrow \infty$. I will also examine the cause of pressure oscillations when a three-field mixed finite element method is used. Based on the results of my study on the causes of the two modes of locking, I will propose a new family of mixed finite elements that are free of both pressure oscillations and Poisson locking. Some numerical results will be presented to validate the theoretical results.

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O267

Non-hydrostatic projection method for dispersive wave modeling with discontinuous Galerkin methods

The shallow water equations are a good first approximation to describe large-scale wave phenomena such as tsunamis and storm surges. To accurately model also smaller wavelengths, an additional non-hydrostatic pressure component has to be considered. Our approach to model these dispersive waves is the depth-averaged non-hydrostatic extension for shallow water equations, where we consider different approximations to the vertical profiles for the non-hydrostatic pressure. For the first time, a Runge-Kutta discontinuous Galerkin method is used to discretize the dispersive equation set. The numerical scheme is based on a projection approach. In each timestep, an explicit predictor step solves the hydrostatic shallow water equations. A correction step follows comprising the solution of a first order elliptic system for the non-hydrostatic pressure. This system is discretized using a discontinuous Galerkin method as well. Numerical tests validate our model concerning accurate representations of analytical solutions and experiments. We discuss the impact of the vertical profile of the non-hydrostatic pressure on our numerical results.

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O268

High-resolution baroclinic modeling using discontinuous Galerkin method

We apply the discontinuous Galerkin method to the three-dimensional hydrostatic equations of coastal ocean circulation. A number of applications that require high spatial resolution in barotropic and baroclinic modes are presented including wetting/drying and dynamically varying vertical mesh resolution.

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O269

Soret and dufour effects on thermohaline convection in rotating fluids

Using linear and nonlinear stability theory, the effects of Soret and Dufour parameters are investigated on thermohaline convection in a horizontal layer of rotating fluids, specifically the ocean. Thermohaline circulation is important in mixing processes and contributes to heat and mass transports and hence the earth's climate. A general conception is that due to the smallness of the Soret and Dufour parameters their effect is negligible. However, it is shown here that for stationary convection, the Soret parameter, salinity and rotation stabilise the system, whereas temperature destabilises, and Dufour parameter has minimal effect. For oscillatory convection, the analysis is difficult as it shows that the Rayleigh number depends on six parameters, and we discuss the effects of each of these parameters herein. We demonstrate the interplay between these parameters and their effects on oscillatory convection in a graphical manner. We believe that these results have not been elucidated in this way before for large-scale fluids. Furthermore, we investigate weakly nonlinear stability and the effect of cross diffusive terms on heat and mass transports. We show the existence of new solution bifurcations not previously identified in literature.

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O270

Simulating mesoscale eddies on unstructured meshes

Mesoscale eddies are an important ingredient of ocean dynamics.

Resolving them in the context of global ocean simulations is still a challenge since the internal Rossby radius decreases with latitude and can be as small as several km. Ocean circulation models formulated on unstructured meshes provide a possibility to resolve eddy dynamics locally. However questions on how to select

the resolution, and how does the mesh variability affect the eddy dynamics are still open. We discuss them showing that (i) the observed variability and the information on the behavior of the Rossby radius can be one of the criteria helping in mesh design, but that (ii) the proximity of coarse and fine domains may imply that eddies are damped

over a portion of fine mesh. The implication is that the size of refined patches has to be sufficiently large.

In a broader context, even locally eddy-resolving global meshes are large (1M or more surface vertices), which means massively parallel runs. Good parallel scalability of unstructured-mesh codes on large meshes ensures a very competitive throughput with respect to that of regular-mesh models, with only a moderate increase in computational resources. We provide examples based on the global simulations with FESOM.

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O271

High order compact mimetic methods

High order mimetic difference operators are currently being used to solve partial differential equations in a variety of science and engineering applications. However, the bandwidth of computing stencils increases with the order of accuracy, making high order mimetic discretizations more complex and less efficient specially for boundary conditions. An alternative is to apply high order mimetic differentiation by means of equivalent compact operators with lower bandwidth. In fact, fourth order and higher mimetic operators can be reformulated in terms of the second order counterparts.

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O272

Applications of mimetic methods to geophysical imaging

Geophysical imaging applications require solving very large-scale 3D simulations in order to either locate or invert for geological structures. Due to the size of the simulations involved, we are required to find compromises between accuracy and compute time. We will present some of our recent applications related to migration and full waveform inversion for both acoustic and elastic approximations in the seismic case. We will also show the impact of incorporating mimetic approaches to physical boundaries for the aforementioned applications.

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O273

An intragranular microfracture model for geologic sequestration of CO₂

A model for simulating microfracture evolution in reservoirs used for geologic sequestration of CO₂ is presented. The model is coupled to a reactive transport simulator that models the solid mineral composition as a collection of spherical grains. Seed fractures are randomly assigned to these spherical grains in each volume cell of a finite volume domain modeling a brine saturated reservoir with a shale caprock layer. These seed

fractures are allowed to propagate according to the Griffith fracture criterion. Stress intensities induced by CO₂ injection are determined via a poroelastic finite element model. The discrete microfracture data generated by the model is coupled to geophysical and geochemical models. For geophysical properties, we utilize Ogas permeability tensor to upscale the incremental effects of microfractures on the reservoir and caprock permeability. The surface areas of modeled microfractures increment the reactive surface area of minerals in the geochemical model, altering the rate of dissolution and precipitation of minerals on the grain surfaces. Results of a CO₂ injection simulation are presented.

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O274

Regularization schemes in the CSEM inversion problem

The inversion of CSEM data is posed as a nonlinear optimization problem of a misfit functional. In particular, it consists in finding the electromagnetic model, i.e. the subsurface conductivity, that minimizes a weighted distance between collected data and numerical electromagnetic fields at the receiver positions. However, in order to stabilize the ill-posed/overdetermined minimization process, the misfit functional in CSEM problems also requires of regularization, penalizing large differences between inverted models and an initial reference model. We explain the mathematical formulation of the CSEM inversion problem and compare different regularization approaches and their effect in describing a synthetic geologic target.

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O275

Quantification of decision uncertainties

Decision analyses related to complex environmental management problems frequently fail because the occurrence of unanticipated adverse events occurring. This is driven by many factors including that (1) the applied models are typically simpler than reality and do not account for all the important governing processes, (2) probability distributions are assigned to critical performance parameters even though some of these parameters might be unknown or not be very well constrained. Recently, we have developed a novel decision analysis methodology and a computational tool based on Bayesian Information-Gap Decision Theory (BIG-DT) that are designed to mitigate the shortcomings of the traditional probabilistic decision analyses. We demonstrate BIG-DT to a representative synthetic groundwater remediation scenario where different options for hydraulic containment and pump & treat are being considered. BIG-DT is implemented in MADS (Model Analyses & Decision Support) framework (<http://mads.lanl.gov> and <http://madsjulia.github.io/Mads.jl>).

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O276

Fast and scalable bathymetry inversion in riverine and near-shore environments

Reliable high-resolution prediction of riverine and nearshore hydrodynamics requires detailed characterization of bathymetry. While in situ measurements are generally straightforward, maintaining up-to-date bathymetric surveys remains impractical or impossible in many areas. As a result, there is increasing interest in remote sensing techniques for estimating bathymetry. Here, we present low-rank approximation-based inverse modeling approaches, Compressed State Kalman Filter for sequential data assimilation and Principal Component Geostatistical Approach for batch data inversion. We show the efficiency and accuracy of the proposed methods compared to Ensemble-based methods.

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O277

Goal-oriented adaptive sampling for groundwater problems

When performing uncertainty quantification studies of groundwater problems, sampling strategies have a large effect on computational cost. We prove that a sample based, non-intrusive, computational algorithm produces exact solutions to the stochastic inverse problem using a certain class of surrogate response surfaces. We use adjoint-based techniques to estimate and correct for numerical error in the surrogate while simultaneously increasing the local order of the surrogate

response surface. The use of the resulting enhanced surrogates are two-fold where we observe an increase in accuracy and decrease in computational complexity in computation of probabilities of specified events. The methodology can also be utilized in adaptive error control.

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O278

Do we need to include short length scale variability in reservoir models?

Reservoir modeling workflows typically produce models in which rock properties such as porosity and permeability are represented on simple Cartesian or cornerpoint grids. The geostatistical methods used to populate the grid blocks with rock property values yield models in which every grid block contains a different value from its neighbour. Yet the size of the grid blocks is not related to the actual length scales over which the rock properties vary; consequently, the variability seen in these models is an artefact of the modeling process and not representative of the modelled rocks.

A simple numerical algorithm is developed that captures key geometric heterogeneities with an associated averaged petrophysical property. These rock property domains, which now have a longer correlation length, are also internally homogeneous. A quantitative assessment on both synthetic and real models showed that eliminating short correlation length variability had a very limited impact on flow. These results lend weight to the idea of surface-based models i.e. geologically constrained domains with uniform petrophysical properties.

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O279

Characterization of modern river deltas using remote sensing data

Many researchers have over the past decades argued for using more prior geological information in geophysical subsurface modeling. But traditional geostatistical simulation methods do not in general incorporate easily interpretable prior distributions. Satellite imagery and other remote sensing data represent abundant sources of information for this purpose. In a deltaic setting, quantification of properties through graph theory has recently been revived by Tejedor et al. (2015). A workflow is proposed to extract channel graph structure, width and sinuosity distributions from a set of 110 modern deltas

from satellite imagery with methods from signal processing and machine learning. Although modern depositional environments may not necessarily be representative reservoir analogues, the aggregated results show that traditional empirical classification methods, such as the diagrams by Galloway (1975) and Orton & Reading (1993), may place disproportionate attention on the extreme cases. For subsurface simulation, formulating a representative prior distribution of the parameters of interest may yield more realistic realizations.

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O280

Assimilation of satellite humidity information within the ICON EnVar system at the DWD

Polar orbiting satellites provide valuable insight into the earth's atmospheric humidity distribution that most prominently influences atmospheric motion and hence weather. At the German Meteorological Service (DWD) we are currently in the process to include such remote sensing information into the assimilation system for the global numerical weather prediction. In my talk, I will describe our global model ICON with its hybrid ensemble variational data assimilation (EnVAR) that combines a classical 3DVar assimilation technique with dynamical information on the current atmospheric state extracted from an Ensemble Kalman Filter. Thereon, I will present the steps taken towards the operational assimilation of humidity information of microwave imagers and sounders at the DWD.

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O281

Hydrological data assimilation using the Particle Batch Smoother

Two case studies will be used to demonstrate the advantages of data assimilation using the Particle Batch Smoother (PBS) in terrestrial hydrosystems. The PBS is an extension of the Particle Filter (PF) in which the states and/or parameters in a time window are updated using all observations in that window. First, the PBS was used to assimilate series of in-situ temperature observations from Passive Distributed Temperature Sensing into Hydrus-1D. In addition to soil moisture and temperature profiles, this approach yields reliable estimates of thermal and hydraulic properties at high resolution (1m) over long transects (km).

Second, a series of Land Surface Temperature (LST) and soil moisture observations were assimilated to estimate the neutral bulk heat transfer coefficient and evaporative fraction (EF). Resultant flux estimates improved at daily and half-hourly timescales. Soil moisture observations proved particularly useful when the surface heat flux partitioning was energy-limited or when LST observations were sparse.

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O282

Effects of subsurface conceptualization on the assimilation of soil moisture data – An example from the Rur catchment

In this study, data assimilation experiments are performed with a regional-scale hydrological model of the Rur catchment (Germany) using the land surface-subsurface part of the integrated terrestrial system modeling platform TerrSysMP. Within the catchment, soil moisture data from a network of cosmic-ray stations are available for assimilation. This model set-up is used to investigate the influence of subsurface conceptualization on the effectiveness of soil moisture assimilation for improving model predictions and parameter estimation. Subsurface conceptualization is compared in terms of the process description of subsurface flow (1D vertical flow with free drainage boundary condition versus 3D topographically-driven flow coupled to surface water flow) and in terms of different available subsurface parameter sets. Results show that especially the simpler representation of subsurface processes leads to a less accurate prediction and updating behaviour of the forward model which, however, could partly be compensated through a simultaneous update of subsurface parameters.

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O283

Determination of the relevant spatial scale for reservoir simulation

Under-sampling of the subsurface combined with scale differences in observations cause the estimation of geological parameters to be an ill-posed problem. As a result only a subset of theoretically possible models can truly depict the reality. In reservoir modeling, we capture complexity and heterogeneity by representing the solution space with a large number of high-resolution models, whose spread represents uncertainties in permeability. This ensemble of models is simulated forward in time to represent fluid flow and associated uncertainties in its response. Based on the sensitivity to flow response, we estimate the optimal spatial scale for simulating subsurface processes. For this, a high fidelity model is upscaled hierarchically in the ensemble members. By quantifying the coarsening

effect, we estimate at which spatial scale numerical errors and model predictability outweigh computational gain. We analyse dynamic model behaviour and static characteristics of simulated rocks as a function of mesh size. This can lead to a more efficient simulation and clarify the evolution of uncertainty across various model scales.

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O284

An analysis of variance reduction methods in stochastic homogenization

The theory of stochastic homogenization of elliptic PDEs predicts that Darcy flow in a medium whose permeability varies randomly on a small scale behaves on large scales like Darcy flow in a medium with an effective permeability. An important approach for the computation of such effective coefficients in stochastic homogenization is the so-called representative volume element (RVE) method: A sample volume of the random medium is chosen, say, a cube with side length L ; by solving the equation of the homogenization corrector on this sample volume, one may obtain an approximation for the effective coefficient. However, the resulting approximation for the effective coefficient is a random quantity, as it depends on the sample of the random medium. It turns out that the leading-order contribution to the error of this approximation is actually caused by the random fluctuations of the approximation around its expected value. To increase the efficiency of numerical methods, it is therefore desirable to reduce the variance of the approximation. We provide an improved rigorous analysis of the variance reduction approaches in stochastic homogenization introduced by Blanc, Le Bris, Legoll, and Minvielle.

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O285

Stochastic homogenization of porous visco-plastic materials based on a measure theoretic approach

In this work we deal with the stochastic homogenization of the quasi-static initial boundary value problems modeling the nonlinear behaviour of porous visco-plastic materials. In the first part of the talk I am going to present a general framework for the analytical treatment of inelastic models of the solid materials possessing microstructures which can be characterised by random measures (including random porosity). After that we shall look at the asymptotic behaviour of convex functionals associated with our models within an ergodic and stationary setting. The derivations of the homogenisation results presented in the talk will be then based on the stochastic two-scale convergence in Sobolev spaces with random measures.

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O286

Stokes flows in rough fractures

Surface roughness is a key property affecting fluid flow in bounded domains. Its effect on bulk flow is usually quantified by means of an empirical roughness coefficient which is introduced into models that treat bounding surfaces as smooth. We present a new approach, which treats the irregular geometry of rough walls as a random field, whose statistical properties (mean, standard deviation, and spatial correlation) are inferred from measurements. The subsequent stochastic mapping of a random flow domain onto its deterministic counterpart and stochastic homogenization of the transformed Stokes equations yield an expression for the roughness coefficient in terms of the wall's statistical parameters. The analytical nature of our solutions allows us to handle random surfaces with short correlations lengths, which cannot be treated by numerical stochastic simulations.

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O287

Boundary layers in periodic homogenization

In this talk, I will review recent progress on the homogenization of linear elliptic divergence form equations with oscillating coefficients and oscillating boundary data (Dirichlet, Neumann). The oscillations on the boundary lead to concentration effects near the boundary. Moreover interaction between the geometry of the domain and the microstructure leads to an intricate dynamics of the solution. The talk is based on results by Armstrong, Kuusi, Mourrat and Prange, as well as Shen and Zhuge.

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O288

Analysis and simulation of the Newman model

Electrochemical systems like batteries are typically modelled as porous media with electric potentials. The Newman equations represent a very popular model for such systems. I will present analytical and simulations results including well-posedness, spectral properties and singular limits with fast and slow forcing.

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O289

Homogenisation of thin periodic frameworks with high-contrast inclusions

We analyse a problem of two-dimensional linearised elasticity for a two-component periodic composite, where one of the components consists of disjoint soft inclusions embedded in a rigid framework. We consider the case when the contrast between the elastic properties of the framework and the inclusions, as well as the ratio between the period of the composite and the framework thickness increase as

the period of the composite becomes smaller. We show that in this regime the elastic displacement converges to the solution of a special two-scale homogenised problem, where the microscopic displacement of the framework is coupled both to the slowly-varying "macroscopic" part of the solution and to the displacement of the inclusions. We prove the convergence of the spectra of the corresponding elasticity operators to the spectrum of the homogenised operator with a band-gap structure.

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O290

An optimization approach for flow simulations in 3D poro-fractured media

Flow simulations in the subsoil are challenging for the geometrical complexity and multi-scale nature of the problem. In the Discrete Fracture Model (DFM) the issue of the different scales is faced resorting to dimensionality reduction. The three dimensional Darcy law for the flow in the porous matrix is coupled to a reduced two-dimensional Darcy law for the flow in the fractures with suitable matching conditions at the fracture-matrix and fracture-fracture interfaces. When the number of fractures is high, the imposition of such conditions might be cumbersome, especially if it requires the conformity of the meshes at the interfaces. In this work a new method is proposed, based on the weak imposition of the conditions at the interfaces, in order to relax any kind of conformity requirement on the mesh. A cost functional expressing the error in the fulfillment of the coupling conditions, is introduced and minimized constrained by the three dimensional Darcy law in the matrix and by the reduced Darcy law in the fractures. Here the mathematical basis of the method are described and numerical results are presented to show its applicability and effectiveness.

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O291

Conditioned simulation of discrete fracture networks using structural and hydraulic data from the ONKALO underground research facility, Finland

Discrete fracture network (DFN) models offer a natural framework for integrating geological, mechanical and hydraulic descriptions of fractured rock. Typically such characterisation takes the form of statistical distributions and correlations of fracture properties inferred from structural mapping, geophysics and hydraulic tests. DFN models are used to make probabilistic predictions of likely stability, flow or solute transport conditions for a range of applications in underground resource and construction projects. Where accurate predictions are required for a specific subsurface volume, models need to be conditioned to honour individual observations of fracture geometries and flows. Predicting conditions in disposal volumes for hazardous materials is one such application.

This paper demonstrates conditioning of a DFN model against

mapping data and hydraulic tests performed in the crystalline rock of the ONKALO underground research facility. The effects of conditioning using different types of data in predicting inflows in subsequent excavations and post-closure flows are quantified, and implications for model reliability are discussed.

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O292

Flow channelling in discrete fracture networks with connected and disconnected permeability fields

We present recent analysis of flow and transport in fracture networks with in-plane single-fracture heterogeneity. A coherent triad of fields with near-identical correlation length and variance are created but which greatly differ in structure, and correspond to textures with well-connected low, medium and high permeabilities. The latter texture is known to enhance flow dispersion and channelling in 2D porous media and we investigate these effects within the context of fracture networks. Through numerical modeling of multiple scales in a stochastic setting we quantify the relative impact of texture correlation length and type against network topological measures, and identify key thresholds for cases where flow dispersion is controlled by single-fracture heterogeneity versus network-scale heterogeneity. This is achieved by using a recently developed novel numerical discrete fracture network model (DFNWorks). Furthermore, we highlight enhanced flow channelling for cases where correlation structure continues across intersections in a network, and discuss application to realistic fracture networks using field data of sparsely fractured crystalline rock from the Swedish candidate repository site for spent nuclear fuel.

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O293

Modeling of fluid flow and solute mixing in 3D rough-walled rock fracture intersections

Rock fracture intersections allow different fluids and solute to mix along flow paths, which significantly affect the fluid flow and solute transport processes in fractured rocks. Traditional models (i.e. complete mixing and streamline routing models) are based on simplified 2D intersection models formed by two smooth parallel plates, which may lead to unknown uncertainties in large scale discrete fracture networks (DFN) modeling. This study presented numerical modeling results of fluid flow and solute transport in a 3D rock fracture-matrix system with an orthogonal intersection of two rough-walled rock fractures. The fluid flow in the two intersected fractures and solute transport in the fracture-matrix system were simulated by solving the Navier-Stokes equations (NSE) and transport equation. The channeling flow at 3D rough-walled fracture intersections caused by the irregular geometry conditions of the fracture surface roughness and spatially variable apertures, significantly enhance the solute mixing process at the intersection. It is important to consider the fracture surface roughness, channeling flow patterns, Pe-dependent transport behaviors and flow directionality in modeling of solute transport in natural rock fractures.

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O294

Virtual Element Methods (VEM) for Porous Media Flow

Virtual Element Method (VEM) is a novel technology for the discretization of partial differential equations responding to the interest of using general polyhedral and polygonal meshes. Indeed, making use of general polytopal meshes, it allows for more efficient and accurate meshing of domain and material data features, for more advanced and cost-efficient refinement and de-refinement techniques, in addition to other problem-dependent features such as better treatment of anisotropic elements and improved robustness with respect to mesh deformation. Finally, by avoiding the explicit integration of the shape functions that span the discrete space and introducing an innovative construction of the stiffness matrices, the VEM acquires advantages in terms of accuracy, efficiency and flexibility on complex polytopal meshes, still keeping essentially the same coding complexity as more standard Galerkin methods (on tetrahedral meshes). All these features make VEM very promising for the treatment of porous media flows.

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O295

A primal-dual finite element method with application to fluid flow in porous media

The speaker will introduce a primal-dual FEM for variational problems where the trial and test spaces are different. The essential idea behind the primal-dual method is to formulate the original problem as a constrained minimization problem. The corresponding Euler-Lagrange formulation involves the primal equation and its dual. The two equations are linked together by using properly-defined stabilizers commonly used in weak Galerkin (WG) FEMs. WG is a numerical method for PDEs where the differential operators in the weak forms are approximated by discrete generalized distributions. The fundamental difference between WG and other existing methods is the use of weak functions and weak derivatives (locally reconstructed differential operators) in the numerical schemes based on existing weak forms for the PDEs. The goal of this talk is to demonstrate the advantages of WG in numerical PDEs. In particular, the speaker will present a cell-centered finite volume/element scheme by applying the primal-dual technique to the model PDEs arising from the simulation of porous media flow. Optimal order error estimates in L2 and H1 will be discussed, and some numerical experiments will be demonstrated.

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O296

A generalized multiscale method with Robin boundary conditions for porous media flows

We are concerned with the development of a new multiscale mixed method that results from the use of the Robin interface condition within a non-overlapping domain decomposition procedure. The proposed method is given by a variational formulation and can be seen as a generalization of a so called Two-Lagrange-Multiplier Method. We compare the new procedure to existing multiscale methods through simulations in realistic, high-contrast, channelized porous formations. These simulations indicate that the scheme can produce very accurate approximations of velocity fields.

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O297

On implicit finite volume WENO schemes for convection diffusion equation

The implicit Weighted Essentially Non-Oscillatory (WENO) scheme was proposed by Gottlieb et al. in 2006. They concluded that the success or failure of the flux-implicit WENO depends heavily on the time-discretization used, as well as the numerical problem. We studied schemes with various implicit Runge-Kutta time-stepping procedures coupled with implicit WENO reconstructions. We concluded that the scheme is more stable when Runge-Kutta fluxes are computed only explicitly. For a third order scheme, we accomplish this by replacing the Runge-Kutta fluxes at the end of the time interval with the unknown solutions of the equation at the same time level. Therefore, the only computed Runge-Kutta fluxes are at known time levels and computed explicitly. A natural continuous extension (NCE) of the Runge-Kutta method is then used to achieve third order accuracy in time. In order to make the scheme more desirable, we take the Eulerian-Lagrangian approach. A larger time step is allowed, since the errors along characteristics are small. For problems with small diffusion, we show that the new schemes maintain third order accuracy for smooth tests. The schemes also maintain the essentially non-oscillatory property in the presence of shocks.

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O298

Simulating polymer flooding using implicit high-resolution methods

Polymer flooding, a widely used enhanced oil recovery (EOR) strategy, can be highly affected by numerical diffusion. We investigate fully implicit, high-resolution schemes, and show that using second-order TVD or WENO reconstructions will counteract the numerical dissipation imposed by the implicit temporal discretization. This ensures displacement profiles that are significantly sharper than what can be computed with a first order scheme. High computational cost is a key argument against using higher-order schemes in a fully implicit formulation. To meet this challenge, we demonstrate that using lagged evaluation of slope limiters and WENO weights alleviates the nonlinearity of the discrete systems and improves the computational efficiency, without having an adverse effect on the stability and accuracy of the schemes.

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O299

Mathematical and computational efficiency for the subsurface solute transport under a radial flow field

In this study, the mathematical modeling for transport either under a uniformly or radial flow field were developed. The computational study based on numerical accuracy and the computational efficiency of the inverse Laplace transform methods will be applied to solve the problem. Two commonly used numerical inverse Laplace transform methods to evaluate their performance for dealing with solute transport in the subsurface under uniform or radial flow condition. These methods included the Riemman sum and Stehfest method. This study revealed that some commonly recommended values of the free parameters in previous studies did not work very well, especially for the advection-dominated problems. Instead, we recommended new values of the free parameters for some methods after testing their robustness. For the radial dispersion, the de Riemman sum worked very well, regardless of the dispersion-dominated or advection-dominated situations. The Weeks method can be used to solve the dispersion-dominated problems, but not the advection-dominated problems. The Stehfest was recommended for the dispersion-dominated problems.

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O300

Chemical enhanced oil recovery driven models and methods for multiphase multicomponent Newtonian and non-Newtonian/viscoelastic porous media flows.

The speaker will give an overview of flow equations arising in the context of chemical enhanced oil recovery. Chemical enhanced oil recovery techniques involve multi-phase multi-component multi-physics flows of complex fluids using a variety of flooding schemes. Fluid dynamics of these complex fluids through porous media which takes into all possible effects present in such flows are poorly understood and are difficult to model accurately. We will discuss various issues involved in accurate physical modeling and discuss development of modern numerical methods to solve complex systems of PDEs in these models. Fundamental results on models of various flooding schemes used for the purpose of stabilizaion will also be presented.

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O301

Nonstandard models for two-phase flow in porous media

Equations currently used for modeling two-phase flow are basically diffusion-type equations. They prescribe stable fluid displacements and don't admit any nonmonotonic distribution of saturation or pressure, which are known to occur in many applications. These equations assume the difference between fluid pressures to be equal to capillary pressure, which is assumed to be an algebraic function of saturation. But, various studies have shown that the capillary pressure is not only a function of saturation but also of amount of fluid-fluid inter-

facial areas. Secondly, the difference between fluid pressures depends on the time rate of change of saturation. This is known as the dynamic capillarity effect. This presentation concerns mathematical modeling of fluids flow in permeable media, with emphasis on non-equilibrium effects and the role of fluid-fluid interfacial areas as a new state variable. First, governing equations of two-phase flow involving new terms are presented. We show that non-equilibrium two-phase flow models result in a set of partial differential equations containing mixed time and spatial derivatives, which result in nonmonotonic solutions. Then, the significance of these extra terms and their ability to model experimental results will be discussed.

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O302

Numerical methods for the Darcy-Brinkman two phase flow in porous media

The main purpose of this work is to propose and analyze a finite volume-nonconforming finite element scheme on general meshes to simulate the displacement of two incompressible phases in a Darcy-Brinkman flow in a porous media. The diffusion term, which can be anisotropic and heterogeneous, is discretized by piecewise linear nonconforming triangular finite elements. The mobility of each phase is decentered according to the sign of the velocity at the dual interface. We present numerical simulations to show the efficacy of the combined scheme.

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O303

Application of water-induced, self-conforming and multifunctional stimulation of gas wells – Fundamentals and case histories

The primary aim of the research project was to develop an efficient technology to control excessive water production in gas wells. As a novelty, water sensitive petroleum-based microemulsions were developed, which spontaneously form extremely high viscosity barrier under reservoir conditions contacting with water. Until now, more than 16 well treatments had been carried out in gas producers. As a results of field project the water production dropped significantly, meanwhile the gas production tripled. Surprisingly, all treated gas producers operating in gas cap over a depleted oil field, started to produce substantial amount of oil. These positive results could be attributed to effective barrier formation against water influx, bottomhole clean-up, reducing skin factor, and opening new flow paths from entrapped oil bodies existing below the gas cap. Thus, the treatment technology was qualified as a "multifunctional well stimulation" method. Recently, the extensive fundamental research is aimed at developing concepts for adequate mathematical simulation of method helping the well selection and predicting the well response.

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O304

Enhancing subsurface transport by Lagrangian chaos

Enhanced oil/gas/heat recovery from subsurface reservoirs by production fluids is a promising concept to explore unconventional gas/oil fields and geothermal resources. However, in current systems often only part of the reservoir is accessed by the fluid, yielding suboptimal performance. Recent studies demonstrated that well configurations and pumping schemes designed on the basis of chaos theory enable efficient distribution of the production fluid by Lagrangian chaos. However, this concerns isotropic reservoirs, while these often are highly anisotropic.

The present study investigates the impact of anisotropy on subsurface transport and reveals that this generally promotes Lagrangian chaos through symmetry breaking. However, symmetries persist for well configurations aligned with the anisotropy and may thus cause an intriguing order within chaos: prolonged confinement of fluid to subregions of chaotic areas. First examinations of the associated advective-diffusive scalar transport by spectral analysis reveal that, contrary to closed flows, enhanced scalar transport is in subsurface reservoirs not automatic with Lagrangian chaos.

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O305

Assessment of feasible strategies for seasonal underground hydrogen storage in a saline aquifer

Renewable energies are unsteady, which results in temporary mismatches between demand and supply. The conversion of surplus energy to hydrogen and its storage in geological formations is one option to balance this energy gap. This study evaluates the feasibility of seasonal storage of hydrogen produced from wind power in a saline aquifer in Castilla-León region (northern Spain). A 3D multiphase numerical model is used to test different extraction well configurations during three annual injection-production cycles. Results demonstrate that underground hydrogen storage in saline aquifers can be operated with reasonable recovery ratios. A maximum hydrogen recovery ratio of 78%, which represents a global energy efficiency of 30%, has been estimated. Hydrogen upconing emerges as the major risk on saline aquifer storage. However, shallow extraction wells can minimize its effects. Steeply dipping geological structures are key for an efficient hydrogen storage.

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O306

Mimetic discretization methods in geoscience and advances in geologic carbon sequestration modeling

The energy method has been shown to produce well-posed solutions to hyperbolic initial value problems. This analysis has previously been completed for the first order elastic wave equation with a perfectly matched layer (PML) and its discrete numerical approximation using summation-by-parts finite difference operators. We extend this analysis of the first order elastic PML system to a different discretization scheme. Specifically, we implement a well-posed numerical model on the 3D standard staggered grid using Castillo-Grone mimetic finite difference operators with strongly imposed boundary conditions.

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O307

Modeling multiphase buoyancy driven plume migration during geologic CO₂ injection

Geologic CO₂ sequestration requires that no more than 1% of injected CO₂ escape within 1,000 years after injection. To predict long-term retention of CO₂ in a reservoir, the interaction of geochemical and geomechanical effects of injection must be investigated through numerical simulation. The transport of gas phase CO₂ through micrometer scale fractures in porous sandstone and shale caprock is one concern that could lead to unwanted release of injected CO₂ into the atmosphere. We model the buoyancy driven flow of a two-phase system consisting of a CO₂-H₂O vapor mixture phase and an aqueous phase. This two-phase system forms a plume of CO₂ that can migrate upward due to differences in density between CO₂-rich phases and the surrounding formation fluid. We model the gas phase CO₂-H₂O composition using a Redlich and Kwong equation of state (EOS) with mixing rules, and the aqueous phase composition using the revised Helgeson Kirkham Flowers model for approximating thermodynamic properties of aqueous electrolytic solutions at high temperature and pressure. To perform this model efficiently we offload numerical integration to compute aqueous molar volume onto Tesla K80 GPU Accelerators.

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O308

Mimetic discretization methods on overlapping grids

Overture is a portable and flexible object-oriented framework for solving partial differential equations (PDEs). One of its features is the composite overlapping grid generation for solving problems that involve the simulation of complex moving geometry. Overlapping grids are a type of block structured body-fitted conforming grids that are used to resolve fine-scale features in a particular domain. One of the most prominent advantages of using these grids is the high efficiency for high-order methods. In this talk, we examine the viability of overlapping grids on mimetic operators, by solving representative PDEs problems using these operators on overlapping grids generated by Overture, while exploring different interpolation techniques on these grids (both implicitly and explicitly).

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O309

Simulation of hydrocarbon pollution removal from subsoil by bioventing

The multiphase mathematical model describes the pollutant decay and the oxygen circulation. Oxygen is treated as a compressible gas, it is injected in some points of the polluted domain and it is consumed from the biodegradation process. The model comprehends a bacteria equation and their growth is limited by the availability of oxygen and pollutant and also by a logistic limiting term. The model includes bacteria metabolic terms describing the oxygen and pollutant consumptions due to the biochemical decontamination process. The correct functionality and the effects of the terms describing the bacterial growth and the oxygen and pollutant consumptions will be shown. Moreover, some simulations of the complete model will be presented.

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O310

Large-scale multi-physics simulation of the 2004 Sumatra-Andaman earthquake

The M 9.1–9.3 Sumatra-Andaman earthquake of 26 December 2004 caused violent shaking and generated a tsunami wave that was up to 30 m high. Here we present a physically realistic dynamic rupture model of the megathrust earthquake using SeisSol, a highly parallelized software package that runs on modern supercomputers. SeisSol follows an ADER-DG scheme to solve the spontaneous dynamic earthquake rupture problem with high-order accuracy in space and time. Use of unstructured tetrahedral meshes increases computational efficiency by allowing for a high-resolution mesh where required, including along the non-planar subducting interface and the high-resolution topography, and a lower resolution mesh in

other regions. The slip interface follows the geometry of Slab 1.0 to the south and is extended to the north based on the fault surface trace and expected dip. Material properties for 4 oceanic and 3 continental layers are taken from Crust 1.0. The model returns surface displacements in good agreement with those recorded by GPS, as well as capturing the observed slip length, propagation speed, and earthquake magnitude. We resolve the influence of source dynamics on ground displacement and the potential impacts on tsunami generation.

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O311

Physics-based numerical simulations of earthquake ground motion in the Beijing area

In this work, we present a large set of earthquake scenarios with magnitude ranging between 6.5 and 7.3, occurring in the proximity of the megacity of Beijing (China). Massive numerical simulations of ground shaking for the Beijing area have been performed through a 3D numerical model that takes into account possible realizations of characteristic earthquakes breaking either the Shouyu and the Tongxian faults. Overall, about 60 earthquake scenarios have been simulated by varying the distribution of the co-seismic slip, the hypocenter location and location of the rupture area. Numerical simulations are carried out using the high-performance computer code SPEED (<http://speed.mox.polimi.it/>), while a novel approach based on Artificial Neural Networks has been employed for generating broadband ground motions for the frequency range (0–25 Hz). We also describe how the previous simulations can be introduced in a probabilistic seismic hazard analysis, enhancing on one hand the comprehension of the variability of ground motion, and preserving on the other the full spatial correlation necessary for risk modeling purposes.

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O312

Modeling rupture of Dip-Slip Faults with variable Dip and heterogeneous stress fields – Implications for corresponding tsunamis

The asymmetric geometry of dip-slip faults leads to greater slip and greater peak slip rate near the free surface than farther downdip. As rupture travels updip along a dip-slip fault and reaches the free surface, a breakout phase results (the rupture front “breaks out” of the elastic material). Properties of the breakout phase are related to the fault geometry, stress distribution, and slip distribution. Using numerical models, we compare traveling wave breakout amplitudes with a variety of fault geometries and prestress conditions to investigate implications for corresponding tsunamis.

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O313

Large scale dynamic rupture simulations of the 2004 Sumatra earthquake

The 2004 Sumatra-Andaman earthquake is an extreme event, regarding magnitude, fault size (over 1000km), and rupture duration. Due to the large dimensions, accurate dynamic rupture simulation of this event are a challenging task, which require petascale computing. In this presentation, we focus on tuning the software SeisSol, which uses an ADER-DG method on unstructured tetrahedral meshes. We present optimizations such as tuning the innermost kernels, decomposing matrices for cache efficiency, and asynchronous output. Furthermore we demonstrate that enabling local time stepping with dynamic rupture leads to a significant speedup.

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O314

A well-balanced meshless tsunami propagation and inundation model

We present a novel meshless tsunami propagation and inundation model. We discretize the nonlinear shallow-water equations using a well-balanced scheme relying on radial basis function based finite differences. The inundation model relies on radial basis function generated extrapolation from the wet points closest to the wet–dry interface into the dry region. Numerical results against standard one- and two-dimensional benchmarks are presented.

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O315

Challenges and issues of data assimilation for Richards equation-based integrated hydrological models

The ensemble Kalman filter (EnKF) has been recently the focus of much attention for physically-based integrated hydrological models, whereby multiple terrestrial compartments (e.g., surface water and groundwater) are solved simultaneously in a holistic approach.

Although the EnKF has been specifically developed to deal with nonlinear models, integrated hydrological models based on the Richards equation still represent a challenge, due to the strong nonlinearity of soil water retention curves that may significantly affect the filter performance. Thus, more studies are needed to investigate the capabilities of EnKF in cases where the unsaturated zone dynamics are dominant. Here, the model CATHY (CATchment HYdrology) is applied to reproduce the hydrological dynamics observed in an experimental hillslope, equipped with sensors to monitor the pressure head, soil moisture, and outflow responses to a series of generated rainfall events. We assimilate pressure head, soil moisture, and subsurface outflow with EnKF in a number of assimilation scenarios and discuss the challenges and issues arising from strong nonlinearities in the Richards equation.

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O316

Data assimilation in integrated groundwater – surface water hydrological modeling

Hydrological data assimilation (DA) that combines observation data with hydrological models offer great potential for improving monitoring and forecasting of water resources systems. The immensely increasing availability of hydrologically relevant data from different sensors offer new opportunities for DA in integrated groundwater - surface water hydrological modeling. A major challenge in this regard is to combine the various data sources that represent different temporal dynamics, different supporting scales, and different uncertainties. A multivariate DA system has been developed with the MIKE SHE integrated hydrological model. It supports use of different ensemble-based Kalman filter algorithms, and includes procedures for localisation, joint state-parameter estimation, and bias-aware filtering. Results are presented of application of the MIKE SHE DA system in different studies investigating assimilation of multiple data sources in catchment-scale integrated hydrological modeling.

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O317

Simplified subsurface modeling – Data assimilation and violated model assumptions

In the presented work we consider the combined groundwater and unsaturated zone, which can be modelled in a physically consistent way using 3D-models solving the Richards equation. For use in simple predictions, however, simpler approaches may be considered. The question investigated here is whether a simpler model, in which the groundwater is modelled as a horizontal 2D-model and the unsaturated zones as a few sparse 1D-columns, can be used within an EnKF to give useful predictions of groundwater levels and unsaturated fluxes. This is tested under conditions where the feedback between the two model-compartments are large (e.g. shallow groundwater table) and the simplification assumptions are clearly violated, e.g. steep hill-slope or pumping wells creating lateral fluxes in the unsaturated zone, or strong heterogeneous structures creating unaccounted flows in both compartments. Under such circumstances, direct modeling using a simplified model will not provide good results. However, a more data driven (e.g. grey box) approach, driven by the filter, may still provide an improved understanding of the system.

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O318

Generic approaches to reducing data-assimilation Monte-Carlo error for subsurface applications

Due to the computational cost of evaluating the forward model, ensemble based data assimilation (EBDA) for subsurface applications such as reservoir history matching is generally restricted to use a moderate ensemble size, E . Large Monte-Carlo (MC) errors – particularly variance errors - may therefore result from use of standard EBDA on such problems. (Distance-based) localization is often applied in an attempt to avoid artifacts induced by large MC errors, but at least for subsurface applications it is very difficult to define a generic approach along these lines. Coarse-scale EBDA with a large E was recently proposed as a generic alternative to localization, but since coarse-scale EBDA results in larger model error than standard EBDA bias errors may increase. In an attempt to reduce also bias errors, we consider a multilevel method for EBDA, where discretized reservoir models with a variety of resolutions are applied as forward models. A proper strategy for allocating computational resources, i.e., E_l for each level l , is then required. Multilevel EBDA is compared to localization and to coarse-scale EBDA on numerical examples where standard EBDA fails.

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O319

The transversal method of lines for the numerical solution of 1D Richards' equation

In the context of unsaturated zone flow modeling, here a tool for tackling the practical problem of getting hydrological data from the subsurface soil is proposed, based on the transversal method of lines for integrating 1D Richards' equation, that models water infiltration into unsaturated soils. By approximating the time derivative, the system is integrated forward in space as a system of ODEs. The approach here proposed presents some advantages: 1) the chance to replace any bottom boundary condition by knowing what happens at the top of the column; 2) this technique allows to treat the integration of Richards' equation over two layered soils by Filippov theory, a widely used approach for dealing with discontinuous differential systems, originally developed in control theory. The result of this approach is that it allows to study further phenomena related to infiltration, which are very natural concepts in Filippov theory, such as the so called sliding.

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O320

Upscaling for flow in porous media

Modeling flow in heterogeneous porous media requires incorporating data from a wide range of length scales from centimetres to hundreds of metres. This is computationally impractical and so requires some form of coarse gridding. Furthermore, our lack of detailed knowledge of the subsurface structure means that multiple stochastic reservoir models must be sampled, again leading to computational impracticalities. In this talk a number of efficient upscaling methods (like real space renormalisation, Haar wavelet transforms) will be applied to this problem and in particular recent developments in using a path integral formulation as a way to speed up Monte Carlo simulation will be introduced. It is shown that these offer practical ways forward for computing coarse scale properties from finer grids.

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O321

A robust implicit scheme for two-phase flow in porous media

Efficient numerical modeling of multi-phase flow in porous media is the key to accurate simulation of a wide range of applications in geoscience. In this work, we present a new implicit scheme for two-phase flow. The proposed scheme is based on the iterative IMPES (IMplicit Pressure Explicit Saturation) method and, therefore, preserves its efficiency in treatment of nonlinearities, while relaxing the time step condition common for explicit methods. At the same time, it does not involve costly computation of Jacobian matrix required for generic Newton's type methods.

Implicit treatment of capillary pressure term ensures stability and convergence properties of the new scheme. This choice of stabilization is supported by mathematical analysis of the method which also includes rigorous proof of convergence. Our numerical results indicate that the scheme has superior performance compared with standard IMPES and fully implicit methods on benchmark problems.

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O322

Hybrid discretization of multi-phase flow in porous media in the presence of viscous, gravitational and capillary forces

Multiphase flow in porous media in the presence of viscous, gravitational and capillary forces is described by advection diffusion equations with nonlinear parameters of relative permeability and capillary pressures. The conventional numerical method employs an upwind direction based on phase potential differences in computing the transport terms between two adjacent cells in finite volume approximation. The numerical method, however, often experiences non-convergence in a nonlinear iterative solution due to the discontinuity of transmissibilities, especially in transition between co-current and counter-current flows.

In this paper we derive the hybrid upwind scheme to include viscous, gravitational, and capillary forces. We present the hybrid-upwind formula in a generalized form that describes two- and three-phase flows. We demonstrate this new model always admits a consistent solution that is within the discretization error. This new generalized hybrid scheme yields a discretization method that improves numerical stability in reservoir simulation.

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O323

Consistent non-local flow formulation and stochastic transport

In the context of flow and transport in porous and fractured media, Darcy-based continuum models, while computationally inexpensive, are of limited use when the scale of interest is of similar size or smaller than the characteristic network connection length. Recently, we have outlined a non-local Darcy model that bridges the gap between network and Darcy-based descriptions. This formulation is able to account for non-local pressure effects that are not accounted for in a classical Darcy description. At the heart of this non-local flow formulation is a conductivity distribution or kernel that is related to the scalar permeability in the classical Darcy law.

In this paper, ensembles of flow networks are considered, of which the necessary statistical information is assumed to be known. In order to relate the conductivity distribution with the flow statistics, a Boltzmann equation for the evolution of fluid "particles" is devised. An important outcome of the analysis is an expression relating the joint probability density function of velocity and connection length in the networks with the conductivity kernel. Finally, this relationship is applied to a stationary flow example demonstrating how the conductivity kernel can be extracted from the flow statistics.

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O324

Upscaling of finite volume discretizations using graph-based spectral multigrid algorithms

We present systematic coarsening procedures for finite volume discretizations, where the coarsening is based on a graph Laplacian interpretation of the discretization. The volumes of the discretization can be identified with the vertices of a graph, and fluxes correspond to graph edges. We then consider the related graph Laplacian problem in a mixed saddle-point form. Coarse basis functions for both flux and pressure are selected as certain eigenvectors of local graph Laplacians associated with aggregated finite volumes. The resulting up-scaled discretization has provable inf-sup stability on coarse levels and good approximation properties.

We present numerical results for several benchmark problems, showing that our method can systematically deliver consistent and accurate coarse-scale models of a fine-scale problem.

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O325

Multiscale simulation of flow through fractured porous media under elastic deformation

The consideration of stress-induced rock deformation is crucial for accurate production forecasts of subsurface resources from fractured formations [Hettema et al, 2000]. Despite this, the leading reservoir simulators mainly focus on the flow and transport of the trapped fluids.

This work introduces a coupled poromechanics framework for efficient simulation of fluid production from fractured media. A conforming grid is first defined, where fractures are confined at the interfaces between matrix cells. Then, a three-stage sequentially implicit solution strategy is employed, where the finite-element displacement (FEM), multiscale finite-volume pressure (F-AMS, Tene et al, 2016) and finite-volume saturation (FV) equations are solved, at each time step.

The stability and performance of the method is investigated on test cases with various degrees of heterogeneity and matrix-fracture property contrasts. The results recommend it as an efficient and accurate model for flow through fractured porous media. Moreover, its modular algebraic structure allows straightforward implementation into existing and next-generation reservoir simulators.

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O326

Coupled thermo-mechanical-numerical framework for highly fractured formations

Accurate modeling of recovery processes in naturally fractured reservoirs requires dynamic simulation of coupled fluid flow, thermal, and deformation processes. To our knowledge, there are no general-purpose simulation frameworks that can deal with this challenge. In this study, we present a numerical framework that allows us to simulate complex thermo-elasticity deformations for fractured reservoirs based on the discrete fracture model. The formulation employs the Darcy-based approach for flow and the fracture mechanics include dealing with the so-called contact problem.

We consider a cold-water injection process and the response of the multiscale network of natural fractures. We demonstrate that complex deformation dynamics due to pressure and temperature changes can change the conductivity of the fractures by significant amounts even when the overall temperature difference between the injected and resident fluids is small. The behaviors are related to thermal contraction of the rock near the injection site and induced shear-slip of the fractures.

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O327

Mixed-dimensional approach to flows in fractured, deformable media

The mixed-dimensional representation of a fractured medium is a flexible strategy which handles a wide variety of fracture networks in a robust manner. In such a representation, the fractures and intersections are considered as lower-dimensional manifolds and the associated, governing equations are fully coupled.

In this work, a mixed-dimensional model is formed by combining Darcy flow with linear elasticity in a fractured medium. Keeping later purposes such as transport problems and fracture propagation in mind, the main interest is to obtain accurate flux fields and stress states which possess physical conservation properties. For this purpose, mixed finite elements are employed in the dimensionally hierarchical setting. The symmetry of the stress tensor is then imposed in a weak sense, which allows for the use of familiar, conforming, finite elements with relatively few degrees of freedom.

We present theoretical results including well-posedness of the variational formulation, as well as stability and convergence of the mixed finite element discretization scheme. These results are supported by numerical examples in two and three dimensions.

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O328

A general framework for DFN flow simulations with the virtual element method

The simulation of subsurface flows has become subject of great scientific interest in later years. We consider soils that can be seen as poro-fractured media, which are modeled as Discrete Fracture Networks (DFN), supposing that fractures are immersed in an impervious rock matrix. The first quantity of interest in such context is the distribution of hydraulic head, from which one

can obtain the Darcy velocity. This last vector field drives the transport of passive scalars such as the concentration of a contaminant or the distribution of the temperature induced by a geothermal heat pump. The main issues when dealing with such problems are originated by the many geometrical configurations that arise when fractures intersect randomly: in realistic DFN, intersection lengths and angles span many orders of magnitude, so

that the meshing process can become too infeasible. This talk is about some numerical methods exploiting the flexibility of primal and mixed Virtual Elements in dealing with generally shaped polygons to circumvent the cited

geometrical complexities, obtaining the distribution of hydraulic head and simulating the evolution of passive scalars within the fractured medium.

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O329

Fundamental frequency of laminated composite thick spherical shells

Spherical shells are used mainly for storage of gas, petrol, liquid, chemicals, and grains. Shell applications are bodies of transportation structures such as motor vehicles, ships, and aircraft. In other words spherical shells are largely used in several engineering fields. In this paper we are going to use the third-order shear deformation thick shell theory to investigate an analytical solution of frequency characteristics for the free vibration of laminated composite thick spherical shells. The equations of motion are obtained using Hamilton's principle. The finite element technique using the well-known packages MATLAB and ANSYS to confirm the derived equations, in this way we obtain our analytical results. Also we considered the fundamental natural frequencies and the mode shapes for simply supported cross ply laminated composites (0,90), (0,90,0), (0,90,90,0) spherical shells, then we compared the results with the classical theory and the first order shear deformation theory, in this way we combine the higher accuracy and the lower calculation efforts.

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O330

Phase-Field modeling for fracture propagation in porous media

Numerical simulation of hydraulic fracturing in porous media is one of the most challenging applications in petroleum, mechanical, and environmental engineering due to heterogeneous rock properties and fracture interaction. This talk will present phase field modeling approach for fluid-filled fracture propagation in poroelastic media and its applications. Here lower-dimensional fracture surface is approximated by using the phase field function. The two-field displacement phase-field system solves fully-coupled constrained minimization problem due to the crack irreversibility. This constrained optimization problem is handled by using active set strategy. The pressure is obtained by using a diffusion equation where the phase-field variable serves as an indicator function that distinguishes between the fracture and the reservoir. Then the above system is coupled via a fixed-stress iteration. In this study, we demonstrate the capabilities and applicabilities of the approach by simulating the interaction of hydraulic fractures and pre-existing fractures, fracture height growth at a layer interface with different mechanical properties and horizontal stresses.

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O331

A macroscopic modeling of hydraulic fracturing in fully-saturated porous materials

Fracturing of porous materials is a very important subject in various branches. To give some examples, consider in the energy sector the enhanced geothermal systems (EGS), that are applied to generate geothermal electricity. Additionally, hydraulic fracture is used in petroleum engineering to extract shale gas. In this work, the numerical modeling of fracture in saturated heterogeneous materials is carried out using an extended form of the continuum Theory of Porous Media (TPM), which accounts for the crack nucleation and propagation, deformation of the solid matrix and change in the flow of the interstitial fluids. The extension towards fracture modeling succeeds using the energy-based phase-field modeling (PFM) approach. The numerical treatment leads to a strongly coupled system of differential algebraic balance equations (DAE), which demands special numerical schemes for a stable solution. Some numerical examples will be introduced to validate the model.

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O332

Iterative schemes for non-linear poromechanics

We consider a non-linear extension of Biot's model for poromechanics, wherein both the fluid flow and mechanical deformation are allowed to be non-linear. We perform a high order discretization in time and propose two iterative schemes for solving the non-linear problems appearing within each time step: a splitting algorithm extending the undrained split and fixed stress methods to non-linear problems, and a monolithic L-scheme. The convergence of both schemes is shown rigorously. We discretize in space by using MFEM for the flow and Galerkin FE for the mechanics. Illustrative numerical examples are presented to confirm the applicability of the schemes and validate the theoretical results. Furthermore, hyperelastic deformation will be considered in the numerical examples.

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O333

On some algorithms for the coupling of flow with geomechanics in a poroelastic medium

Recently, the accurate modeling of flow-structure interactions has gained more attention and importance for both petroleum and environmental engineering applications. Of particular interest is the coupling between subsurface flow and reservoir geomechanics. Different single rate and multirate iterative and explicit coupling schemes have been proposed and analyzed in the past. Extending the work of Mikelic and Wheeler, Banach contraction was established for iterative schemes, while explicit schemes were shown to be only conditionally stable. However, all previously established results are valid for spatially homogeneous poroelastic media. In this work, we try to bridge this gap, and consider the mathematical analysis of iterative coupling schemes for spatially heterogeneous poroelastic media. We will re-establish the contractivity of the single rate and multirate iterative coupling schemes in the localized case. However, heterogeneities come at the expense of imposing more restricted assumptions for the multirate iterative coupling scheme. Our mathematical analysis will be supplemented by numerical simulations, validating our derived theoretical assumptions.

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O334

An ALE approach to mechano-chemical processes in fluid-structure interactions

Mathematical modeling and simulation of fluid-structure interaction problems are in the focus of research already for a long period. However, taking into account the chemical reactions is a rather new, but for many applications highly important area. In this talk we formulate a model for fluid-structure interactions including chemical reactions. The penetration of chemical substances from the fluid phase into the solid one and their reactions lead to changes of volume and mechanical properties of the solid structure. Numerical algorithms are developed and used to simulate the dynamics of such a mechano-chemical fluid-structure interaction problem. The arbitrary Lagrangian Eulerian approach (ALE) is chosen to solve the systems numerically. As an example, a plaque formation model is derived as a specific model system for this scenario. The investigation has shown that the chosen ALE approach delivers very reliable numerical results, which in case of the plaque formation model are in good qualitative agreement with clinical observations. The mathematical and computational concepts and methods are portable to other situations of multi-physical interactions between fluid and solid phases in biomechanics and geosciences.

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O335

A fully coupled XFEM-EDFM with dual porosity simulator for the fractured reservoir

Unconventional reservoirs are often naturally and hydraulically fractured with characteristically small pores and low permeability within the matrix. The underlying fracture networks can have a wide range of length scales and complex geometries. While hydraulic fractures may be propped, natural fractures are predominantly supported by pore pressure. A timely topic in the simulation of unconventional petroleum resources is in devising models that can accurately capture the coupling between the geomechanics of the fractured media and the multiphase fluid flow and transport. The ability to resolve such coupling is paramount towards the development of a basic understanding of a number of important practical questions including the cause for a loss of productivity in wells when neighboring wells are completed.

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O336

Well-balanced central-upwind schemes

I will first briefly review the central-upwind schemes for hyperbolic systems of conservation and balance laws. Their application to the Saint-Venant system of shallow water equations is not straightforward since the designed scheme should be well-balanced and positivity preserving. The latter property can be achieved either by using a special positivity preserving reconstruction of the water surface or using the draining time step technique. In this talk, I will focus on the well-balanced property, that is, on the ability of the scheme to exactly preserve steady-state solutions. There are several types of steady states, which should be preserved depending on the problem at hand. While in some situations, preserving still-water ("lake at rest") equilibria is sufficient to achieve the desired well-balanced property, one may often need to preserve moving-water equilibria, which is a more challenging task.

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O337

Well-balanced methods for the Shallow Water equations in spherical coordinates – Application to tsunami modeling

The shallow water equations (SWE) are useful to model free surface gravity waves whose wavelength is much larger than the characteristic bottom depth. This is the case of tsunami waves: the characteristic wavelength of a tsunami may be of the order of 100km, much larger than the characteristic ocean depth.

Further, the application of SWE to large scale phenomena makes necessary to consider the curvature of the Earth. The Earth is approached by a sphere and the equations written in spherical coordinates. Thus, new source terms appear related to the deformation due to the change of variables.

Here we present a high order well-balanced method for the SWE in spherical coordinates that considers the source terms related to bottom variations and to the change of variables.

The high order finite volume solver that we present is based on a first order path-conservative scheme and high order reconstruction operator. A parallel GPU implementation has been done to speedup the simulations.

Finally, some numerical tests to check the well-balancing and high order properties of the scheme, and its ability to simulate planetary or tsunami waves over real bathymetries will be presented.

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O338

Numerical simulations for erosion processes

Erosion and sediments transport processes have a great impact on industrial structures and on water quality. Despite its limitations, the Saint-Venant--Exner system is widely used in industrial codes to model the bedload sediment transport. In practice, its numerical resolution is mostly handled by a splitting technic that allows a weak coupling between hydraulic and morphodynamic distinct softwares but may suffer from important stability issues. In recent works, many authors proposed alternative methods based on a strong coupling that cure this problem but are not so trivial to implement in an industrial context. In this talk, we then pursue two objectives. First we propose a very simple scheme based on an approximate Riemann solver, respecting the strong coupling framework, and we demonstrate its stability and accuracy through a number of numerical test cases. But, second, we reinterpret our scheme as a splitting technic and we extend the purpose to propose what should be the minimal coupling that ensures the stability of the global numerical process in industrial codes, at least when dealing with collocated finite volume method. The resulting splitting method is, up to our knowledge, the only one for which stability properties are fully demonstrated.

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O339

A class of staggered schemes for the shallow water equations

We present in this work a original way to design well-balanced numerical schemes for the shallow water equations.

The scheme is explicit in time, scalar variables are defined on a primal mesh, while the velocity is defined on a dual mesh centered around the edges of the first mesh. A classical finite volume discretization is used for the discrete convective terms. Thanks to a CFL condition, the scheme preserves the positivity of the water height. Besides important steady states are preserved by our scheme. A discrete kinetic energy balance is derived on the dual mesh, from the momentum balance equation, with positive residual terms. Likewise a discrete elastic balance is established on the primal cells. The scheme is Lax-consistent, which means that the limit of a converging sequence of discrete solutions is a weak solution of the continuous equations. Furthermore, such a limit satisfies a weak entropy inequality. In our numerical experiments, several standard tests are performed, like problems involving shocks, vacuum, discontinuous topographies or even steady states at rest. Error and convergence rate computations show good results for the staggered scheme.

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O340

Shallow water solvers and the wet-dry front

A key difficulty for discontinuous topographies is the non-conservative product of measures due to the gravitational force acting on a sloped bottom. Solutions may be non-unique, and numerical schemes are not only consistent discretizations of the shallow water equations, but they also make a decision how to model the physics. We present a refinement of the hydrostatic reconstruction method [Audusse, Bristeau, Bouchut, Klein, Perthame, SISC 2004], which improves the resolution for very shallow flows [Chen, Noelle, SINUM 2017]. Then we show experiments where both a continuous [Bollermann, Chen, Kurganov, Noelle, JSC 2013] and the present discontinuous bottom reconstructions exhibit difficulties near the wet-dry front. We discuss a new reconstruction technique which promises to solve these problems.

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O341

Challenges for enhanced solutions in large scale data assimilation

Enhanced solutions of large scale Data Assimilation (DA) simulations require mathematical models describing the physics of the application and numerical algorithms designed to solve the model on target computing architectures. As sustained computer performance is becoming increasingly dependent on how efficiently simulations run, an intensive collaborative effort between application scientists and computing scientist is a key step for providing DA solutions able to exploit the resources that will be able in the next future. Nevertheless, many approximations are still used to make the computational load of the proposed solutions lighter instead of integrating – ab initio – high performance into numerical simulations. Main focus should be on the model’s nonlinearity, solution’s sensitivity analysis and algorithm’s scalability (also in the H2020-MSCA-RISE-2015-691184-NASDAC project). We discuss why it is crucial to assess and preserve such essential requirements.

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O342

Rapid deployment of adjoint-based data assimilation for large scale problems

Sensitivity analysis is crucial to identify the most influential parameters in simulations, to describe the behavior of dynamical models, and to solve dynamic constrained optimization problems. Existing easy-to-implement approaches such as finite-difference and forward sensitivity analysis require a computational effort that increases linearly with the number of sensitivity parameters. In this work, we investigate, implement, and test a discrete adjoint approach, whose computational effort is effectively independent of the number of sensitivity parameters. The approach is highly efficient for calculating sensitivities of larger systems and is consistent with the function whose sensitivity we are seeking. Moreover, our approach includes a consistent treatment of dynamical systems with switching by deriving and implementing the adjoint jump conditions. An efficient implementation of our approach has been developed as part of the time-stepping component in PETSc. Due to the generality of the framework, many other applications, especially existing ones using PETSc for time integration, would be expected to benefit from this development with minimum user effort.

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O343

Ensemble Kalman filter on a reduced model of the North Brazil Current

Atmosphere and ocean coupled models are characterised by their high dimensionality and nonlinearity. Thus, the application of data assimilation techniques over these models is very computationally expensive. Here we utilise a Ensemble Kalman Filter (EnKF) applied on a reduced model (RS). The

study area is the North Brazil Current. Daily inputs from a 10 km resolution hindcast full space ROMS model (FM), during 9-year period are used. The procedure consists of 3 steps: dimension reduction, neural network (NN) training and data assimilation. During the first step, an Empirical Orthogonal Function (EOF) analysis is applied to FM to reduce its high dimensionality. An adequate amount of EOFs are retained. Here, the first 100 EOFs hold 90 of the variability when sea surface temperature (SST), sea surface height (SSH), and U and V current components are considered. In order to create short-range forecasts, the RM is trained using an (NN). An EnKF is then used where the ANN provides short-range forecasts from the ensembles. Observational data is obtained from GHRSSST, AVISO, and GLOBCURRENTS to assimilate and validate SST, SSH, U and V, respectively.

The EnKF in the reduced model is succesful in reducing considerably the RMSE and increasing the spatial correlations in the validation.

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O344

Developing efficient surrogates of coupled flow and geomechanical deformation models for data assimilation applications

Observations of fluid pressure and deformation may offer valuable insight into processes governing the migration of fluids in the subsurface. The worth of information of these data can be unravelled with numerical methods that merge measurements into coupled flow-deformation models. This work presents an application of ensemble-based approaches for the assimilation of pressure and deformation data, in order to reduce parameter and model uncertainties. Since coupled flow-deformation models are

often computationally intensive, data assimilation is practically viable if these models are substituted by surrogates that drastically cut simulation times while preserving model fidelity. With surrogates, the overall computational cost is practically shifted from the data assimilation process to the surrogate construction. Here, a “model-driven” surrogate is proposed that leverages the mathematical structure of the coupled flow-deformation problem and rely on simplifications of the underlying physics based on superposition of effects and linear convolution. The performance of this approach is then compared to that of other “data-driven” surrogates.

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O345

Wavelet-based priors for subsurface parameter inference

A standard inverse problem is the inference of the permeability (as a function of the two- or three-dimensional domain) in a subsurface model given pointwise pressure head measurements polluted by additional measurement noise. Classical methods to solve this ill-posed problem are e.g. Tikhonov regularization or truncated singular value decomposition methods, but a Bayesian point of view is also possible: Here, the prior belief

about admissible permeability functions is coded by a prior probability distribution on an infinite function space. Then, by an application of Bayes' formula, a posterior distribution emerges which reflects the posterior belief about possible permeability functions given the observed data. A main issue is the choice of the prior, often a Gaussian measure with a fractional-Laplacian covariance operator which leads to permeability functions spanned by trigonometric functions. We argue that a wavelet-based prior can more effectively capture realistic properties of subsurface permeability, in particular sharp edges which typically arise when patches of matter with very different permeability are directly neighbored.

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O346

Novel integral equation solver for the large-scale 3D geoelectromagnetic modeling based on polynomials

Electromagnetic methods are widely used in geophysics to obtain the electrical conductivity distribution inside the Earth. However, even a forward problem i.e. calculation of the electromagnetic fields in complex geological structures with a high level of accuracy requires a large number of unknowns and is computationally challenging. The first-ever "high-order" solver for the volumetric integral equations (IE) of electrodynamics is presented. In contrast to previous IE solvers based on piecewise constant approximation of the fields inside anomaly, the novel one is based on the piece-wise polynomial representation. Utilization of Galerkin method for constructing the system of linear equations provides not only guaranteed convergence of the iterative numerical solution, but also ensures that the system matrix is well-conditioned irrespective of the number of unknowns and polynomial orders.

The numerical experiments demonstrate the possibility to decrease number of unknowns in 5–50 times depends on model with corresponding memory saving and speed up.

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O347

Advances in the numerical solution of the time-domain EM inverse problem

The numerical solution of inverse problems arising in the context of time-domain geoelectromagnetic prospecting is a computationally challenging task.

One of the key points is the accurate calculation of the Jacobian of the forward solution or at least the accurate evaluation of matrix-vector products with the Jacobian and its transposed. We address recent advances in how such Jacobians can be obtained. Since the efficiency and feasibility of these computations strongly depend on the chosen forward problem implementation, we present several implementation strategies and discuss their benefits and disadvantages. More precisely, we consider inversion schemes based on the implicit Euler method, rational Arnoldi approximations, and rational best approximations. We illustrate the performance of our algorithms on some numerical examples.

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O348

Electromagnetic modeling of geology cluttered with infrastructure and other thin conductors – a finite element method for hierarchical model parameters on volumes, faces and edges of an unstructured grid

Geophysics in urban and culturally impacted areas is a growing area of research directed specifically at the relationship between society and the natural world. Working in these areas is challenging for several reasons because of logistics, pervasive ambient noise, and the presence of anthropogenic clutter, each of which can strongly impact the data usability. In this study I present a novel finite element method for representing thin, strong electrical conductors in a geologic model in the context of direct current resistivity modeling. These conductors (pipes, sheets, cables) are discretized as material properties on the edges and facets of a tetrahedral mesh, rather than the tetrahedral volumes, which are reserved for representing bulk geology. This hierarchical model accounts for the finite conductivity of thin features and results in a modified stiffness matrix for the finite element system of equations, consisting of a sum of 1D, 2D and 3D element matrices, and is thus simple and efficient to implement in practice. With this model, the reduction in problem size is on the order of several orders of magnitude in comparison to a volume-only representation.

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O349

Efficient and accurate ways of modeling the electromagnetic response of metallic pipelines and well casings

Electromagnetic data recorded in the vicinity of large metallic objects, such as well casings or pipelines, are strongly affected by the presence of the metal. For correct interpretation, metal objects need to be considered in modeling subsurface responses. Here, we compare the capabilities of effective medium, finite-element (FE) and method-of-moments (MoM) approaches to model metal effects. We demonstrate that effective medium techniques may compute EM fields efficiently and fairly accurately if sources and receivers are located relatively far from any metal bodies. FE techniques provide accurate solutions for instruments at any distance from metal objects, and are used for reference here. Yet due to their numerical complexity, FE techniques have limited capability to model complex real-world scenarios, such as producing oil fields with many deviated well casings. Our recently developed MoM approach can handle multiple metal objects of arbitrary geometry more easily, and produces results comparable to the FE solutions. We discuss this method in some detail and present results for realistic scenarios comprising multiple well casings and pipelines.

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O350
Integral equations method for electrical tomography sounding above ground surface relief

One of the leading methods of geoelectric research, used worldwide is the Vertical Electrical Sounding method in the modification of the Electrical Impedance Tomography. The main experimental conditions that influence to the result of EIT measurement are the type of the electrodes array, distribution of the electrical conductivity in the media, and the form of the ground surface relief. One of the efficient and accurate way to calculate the influence of a shape of a ground surface relief on sounding data is the Integral Equations Method. The method is based on representation of the potential of the stationary electric field via potentials of prime layers distributed on the surface of the medium and internal contact boundaries.

We study the impact a ground surface relief to electrical tomography curves. Electromagnetic field and apparent resistivity curves are calculated based on the prime layers potential theory. A system of integral equations for the density of prime layers is derived. Results of experiments above artificial physical models with a surface relief and field experiments are discussed. Numerical experiments above a homogeneous and two layered media with a ground surface relief are presented and compared with result obtained for artificial models.

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O351
Imaging by joint inversion of electromagnetic waves and DC currents

We propose a joint inversion algorithm to solve for electrical permittivity and conductivity of a 2-dimensional model of the subsurface by using observed data from ground penetrating radar (GPR) and electrical resistivity (ER). We model the wavefield generated by the GPR and the electric field generated by the ER DC current, using our own developed computational finite difference time domain and finite volume forward models for GPR and ER respectively. ER captures low frequency variability and is sensitive to conductivity, while GPR captures high frequency variability and is sensitive to permittivity through reflectivity and velocity, and to conductivity through attenuation. Our joint inversion approach exploits this ER-GPR duality in frequency variability by allowing the GPR and ER data to work cooperatively while also honoring the physics of the problem. We show synthetic examples of our proposed joint inversion using an objective function that enables updates on permittivity and conductivity by incorporating both data (GPR and ER) in each iteration of a Newton optimization scheme, and compare with results of inversions using only either GPR or ER.

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O352
Upscaling reactive transport in porous media: Homogenisation and computational approaches in periodic and random media

Surface and bulk reactions appear in several industrial and environmental porous media applications (e.g., batteries, groundwater remediation, catalysis). When the reaction rate is sufficiently high, or in presence of non-linear reaction, the standard upscaling techniques can fail due to the appearance of a coupling between the macroscopic reaction and the transport (advection-diffusion). In this talk, we will present some theoretical results related to the upscaling of fast reactions and practical computational algorithms to overcome some of the closure problems.

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O353
Homogenization of the Stokes problem with application to particle flow

Obtaining a macroscopic equation for the motion of a fluid containing a dispersed solid phase appears to be a challenging issue of mathematical fluid mechanics with regards to several applications (such as the modeling of sprays in different contexts). Different approaches are required depending on the concentration of the solid phase. If this phase is suf-

ficiently dilute but the number of solid particles is large, one approach consists in coupling a classical fluid equation such as the incompressible Navier Stokes equations – for the leading fluid phase – with a Vlasov equation – for the dispersed solid phase. A critical issue is then to compute the terms coupling both equations because they include all the fluid/solid interactions modeling. In this talk, I shall consider the fluid viewpoint, the solid phase being described as holes in the fluid domain. On a simplified stationary problem I shall explain how computing the action of the solid phase on the fluid is related to an homogenization problem and describe results obtained recently on that problem.

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O354

A mixed stochastic–deterministic approach to particles interacting in a flow

In this talk, we present a novel approach to the solution of coupled particle population balance systems. The systems in question consist of particles transported by a fluid flow. Particle-particle interactions and particle-fluid interactions are solved with a stochastic simulation algorithm, while the continuous flow phase is computed with a finite element flow solver. This best-of-two-worlds approach enables the efficient treatment of particle-fluid systems, where the particles are described by multiple internal coordinates. A successful simulation of a flow crystallization process will be presented as a proof of concept.

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O355

Homogenization of nonlinear transmission conditions in porous media

We are concerned with the mathematical modeling and homogenization of nonlinear reaction-diffusion processes in a porous medium that consists of two components separated by an interface. One of the components is connected, and the other one is disconnected and consists of periodically distributed inclusions. At the interface, the fluxes are given by nonlinear functions of the concentrations on both sides of the interface. Thus, the concentrations may be discontinuous across the interface. For the derivation of the effective (homogenized) model, we use the method of two-scale convergence. To prove the convergence of the nonlinear terms, especially those defined on the microscopic interface, we give a new approach which involves the boundary unfolding operator and a compactness result for Banach-space-valued functions.

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O356

Trends and Challenges in Computational Modeling of Giant Hydrocarbon Reservoirs

Giant oil and gas reservoirs continue to play an important role in providing energy to the world. Nowadays, state of the art technologies are utilized to further explore and produce these reservoirs since a slight increase in the recovery amounts to discovering a mid-size reservoir somewhere else. Mathematical modeling and numerical simulation play a major role in managing and predicting the behavior of these systems using large super computers.

Today, with the aid of evolving measurement technologies vast amount data is being collected and consequently high-fidelity numerical models are constructed. However, certain computational challenges remain. These challenges include effective parallelization of the simulator algorithms, cost effective large scale sparse linear solvers, discretization, handling multi scale physics, complex well shapes, fractures, complaint software engineering with the rapidly evolving super computer architectures and effective visualization of very large data sets.

This presentation will cover examples for the giant reservoir models using billion plus elements, model calibration to historical data, challenges, current status and future trends in computational modeling in reservoir simulation.

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O357

An implicit SPH multiscale method for porous media flow

Smoothed particle hydrodynamics (SPH) has been extensively used to model high and low Reynolds number flows, free surface flows and collapse of dams, study pore-scale flow and dispersion, elasticity and for thermal problems. In different applications, it is required to have stable and accurate discretization of the elliptic operator with homogeneous and heterogeneous coefficients. In this paper, an implicit SPH multiscale method for porous media flow is presented. The proposed approach enhances the Brookshaw and Schwaiger schemes used in the SPH community for thermal, viscous, and pressure projection problems. The numerical results are illustrated by both industrial and academic numerical examples.

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O358

CVD-MPFA with full pressure support for computation of flow in fractured porous media on unstructured grids

We discuss finite-volume control-volume distributed multi-point flux approximation (CVD-MPFA), with full pressure support (FPS) [Edwards 2008, Friis 2011], coupled with discrete-fracture matrix approximations [Martin. 2004, Karimi-Fard 2004, Hoteit 2008] for simulation on unstructured grids. Flow is governed by Darcy's law together with mass conservation both in the matrix and the fractures, where large discontinuities in permeability tensors can occur. We use a cell-centred hybrid-grid method,

where fractures are modelled by lower-dimensional interfaces between matrix cells in the physical mesh but expanded to equi-dimensional cells in the computational domain. The results show that the hybrid-grid FPS method applies to general full-tensor fields and provides improved robust approximations compared to the hybrid-grid TPS method for fractured domains, for both weakly anisotropic permeability fields and very strong anisotropic full-tensor permeability fields where the TPS scheme exhibits spurious oscillations. Furthermore, we also present FPS coupled with a lower-dimensional fracture model, where fractures are strictly lower-dimensional in the physical mesh as well as in the computational domain.

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O359
Localized computation of Newton updates in the implicit time-stepping of Advection-Diffusion-Reaction approximations

A connection is developed relating the infinite- and finite-dimensional Newton updates for the solution of nonlinear ADR equations and their discrete approximations. The connection relies on consistency and stability requirements that are often satisfied in practice. Using this connection, we apply methods in approximation theory (homogenization and domain comparison) to easily compute a conservative support set for the discrete Newton update prior to solving the corresponding linear system. This results in the need to solve significantly smaller linear systems while obtaining the same iterates when using global solves.

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O360
Semi-implicit methods for advection dominated problems
 Transient mathematical models with dominated advection are present in many applications of flow and transport problems in porous media. We propose new class of semi-implicit methods for their numerical solution that are free of stability restriction on the choice of time steps. Such methods are superior to standard explicit methods for computational cases when the CFL condition is too restrictive like nonuniform or locally adapted grids or implicitly defined boundaries or interfaces. At the same time the semi-implicit methods are simpler and more accurate than analogous fully implicit methods. We present some analytical considerations and some numerical experiments and applications that support these conclusions.

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O361
A lightweight numerical model of the generation and expulsion of hydrocarbon in the source rock
 The work involves the study of the generation and primary migration of hydrocarbons inside the source rock. The problem is characterized by a strong coupling among chemical reactions (which may include biological processes), selective retention phenomena, flow of water and hydrocarbons inside the rock and variations in porosity. A numerical model to simulate these phenomena given the sedimentation history and the production chemistry is presented, as well as some results to highlight some of its features.

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O362
Salt reconstruction with full waveform inversion and a parametric level-set method

Seismic full-waveform inversion has become a popular technique for imaging the subsurface from seismic data. The reconstruction of the subsurface medium parameters becomes challenging in the presence of sharp contrasts such as salt bodies. We address the problem by splitting the subsurface model in two parts: a background velocity model and a salt body with known constant velocity but undetermined shape. The salt geometry is represented by a level-set function parametrized by radial basis functions. This leads to a non-linear optimization problem with a modest number of parameters. We improve the convergence speed by utilizing second-order updates from Gauss-Newton Hessian. Tests on the suite of idealized salt models show that the proposed method accurately determines the salt geometry in the presence of a modest amount of noise.

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O363
Using second order information for updating salt body boundaries with level sets

Full Waveform Inversion is generally used to update a continuous earth parameter like density or acoustic velocity. However, we often do not have enough frequency information to resolve features that have sharp boundaries, like salt bodies. It has been shown in previous work that level sets can provide a way to update these types of sharp boundaries. However, non-salt regions are best approximated by continuous rather than discrete updates. This presents a problem of making updates to two domains; both an implicit surface that represents the sharp boundary, as well as the continuous background velocity field. Can we find an approximation of the Hessian

for this new model space that allows us to effectively update both parameters simultaneously? In this work, we show a parametrization based on linearizing our new formulation for acoustic velocity. From this, we derive an approximation for the Gauss-Newton and Full Hessian. We show examples of applying these Hessian operators on example models. We compare the inversion results of solving for the update step against baseline approaches, and find slightly improved updating, but at a higher computational cost.

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O364

A level set method for seismic full waveform inversion in 2D
This work is targeting the estimation of shape-like objects in seismic full-waveform inversion, for example salt-bodies buried in the ground. Since such objects are assumed to have a sharp interface to the background, standard pixel- or voxel-based techniques are not optimal for their reconstruction since usually interfaces are blurred in these approaches. We propose a level set technique for the estimation of such bodies as part of a shape evolution approach. Numerical experiments in 2D are presented that demonstrate the performance of this technique in a variety of situations.

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O365

A level set ensemble Kalman filter method for history matching of production data incorporating electromagnetics

In this work we couple a novel history matching level-set enhanced ensemble Kalman filter (EnKF) algorithm from our previous work with time-lapse EM surveys using a non-linear Kaczmarz-type approach for the estimation of water saturation distributions in a 3D oil reservoir from EM data. Our main focus is on the coupling of the inverse Maxwell problem in geophysical imaging with the fluid flow estimation from production data. The water saturation distribution is inferred from low frequency cross-borehole electromagnetic induction tomography (EMIT) data using the well-known Archie equations. These internal estimates of saturations are then plugged into one step of the Ensemble Kalman filter for matching production data by modifying some reservoir parameters. Numerical results will be presented in the talk that shows that this integrated assimilation of EM inferred internal water saturation data during the EnKF inversion scheme yields in an efficient way improved results compared to history matching without integrating time-lapse EM data

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O366

Joint inversion of gravity and travelttime data using a level-set based structural parametrization

We develop a level-set-based structural parameterization for joint inversion of gravity and travelttime data, so that density contrast and seismic slowness are simultaneously recovered in the inverse problem. Because density contrast and slowness are different model parameters of the same survey domain, we assume that they are similar in structure in terms of how each property changes and where the interface is located, so that we are able to use a level-set function to parameterize the common interface shared by these two model parameters. The inversion of gravity and travelttime data is carried out by minimizing a joint datafitting. An adjoint state method is used to compute the travelttime gradient efficiently. Numerical examples are provided to demonstrate the inversion algorithm.

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O367

Fractional differential operators to detect multi-scale geophysical features

We investigate the feasibility of using fractional differential operators to detect multiscale features in the subsurface. A partial differential equation (PDE) constrained optimization problem is formulated to invert for the fractional coefficient on the temporal operator for the Helmholtz equation. A synthetic prototype demonstrates the mechanics and feasibility. Furthermore, we solve an optimization problem in which the fractional coefficient is on a spatial differential operator, requiring the implementation and solution of a pseudo-time cylinder. A numerical prototype demonstrates the use of a special preconditioner in an attempt to achieve scalable results. Our implementation leverages three dimensional, unstructured finite element, parallel discretizations with embedded optimization interfaces and sensitivity capabilities in C++.

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O368

Linearly implicit extrapolation methods for density driven flow problems

Many problems in porous media science and geophysics comprise interactions of processes, and are typically formulated as a system of coupled PDEs. In most cases, these systems are transient and non-linear. Developing efficient solvers is a delicate task, since one needs to must combine suitable schemes for (i) time integration, (ii) linearization, and (iii) (geometric and/or algebraic) multilevel solvers, finally being employed in a (iv) parallel computing environment.

In this presentation, we focus on the problem class of density-driven-flow of brine in a porous media. Previous studies compared different nonlinear solvers for this problem class. The governing equations form a system of differential algebraic equations and linearly implicit extrapolation methods are applicable. For these methods, when applied as a so called W-method, inexact approximations of the Jacobian are admissible. We investigate different approximations and classify, which are the most favourable w.r.t. multigrid performance and computational effort. We present numerical experiments, report on results, and provide examples where these methods significantly improved efficiency, thus allowing to address new sets of problems.

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O369

Strain localization in a solid-water-air system with random heterogeneity via stabilized mixed finite elements

Unsaturated soils are solid-water-air systems that include a solid skeleton, pore water, and pore air. Heterogeneities in porosity or degree of saturation are salient features of unsaturated soils. These heterogeneities may trigger localized deformation (e.g., shear banding) in such materials as demonstrated by numerical simulations via a pseudo three-phase model. In this article, we formulate a true three-phase mathematical framework implemented via stabilized lower-order mixed finite elements. With this mathematical framework, we study the evolution of pore air pressure and its role in the inception of strain localization triggered by initial heterogeneities either in porosity or suction. The numerical simulations show that pore air pressure is non-zero and non-uniform in the process of progressive failure in unsaturated soils. The heterogeneity of pore air pressure may also play a significant role in the onset of localized deformation of unsaturated soils. Therefore, a three-phase model considering the pore air phase is physically more appropriate for modeling strain localization in unsaturated soils.

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O370

Modeling multiscale behavior of hydraulic fractures via analytical and numerical approaches

Hydraulic fractures are known to feature the multiscale near-tip behavior due to the interplay of the fluid viscosity, fracture toughness, and leak-off. From mathematical perspective, the near-tip behavior is governed by the problem of a semi-infinite hydraulic fracture that propagates steadily under plane strain elastic conditions. This talk presents an approach to obtain the efficient numerical solution for the tip region problem and to construct the accurate approximate solution. The solution to this simpler problem unmasks the multiscale nature of the solution that governs both the local behavior of the fracture opening as well as the location of the fracture's free boundary. As a result, it is used in the Implicit Level Set Algorithm as a propagation condition to effectively incorporate the near-tip behavior into the numerical solution. In addition, this near-tip solution is used to develop approximations for the problems of a radial and plane strain hydraulic fractures. Since these solutions are able to provide the result virtually instantly for the considered fracture geometries, they can be used for sensitivity analysis or to tackle inverse problems.

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O371

Coupled hydromechanical numerical simulations of the production of tight reservoirs in complex discrete and deformable fracture networks

Characterization of unconventional reservoirs implies the conciliation of several scales, integrating a potentially large fracture information database. It normally results in the modeling of a large Discrete Fracture Network (DFN) that includes many fracture planes. Using a realistic example inspired from field data, we show how the construction of a fracture model using a consistent Discrete and Deformable Fracture Network (DDFN), tractable for multiphase flow reservoir simulations, can help describing a complex fracturing case. This explicit description of the fracture geometry is coupled to a non-discretized matrix refinement function accounting for matrix heterogeneities, well-adapted to the dynamic pressure behavior observed in such reservoirs. A generalized multiple interacting continua formulation (named "transient transfer influence function") is used within the matrix medium, allowing the simulation of a longer transition period, typical of many unconventional reservoirs (Ricois et al., 2016). The fluid flow numerical simulation model is coupled to a mechanical elastic model to account for the change in aperture of fractures due to the pressure drop in the fracture network during the production of stimulated wells.

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O372

A non-local integral Ehlers plastic-damage model for shales

We propose a model coupling Ehlers plasticity and isotropic damage mechanics. We implemented an integral non-local formulation of the damage driving variable to avoid pathological mesh-dependency. Furthermore, as plasticity can still localise excessively, the formulation of the integral averaging is over-non-local. The model is implemented in the FEM code OpenGeoSys-6. We performed three-point bending numerical simulations of a notched beam with random-field initialisation to account for heterogeneities in the specimen. We compared results from the numerical simulations against experimental results on Opalinus Clay samples available from literature. Results show that the model can adequately predict the quasi-brittle localised failure pattern observed in shales.

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O373

Hybrid finite-volume/finite-element simulations of fully-nonlinear/weakly dispersive wave propagation, breaking, and runup on unstructured grids

This talk presents an efficient method to numerically model fully nonlinear, weakly dispersive free surface hydrodynamics on unstructured meshes. The model is based on a hybrid approximation of a particular form of the so-called Serre-Green-Naghdi equations. The PDE system is recast as the hyperbolic shallow water equations plus an algebraic correction term obtained as the solution of a coercive elliptic grad-div type problem. The method proposed relies on a second order P1 Galerkin approximation of the elliptic problem, while the hyperbolic step is solved by means of a third or fourth order node-centered finite volume method. This approach is justified by looking at the contributions of the two different operators to the overall truncation error, and by a quantitative spectral analysis. Wave

breaking is embedded in the model by locally turning off the dispersive correction.

Thorough numerical validation on benchmarks involving wave propagation, transformation, breaking, overtopping, and runup will be shown.

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O374

Numerical simulation of shallow water flows with sediment transport and variable density

Environmental free surface shallow water flows have numerous applications in transport of debris and suspended sediment especially over a sloped bed. When such flows enter larger rivers or other types of water bodies such as lakes, significant difference between the densities of the two systems need to be accounted for in order to ensure accurate simulation results. In this study, the central upwind scheme developed by Bryson et al. (2010) is applied and extended to variable density shallow water equations following the work of Brice et al. (2010). Due to the use of the Boussinesq approximation in the formulation suggested by Brice et al. (2010), it is assumed that the density gradients are small. Therefore, the methodology used here is more efficient compared to similar works by other investigators, when the concentration of the sediment in suspension is not very high. This scheme considers the well-balanced and positivity-preserving characteristics of the dense flows. In this regard, the analytical solution is presented over a triangular grid, using a high order temporal and spatial numerical scheme which is discussed in detail.

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O375

An all-flow confluence condition for 1-dimensional river systems

Simulation of two-dimensional river system models can become very complex. We consider reducing this complexity in a region containing the confluence of a river and a tributary. In each uninterrupted stretch of river, one may reduce the model to a one-dimensional flow model without sacrificing accuracy. It is not obvious, however, how to model the confluence if one does this. We wish to mathematically connect the river and the tributary in a way that 1) Reflects the river junction geometry and bottom topography, 2) Captures sub- and supercritical flow, and 3) Does not increase the complexity of the model. We achieve these goals by defining a two-dimensional confluence region at the river junction. Numerical examples illustrate the ability of our model to handle a variety of junction geometries and flow regimes.

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O376

Dynamically adaptive data-driven simulation of extreme hydrological flows

Hydrological hazards such as storm surges and tsunamis are physically complex events that are very costly in loss of human life and economic productivity. Such disasters could be mitigated through improved emergency evacuation in real-time, and through the development of resilient infrastructure based on knowledge of how systems respond to extreme events. Data-driven computational modeling is a critical technology underpinning these efforts. Our investigation will focus on the novel combination of methodologies in forward simulation and data assimilation. The forward geophysical model will be based on adaptive mesh refinement (AMR), a process by which a computational mesh can adapt in time and space to the current state of a simulation. The forward solution will be combined with ensemble based data assimilation methods, whereby observations from an event can be assimilated to improve the veracity of the solution. The novelty in our approach is the tight two-way coupling of AMR and ensemble filtering techniques. The technology will be tested with twin experiments and using actual data from the event of Chile tsunami of February 27 2010.

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O377

Modeling shallow water flows through solid obstacles with Windows

When floodings occur in urban areas water may flow into houses and other objects through windows. In order to model such situations, we study water flows through solid obstacles with windows. In a simplest situation with just one window

we assume that the obstacle is solid and cannot be moved or deformed by the water flow and is infinitely thin. Such flows can be accurately modeled by the Saint-Venant system as long as the water level near the window does not rise up to its upper edge. However, when the water level is above the upper edge of the window, none of the existing shallow water systems is valid (to the best of our knowledge). In this talk, we will introduce a new shallow water model based on locally multilayer approximations used in the vicinity of the window and present an accurate and robust numerical method for simulating flows through obstacles with windows.

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O378

Preliminary results on seismic data assimilation in geomechanical modeling

Fault reactivation due to injection and/or production of fluids into and/or from the subsurface is affected by high uncertainty. This work develops a mathematical framework to quantify and reduce the prior modeling uncertainties by assimilation of seismic data. The fault mechanics is simulated by a Lagrangian approach used into a Finite Element (FE) numerical model. First, a global sensitivity analysis based on Sobol's indices is carried out to estimate the influence of the input on the model solution. Then, a Markov Chain Monte Carlo (MCMC) sampling technique based on the Polynomial Chaos Expansion (PCE) surrogate solution is used to update the prior information conditioned on seismic observations. The methodology is tested on a 3D synthetic test case. A good reduction of the prior uncertainty is obtained, showing that the assimilation of seismic and micro-seismic data can have a promising potential to improve the subsurface characterization.

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O379

Parameter estimation in subsurface flow using ensemble data assimilation techniques

Predictions of subsurface flow models depend extensively on accurate estimations of the parameters defining geological properties. We deal with the problem of estimating the permeability of a two-dimensional groundwater reservoir by implementing Ensemble Kalman Filter and a novel method, Ensemble Transform Particle Filter. The latter method is developed on the backbone of sequential Monte Carlo with the framework of linear transport problem and has proved to be highly beneficial for system with non-Gaussian distributions.

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O380

Multi-level ensemble data assimilation

Ensemble based data assimilation (DA) for high-dimensional geophysical problems are generally restricted to use a moderate number of ensemble members. This is due to the high inherent cost of running a complex reservoir simulator. It is well known that without modification the DA methods fails for this problem type. The DA algorithm can be modified by methods such as distance-based localization, however, for many cases, it is difficult to define the localization in a suitable manner. In a recent work, it was shown that by using a computationally less intensive proxy model the ensemble size could be increased sufficiently to avoid localization. However, utilizing any proxy model will increase the bias in the posterior estimate. Here, we investigate multi-level strategies for ensemble based DA. By discretizing the reservoir model equations on a variation of grids we generate a large family of proxy models, where the computational complexity and the numerical accuracy for each proxy model varies and depends on the grid. With fixed computational resources one must decide how to allocate resources for the multi-level strategy. The multi-level strategy is designed to find the optimal balance between the proxy models to minimize the sum of variance and bias.

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O381

Domain decomposition approaches for data assimilation in large scale models

Data Assimilation (DA) are large scale problems. This mandates to design and develop DA models to be solved by exploiting High Performance Computing environments. We discuss DA models that we are developing (also in the H2020-MSCA-RISE-2015-691184-NASDAC project) based on Domain Decomposition (DD) approaches. The main outcomes of the DD approaches are that they preserve the solution accuracy, as no approximation and no parameters must be selected a priori, and they improve the algorithm's scalability.

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O382

A computational framework for uncertainty quantification in CSEM with stochastic conductivity models

We present a computational framework for uncertainty quantification (UQ) in controlled source electromagnetic (CSEM) measurements using stochastic conductivity models. Unlike the deterministic models that can predict the model's response to a particular profile of the electrical properties, a stochastic model provides statistical information on the expectation and covariance of the measurements, derived from the adopted prior information assumptions on the conductivity parameter. Our methodology combines elements of sparse quadrature for the efficient calculation of the UQ integrals, as well as

model reduction methods for expediting the model evaluations. Our numerical results show that subject to some mild assumptions on the smoothness of the random conductivity fields, our algorithm outperforms the convergence of the conventional Monte-Carlo method. Numerical results to illustrate the method are presented from three-dimensional CSEM simulations.

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O383

Numerical approximation of single faults with rate-and-state dependent friction

We present a variational formulation and mathematically consistent numerical algorithms for the simulation of earthquake rupture with rate- and state-dependent (RSD) friction. Its main features are adaptive time-stepping, a priori mesh-adaptation, and a novel fixed point iteration for the rate and state decoupling.

Numerical simulations involve a lab-scale subduction zone and strike-slip faults. Possible extensions to fault networks involving multiple spatial scales will also be discussed.

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O384

A new discontinuous Galerkin spectral element method for elastic waves with physically motivated numerical fluxes

The discontinuous Galerkin spectral element method (DGSEM) is now an established method for computing approximate solutions of partial differential equations in many applications. Unlike continuous finite elements, in DGSEM, numerical fluxes are used to enforce inter-element conditions, and internal and external physical boundary conditions. For certain problems such as elastic wave propagation in complex media, a standard numerical flux may not be compatible with the physical boundary conditions.

We present a stable and arbitrary order accurate DGSEM for elastic waves with a physically motivated numerical flux. Our numerical flux is compatible with all well-posed, internal and external, boundary conditions. By construction our choice of penalty parameters yield an upwind scheme and a discrete energy estimate analogous to the continuous energy estimate. The spectral radius of the resulting spatial operator has an upper bound which is independent of the boundary and interface conditions, thus it is suitable for efficient explicit time integration. We present numerical experiments verifying accuracy and numerical stability.

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O385

Adaptive simulation of the tsunami resulting from the 2004 Sumatra-Andaman earthquake – dynamic rupture vs. seismic inversion source model

Simulations of historic tsunami events such as the 2004 Sumatra earthquake are usually initialized using earthquake sources resulting from inversion of seismic data. The associated tsunami event can often be well simulated, but it is unclear how the derived source model compares to the particular earthquake event.

In this study we use the results from dynamic rupture simulations. The tsunami model is based on a second-order Runge-Kutta discontinuous Galerkin (RKDG) scheme on triangular grids and features a robust wetting and drying scheme for the simulation of inundation events at the coast. Adaptive mesh refinement enables the efficient computation of large domains, while at the same time it allows for high local resolution. The results are compared to measured data and results using earthquake sources based on inversion. With the approach of using the output of actual dynamic rupture simulations, we can estimate the influence of different earthquake parameters.

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O386

Robust adaptive simulations for the 2011 Tohoku tsunami

This talk describes some recent work done in building an adaptive unstructured grid model for the simulation of tsunami propagation and inundation. We will present the main elements of the model which include an Arbitrary Lagrangian Eulerian (ALE) of the rotating shallow water equations in curvilinear coordinates accounting the effects of the planet's curvature on oceanic scales, an adaptive moving mesh method based on the solution of the Laplace-Beltrami equations in curvilinear coordinates, and a high order residual based discretization of the resulting equations, with a mass conserving mapping of the topographic data. The talk will discuss the sensitivity of the results to the mesh adaptation procedure as well as to the parametrization of the tsunami source for the 2011 tohoku event.

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O387

Hydrostatic vs non-hydrostatic NLSW tsunami modeling: some comments to the light of the numerical results

There is some controversy about the use of hydrostatic models vs. non-hydrostatic models in tsunami simulations, but this controversy is increased when the tsunamigenic source is

a landslide, either subaerial or submarine. In any case, the role of dispersive effects in shallow water models remains a subject of current investigation.

In our presentation we intend to give some clues on this question in the light of diverse numerical simulations. How runup or arrival time is affected or if dispersion is mandatory required in hazard assessment studies are some of the issues that we intended to address. Several state of the art benchmark tests will be considered and several versions of Tsunami-HySEA numerical model used for this purpose.

Physics-based Rupture and Tsunami simulation

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O388

The impact of numerical schemes on time to solution in adaptive shallow water equations

Optimizing PDE solvers for time to solution is a highly complex endeavor. Elementary parts of a solver, such as the order of representation, time stepping or the algorithm used for adaptive mesh refinement have a fundamental influence on performance. Algorithms addressing the same problem are often efficient in opposing application domains. E.g. low order methods are well suited to simulate discontinuous solutions, though they are expected take more operations for the same accuracy in the smooth case, than a high order method. The choice of algorithms is also constrained by modern hardware architectures. Methods that adapt well to these constraints, such as hidden communication or exploited SIMD instructions, contribute to a low time to solution. We attempt a comparison of time to solution utilizing the software package sam(oa)² for solving Shallow Water Equations (SWE), motivated by tsunami simulations. By using a series of common SWE benchmark cases a comparison of Finite Volume and discontinuous Galerkin methods on tree structured triangular meshes, that may include regular grid patches, will be presented. We will discuss the performance of both methods and show various hybrid implementations.

We will present results for different choices in adaptivity (block-adaptive and tree structured approaches) and time stepping (Runge Kutta and ADER-DG).

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O389

Quality assurance in scientific software frameworks and automated system testing in DUNE

Many modern publications contain results of numerical simulations. However, the code is almost never peer-reviewed. Software quality and reproducibility of results are important. Scientific software frameworks can improve software quality with many developing researchers. Continuous testing of such frameworks remains difficult.

We developed a concept for system testing for the numerical software framework DUNE, used through the modules dune-

pdelab and DuMux. The concept focuses on a fast implementation of system tests with a limited number of variations, rather than an exhaustive combinatoric approach. We present a concept for automating testing in a modular framework resulting in a continuous integration work-flow using modern tools like CTest, GitLab / GitLab-CI, Docker.

We show how the concept can be integrated into the build system becoming an integral part of the developer's work flow. Testing and in particular system testing is inevitable to assure research software quality sustainably. Continuous integration has to be tailored for a typical developer's work-flow of a specific project to minimize development and maintenance time.

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O390

Code-driven automated test environments and workflows
 Simulation software in the geosciences is getting more complex due to its increasing functionality and due to the growing amount of input and output data to process. Handling this complexity requires strict quality assurance by using automated tests and quality checks especially in the context of a distributed developer team diverse in professional backgrounds. The QA process itself as well as its required hard- and software needs to be strictly defined and should be transparent. We propose to formalise and automate the entire QA process by using domain specific languages for test infrastructure (Terraform + Ansible), test environments (Dockerfile) and continuous integration (Jenkins Pipeline). Peer-reviewed and version-controlled changes to the process are handled by GitHub pull requests and are executed by Jenkins CI with the click of a button inducing a code-driven automated test environment and workflow.

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O391

Maintaining quality assurance within software evolution: lessons learned with PFLOTRAN

Software evolution poses a major challenge to a geoscientific simulator. Keeping pace with the frequent advances in subsurface science and high performance computing technology requires continual development, in order to remain competitive. New scientific process models implemented and increasingly efficient numerical methods and programming

paradigms adopted, there is likely an arduous union to be made with some measure of legacy code. But software evolution also has a positive side. With robust software engineering and a plan for long-term maintenance, a simulator can evolve over time incorporating and leveraging these advances in the computational and domain sciences. In this positive light, what practices in software engineering and code maintenance can be employed within simulator development to maximize the positive aspects of software evolution while minimizing its negative side effects? This presentation discusses steps taken in the development of PFLOTRAN (www.pflotran.org) to better ensure sustainable software development within the context of quality assurance within an evolving software framework.

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O392

OPM – Open source software for reservoir simulation and visualization

The Open Porous Media (OPM) initiative facilitates open software development in the geosciences. The initiative provides an open community, open data, open source code and open license to enhance the collaboration, speed up the development and ensure reproducible research. This lecture focus on the current development of the reservoir simulator Flow. Flow is a three-phase black-oil simulator that are capable of handling realistic reservoir models. Flow reads and writes standard industry formats, supports fully-unstructured grids, state-of-the-art linear solvers, basic modeling capabilities and fluid and rock properties. Field case demonstrations shows results and performance comparable with industry-standard simulators. An important use case for the Flow simulator is CO₂-EOR studies. In order to model CO₂ injection in an oil reservoir the Flow simulator is enhanced with an additional equation for the CO₂ component where a Todd-Longstaff type model accounts for the mixing of the CO₂ with the hydrocarbons. The CO₂-EOR simulator is demonstrated with field case examples.

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O393

Development of an open-source, community hydrology model – discussion of best software practices

The integrated hydrology model, ParFlow solves the simplified shallow water equations implicitly coupled to Richards equation using the KINSOL nonlinear solver package from the SUNDIALS library and multigrid preconditioners from the hypre library and is developed by an international community. It is massively parallel and has been ported to a wide range of architectures. The model is coupled to the CLM 4.5 and CoLM land surface models, the COSMO and WRF mesoscale atmospheric systems and the reactive transport code CRUNCH. ParFlowE has been developed for coupled flow and energy

transport. ParFlow is available under the GNU LGPL license on Github and has well over 100 active users. The model has been extensively benchmarked, has more than 70 publications, has been applied continental US and European domains and more than a dozen watersheds worldwide. This active community development presents interesting challenges and we have implemented software standards, regression tests (more than 200 serial and parallel benchmark problems) that allow a user to check proper build and help manage development and educational materials and short courses.

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O394
Comparison of linear reconstructions for second order finite volume schemes on polyhedral grids

Polyhedral grids play an important role in subsurface modeling of flow and transport processes and the application of higher order accurate schemes is important to reduce effects of numerical diffusion. In realistic applications such higher order methods are typically not used because no straight forward extension to polyhedral or corner point grids exists. In this work we compare different approaches to construct linear reconstructions for second order Finite Volume schemes on polyhedral grids. A variety of second order Finite Volume exists and have been successfully applied to different applications on mostly structured or simplicial grids. For polyhedral

grids the absence of a reference element mapping and a possibly high number of neighboring cells make the application of higher order schemes more complicated. We present several different possibilities to construct second order schemes on polyhedral grids. The different schemes are compared in terms of accuracy, runtime, and feasibility of implementation. The implementation of the presented schemes is based on DUNE (www.dune-project.org) and OPM (www.opm-project.org).

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O395
Optimal reconstruction of constitutive relations for porous media flows

Comprehensive full-physics models for flow in porous media typically involve parameters to be reconstructed from experimental data. Special complexity is seen when the reconstructed parameters are considered as state-dependent functions, e.g. the relative permeability coefficients krp . Modern petroleum reservoir simulators still use simplified approximations of krp as single variable functions of p -phase saturation sp given in the form of tables or simple analytical expressions. This form is hardly reliable in modern engineering applications used, e.g., for enhanced oil recovery, carbon storage, modeling thermal and capillary pressure relations. Thus, the main focus of our research is on developing a novel mathematical concept for building new models where krp are approximated by multi-variable functions of fluid parameters, namely phase saturations sp and temperature T .

Reconstruction of such complicated dependencies requires advanced mathematical and optimization tools to enhance the efficiency of existing engineering procedures with a new computational framework generalized for use in various earth science applications.

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O396
Improvement of numerical approximation of coupled two-phase multicomponent flow with reactive geochemical transport in porous media

In the context of the simulator DuMuX, we have developed and implemented a parallel code coupling approach for two-phase flows and reactive transport simulation. Modeling such problem leads to a highly nonlinear coupled system of PDEs to algebraic or ordinary differential equations requiring special numerical treatment. In this talk, we will discuss a sequential approach solving firstly a two-phase flow problem and then a direct substitution approach (DSA) is employed to solve the

reactive transport problem. Both subsystems are discretized by a fully implicit cell-centred finite volume scheme and then an efficient sequential coupling has been implemented in DuMuX. The accuracy and effectiveness of the approach is demonstrated through 2D and 3D numerical simulations. Numerical results for gas migration in a nuclear waste repository and long-term fate of injected CO₂ for geological sequestration will be presented. The numerical results have demonstrated that this approach yields physically realistic flow fields in highly heterogeneous media and showed that this approach performs significantly better than the sequential iterative approach (SIA).

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O397

Application of the multirate TR-BDF2 method to the time discretization of non-linear conservation laws

In this work, we propose a multirate TR-BDF2 method to discretize in time hyperbolic non-linear conservation laws whose components have largely different characteristic time scales. Multirate methods use different time steps for each component to reduce the computational costs while keeping the total error below a desired tolerance. The study of numerical methods for the resolution of this type of non-linear hyperbolic partial differential equations has numerous applications, in particular in the study of multiphase and reactive underground flows. Applying it to some benchmark cases, we found that our multirate method is able to capture automatically the complexity of the problem, thanks to an appropriate error estimator, which allows to identify the components of the solution that need smaller time step to ensure the desired accuracy. Furthermore, an approach that allows to guarantee mass conservation has also been analyzed and tested.

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O398

A relaxed Gauss-Newton algorithm for low frequency EM data inversion with applications in geophysics

Low frequency electromagnetic (EM) induction techniques are often used for non destructive investigation of soil properties. The need for correctly representing the effect of strong conductors in the subsoil requires the adoption of nonlinear mathematical models. The strong propagation of experimental errors, due to ill-conditioning, makes it necessary to approximate the solution by suitable regularization methods. We will describe a relaxed Gauss-Newton method, regularized by means of a low rank approximation of the Jacobian of the forward model. The relaxation parameter is used to ensure convergence to a positive solution, while a regularization parameter adjusts the amount of smoothing. Both parameters

are automatically estimated. The algorithm is designed to process the quadrature as well as the in-phase component of the measured signal, and to determine the value of both the electrical conductivity and the magnetic permeability in the ground layers. Numerical experiments on synthetic and experimental data sets will be illustrated.

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O399

Large-scale 3D controlled-source EM modeling with a block low-rank multifrontal direct solver

We propose a Block Low-Rank (BLR) multifrontal direct solver to efficiently solve the linear systems arising from a 3D finite-difference discretization of the Maxwell equations. The solver uses a low-rank representation for the off-diagonal blocks of the intermediate dense matrices arising in the multifrontal method. Simulations were carried out over large-scale 3D resistivity models typical for marine controlled-source EM surveys, e.g. for the SEG SEAM model. The flop count, size of factor matrices and run time for matrix factorization using BLR representations go down to, respectively, 10%, 30% and 40% of their full rank values for our largest system with $N=20.6$ million unknowns. The BLR savings increase for larger systems, which reduces the factorization flop complexity from $O(N^2)$ for the full-rank solver to $O(Nm)$ with $m=1.4-1.6$. The BLR savings are significantly larger for deep-water environments that exclude the highly resistive air layer from the computational domain. It is shown that the BLR solver can outperform iterative solvers as an engine for 3D CSEM Gauss-Newton inversion that requires forward modeling for a few thousand right-hand sides.

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O400

Adaptive regularization in variable exponent Lebesgue spaces for microwave subsurface prospecting

Electromagnetic prospecting of buried targets involves the solution of an ill-posed inverse problem, since the dielectric properties of the targets and the (measured) scattered field are related by a nonlinear integral operator.

We solve the inverse problem of subsurface prospecting by means of an iterative regularization method developed in variable exponent Lebesgue spaces $L_p(\cdot)$. A variable exponent Lebesgue space $L_p(\cdot)$ is a direct generalization of classical Lebesgue space L_p , where now the exponent is not constant, but rather it is a function of the domain.

The formulation of the ill-posed problem in a variable exponent Lebesgue space allows us to adaptively assign different regularization parameters, related to different values of the function parameter $p(\cdot)$, on different regions of the subsurface domain. Different pointwise regularization is useful because background, low intensity, and high intensity values of the dielectric of the targets usually require different filtering (i.e., regularization) levels.

A numerical evidence of the proposal will be also discussed.

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O401

Analysis of a statistical descriptor for classification of seismic scatterers

Seismic diffractions are mainly induced by discontinuities and small structures, so diffraction imaging can extract valuable information to identify subsurface scattering features. We investigate the possibility to image and characterize diffractions using pattern recognition methods.

To this end, we look at kinematical and dynamical aspects of diffraction operators and we propose a set of statistical attributes that better distinguish diffractions from reflections. These attributes are used as descriptors for image points of a seismic section to perform automatic classification of scatterers using Support Vector Machines with a radial basis function kernel. We evaluate the method using synthetic seismic models and a GPR dataset.

Results indicate that the method can identify scatterers even in low signal to noise ratio situations. This is an important result, since diffractions amplitudes are usually of the same order of the noise. The method depends on velocity model, but it is robust to small velocity model variations.

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O402

The analysis and implementation of a vorticity-divergence-based numerical scheme for the shallow water equations

Unstructured meshes have been gaining popularity in recent years, because they are free of polar singularities, and appear better suited for petascale and eventually for exascale HPCs. New schemes are required in order to unleash the full potential of these meshes. The classical C-grid scheme, which is widely popular on structured meshes, has serious issues concerning the reconstruction of the tangential velocity component. This talk presents a new numerical scheme based on an old idea, namely the collocated vorticity-divergence formulation (so-called Z-grid), for large-scale geophysical flows on unstructured centroidal Voronoi meshes. Using the finite-volume discretization technique, the scheme conserves the mass and the absolute vorticity locally, and the potential enstrophy globally. It is also shown that, in an area-averaged sense, the scheme reproduces the Lagrangian transport property for potential vorticity, which is fundamental to the understanding of the dynamics of large-scale geophysical flows. An efficient execution of the numerical scheme is made possible through the use of an iterative scheme for the linear system, coupled with a specialized pre-conditioner and an initialization procedure based on the geostrophic balance.

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O403

A new coastal ocean modeling framework with applications in renewable energy

Increased human activity of the coastal zone has led to a growing demand for modeling tools to evaluate the engineering, economic and environmental aspects of various coastal developments, such as renewable energy generation and waste water disposal. These tools need to combine the reliable simulation of the physical processes typical of the coastal ocean with the ability to accurately represent the flow around engineering structures, often at a wide range of scales. We present a new ocean model that offers the required numerical flexibility, and in addition, the capability to incorporate these simulations in an efficient optimisation framework. We demonstrate this functionality for the purpose of modeling tidal energy projects where we simulate in an integrated sense both the large scale tidal flow and the small scale 3D flow through and around tidal turbines and show the effectiveness of the optimisation capabilities to maximise energy extraction or minimise environmental impact.

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O404

Modeling of random ocean waves in an irregular shaped harbor with variable bathymetry by using 3D boundary element method

A 3D mathematical model is presented to predict the ocean surface wave field in an irregular domain due to the diffraction

and refraction of multidirectional random incident waves. A 3D Boundary Element Method (BEM) is used to solve the Laplace equation in the irregular bounded domain (i.e. Harbor) with depth variation. Further, the Green's function is utilized to solve the Laplace equation in the irregular bounded domain. The convergence of the numerical scheme is conducted for the rectangular shaped harbor for the validation. Then, the current numerical model is applied to the realistic Paradip Port to analyze the resonance phenomenon. Six record stations have been chosen Paradip port to estimate the wave height ratio for the multidirectional random waves. Further, the surface wave field is also analyzed for the incident waves with different directions and wave frequencies. Some tactic such as additional breakwaters were implemented based the simulation results to reduce the wave oscillation. The present numerical model can be applied to any realistic harbor connected to open sea to the analysis of wave oscillation.

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O405

DG-based simulation of coupled surface subsurface flow

The simulation of coupled surface subsurface flow is a topic of high scientific and social relevance for flood protection, agriculture and weather prediction. Most existing numerical models use a kinematic wave approximation for the simulation of the surface runoff. We present an approach based on the diffusive wave approximation for surface and Richards' equation for subsurface flow. An operator splitting approach is used with a kind of Dirichlet Neumann coupling for surface and subsurface flow. Spatial discretisation of both flow equations is done with a Weighted Interior Penalty Discontinuous Galerkin scheme, while for the temporal discretisation a semi-implicit scheme is used for the surface runoff and a diagonally implicit Runge-Kutta scheme for the subsurface flow. We present first results obtained with the parallel numerical solver based on DUNE-PDELab.

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O406

A new scheme for water flow-driven stratigraphic forward modeling

Stratigraphic forward models are essential tools to understand the nature of subsoil rocks and the architecture of sedimentary basins. In these models, sediment transport is governed by a linear diffusion law at the continuous level while water flow is described through an ad hoc algorithm at the discrete level, such as MFD (Multiple Flow Direction). In this work, we propose

a new model that enables us to couple sediment transport with water flow at the continuous level. The resulting water and sediment fluxes are nonlinear and involve p-Laplacians in order to get more realistic landscape evolutions, ensuring finite speed of propagation for knickpoints. Our model also considers several diffusion coefficients in order to distinguish between marine and continental domains. To approximate the system of equations, our numerical scheme is based on the Finite Volume method. Due to the p-Laplacian, it requires an approximation of the gradient norms to be built at each interface between cells.

To illustrate the model and to show the capabilities of the numerical scheme, various configurations in several test cases are presented.

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O407

Modeling and simulation of fracture aperture

DNF (fracture-only) and DFM (fracture and rock matrix) simulation is a rapidly growing field. While more and more geometrically realistic models are being published, fracture aperture is often assumed constant or varied only set by set. This is incompatible with field observations of large aperture variations, log-normal or multi-modal distributions, and-or partial annealed fractures. This presentation explores how aperture distributions in multiple sets of intersecting fractures can be computed taking into account geometry (orientation, length versus frequency distributions, abutting relationships), mechanical properties of the fractured rock, in situ stress, and pore pressure. New aperture calculation algorithms trying to account for mechanisms like dilatation, asperity gliding, asperity crushing, and dissolution-precipitation annealing in complex fracture patterns are presented and assessed in terms of their physical realism. Results highlight the first-order control that aperture exerts on permeability, anisotropy and flow localisation. Mechanical fracture-fracture and rock fragment interactions are identified as a key challenge.

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O408

Prediction of fracture aperture in fragmented rocks

In fractured rock masses open fractures tend to act as the main pathways of fluid flow. The permeability of a rock fracture depends on its aperture. The change of aperture with

stress can cause a many-orders-of-magnitude change in the hydraulic conductivity at moderate compressive stress levels. In this study, the change of aperture in fragmented rocks is investigated using finite element analysis. A full 3D mechanical model of a simplified version of an outcrop analog is created and studied. A constant initial aperture value is applied to all fractures. Different far field stresses are applied and the change of aperture is monitored considering the block to block interaction. The fragmented rock layer is assumed to be sandwiched between softer layers. Frictional contact forces are defined at the layer boundaries as well as among contacting rock blocks. For a given in situ stress, the blocks slide and contact each other, resulting in new aperture distributions. A map of changed aperture is produced after applying the in situ stress and compared to the initial apertures. Subsequently, the permeability of the system before and after the stress application is compared.

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O409

Impact of natural fracture reactivation on gas production from shale gas plays

Shales play an important role for future energy supply and productive horizons tend to contain abundant natural fractures that are completely or partly sealed, but may get reactivated by hydraulic stimulation. To investigate the impact of hydraulic re-opening of sealed fractures on gas flow, our analysis departs from a geostatistically conditioned discrete fracture model with a horizontal well. Initial fracture aperture is calculated using a combination of geomechanical, surface-roughness and in situ stress based techniques. The fractures are partially sealed by application of a simulated annealing algorithm. Then, injection is simulated allowing sealed fractures to re-open when their tensile strength is exceeded. The post-stimulation gas flow is monitored, while an effective-stress dependent fracture aperture permits progressive fracture closure. Comparing the gas flow of the (sealed) base case with the stimulated cases, the recovery potential and the longevity of fracture reactivation are evaluated.

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O410

Flow and tracer transport in coupled fracture and porous block – code comparison and singularity study

The real-case benchmark problem is defined by geometric simplification of real hydrogeological conditions of the tunnel inflow in fractured granite and the natural tracer transport from the surface to the tunnel at Bedrichov site, Czech Republic. Its feature is explicit representation of a single fracture of fault and an equivalent continuum block. This part of presentation will be based on the author’s recently published paper (Hokr et al, *Envir.Earth.Sci.* 2016), where three numerical simulators Flow123d, OpenGeoSys, and PFLOTRAN are compared, as part of the DECOVALEX project. The effects of e.g. different numerical schemes, options for coupling of 2D and 3D domains, and of numerical dispersion will be discussed. Additionally, the problem involves a configuration close to a singular problem – the block and fracture connection is similar to a point borehole injection/pumping. We demonstrate the mesh-dependent results and show how they are related to a simplified problem analytical solution with parametrized geometry.

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O411

GeoClaw software development and testing

The GeoClaw software for modeling flow over topography with depth-averaged fluid equations was originally developed for tsunami modeling, and has also been extensively used for related applications such as storm surge and flooding due to dam breaks. It is part of the open source Clawpack suite of software that is actively developed on Github. Recent extensions include coupling GeoClaw to ForestClaw, allowing adaptive mesh refinement to scale well on supercomputers, and the D-Claw code of David George for modeling debris

flows and landslides. Our workflow for developing and testing code and testing will be briefly described. In particular we use Travis Continuous Integration to perform regression tests with each pull request on Github.

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O412

Reaktoro – an overview of its software design and algorithms for geochemical and reactive transport modeling

Modeling fluid flow in subsurface porous media involves many physical and chemical processes. In many cases, the chemical processes, i.e., the geochemical reactions among the chemical species composing the fluids and the minerals composing the rock, can play a major role in how the entire system behaves. Efficient and robust computational methods for chemical equilibrium and kinetic calculations are essential for modeling such geochemical reactions. These calculations require thermodynamic properties of the species and reactions, as well as thermodynamic models to account for the non-ideal behavior of the fluid phases (e.g., activity models such as Pitzer, Debye–Hückel for aqueous fluids, or equations of state such as Peng–Robinson for gaseous fluids). In this talk, we present an overview of how the numerical methods and thermodynamic and reaction models are implemented in Reaktoro (reaktoro.org), a unified framework written in C++/Python for modeling chemically reactive systems and processes. More specifically, we present the design and implementation techniques that allow Reaktoro to be easily extended with new thermodynamic models and to be applied to a variety of chemical systems of interest.

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O413

Dumux-Pub – enhancing the transparency of simulation results

Dumux is an open-source porous-media simulator that is mainly developed at the Department for Hydromechanics and Modeling of Hydrosystems (LH2) at the University of Stuttgart. Since 2015, the LH2 has the internal policy that every publication such as bachelor, master and doctoral theses as well as journal articles has to be accompanied by the code that was used to calculate the simulation results that are presented in the publication. This talk will present the steps undertaken to achieve this for a particular publication. Archivability and reproducibility aspects of the approach are discussed.

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O414

Multi-physical process modeling and validation for the deep geological disposal of nuclear waste in the DECOVALEX project

The safe long-term deposition of radioactive waste in deep geological repositories requires a knowledge-based assessment of potential environmental impacts of the repository and hence a reliable quantification of the coupled physical and chemical processes occurring before, during, and after emplacement. This quantification along with scenario analyses can only be performed with the necessary scientific rigor and complexity using numerical simulations. The long time scale considered as well as safety concerns raised by authorities and the public, place strong demands on validation, documentation and quality assurance of the employed methods. The international project DEvelopment of COupled models and their VALidation against EXperiments (DECOVALEX) is dedicated to code comparison and experimental validation for process understanding and confidence building. In this context, we highlight recent developments in the simulation platform OpenGeoSys. Exemplarily, we will address the modeling of THM processes in clay rock as well as of hydraulic fault reactivation along with the integration into a development workflow for code-quality assurance.

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P1

Detecting break points in the Arctic Sea Ice Decline and linked atmospheric moisture sources

Recent years have seen important reductions in Arctic sea ice, with downward trends in both the extent of sea ice extent and its concentration over the Arctic Ocean. In particular, considerable attention has been devoted to the years 2007 and 2012, which contained maxima in the loss of sea ice. Understanding the causes of this loss of sea ice is key to the analysis of how future changes in the global climate could affect the Arctic system. Understanding changes in atmospheric moisture transport have been proposed as a means of interpreting some of the most significant changes in the Arctic region (Gimeno et al, 2015 doi:10.5194/esd-6-583-2015). To this end, we applied the Lagrangian FLEXible PARTICle dispersion (FLEXPART) model to study the transport of moisture from the main sources for the Arctic, as detected by Vázquez et al. (2016, doi:10.1002/2016JD025400), towards target regions over the Arctic that are known to be suffering anomalous ice melting. We use indicator saturation methods (Castle et al, 2015, *Econometrics*, 3, 240–264.) to detect breaks in the annual series of Arctic Sea Ice extent month-by-month, together with the associated moisture sources, in the search for common patterns.

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P2

Probability distributions of summer Arctic Sea extension variability driven by the atmospheric circulation and moisture transport

Variations in the transport of moisture from extratropical to the Arctic has been proposed to have an important role on the Arctic atmospheric hydrological system [e.g., Gimeno et al., 2015] with implications for the Arctic Sea extension. Variations in moisture transport can be due to a) changes in general circulation patterns, b) increases or reductions in moisture supply from particular sources caused by changes in evaporation, or c) a combination of these two effects. Here we use monthly data of summer Arctic sea extension from the NSIDC (http://nsidc.org/data/seaice_index/archives.html) for the period 1980–2016 and frequency of both Lagrangian moisture transport patterns and circulation patterns to estimate the probability distributions of summer Arctic Sea extension variability driven by the atmospheric circulation and moisture transport. We use a cluster analysis of daily moisture transport to the Arctic from the four major summer moisture sources as identified by Vázquez et al (2016): the subtropical and southern extratropical Pacific and Atlantic Oceans, North America, and Siberia and the methodology developed by Fettweis et al. [2011] to group individual days into five circulation types.

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P3

Impact of the North Atlantic Oscillation on the synoptic processes in Europe: Continuous wavelets transform approach

The North Atlantic Oscillation (NAO) is usually considered as a dominant type of European climate variability. Much less attention is paid to an impact of the NAO on synoptic scale processes with time scales from a few days up to two weeks. The lack of knowledge can be conditioned by the high level of noise in the data with the one-day discreteness. The continuous wavelet transforms provide useful decompositions of original time series, so that wavelet-transformed data improves the ability of analyzing model by capturing useful information on various resolution levels, and the cross-wavelet transform of two time series allows revealing their common features in time-frequency space. Here, we used the wavelet analysis in order to (i) identify a total ozone response to NAO-induced weather pattern, and (ii) to investigate the role of the NAO in spatial propagation of heat wave in Eastern Europe occurred during the summer 2010. Our results allow concluding that there are local time lags for variability of the total ozone column over Europe depend on the distance from the NAO as well as spatial propagation of extreme warm temperatures over Europe during heat waves.

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P4

Assimilation of cloud-affected radiances in deep convection – a case study

The COSMO-KENDA data assimilation system was applied successfully for a number of realistic atmospheric conditions such as stratus clouds (Schomburg et al., 2015), a weather situation with weak convection (Schraff et al., 2016), or in idealized conditions with deep convection (Lange and Craig, 2014). To calculate synthetic satellite images from the simulation, we apply the radiative transfer model RTTOV (Schomburg et al., 2015). In contrast to Schomburg et al. (2015), we assimilate cloud-affected radiances and not retrieved cloud properties, such as cloud-top height. Directly assimilating the cloud-affected radiances has several advantages, e.g., we do not need to estimate a background potential temperature profile. That advantage is especially beneficial for convective clouds, where the ambient temperature is affected by the turbulence initiated by the cloud. Compared to the assimilation of conventional parameters, a larger number of (> 6000) BT values is typically assimilated every hour in the numerical domain (Harnisch et al., 2016). Our goal is to better understand the limits of the forecast skill at the convective scale by assimilating the cloud-affected radiances, e.g., in the idealized setup (Lange and Craig, 2014).

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P5
Large-eddy simulations of a wind turbine wake above a forest

Since the pioneering large-eddy simulations of Shaw and Schumann (1992), the forest stands have been treated as a porous body of horizontally uniform (leaf) area density with constant drag coefficient. This approach is sometimes called field-scale approach. Current finer scale applications and field campaigns consider the heterogeneity of the canopies at the plant-scale (Schrottle and Dörnbrack 2013). We present results from plant-scale simulations of flow through resolved tree structures originating from laser scans. Simulating the wake of one wind turbine, e.g., above a forest requires a new computational approach. For this purpose, EULAG (Prusa et al. 2008) is modified to accommodate two independent hydrodynamic solvers. The two solvers are integrated simultaneously. The turbulence structure above a forest is simulated in the first solver at the field scale and acts as inflow for the wind turbine wake flow.

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P6
Thermoconvective instabilities for the formation and tilt of the eye in a dust devil-like vortex

We show numerically that thermoconvection is behind the formation and tilt of the eye in a dust devil-like vortex. The analysis is done using nonlinear simulations. By considering a cylinder non-homogeneously heated from below we prove that an intense localized heating on the ground generates a convective stationary axisymmetric flow that begins to spiral up around a central axis when perturbation vertical vorticity is permitted and a critical vertical temperature gradient is exceeded, thus forming an axisymmetric vortex. If the intense heating on the ground is not too localized and the temperature gradient continues increasing, central downdrafts appear in the vortex and an eye is formed. We show that the axisymmetric vortex loses stability toward a new state for which the axisymmetry is broken, the axis of rotation or proper eye displaces from the center and tilts. The vortical states found are comparable to dust devils. These findings establish the relevance of thermoconvection on the formation and evolution of these atmospheric phenomena.

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P7
Moment approximations for shallow flow

Shallow flow models are used for a large number of applications including weather forecasting, open channel hydraulics and simulation-based natural hazard assessment. The apparent shallowness of the process motivates a depth-averaged formulation of reduced dimension that results in a mathematical system of (conditionally) hyperbolic type. While the shallow flow formulation is advantageous in terms of computational efficiency, it also comes at the price of losing vertical information such as the flows velocity profile. This gives rise to model error that is typically not quantified, and limits the predictive power. We propose the use of vertical moments to overcome this problem. It allows us to preserve information on the vertical flow structure while we can still make use of the simplifying and complexity reducing framework of depth-averaging. In this contribution, we describe a generic shallow flow moment system, and specify it for 1d Newtonian flow. We also describe a depth-projected, yet fully resolved reference model. Finally, we present numerical results for a hierarchy shallow flow moment models and discuss their proficiency with respect to the reference solution.

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P8
Numerical and computational strategies for the EULAG conservative dynamical core of COSMO NWP framework

Advancing the robust and efficient hydrodynamical solver for high-resolution Alpine weather prediction relies on multidisciplinary research that combines, among others, application of the efficient numerical methods, choice of software design for portability and maintainability and computationally and energy efficient implementation for the modern supercomputers. In this contribution we present recent progress towards the operationalization of EULAG conservative dynamical core for the numerical weather prediction framework of COSMO Consortium. In particular, we elaborate on computational efficiency of Fortran and the prototype C++ implementation of EULAG components using Domain Specific Embedded Language. Furthermore, we discuss the strategies for the computational realization of the eddy diffusivity in EULAG model in the context of weather modeling.

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P9

Multiscale reconstruction of compositional transport

A compositional formulation is a reliable option for understanding complex subsurface processes. However, this type of model has a great computational cost, since the number of equations (N_c) to be solved for each grid block increases proportionally to the number of components employed.

A compositional-space parameterization approach was proposed to speed up the phase-behaviour calculations by replacing the flash calculation with interpolation in the parameter space of the problem. The phase behaviour of gas-injection processes is predominantly controlled by the properties of the key tie-lines, and hence it is convenient to parameterize the problem based on them.

Here we utilize this technique to develop a multi-scale reconstruction of compositional transport. Initially, the modified conservation equations are used for a reconstruction of the leading and trailing shock positions in space and it is performed on a coarse-scale mesh since the structure of the transport solution outside of the two-phase region is relatively simple. Next, the structure of the entire solution for N_c components is reconstructed between these two shocks by solving only two equations. Using this approach, simulation time is appreciably reduced without significant loss of accuracy.

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P10

Multiscale gradient computation for sequentially coupled flow and transport in heterogeneous porous media

Multiscale (MS) methods provide efficient and accurate subsurface flow simulation strategies. In order to fully take advantage of MS techniques in gradient-based inverse and optimization problems, both forward model and gradient computation can benefit from MS strategies. After the development of a MS gradient for single-phase flow [Moraes et al., JCP, 2017], extensions to multiphase flow require two major developments: (1) Direct and Adjoint formulations for sequentially coupled flow-transport, and (2) consistent integration of MS procedures within the forward and derivative computation frameworks.

In this work, these two developments have been achieved for an IMPES formulation. To this end, an implicit differentiation strategy is followed, where model equations and state vector are augmented to include all stages involved in MS, including reconstruction of conservative velocity.

Our results show that MS gradients applied to data assimilation studies are close to fine-scale gradients, and hence provide similar results for parameters update and data matching.

As such, MS gradients can be successfully applied to data assimilation studies. Also, the framework provides a flexible strategy to compute derivative information to any optimization problem.

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P11

Multiscale finite volume method for sequentially coupled flow-heat system of equations in fractured porous media: application to geothermal systems

Modern geoscience challenges motivate the development of advanced simulation methods for large-scale geothermal fields, where single- or multi-phase flow is coupled with heat transfer equation in heterogeneous fractured formations. The state-of-the-art multiscale formulation for fractured media (F-AMS; Tene et al., JCP, 2016) develops an efficient approach for flow equation only. Here, for the first time, the F-AMS formulation is extended to coupled flow-heat equations arising from single-phase flow in enhanced geothermal reservoirs. To this end, the nonlinear multiscale operator is obtained based on elliptic basis functions for both P and T, for simplicity and efficiency of the method. ILU(0) 2nd-stage smoother is then used to guarantee convergence to any desired accuracy. Numerical results are presented to systematically analyse our multiscale approximate solutions compared with the fine scale ones for many challenging cases, including the outcrop-based geological fractured field. These results show that the developed multiscale formulation casts a promising framework for the real-field enhanced geothermal formations.

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P12

Geoscientific application of the reduced basis method and high-performance simulations

Geoscientific tasks are usually highly parameterized and associated with a huge amount of degrees of freedom, resulting in high-dimensional problems. Accordingly, they are computationally intensive, often requiring high-performance computing (HPC) infrastructures to solve.

Consequently, one seeks a method to construct low-order approximations with a much smaller number of degrees of freedom. We consider here the reduced basis (RB) method, a model order reduction technique, and implement it using the Multiphysics Object-Orientated Simulation Environment (MOOSE). We present the advantages of the RB method; in particular, we demonstrate that it leads to a considerable speed-up allowing, in turn, simulations to be performed on non-high-performance infrastructures or the solution, for instance, of problems involving model calibration or inversions with several parameters.

For the numerical test, we apply the method to a thermal conduction problem. Additionally, we show the merits of combining the RB method and HPC. We investigate the method's scalability and parallel efficiency, two measures for its performance of clusters.

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P13

Surface-based reservoir modeling using NURBS surfaces

Here a surface-based geological modeling approach is presented that generates bounding surfaces to represent geological heterogeneity of interest without imposing it on a predefined grid. It can preserve complex input geometry from geological modeling to fluid flow simulation across a broad range of heterogeneity types and length scales. Using a NURBS representation enables accurate modeling of complex geometries. Different length scales of heterogeneity can be switched on/off easily, because no grid is present that would otherwise have to be modified. Many geological features that form heterogeneities can be described and quantified by their cross section, and can be conveniently translated into a NURBS description. NURBS surfaces can also represent geometries that are typically defined by geostatistical input. The efficiency of NURBS enables rapid generation of multiple surface-based model realizations. Surface metadata adds meaningful geological information to surfaces for automated assemblage into full geological reservoir models for which an unstructured tetrahedral mesh is created only when required for flow simulation.

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P14

FESTUNG – The Finite Element Simulation Toolbox for Unstructured Grids

We develop FESTUNG, the Finite Element Simulation Toolbox for UNstructured Grids, as a free and open source MATLAB/GNU Octave toolbox aimed at research oriented users and students. It is centered around Discontinuous Galerkin Finite Element methods and offers a rapid prototyping framework for application and algorithm development. Careful documentation, a clear code structure, and intuitive interfaces make the usage of the software package simple. At the same time, fully vectorized matrix/vector operations deliver optimal performance for small to medium scale problems.

The current set of features includes among others support for unstructured triangular grids, LDG- and HDG-discretizations, higher order explicit and implicit Runge-Kutta time stepping methods, vertex based hierarchical slope limiters, a generic solver formulation that allows for easy coupling of multi-physics problems, and VTK/Tecplot-compatible output. Example implementations of advection- and diffusion-type operators are readily available.

In this poster we present the current state of the toolbox, demonstrate its use, and present some implementation details.

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P15

Numerical computation of effective parameters in an evolving porous medium

Homogenization theory is a well-known upscaling technique. It allows for investigation of large scale applications while incorporating informations that originate from the pore scale. More precisely effective parameters of a macro-scale model are obtained from solutions of auxiliary cell problems. Homogenization theory has been applied to subsurface flow and transport problems in the last decades. However, related research was mainly restricted to rigid porous media. In this research we contrarily consider the alteration of the porous medium. We apply a level set formulation and implement numerical schemes for its solution. Moreover, on the resulting geometries cell problems and related effective parameters are computed. We further discuss their coupling into macro-scale simulations.

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P16

Effective models including dynamic Wentzell-type transmission conditions for domains separated by a thin heterogeneous layer

We are dealing with a system of non-linear reaction-diffusion equations in a domain consisting of two bulk regions separated by a thin layer with a periodic structure. The thickness of the layer ϵ , and the equations inside the layer depend on the parameter ϵ , as well as on an additional parameter $\gamma \in [-1, 1]$, describing the size of the diffusion in the layer. We derive an effective model for the limit $\epsilon \rightarrow 0$, when the layer reduces to an interface Σ between the two bulk domains. The macroscopic problem depends on the choice of the parameter γ . For $\gamma=1$, the effective problem was derived in [Neuss-Radu, Jäger (2007)], and consists of reaction-diffusion equations in the bulk regions coupled by transmission conditions involving jumps in the solution and the normal fluxes. These transmission conditions are formulated by means of solutions to local problems in the layer. We consider here the cases $\gamma \in [-1, 1]$, where different types of transmission conditions are obtained at the interface Σ . For these values of the parameter γ , the effective solution is continuous across Σ . In the case $\gamma \in (-1, 1)$, the jump in the normal fluxes is given by a non-linear ordinary differential equation on Σ . In the critical case $\gamma=-1$, a dynamic transmission condition of Wentzell-type arises.

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P17

An upscaled model for permeable biofilm formation in a thin strip

The purpose of microbial enhanced oil recovery is the use of bacterial products to improve the oil extraction. After some time of injecting water to a reservoir, the water will flow through main paths and the oil production will stop. We can use the biomass in order to clog these main paths. Then, the water will flow through new paths, increasing the oil recovery. A mathematical model that realistically describes the biologically regulated mechanism of adaptive bio-plugging is needed to qualify the technology for field implementation. The focus of this work is the derivation of a core-scale model for permeable biofilm formation with variable biofilm density. We start building a pore-scale model in which the local geometry of the pore is represented as a thin strip. We apply homogenization techniques to obtain the upscaled model. We perform numerical simulations with both models (we implement the pore-scale model in COMSOL Multiphysics and the core-scale model in MRST) and we compare with laboratory experiments. We discuss all the results and propose further work.

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P18

Numerical model for phase transitions at pore-scale

In various subsurface flow and transport processes the pore geometry changes due to the phase transitions. The question is how accurate do the numerical models of phase transitions at pore-scale have to be depending on the scale of interest? Our methods and results are as follows. We study two model problems of (i) biofilm growth, and (ii) solid phase appearance such as ice or hydrate. Both models are based on a parabolic variational inequality, and we take into account the walls of the pore-scale. We analyze convergence of the models, and we test different solvers such as semismooth Newton methods with the Nonlinear Complementarity constraint, as well as relaxation methods. Separate issue is the upscaling to core-scale, and how the accuracy of the phase transitions model affects the upscaled results.

We conclude that, while the accuracy of a numerical pore-scale model clearly affects the core-scale quantities, modeling at the scale of interface is generally not needed, especially if validation with experiments at core-scale is desired. On the other hand, modeling coupled phenomena may require the study of interfaces modeled with highly accurate numerical phase transitions models.

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P19

Microbial metabolic lag in a bio-reactive transport model for underground hydrogen storage

Intermediate storages for electrical energy can be established by injecting hydrogen into porous geological formations. The fact that hydrogen is a favored substrate for several anaerobic microbial species, which are present in the subsurface, stimulates their growth and the stored gas could be partially transformed into other substances. However, the growth of microbial populations is usually not instantaneous when changes in the substrate availability occur. The microbial cells need a certain time to adapt themselves until they are able to utilize the newly introduced substrate. This temporal phase is referred to as metabolic lag and can last up to several months. Mathematically the metabolic lag phase can be modeled by a convolution integral equation incorporating a specific memory function. In the present work such a model was introduced into a coupled bio-reactive transport model. The integro-differential equation system was transformed into an equivalent system out of partial and ordinary differential equations which were numerically implemented on the basis of DuMuX. Storage cycles were simulated to show the importance of the metabolic lag.

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P20

Simulation of microbial growth in complex geometries

Denitrification is a potential source of nitrous oxide, an important greenhouse gas. It has been shown, that denitrification is also occurring in well aerated soils. The common assumption is, that anoxic zones are located within dense aggregates in the soil. To test this theory, experiments with an ensemble of artificial aggregates from sintered glass have been conducted. The aggregates were inoculated with bacteria from a strain capable of denitrification. To evaluate the experiments, simulations of microbial growth and sustenance in the aggregates are conducted using the complex geometry of the pore space obtained from X-ray micro-tomography. For this, a reaction-diffusion problem with high spatial resolution on a complex domain is solved numerically on a sufficiently powerful parallel computer. First results are presented and compared to experimental results.

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P21

Impact of transport pathways in radionuclide accumulation under groundwater discharge areas

Radionuclide accumulation patterns in near surface quaternary sediments is evaluated considering three modelling approaches: (1) a 3D hydrogeological model with a Kd-based retention approach; (2) a 1D comprehensive mechanistic geochemical model and (3) a combination of the other two, i.e., a 3D hydrogeological model with a mechanistic geochemical model. These models lead to different concentration patterns as a result of their underlying simplifications.

The Kd depends on soil properties and it is constant in time. Thus, accumulation responds to the materials Kd values and their proximity to the radionuclide source. In the 1D mechanistic geochemical model, immobilization occurs through precipitation and sorption in the sediments close to the source. Finally, in the 3D reactive transport model, chemical reactions, i.e., retention, are driven by mixing and controlled by the three dimensional groundwater flow field. Results evidence the importance of understanding transport pathways to predict accumulation patterns and fluxes of radionuclide bearing groundwater.

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P22

Understanding the physics of the Yellowstone magmatic system with geodynamic inverse modeling

The Yellowstone magmatic system is one of the largest magmatic systems on Earth. Thus, it is important to understand the geodynamic processes that drive this very complex system on a larger scale ranging from the mantle plume in 100 km depth up to the shallow magma chamber in the upper crust. For example, why melt stalls at different depth levels above the Yellowstone plume, whereas dikes cross-cut the whole lithosphere in the nearby Snake River Plane is puzzling. Therefore, we employ parallel visco-plastic lithospheric-scale 2D and 3D models to test the influence of different parameters, such as

the geometry of the magma chamber, the melt fraction, the rheological flow law, the densities and the thermal structure on the dynamics of the lithosphere. Our model predictions can be tested with available geophysical data (uplift rates, melt fractions, ...). By framing it in an inverse modeling approach, using the adjoint equations, we can constrain which parameters (melt fractions, viscosities, geometries) are consistent with the data.

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P23

Determining scaling laws from geodynamic simulations using adjoint gradients.

Whereas significant progress has been made in modeling geological processes in recent years, understanding it often remains a challenge to understand which of the model parameters is of key importance for a particular simulation. Determining this is usually done by manually changing the model input parameters and performing new simulations, which is computationally expensive. For certain (simple) cases, analytical solutions exist that give some insights in the underlying physics. Yet, for more general cases with more input parameters this does not exist. Here, we test a different approach which computes gradients of the model parameters versus a reference solution using adjoint based methods. A key advantage of this is that the computational speed of the approach is nearly independent on the number of model parameters and that it allows computing and analysing the covariance matrix and the gradient of the parameter space. We give examples of using the method to obtain insights in processes such as subduction dynamics and crustal-scale folding.

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P24

Uncertainty estimation of onset arrival times using parametric bootstrap of statistical time series models

The time, geolocation, type, and size of a measured seismic event all come from the processing of the raw seismic waveforms that record ground motion at various sensor locations. Many types of measurements are made on the waveforms, but perhaps the most fundamental are the estimated arrival times of the various seismic phases. While considerable effort has been placed into the research of accurately estimating arrival times, relatively little has been done to quantify the uncertainty of these estimates. We extend the state-of-the-art auto-regressive time series methods of phase onset estimation to include a full estimation of the probabilistic uncertainty of the onset estimate. We propose a parametric bootstrap methodology to obtain a full posterior probability distribution to describe the signal onset detection estimates. We demonstrate our approach on both synthetic and real ground motion data, and discuss the substantial implications that a full uncertainty description affords the subsequent stages of downstream analyses.

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P25

Image processing for mass transport deposit retrieval in seismic data

Understanding ancient buried mass transport deposits (MTDs), marks of slope instabilities, is crucial for natural and industrial risk mitigation on continental passive margins. On seismic data, MTDs appear as specific objects with chaotic visual texture. A numerical workflow has been developed for detecting them in a computer vision framework.

MTDs are detected in seismic images via an object retrieval approach. Firstly, we assign to each pixel of an image a selection of textural attributes involving scale and orientation information. A classification algorithm then segments the image into regions similar to MTDs in texture. Lastly, a contour algorithm is applied to retrieve geometrically-closed objects, interpreted as MTDs. The whole workflow is first trained on a few seismic images where MTD contours are known; it can then be applied to a batch of data, yielding fast MTD contour detections.

This object retrieval is applied to seismic data from the Amazon basin. Each MTD is then described in terms of spatial extension and internal features, which will serve to derive interpretations on physical processes and controls on the mass transport event itself.

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P26

LaMEM – A massively-parallel code for 3D modeling of visco-elasto-plastic lithosphere

LaMEM (Lithosphere and Mantle Evolution Model) is a three-dimensional thermo-mechanical numerical code to simulate crustal and lithospheric deformation. The code is based on a staggered finite difference (FDSTAG) discretization in space, which is a stable and efficient technique to solve Stokes equations. FDSTAG discretization has considerably less degrees of freedom than quadratic finite elements, providing the same accuracy level for the nonlinear problems with viscosity variations.

LaMEM is build on top of PETSc library and uses the particle-in-cell technique to track phases and history variables. A coupled set of nonlinear momentum, mass, and energy equations, combined with visco-elasto-plastic rheology is treated by the Newton-Raphson solver with matrix-free analytical Jacobian. Customized coupled Galerkin multigrid preconditioner is implemented which results in a good parallel scalability of the code.

We have successfully scaled LaMEM on an IBM Blue Gene/Q machine with up to 458'752 cores and ~1000³ grid points.

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P27

H(div) mixed finite elements of minimal dimension on quadrilaterals and hexahedra

We present two new families of mixed finite elements defined on general convex quadrilaterals and hexahedra. The new families are inf-sup stable, and they approximate optimally the velocity, pressure, and divergence of the velocity. The spaces are of minimal dimension subject to the approximation properties and finite element conformity (i.e., they lie in H(div) and are constructed locally). The two families give full and reduced H(div) approximation, like Raviart-Thomas and BDM spaces. The two families are identical except for inclusion of a minimal set of vector and scalar polynomials needed for higher order approximation of the divergence of the velocity and pressure, and thereby we clarify and unify the treatment of finite element approximation between these two classes on quadrilaterals and hexahedra.

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P28

ROFMP – An iterative algorithm for the solution of inverse problems

The Regularized Orthogonal Functional Matching Pursuit (ROFMP) is a greedy algorithm for the solution of inverse problems as they appear in the geosciences. It is able to expand the solution in a combination of arbitrary trial functions. The functions are iteratively picked out of a dictionary which can be particularly tailored for different applications. By considering appropriate time-periodic trial functions, for instance, it is possible to extract periodic tidal signals out of geomagnetic field data. In order to stabilize the solution, a Tikhonov regularization with a particular (spherical) Sobolev norm is used. Moreover, there is neither a system of linear equations nor any integration problem involved, such that the method provides the ability to handle extremely scattered data sets.

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P29

Multi-physics inversion through joint sparsity

Joint inversion of multi-physics (e.g., seismic and EM) data is a promising technique aiming to reduce the uncertainty of geophysical inversion. Major challenges associated with it are (i) defining the constraints coupling different physical models and (ii) handling the complexity of the composite objective function (most apparent when more than two models are present). I show that both challenges can be addressed by using the constraints, promoting joint sparsity of some transforms

of the models. A well-known example of such constraint is the joint total variation – a mixed L1,2 norm of the models' gradients. I present another example based on the minimum gradient support functional. Both functionals are convex, provide regularization and structural coupling of any number of the models, thus greatly simplifying the objective function. While sparsity of the gradient implies that the models are piecewise-constant, using discrete wavelet transform instead of the gradient provides generalization for smooth models. 2D joint inversion of seismic traveltime, magnetotelluric and gravity data is considered as an example.

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P30

A discrete, conductive fracture model of single phase flow in porous media using non-conforming grids

The talk is concerned with a novel discrete fracture model for single-phase flow in aquifers with highly permeable fractures, which are assumed to be filled with a porous medium different from the porous medium in the surrounding matrix rock. The fractures are treated as a $(n-1)$ -dimensional interface in a n -dimensional domain. Based on a fictitious domain finite element method the flow in the fracture and the matrix is coupled (weakly) by a Lagrange multiplier representing the jump of the pressure derivative normal to the fracture. By this means it is particularly possible to consider non-conforming and non-matching fracture-matrix meshes. The performance of the method is shown for various test cases of different complexity. Moreover stability issues and convergence properties are addressed.

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P31

A topology based simulated annealing framework to generate fracture networks for geothermal systems

The presence of a well connected network of fracture is of paramount importance in the exploitation of geothermal energy. Although a statistical framework is the only practical means to describe large numbers of fractures, it is not clear which data representation best preserves the flow properties of fracture networks. In particular, in light of the critical role played by percolation properties, parameterizations that include topological information can be expected to be superior to purely geometric representations. We present a simulated annealing procedure to clarify the relative performance of the different data representations, domains with deterministic fractures will be used as base cases for calculating statistics, after which ensembles of cor-

responding stochastic fractures will be generated matching the real topological information. Different numerical techniques are used to verify the crucial role played by the latter in different scenarios.

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P32

Pilot-point ensemble Kalman filter for permeability estimation tested in synthetic tracer-test

The estimation of permeability values alongside their uncertainty is vital in the assessment of groundwater flow and heat transport. The Ensemble Kalman Filter (EnKF), an efficient tool for sequential data assimilation, has proved to be useful in the estimation of parameters that display complex spatial patterns. Such spatial patterns can also be estimated by the Pilot-Point method, interpolating a full spatial permeability field according to values at specific locations (the Pilot-Points). We interpret this interpolation as a projection of a full parameter field onto a subspace determined by the covariance structure of the parameters. Both methods are merged to yield a Pilot-Point EnKF. By reducing the parameter space, smoothing the covariance structure, and leaving invariant the kernel of the projection, this filter potentially removes artifacts that, otherwise, would have made necessary variance inflation or localization. We compare the new filter to eight EnKF-variants through synthetic tracer tests in a 2D heterogeneous flow and transport model for runs with 50 to 2000 ensemble members.

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P33

A newly derived one step computational algorithm for the solution of initial value problems

Abstract In this paper, a one-step numerical method was developed and the implementation of this method was carried out on some initial value problems of ordinary differential equations. Problems in Geophysics which can be modeled mathematically can be in the form of initial value problems which can be solved with this newly computed scheme. The derivation and the full characterization of this method from a given interpolating function were fully presented. The new method compares favourably with exact/analytical solution and some existing methods. The newly derived scheme converges and was found to be computationally time friendly.

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P34

Reactive transport simulations with iCP (Interface Comsol-Phreeqc) v1.3.1 and iCP Apps

Many natural phenomena involve coupled systems where multiple physical processes interact. At present, there are limited number of multidimensional codes able to model complex coupled (THMC) phenomena in the subsurface environment. iCP (Nardi et al., 2014) is a software that couples two stand-alone programs: COMSOL Multiphysics and the geochemical simulator PHREEQC (Parkhurst & Appelo, 2013). iCP maximizes the synergies between both codes; being of great benefit in applications where geochemistry is linked to other physical processes.

Its flexibility and wide range of applicability make iCP suitable for many modeling challenges in various fields of Earth Sciences. It has been successfully applied to model complex natural and engineered environments (Sainz-Garcia et al., 2017; Karimzadeh et al., 2017). Furthermore, iCP incorporates the capability of creating computational Apps, user-friendly interfaces tailored for specific physical configurations in which the chemical system can be adapted. iCP Apps allow the users to focus on the aspects that matter without requiring a high level numerical computation foreknowledge.

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P35

Finite volume discretizations for coupled thermo-mechanical problems

The stimulation of and production from geothermal energy systems involve strong interactions between thermal, hydro-

logical and mechanical processes and are furthermore often highly influenced by the presence of fractures. To model these problems in an efficient yet consistent manner, we rely on mathematical models for governing processes in addition to good numerical methods. It is important to investigate the relative importance of the different processes and couplings. Focusing on the thermo-mechanical coupling we extend existing FV discretizations for both the thermal and mechanical problem, using multi-point approximations. The main motivation for using a FV discretization for the mechanics is the coupling to fluid flow. If a FV scheme is chosen to obtain conservation of the fluid, there are considerable advantages to exploiting the similarity of data structures to develop efficient simulation codes.

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P36

Time adaptive domain decomposition method for non-linear reactive transport problems

Numerical simulation of reactive, flow and transport in porous media requires that increasingly non-linear models be solved in an accurate and computationally efficient manner. However, the time step sizes associated with each of these processes differ greatly. For example, kinetic reaction rates varying over order of magnitudes or layered reservoirs with fast and slow concentration changes in high and low permeability layers, respectively. We present a mass conservative, adaptive time-stepping scheme with different time step sizes in different spatial subdomains. A fully implicit solution algorithm is also described for the coupled reactive Darcy's flow and transport model. Preliminary numerical results indicate a reduced error in fine time step subdomain compared to the benchmark case of fine time steps over the entire domain.

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P37

Mathematical modeling of reactive transport in porous media with mineral precipitation-dissolution: uniqueness and nonnegativity of solutions

We consider models of reactive transport problems in porous media consisting of partial and ordinary differential equations. When mineral reactions are involved, some specific challenges arise: First, for minerals (constant activity species) it has to be distinguished between the two cases of a mineral being present, which allows for dissolution, and the mineral being completely dissolved, which prohibits any further dissolution. In a mathematical model these two cases can be formulated in an elegant way by a so-called complementarity condition. This formulation guarantees nonnegativity of solutions. Second, often the assumption is made that the reaction rate depends on the size of the reactive surface area, which again is related to the mineral volume. Measurements may lead to assumptions such as $A(m) \sim m^\alpha$ with $0 < \alpha < 1$, where

m is the mineral volume or mass and $A(m)$ is the surface area. Geometric arguments may lead to $\alpha=2/3$. However, such assumptions lead to models with non-unique solutions (ill-posed problems) and numerical results are not reliable. We show how to avoid this severe issue, i.e., we present a reformulation of the model in a well-posed form, providing uniqueness and non-negativity of the solution.

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P38
StoichPack – A general C++-library for treating stoichiometries in multi-species transport problems

The aim of our C++-library StoichPack is to provide a general interface for reactions in multi-species transport problems with a maximum of reusability, flexibility and maintainability. This can be achieved with strict adherence to only a few design guidelines. A particular advantage of StoichPack is the possibility to apply preprocessing schemes in order to decrease the computational complexity resulting from the multi-species nature of the problem, using only a few lines of additional source code. The usage and the benefits of those schemes, as well as the underlying design guidelines and the resulting software architecture, will be presented on this poster.

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P39
First steps towards a simulation tool to predict the long-time performance of geothermal plants – changes in permeability by dissolution and precipitation

At LIAG, geothermal energy utilization is a main area where we use numerical models to develop and enhance process understanding and to predict the dynamics of the system under consideration.

To this purpose we develop oops!™ (open object-oriented parallel solutions), a C++ class library for the numerical solution of mathematical models of coupled thermal, hydraulic and chemical processes. This library implements a finite-volume solver for transport equations and structures and algorithms to realise the coupling between different processes.

A major concern for the long-time performance of geothermal plants is the change of permeability in the transport path between injection and production borehole through dissolution and precipitation of minerals. We present first results from simulations with oops!™ for a calcite system.

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P40
Numerical model of coupled free gas and hydrate

In the flow of methane gas within the gas- and hydrate bearing sediments, one considers two zones of interest, separated by an interface. The upper zone where the temperature is low enough is the hydrate zone. The lower zone is where the temperature is too high for hydrate to be stable. When the amount of gas dissolved in the liquid phase exceeds the maximum allowed by thermodynamic constraints, the gas either forms the solid hydrate phase, or it exists in the free gas phase. The computational model for gas transport has to couple these two zones together, and consider two dramatically different mechanisms of transport. In the presentation we show our recent results on convergence of the numerical model for this complex process.

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P41
A pseudo-vertical equilibrium model for slow gravity drainage dynamics

Vertical equilibrium models are computationally efficient and have been widely used for modeling fluid migration in the subsurface. However, they rely on the assumption of instant gravity segregation of the two fluid phases which may not be valid especially for systems that have very slow drainage at low wetting phase saturations. In these cases, the time scale for the wetting phase to reach vertical equilibrium can be several orders of magnitude larger than the time scale of interest, rendering conventional VE models unsuitable. We present a pseudo-VE model that relaxes the assumption of instant segregation of the two fluid phases by applying a pseudo-residual saturation inside the plume of the injected fluid that declines over time due to slow vertical drainage. Comparisons with a conventional VE model and a full multidimensional model show that the pseudo-VE model has much wider applicability than the conventional VE model while maintaining the computational benefit of the conventional VE model.

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P42

The “Open Porous Media Initiative” (OPM) Software

We describe the “Open Porous Media Initiative” (OPM, <http://opm-project.org>) software and open data modules. It is a collaborative effort of both academia and industry to foster collaboration between both and facilitate innovation. The development focus is CO₂ sequestration and improved and enhanced oil recovery.

The OPM software, based on DUNE, contains various solvers for porous media flow (IMPES, two-phase incompressible transport, a reordering-based two-phase polymer solver, and a parallel fully implicit black-oil solver). In addition solvers for flow-based upscaling of both permeability (single-phase upscaling) and relative permeability (two-phase upscaling), including capability for steady-state upscaling are included. For the fast and easy visualization of reservoir simulations it also provides the tool ResInsight. Together with the software OPM provides various SPE test data sets, and the data of the Norne oil field as open data to allow easy experiments and benchmarking.

The software is licensed under GNU General Public License (GPL) version 3 and the data under the Open Database License.

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P43

Implementation of efficient global optimization algorithm for well placement optimization

Well placement optimization procedures are used to augment planning and field design workflows within subsurface engineering domains such as groundwater resource management and petroleum field development. Well placement procedures usually rely on derivative-free methods, since gradients are often not available from black-box simulators. However, procedures based on derivative-free methods are often not practical because they involve a large number of sampling points, each one requiring a time-consuming reservoir simulation. Efficient global optimization (EGO) is a global derivative-free method shown to be efficient in terms of reducing the number of trial points needed to find an optimum. The method is based on fitting a response surface to sampled points and refitting it at subsequent iterations using trial points obtained by optimizing a utility function. This meta-optimization process generates trial points with a high probability of either improving the objective or reducing the uncertainty in the search model. Results from the EGO algorithm are compared to other global optimization algorithms, such as particle swarm optimization.

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P44

A shallow water model for roof modeling in free surface flow

This work is devoted to the modeling and the numerical resolution of a shallow water model with a supplementary congestion constraint describing a roof, see [1]. For example, the model can be applied to flows under the ice floe or the production of sustainable energy from wave power using buoys.

The model is derived from the Navier-Stokes equations and to overcome the difficulty of taking into account the congestion constraint numerically, a pseudo-compressibility relaxation is used. Eventually, a numerical scheme based on a Finite Volume method is proposed. In spite of the large celerity of the potential waves, the well-balanced property and the dissipation of mechanical energy, acting as a mathematical entropy are ensured under a non-restrictive CFL condition. Simulations in one dimension for transcritical steady flow are carried out and numerical solutions are compared to several analytical solutions (stationary and non-stationary) for validation. [1] E. Godlewski, M. Parisot, J. Sainte-Marie, and F. Wahl. Congested shallow water type model: roof modeling in free surface flow. working paper or preprint, September 2016.

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P45

Multi-scale numerical simulation of a tsunami using mesh adaptive methods

Since the millennium two particular tsunamis, impacting the Indian Ocean rim in 2004 and Japan in 2011, caused enormous destruction and claimed very many lives. How can numerical modeling of tsunamis be made more efficient in order to provide better early warning systems?

One possible approach is to make use of adaptive meshes for use in solving the shallow water equations by the finite element method. Through adaptivity we can focus computational power where it is needed, accurately resolving the tsunami waves and especially those at important coastal locations, using a fine mesh. Using a coarser mesh elsewhere, we can keep the overall computational cost of the algorithm low.

My preliminary experimentation in solving the shallow water equations over the ocean domain surrounding Fukushima has been so far successful. I hope to illustrate the efficiency of a mesh-adaptive approach to the finite element method when

solving this during the coming months. Adaptivity has been shown to be effective in solving tsunami-type problems by [Behrens et al., 14] and [Davis and LeVeque, 16] and I hope to be able to reach similar conclusions within the period of my MRes project.

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P46
Dynamical reconstruction of AMOC variability at the mouth of the South Atlantic

The two main dedicated Atlantic meridional overturning circulation (AMOC) observing systems (RAPID and OSNAP) are located in the Northern hemisphere. Insights from these systems have motivated a recent focus on the South Atlantic, where water masses are exchanged with neighboring ocean basins. In a numerical study, we compute linear sensitivities of the AMOC at 34°S to global atmospheric forcing with the adjoint of the MIT general circulation model, which is fit to 20 years of ocean observation data. We attribute the influence of each atmospheric state variable on the monthly mean AMOC and find that wind (particularly the zonal component) dominates variability on monthly and interannual timescales. In contrast to past studies in the Northern hemisphere where sensitivity patterns are mostly confined to the Atlantic, atmospheric forcing perturbations over the Pacific, Southern, and Indian ocean basins have a notable influence over the South Atlantic MOC even at lead times of one month. These results emphasize the importance of continuous widespread observations of the global atmospheric state for (eventually) forecasting SAMOC variability.

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P47
A comparison between intrusive and non-intrusive spectral projection method with implementation on shallow water system.

Nearshore surge elevation plays an important role in the field of hazard assessment. However, uncertainties from wind fields, bottom friction and tidal boundary can cause inaccuracy in the simulation of surge elevation, thus understanding the propagation of uncertainties in the shallow water system is essential. A systematic comparison between intrusive and non-intrusive spectral projection methods is carefully conducted on the same 2D problem of viscous Burgers' equation, in order to test their accuracy of each method. For intrusive method, high-order generalized polynomial chaos expansion is utilized for the discretization of random space, and high resolution continuous galerkin method is utilized for the discretization of physical space. For non-intrusive methods, we test various collocation approaches. Finally, Monte Carlo method is used to verify the quality of the two series surrogate models. This study is presented as a pre-study for shallow water system, and it's also important when applies to an advanced circulation model ADCIRC with its inherent uncertainty in wind drag coefficient, bottom friction coefficient and tidal boundaries.

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P48
A new D-Flow FM (Flexible Mesh) shallow water model for Lake Marken

Forecasting of flooding, morphology, and water quality in coastal areas, rivers, and lakes is of great importance for society. To tackle this, the modeling suite Delft3D was developed by Deltares. Delft3D is open source and used worldwide. Currently there is a transition to the shallow water solver D-Flow FM (Flexible Mesh) for unstructured computational meshes in the Delft3D suite. A new model with D-Flow FM is being developed for the Lake Marken area in the Netherlands. We aim for an integrated approach in which the new model can be used for the different societal aspects. A key idea is to have the triangular mesh optimized for required local resolution and computational time. In this poster we will illustrate different aspects of the modeling stages:

- grid generation by following local structures and coarsening resolution where possible,
- proper projection of topography on grid and subtle changes to improve the model performance,
- use of simplified test cases to understand the characteristic dynamics,
- parallel performance,
- calibration and validation.

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P49
Towards an integrated hydrodynamic, waterquality, and ecological modeling approach for Lake IJssel and Lake Marken.

For Lake IJssel and Lake Marken, the two big shallow lakes in the Netherlands, various societal aspects are of importance:

- safety assessment of the dikes,
- operational forecasting of flooding,
- improving water quality and ecology,
- salt intrusion and drinking water quality,
- maintenance of the navigation channels.

Despite the diversity of aspects, they are related to common underlying physical and biological processes like wind driven waves, suspended sediments, and mussels. We will show with several illustrative real-life applications that deal with these aspects, how hydrodynamic, waterquality, and ecological modeling plays a central role.

In the near future, we aim for an integrated approach in which common computational components for modeling the underlying processes are used for different applications. This consists of a modeling chain of meteorological model, shallow water model, near shore wave model, and advection-diffusion-reaction model (including an extensive set of process definitions for suspended sediments, water quality, and ecology). On the poster we show how we work towards this aim by a step by step approach.

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P50

Derivation of a bedload transport model with nonlocal effects

The simulation and prediction of sediment transport are relevant for environmental engineering purposes. Two transport modes exist: bedload transport, and suspended load transport. We deal here with the former. The Shallow Water-Exner system is commonly used to model it. However, this model requires an empirical closure relationship for the sediment discharge. Our model is deduced from a fluid description of the sediment layer. It is obtained by performing simultaneously the Shallow-Water approximation and the diffusive limit in the Navier-Stokes equations. Different scalings of the viscosity coefficient allow to obtain a nonlocal equation for the solid discharge. The bilayer model (water and sediment layer) has an associated energy and does not need a closure relationship. In the inviscid case, the correspondence with classical solid discharge formulas used in hydraulic engineering is shown. Preliminary mathematical analysis of the equations is performed. 1D numerical results are presented.

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P51

Space-time domain decomposition methods and a posteriori error estimates for the subsurface

We present a posteriori error estimates and stopping criteria for global-in-time, nonoverlapping domain decomposition methods to model flow and transport problems in a porous medium. The method considered uses the optimized Schwarz waveform relaxation method with Robin or Ventcell transmission conditions whose coefficients can be optimized to improve convergence rates. The different error components given by the space-time DD method, the spatial discretization, the time discretization as well as the linearization are estimated separately. Consequently, an effective criterion to stop the DD iterations is developed and a posteriori error estimates help choose the free coefficients. Our a posteriori estimates are based on reconstruction techniques for pressures and fluxes. This work is supported by ANDRA, the ANR project DEDALES, the ERC project GATIPOR and the Labex MME-DII.

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O415

A nonlinear domain decomposition method to couple non-isothermal compositional gas liquid Darcy and free gas flows

A domain decomposition algorithm is proposed to couple at the interface a non-isothermal compositional gas liquid Darcy and free gas flows. At each time step, our algorithm solves iteratively the nonlinear system coupling the non-isothermal compositional Darcy flow in the porous medium, the RANS gas flow in the free flow domain, and the convection diffusion of the species and energy in the free flow domain. In order to speed up the convergence of the algorithm, the transmission conditions at the interface are replaced by Robin boundary conditions. Each Robin coefficient is obtained from a diagonal approximation of the Dirichlet to Neumann operator related to a scalar simplified model in the neighbouring subdomain. The efficiency of our algorithm is assessed in the case of the modelling of the mass and energy exchanges at the interface between the geological formation and the ventilation galleries of geological radioactive waste disposal.

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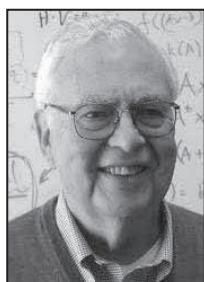
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Gene Golub g2s3 2018 SIAM Summer School

June 17-30, 2018
Breckenridge, Colorado, USA

Inverse Problems: Systematic Integration of Data with Models under Uncertainty



The ninth Gene Golub SIAM Summer School will take place at the Double Tree by Hilton in Breckenridge, Colorado, USA.

The summer school aims to introduce graduate students to the mathematical and computational aspects of inverse problems, particularly modern developments that emphasize the quantification of uncertainty in the inverse solution within the framework of Bayesian inference. The target audience is PhD and appropriate MS students in mathematics and related fields such as computer science, statistics, engineering, and science.

The central question we address is: How do we learn from data through the lens of models? The summer school will feature an integrated and coherent presentation that begins with ill-posedness and regularization, develops the ideas and tools for deterministic inversion via nonlinear least squares optimization, and elaborates formulations and solution methods for the modern Bayesian perspective, building on several of the deterministic tools. The concepts introduced in the morning lectures will be reinforced and put into practice in afternoon hands-on laboratory sessions using open-source software (hippylib, MUQ) implementing state-of-the-art deterministic and Bayesian inversion methods. Students will work together on projects that will be presented on the last day of the school.

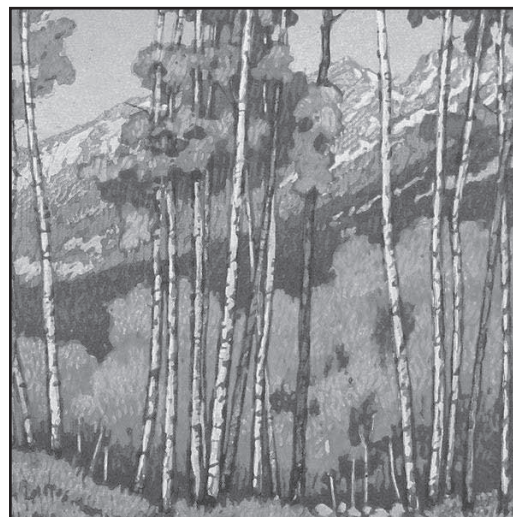
The summer school is being organized by Omar Ghattas (The University of Texas at Austin), Youssef Marzouk (MIT), Matthew Parno (US Army Corps of Engineers), Noemi Petra (University of California, Merced), Georg Stadler (New York University), and Umberto Villa (The University of Texas at Austin).

Applicants selected to participate pay no registration fee. Funding for local accommodations and meal expenses will be available for all participants.

Application deadline: February 1, 2018

As information becomes available on how to apply, it will be posted at:

<http://www.siam.org/students/g2s3/>



Aspen Stand, woodcut by Leon Loughridge

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