

IP1**The Use of Geophysical Methods to Characterize Hydrogeologic Systems**

There is growing use of geophysical methods to obtain information about subsurface properties and processes in hydrogeologic systems. Critical to advancing this use is the need to better understand the link between measurements made remotely of geophysical parameters and the properties and processes governing fluid flow and contaminant transport. Captured in the geophysical data is information about hydrogeologic systems across a range of scales from the pore scale to the facies scale. Laboratory experiments best reveal the complex relationships between geophysical parameters and various physical and chemical properties/processes at the pore scale. Field studies best reveal the relationship between geophysical images and the larger facies-scale hydrogeologic structure. At all scales of measurement we need to develop a quantitative framework that allows us to accurately characterize hydrogeologic systems using data acquired with geophysical methods.

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IP2**Decision and Control with Uncertainty: What Problems Should We Aim to Solve?**

There are four basic types of activity involving combinations of uncertainty and optimisation: * Uncertainty propagation where the problem is to predict the behaviour of an uncertain system, where the uncertainty is in the initial state of the system or factors, such as properties, influencing the system evolution. * Data assimilation, also known as history matching, system identification or inverse problems. * Decision making. Here a choice must be made between competing courses of action. For each choice of action the outcome is uncertain. * Optimal control of an uncertain system. A system is only known in a probabilistic way. One has to design a control policy that optimises the system. The problem is particularly difficult when optimisation of the measurement system is included in the problem. These problems are closely related to one another. However, the subject of decision theory is perhaps the most fundamental and well developed theory as it has a firm axiomatic basis and an extensive literature. In this talk we will examine the formulation of the problems and then discuss the matter of how close we are to solving any of these problems in a satisfactory way. The main points that will be defended are (i) we should always optimise our expected utility and (ii) sequential formulations are the most fruitful for practical progress.

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IP3**Career Awardees Talk: Challenges in Modeling Subsurface Complex Phenomena**

Today we are witnessing the beginnings of an ongoing intellectual paradigm shift in that computational simulations are being (1) included routinely in scientific analyses and (2) used to make engineering design decisions. These developments involve the merging of (1) high performance, ad-

vanced numerical computation and (2) field and laboratory experimental results with a properly validated and verified simulation tool for prediction. This result is a necessary prerequisite for wide-spread acceptance of computational simulation and enhancement of computer driven discovery and innovation in the geosciences, and, ultimately, in geo-engineering. A fundamental difficulty in understanding and predicting large-scale fluid movements in porous media is that these movements depend upon phenomena occurring on small scales in space and/or time. The differences in scale can be staggering. Aquifers and reservoirs extend for thousands of meters, while their transport properties can vary across centimeters, reflecting the depositional and diagenetic processes that formed the rocks. In turn, transport properties depend on the distribution, correlation and connectivity of micron sized geometric features such as pore throats, and on molecular chemical reactions. Seepage and even pumped velocities can be extremely small compared to the rates of phase changes and chemical reactions. The coupling of flow simulation with mechanical deformations is also important in addressing the response of reservoirs located in structurally weak geologic formations. An example of a subsurface grand challenge is the sequestration of carbon in saline aquifers. Here one needs to accurately predict the fate of injected carbon dioxide in conditions governed by multiphase flow, rock mechanics, multicomponent transport, thermodynamic phase behavior, chemical reactions within both the fluid and the rock, and the coupling of all these phenomena over multiple time and spatial scales. In this presentation we will discuss several multiscale and multiphysics approaches for addressing the modeling and simulation of complex subsurface phenomena such as carbon sequestration.

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IP4**Junior Scientist Award Lecture: Geologic Storage of Carbon Dioxide: A Challenge for the Geosciences**

Geologic storage of CO₂ presents the geosciences community with a renewed challenge in terms of spatial and temporal scales, non-linearly interacting physical processes, data uncertainty, and urgency of answers to key regulatory questions. In this talk, we will outline the development and implementation of a modeling approach to CO₂ storage. We discuss dominant processes and temporal scales, properties of numerical methods and analytical solutions, and design of new solution approaches. In the context of applications to real datasets we conclude by opening a discussion on whether simulating CO₂ storage is a well posed challenge.

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IP5**Multiple Scales Analyses for Atmospheric Flows**

Asymptotic techniques generalize the classical approach of scale analysis in theoretical meteorology. Through, e.g., matched asymptotic and multiple scales expansions they allow us to systematically study interactions across separated length and times scales. This will be demonstrated

drawing from recent work on hurricane-like concentrated vortices and on cloud–internal wave interactions. Whereas the classical theory of anelastic motions by Ogura and Phillips (1962) is naturally captured in an asymptotics-based framework, its subsequent extensions, e.g., by Dutton and Fichtl (1969), Lipps and Hemler (1982), Bannon (1996), as well as Durran’s pseudo-incompressible model (1989,2008) pose a particular challenge. I will show that their systematic theoretical justification will require techniques that go beyond scale analysis and single or multiple scales expansions.

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IP6

Sea Ice Modelling

On the geophysical scale sea ice is a thin, broken layer on the polar oceans which is modified in thickness and compactness by dynamic and thermodynamic processes. Sea ice represents the boundary between the two much larger geophysical fluids, the atmosphere and the ocean, and, therefore, influences their interaction considerably. Sea ice is described as a two-dimensional deformable solid material with a specific geophysical rheology. The presentation will focus on the optimization of sea ice dynamics, and on model verification using satellite data and buoy trajectories. Applications to past and current sea ice anomalies will be shown, including the interaction with atmosphere and ocean.

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IP7

Modeling Hurricane Waves and Storm Surge using Integrated Tightly Coupled Scalable Computations

In the wake of recent Gulf of Mexico hurricanes (Katrina, Rita, Gustav and Ike), efforts to accurately model storm surge in the Gulf of Mexico have intensified. A modeling system has been developed that simulates hurricane winds, wind-waves, storm surge, tides and river flow in this complex region. This is accomplished by defining a domain and computational resolution appropriate for the relevant processes, specifying realistic boundary conditions, and implementing accurate, robust, and highly parallel unstructured grid algorithms for both the wind waves and the long wave current/storm surge/tide model.

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IP8

Design of Carbon Dioxide Storage

We propose design strategies for CO₂ injection to maximize storage in aquifers and to maximize both CO₂ storage and enhanced oil recovery (EOR) in oil reservoirs. We propose a carbon storage strategy where CO₂ and brine are injected into an aquifer together followed by brine injection alone. This renders 80-95% of the CO₂ immobile in pore-scale droplets within the porous rock. The favor-

able mobility ratio between injected and displaced fluids leads to a more uniform sweep of the aquifer leading to a higher storage efficiency than injecting CO₂ alone. This design was demonstrated through one-dimensional simulations that were verified through comparison with analytical solutions. We then performed simulations of CO₂ storage in a North Sea aquifer. We then extended our study to oil fields. We propose to inject more water than the traditional optimum that maximizes only oil recovery. This causes the CO₂ to remain in the reservoir, increases the field life and leads to improved storage of CO₂ as a trapped phase. Again, a short period of chase brine injection at the end of the process traps most of the remaining CO₂.

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CP1

A Lagrangian-Averaged Air-Water Coupled System for Wind-Driven Sea Surface Waves

Based on the Lagrangian-averaging modeling concept we formulate equations for the generation of wind-driven sea surface waves. The equations are an air-water coupled system which includes viscosity and the surface tension. We apply the system to simplified two-dimensional laminar flows, and compare the results with those from the models based on the exact Navier-Stokes equations. Especially, we discuss its stability with laminar base profile. Growth rate, the zones of amplification and zones of decay with respect to different wave lengths and wind speeds are found.

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CP1

Parameterization of Turbulent Transport in Random Vortex Models

We employ homogenization theory to develop a systematic parameterization strategy for quantifying the transport effects of mesoscale coherent structures in the ocean which cannot be well resolved by large-scale weather and climate simulations. We work from the ground up with simple kinematic models and study in particular how the effective diffusivity depends on the governing parameters, such as Strouhal number and Peclet number, in a class of dynamical random vortex flows.

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CP1**Modeling Wave Breaking and Its Dissipative Effects on Planetary-Scale Wave-Current Interactions**

The equations for basin scale currents and waves are modified to include wave breaking via velocity perturbations of random strength at random locations. The acceleration field of individual perturbations is parametrized as to fit observations. The statistics of the perturbations are derived from realizations of a Gaussian ocean surface. Simulated wave groups are tracked and their growth rate of wave group energy is computed as a predictor of the onset of wave breaking.

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CP2**A Weak Solution and a Numerical Solution of the Coupled Navier-Stokes and Darcy Equations.**

In this work we propose a multi-numeric scheme for modeling the coupling of the Navier-Stokes and Darcy equations using the continuous finite element method in the incompressible flow region and discontinuous Galerkin method in the porous medium region. We first show existence and uniqueness of a weak solution. We then prove convergence of the numerical scheme and show some numerical simulations.

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CP2**On the Simulation of Flow in Large-Scale Fractured Media**

We propose to simulate flow within fractures lying in an impervious rock matrix. Each fracture is modeled by an ellipse of random distribution of eccentricity, length, position and orientation. For efficiency purpose and easy mesh refinement, fractures are meshed independently. The challenge comes then to guarantee the continuity of the fluxes and heads at the fracture intersections by the means of a Mortar method for any crossing configurations of the fractures.

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CP2**Some Results Concerning a Model for Fractures with Forchheier Flow**

Flow of a single phase, incompressible fluid in a porous medium with a fracture is usually modeled using a conservation law together with Darcy's law both in the fracture and in the surrounding rock matrix. However for some fractures in which the flow is more rapid, the flow in the fracture is more accurately described using Forchheimer's equation. Here we are interested in a model in which the fracture is treated as an interface between two subdomains of rock matrix and in which the flow in the fracture, is governed by Forchheimer's equation, while that in the surrounding matrix is governed by Darcy's law. We show existence and uniqueness of the solution of the resulting system. Some numerical results are also presented.

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CP2**Coupling Multi-Component Porous Media Flow with Free Flow**

Up to now, the coupling of free flow with porous media flow has been often considered only for a single-phase system. We extend this classical concept to two-component non-isothermal flow with two phases inside the porous medium and a single phase inside the free flow region. Our model also takes into account evaporation and condensation processes. We discuss the coupled model and its iterative solution by means of several numerical examples.

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CP3

Downscaling of Pressure and Saturation Maps for An Improved Modelling of 4D Seismic Data

History-matching workflows usually use pressure and saturation maps provided by fluid-flow simulations to compute 4D-seismic attributes. Unfortunately the resolution of these maps is often too coarse to represent precisely the fluid displacements at the geological scale. We introduce here downscaling algorithms which compute fine pressure and saturation maps from geological data and reservoir-simulation results. These algorithms are fast, conservative and improve significantly the 4D-seismic response of the reservoir model.

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CP3

Finite Difference Modeling the Acoustic Logging in Porous Media

A finite-difference time-domain (FDTD) algorithm is proposed to simulate the axisymmetric acoustic logs in fluid-saturated porous formation. In this algorithm, different forms of acoustic wave equations in fluid, solid and porous media are unified as the form of Biot's equations governing wave propagation in poroelastic media. The algorithm is validated by the comparisons with the analytical method. Simulations of the acoustic logging in radial layering and horizontally layering porous formations are given by the algorithm.

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CP3

A Geostatistical Study of Geophysical Data Inside Rock Blocks Bordered by Brittle Structures in Crystalline Bedrock

Interpolated gravity and magnetic maps are used together with elevation models in the interpretation of large geological structures such as folds and faults in crystalline bedrock. In the present study, geophysical data from study sites in southern and eastern Finland were analysed and interpolated to maps inside bedrock blocks bordered by fracture zones which were defined by using geological observations and elevation models. The geophysical data consisted of gravity, magnetic and seismic surveys. As a result, geostatistical measures such as different kinds of variograms

show characteristic anisotropies for different rock blocks in the study areas. The results were applied in analysing the relative movements of rock blocks and, especially, in 3D modelling of discontinuous ore bodies.

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CP3

On Semivariogram Fitting by TLS Adjustment with a New Weighting Scheme for Aeromagnetic Data

In order to fit a nonlinear mathematical model to the empirical semivariogram values that belong to a set of spatially distributed data, the Total Least-Squares (TLS) adjustment method is employed with a new extended weighting scheme. In contrast to the standard Least-Squares (LS) method, TLS approximation is particularly suited in this case since it treats the lag distance and the empirical semivariogram values symmetrically, assuming random errors in both variables. Beside the development of a (simplified) weighting scheme, proper measures for goodness of fit are also considered in this more general case, the applicability and performance of the relatively new method will be demonstrated by using a set of aeromagnetic data.

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CP4

Evolution of Rotation of a Satellite with Cavity Filled with a Viscous Fluid under the Action of Light Pressure Torque

We investigate fast rotational motion of dynamically asymmetric satellite with cavity filled with viscous fluid under the action of gravitational and light pressure torque. This problem is similar to the motion of the planet composed of a liquid core and rigid mantle. The system obtained after averaging with respect to Euler-Poinsot motion is analyzed. Numerical analysis shows that the kinetic energy is monotonically decreasing. Analytical analysis is conducted in neighboring of axial motion.

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CP4**On Resolving Exponentially Large Viscosity Variations in Convective Mantle Flow with High Order Discontinuous Galerkin Methods**

The equations governing planetary mantle convection involve a strongly temperature dependent viscosity coefficient in the elliptic problem for the fluid velocity. The viscosity is typically Arrhenius or more generically $\exp(f(T(x)))$ and needs to be resolved accurately in order to calculate the correct velocity and temperature fields. An analytic discussion showing how viscosity influences numerical calculations is followed by some numerical examples of convective mantle flow solved with the discontinuous Galerkin formulation on unstructured meshes.

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CP4**Generation, Retention and Expulsion of Hydrocarbons**

Hydrocarbon generation and expulsion are strictly interrelated processes and at a first approximation it is reasonable to assume a Darcy flow description of the expulsion process. The proposed modelling combines a two-phase Darcy flow, with time dependent porosity, with a set of Arrhenius reactions to describe hydrocarbon generation and cracking and with a differential retention process in kerogen that affects petroleum fractionation. The modelling approach has been compared and validated with laboratory experiments results.

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CP4**Applications of Full Three-Dimensional Dynamic Structural Modelling**

An innovative full three-dimensional dynamic structural modelling software has been developed in order to model basin geological evolution. The proposed approach is able to mimic the principal geological processes: sediment com-

paction, non-Newtonian behaviour of salt and sedimentary rocks, basement evolution (due to isostasy and/or tectonic movements) and fault induced displacements. Some synthetic and real application examples are used to validate and demonstrate the robustness of the approach.

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CP5**A Local Discontinuous Galerkin Discretization for Incompressible Hydrostatic Flows with Free Surface Using σ -Transformed Coordinates**

The Local Discontinuous Galerkin (LDG) method is a higher order discretization method for advection-diffusion equations. In this talk we present a conservative LDG method for the simulation of incompressible hydrostatic free surface flows using σ -transformed coordinates. The time-dependent computational domain representing the fluid region is transformed onto a domain that is fixed in time. The advantage of solving the resulting transformed system of partial differential equations is that unlike in moving mesh strategies there is no need to smooth the discrete surface elevation for grid adaptation.

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CP5**Representation of Linear Terrain Features in a 2D Flood Model with Regular Cartesian Mesh**

The failure of water control infrastructures leads to potentially destructive floods. Accurate numerical simulation of such flows is fundamental in performing risk analyses and planning for emergency management. This paper describes a cut-cell boundary approach to represent subgrid linear features (dams, rivers,...) inside a 2D structured FV code; a special version of this method is developed to represent river flows allowing the coupling of 1D and 2D computations to simulate levee overtopping floods.

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CP5

Nonlinear Shallow Water Equation in Polar Coordinates

An interaction of two water waves in a circular basin is studied within quadratic approximation. When the polar coordinates are used, the usual perturbation techniques in separation of variables method inevitably lead to a series of overdetermined systems of linear algebraic equations for unknown coefficients (in contrast with the Cartesian coordinates). However, if we formally introduce a new function satisfying the first system of this series, all these overdetermined systems become compatible (remaining overdetermined) for the special case of the nonlinear shallow water equation. Using the new function and quadratic polynomials of the Bessel functions of radius, we explicitly express the coefficients of the resulting harmonics. It gives solutions describing the two-waves interaction which are found with the same accuracy as the nonlinear shallow water equation is derived. As a consequence, a general boundary problem can be explicitly solved in these terms.

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CP6

Numerical Simulation of Multiphase Flows in Porous Media with a Degenerate Parabolic System

In this work is introduced a numerical scheme for solving degenerate parabolic systems for porous media flow by means of mixed finite elements formulation when a distinct number of fluid phases flows in distinct flow regions in the physical domain. By means of an operator splitting and domain decomposition techniques conformity conditions were obtained to bypass such degeneracy in order to obtain a non-singular system for their numerical solution.

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CP6

A Comparison of Two Numerical Models for Secondary Oil Migration and Entrapment

In this work, we compare the solutions obtained by two different methods for a synthetic trapping scenario with realistic input parameters. The first method is an invasion percolation model based on the following assumptions : oil migration is a rapid process limited by oil generation rate and capillary pressure barriers. The second method is a two phase flow finite volume method with a flux definition based on local extended pressure continuity conditions.

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CP6

Outflow Boundary Conditions in Porous Media Flow Equations

To model the flow in porous media one typically uses either the Richards equation if the flow can be described effectively by one phase, or the two-phase flow equations if two phases must be modeled. Due to the wide range of applications, the interest in these two systems is enormous. Rigorous analytical results became available in the 80ies, when strong nonlinearities in time-dependent problems were treated systematically. In most contributions on the subject, the analysis is simplified by restricting to Dirichlet boundary conditions, even though a physically more appropriate boundary condition is the outflow condition. After motivating and explaining this condition we present the corresponding qualitative analytical problems, a regularization technique and existence results.

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CP6

Formulation of Compressible Immiscible Two-Phase Flow Model by Means of Global Pressure

We consider a compressible immiscible two-phase flow model in porous media formulated in terms of a global pressure. Two possible definitions of global pressure are considered: a simplified one which is a generalization of incompressible flow global pressure, and based on an approximative calculation of mass densities, and a new one introduced by B. Amaziane and M. Jurak which does not assume any approximation. We present analytical and computational comparison of the two models.

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CP7

Numerical Modelling of Dispersion in Complex Systems

We consider dispersion processes taking place in complex systems where particles can be transported over large distances by the fluctuations of the velocity field (e.g. turbu-

lent flows) or the heterogeneity of the of system (e.g. sub-surface hydrology). For such situations, dispersion models based on Ficks law might not be accurate. These models implicitly assume that the particles are following a Brownian motion, where the dispersion of a cloud of particles is only driven by the local interactions between particles. Such a model prevents random displacements of large amplitude that could result from external forcings or heterogeneities. A more accurate dispersion pattern can be obtained by assuming that random fluctuations follow a Levy distribution, which results in so-called Levy flights. In that case, the distribution of particles is no longer the solution of a second-order diffusion equation. Instead, it can be shown that it is the solution of a fractional-order equation whose exponent is generally comprised between 1 and 2. Fractional-order differential operators are global differential operators in the sense that they take the whole behavior of the function into account and not just the local value of the slope or convexity. In this work, we discuss numerical methods to solve the fractional-order dispersion equation. Numerical methods like the finite difference and finite element methods are not well suited to solve this equation as they are generally of low order and thus require a lot of grid points to obtain an accurate solution. For local differential operators, this results in large sparse matrices that can be handled easily. However, for global differential operators, like the ones considered here, the resulting matrix is full since the global behavior of the function has to be taken into account. High-order, global numerical methods like the spectral method therefore appear to be a better choice to solve this problem as they naturally take the global behavior of the solution into account and use a limited number of degrees of freedom. Both approaches will be compared in terms of accuracy and computational efficiency.

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CP7

Attractor for Random Boussinesq-Glover Equation with Colored Noise

We consider the random Boussinesq-Glover equation with monotone operators in Banach or Hilbert spaces, driven by a colored noise and with random initial condition. The noise is defined as stationary solution of a stochastic differential equation in finite dimensional (or Hilbert) spaces. Under suitable assumptions, we prove the existence of global attractor. This attractor is independent on probabilitary variable. Similar results arise in random reaction-diffusion equations.

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CP7

The Simulation of Contaminant Transport in Groundwater and Environmental Risk Assessment

The problem of assessing groundwater pollution has be-

come a matter of considerable concern. For proper groundwater management, it is necessary to model the contamination mathematically in order to assess the effects of contamination and predict the transport of contaminants. Several deterministic models have been proposed and numerical procedures developed. Because of aquifer heterogeneity, the the spatial variation of flow properties is erratic. Therefore a stochastic model of flow regime and transport processes is more realistic. In this talk we use a new method (*A. Beskos and G.O. Roberts*), Exact simulation of diffusions, *The Annals of Applied Probability* 2005, vol. 15(4), 2422-2444) for modelling contaminant transport. Furthermore we adress sensivity analysis of exceedance probabilities with respect to variations of the transmissivity field, porosity and dispersivity

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CP7

Models for Transport in Porous Media

Tracer transport is most commonly described with the advection/dispersion equation (ADE). However even in simple experiments on homogenous systems, the ADE may demonstrate incorrect behavior. In context of a specific experiment, data is compared with numerical solutions of advection/dispersion and dual-permeability models. A pore scale network model introduces a numerical laboratory for transport in homogeneous porous media with time dependent boundary conditions. Finally we discuss a model based on the continuous transport that covers general transport phenomena in porous media.

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CP8

Ensemble Kalman Filter (enkf) for An Oregon Coastal Transition Zone (octz)

A primitive-equation numerical ocean model is used to study the upwelling circulation of OCTZ where shelf flows interact with the northern California Current. The present OCTZ simulation results show realistic features such as coastal jet separation and eddy formation offshore of Cape Blanco. An Ensemble Kalman Filter is formulated to improve forecasts and representations of the flow, and to study sensitivities to uncertainty in forcing and boundary conditions.

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CP8

Uncertainty Quantification for An Oregon Coastal Transition Zone Ocean Model

We explore the practical effect of perturbing the boundaries and wind forcing in a realistic-grid model of the Oregon Coastal Transition Zone, a region in which mesoscale eddies play an important role. The shelf flow is strongly wind-driven, and dynamically balanced perturbations of the boundary data produce different solutions in various perturbed model simulations. Integrated effects on the simulation results are assessed, and the predictability and uncertainty are quantified both in a Bayesian framework and by other standard statistical quantities.

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CP8

Effect of Island Shape on Oceanic Wake Formation

Numerical studies using Regional Ocean Modeling System are presented. We investigate the formation of oceanic wakes, generated by obstacle of the shape of Madeira Island without consideration of bathymetry (i.e., with vertical sides). The results are compared with ones, obtained by [Dong, McWilliams, Shchepetkin, 2007: Island Wakes in Deep Water. *J. Phys. Oceanogr.*, **37**, 962-981] where they investigate the formation and evolution of wakes around an idealized cylindrical island.

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CP8

Numerical Method for Solving the Unsteady Gravity-Capillary Wave Problem

The Boundary Integral Equation Method (BIEM) based on the Mixed-Eulerian-Lagrangian (MEL) approach is presented in this talk. We apply the method to numerically solve the unsteady free surface flows in water of finite depth. Here, the fluid is assumed to be inviscid and incompressible, while the flow is irrotational. The gravity and surface tension effects are included in the dynamic boundary condition. The main propose is to study the stability of steady gravity-capillary waves. Some numerical results for both steady and unsteady flows are shown.

Connections between them are also made.

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CP8

On Some Models of the Equipotential Gravity Surfaces in the Coastal Areas.

This presentation deals with mathematical models of the geoid equipotential surfaces in the coastal areas. At this moment the greatest errors in the local (small scale) Geoid determination are either in the complex mountain terrains or in the coastal areas, and it is quite important to evaluate precise Geoid in the short wavelength (small scale) for the local communities in the coastal areas as to predict impacts of tropical storms and floods. Recent studies and models of the Geoid demonstrated that the greatest errors in the Geoid surface have been made in the coastal area where there are border lines between two huge volumes of masses with rather different densities. In this presentation of the ongoing research we are considering some statistical models based on the observed anomaly data as well as the model based on the Stokes-Helmert integral for the potential of the gravitational field in the neighborhood of the shoreline, namely, we consider some ideal boundary of the water and the land masses. We have used MatLab software to simulate some models and to visualize equipotential surfaces.

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CP9

Using Energy Minimizing Basis Functions As a Multiscale Method, with Applications to Multigrid and Domain Decomposition Solvers

We demonstrate the applicability of energy minimizing basis functions for two-phase flow simulations, and we highlight their numerous benefits. We show how they can be implemented to obtain efficient serial (algebraic multigrid) and parallel (Additive Schwarz with coarse space correction) linear solvers for large-scale heterogeneous problems. Moreover, they possess the same advantages of other multiscale techniques, but without the need of constructing a coarse mesh, and they are well-suited for adaptive algebraic coarsening.

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CP9

An Unfitted Discontinuous Galerkin Finite Element Method for Numerical Upscaling in Porous Media

Porescale simulations usually require a trade-off between computational costs, simplification of the model or the geometry. A new scheme is presented, avoiding most of these drawbacks. It combines the idea of Unfitted Finite Elements with Discontinuous Galerkin methods. The minimal number of unknowns is not determined by the shape of the domain, still a maximum of the geometric information is accounted. The method is verified by computing the permeability for a domain with known properties.

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CP9

Iterative Multiscale Finite Volume Method for Compressible Multiphase Flow in Porous Media

We introduce an iterative MSFV (i-MSFV) method for parabolic problems arising from compressible multiphase flow in porous media as an extension of recently published i-MSFV method for incompressible (elliptic) problems. Convergence studies are presented including applications for multiphase flow. We show that only a few iterations per time step are sufficient in order to obtain good results; even for highly anisotropic heterogeneous reservoirs. In any case, however, the resulting solution is conservative at the fine scale.

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CP9

The Heterogeneous Multiscale Finite Element Method for Advection-Diffusion Problems with Rapidly Oscillating Coefficients and Large Expected Drift

In this contribution we analyze a new version of the heterogeneous multiscale finite element method (HM-FEM; originally introduced by E and Engquist [1]) for solving multiscale advection-diffusion problems. These types of problems have a variety of applications in geoscience, especially in modelling transport of solutes in groundwater and surface water. We give a-priori and a-posteriori error estimates for the method and provide corresponding numerical experiments that underline the analytical results. For details see [2,3,4]. [1] W. E and B. Engquist. The heterogeneous multiscale methods. *Commun. Math. Sci.* 1 (2003), no. 1, 87–132. [2] P. Henning, M. Ohlberger. The heterogeneous multiscale finite elements method for advection-diffusion problems with rapidly oscillating coefficients and large expected drift. Münster University, in preparation. [3] P. Henning, M. Ohlberger. The heterogeneous multiscale finite element method for elliptic homogenization problems in perforated domains. Münster University, Preprint 01/08 - N. [4] M. Ohlberger. A-Posteriori error estimates for the heterogeneous multiscale finite element method for elliptic homogenization problems. Multi-

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CP9

A Multiscale Mass Conservative Domain Decomposition Preconditioner for Solving Elliptic Problems on Perturbed Grids

We present a multiscale mass conservative domain decomposition preconditioner for solving elliptic problems on perturbed grids. An important feature for the multiscale methods, is the localisation approximations, for reducing the size of the global problem. We study different properties of the fine scale solution. We have looked at lack of monotonicity on the coarse scale, and studied circulations in fine scale velocity field.

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CP10

Hybrid Method for Low-Frequency Electromagnetic Scattering from a Resistive Underground Target

We present a fast and accurate hybrid method for computing low-frequency electromagnetic scattering from a resistive underground target. The method consists of solving a finite volume problem in a localized region containing the target, and using the integral equation (IE) method to obtain the field outside that region. The hybrid method thus replaces the dense-matrix part of the rigorous IE method by sparse-matrix calculations based on an approximation of Maxwell's equations.

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CP10

Impact of Time-Lapse Seismic Data on Permeability Estimation

Time-lapse pseudo-seismic (saturation) data are integrated with production data to estimate the permeability field. We investigate the impact of pseudo-seismic data with fairly large uncertainty on the final estimates by apply-

ing an error analysis to a particular estimation technique. Numerical experiments show that the over-parametrization problem is more due to measurement errors than representation bias. A quantity is derived to study the impact of perturbations in different types of measurements on the estimate.

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CP10

Locating Point Diffractors in Layered Media by Spatial Dynamics

We present a new approach to the problem of detecting point diffractors from active source surface seismic data. We formulate an optimization problem in the configuration space of possible collections of scatterers and construct a birth-and-death spatial dynamic, which converges to the optimal solution. By design, this dynamic does not have resolution limits typical of migration based techniques, which allows for subwavelength sensing.

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CP10

Non-Invasive Methods and Modelling Approaches to Study the Impact of Subsurface Structures on Flow and Transport

Geophysical methods may play an important role in managing our terrestrial environment and in maintaining ecosystem functioning and services. Especially, the application and further development of hydrogeophysical methods combined with mathematical models seem very promising to maintain and protect soil and groundwater quality. Hydrogeophysical methods may help to improve our control on storage, filter and buffer functions of soils and groundwater systems. Moreover, methods are needed that will help us to bridge the gap between the scale of measurements and observations and the scale at which management of terrestrial systems takes place. In this presentation several examples will be presented showing how hydrogeophysical research can contribute in meeting these challenges and may be used to characterize subsurface water flow and transport.

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CP10

Recovery of Active Faults from Surface Displacement Fields.

The goal of this research project is to process measurements of surface displacements in such a way to use them as data for the inverse problem consisting of locating faults and portraying their geometry. Our research is also aiming at determining whether a measured displacement field on the surface is indicative of the onset of a destabilization phase. We have already entirely solved a two dimensional problem associated to the strike slip model, which essentially reduces displacement fields to two dimensional scalar fields. Deriving the inversion method involved a rigorous mathematical eigenvalue asymptotic analysis, leading to closed form inversion formulas. Those formulas were then tested for robustness in numerical simulations. As the strike slip model is limited in scope (it captures only one of the textbook examples of faults), we have worked on extending our results to fully three dimensional fault problems. In this much more difficult case, we have already obtained very promising closed form formulas (valid for the dominant part of the asymptotic behavior), and we have tested their use on numerical data. Nonetheless, a complete mathematical analysis of the eigenvalue problem obtained by studying destabilization is still being investigated. This is joint work with I. R. Ionescu, with the support of NSF grant DMS 0707421.

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CP11

An Experimental Setup of Ground-Based and Airborne Systems to Study Spatio-Temporal Structures in Atmosphere-Land Surface Energy, Water and CO₂ Exchange

Exchange processes between land surface, vegetation and atmosphere over structured, inhomogeneous regions are investigated in an experimental approach. For that purpose ground-based long-term monitoring and dedicated campaigns are combined within the Rur catchment, Germany. Four campaigns covering different vegetation periods have been performed with instrumentation ranging from leaf level gas exchange, eddy correlation, scanning remote sensors to aircraft observations. Synergistic data analysis shall reveal spatio-temporal structures in the exchange processes and their relation to external parameters.

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CP11

One-Shot Parameter Optimization in Climate Modeling

We present an iterative method to solve data assimilation problems to identify parameters of parts of the climate system as for example ocean or atmospheric models. The goal is to obtain feasibility and optimality by simultaneously updating the state, adjoint and parameter values. Numerical results are shown on the basis of a least-squares fit of the Rahmstorf North Atlantic THC box model to given data.

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CP11

Three-Dimensional Dynamics in Non-Parallel Shear Stratified Flows

The instabilities of non-parallel flows such as those induced by polarized inertia-gravity waves embedded in a stably stratified environment are analyzed in the context of the 3D Euler-Boussinesq equations. We derive a sufficient condition for shear stability and a necessary condition for instability in the case of non-parallel velocity fields. Three dimensional numerical simulations of the full nonlinear equations are conducted to characterize the respective modes of instability, their topology and dynamics, and subsequent breakdown into turbulence. We investigate three-dimensional characteristics and present computational results on Lagrangian particle dynamics.

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CP11

Evaluation of Numerical Schemes Intended for Global Atmospheric Climate Models

The products of climate models are temporal statistics based on a calculated evolution of an atmosphere model in a forced-dissipative equilibrium. Evaluation techniques beyond deterministic test cases are needed. Because of uncertainties in the nonlinear, interactive forcing, absolute errors of the statistics are difficult to attribute to the dynamics. However comparative statements can be made which address the question: from a set of schemes which produce the same quality statistical solution, which requires

the least computer time.

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CP12

A Priori Convergence Analysis of a Coupled Geomechanics and Reservoir Flow Model with Stress-Dependent Permeability

We consider the numerical solution of a coupled geomechanics and a stress-sensitive reservoir flow model. We combine a mixed finite element for Darcy flow and Galerkin finite element for elasticity. This work focuses on deriving convergence results for the numerical solution of this nonlinear partial differential system. The CG/mixed method produces optimal convergence rates with respect to regularity. The theoretical error estimates we derived include the possibility for the displacement and the flow variables being calculated on different grids. We perform numerical experiments for verifying our theory and modeling some engineering applications.

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CP12

Large Deformation in Viscoelastic Solid Bodies – Numerical Simulation of Salt Migration.

We consider instability of a two layered solid body of a denser material on top of a lighter one. This problem is widely known to geophysicists in sediment-salt migration as salt diapirism. In the literature, this problem has often been treated as Raleigh-Taylor instability in viscous fluids instead of solid bodies. In this presentation, we propose a successive incremental method for large deformation in viscoelastic solids as a model for salt migration.

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CP12

An Asymptotic Model of Carbon Dioxide Dissolution and Mineral Carbonation Kinetics

We formulate a nonlinear o.d.e. model that describes the kinetics of the dissolution of carbon dioxide in water, and subsequent chemical reactions through to the formation of

calcium carbonate, a process central to CO₂ sequestration. An asymptotic analysis reveals seven different timescales within this system, and approximate expressions for the evolution of each species on each timescale. These approximations are used to derive uniformly valid composite expressions for the evolution of the system to equilibrium.

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CP12

The Riemann Solution for the Injection of Supercritical Carbon Dioxide and Steam in a Porous Medium

We solve a model for flow of CO₂, vapor and water in porous media, neglecting compressibility, heat losses and capillary effects. We study the dynamics of CO₂ sequestration in brine aquifers assuming constant pressure and temperature, emulating long time scale scenarios. Due to high pressures and temperatures, CO₂ appears in supercritical state. To solve the Riemann Problem, we analyze mathematical structures such as rarefactions, shock waves and their bifurcations.

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CP12

Capillary Effects on the Dynamic Sequestration of CO₂

We present a series of models of the dynamics of a plume of CO₂ being sequestered in a confined inclined permeable rock. We describe the effects of capillary retention in the pore spaces both on the advancing CO₂ front and, in the late stages, on the receding CO₂ front. We also discuss the role of capillary forces in controlling the entry pressure of CO₂ into a neighbouring, lower permeability layer, and how this can enhance the lateral dispersion of the flow as it thins. Simplified analytical models are presented along with numerical solutions of the governing equations to illustrate the key effects.

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CP13

On An Optimal Number of Time Steps For a Sequential Solution of An Elliptic-Hyperbolic System

We are interested in efficient sequential solution of the pressure-saturation formulation of two-phase flow equations in porous media. We estimate an optimal number of pressure updates in sense of saving computational efforts at given accuracy. An analytical solution to a special initial boundary value problem for the 1D formulation

of the coupled elliptic-hyperbolic system is used for such optimization. We show that global and local optimization procedures yield better results than with equidistant steps.

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CP13

An Efficient Algorithm for Modelling Dynamic Drainage

The high computational cost involved in modelling viscous effects in multiphase flow simulations using large pore network models comes from the requirement to solve a new large linear system every time one phase displaces another from a pore. To address this problem, we propose the use of an algorithm that performs a low-rank sparse Cholesky update. This direct sparse solver is faster than the preconditioned conjugate gradient (PCG) iterative solver, and eliminates the slowing down associated with the PCG in the case of adverse viscosity ratios. We apply the method to a simple description of two-phase dynamic drainage in unstructured pore network models.

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CP13

Central Schemes for Porous Media Flow

We discuss the development of a new, genuinely multi-dimensional second order semi-discrete central scheme for solving hyperbolic conservation laws arising in the simulation of multiphase flow problems in heterogeneous porous media. The scheme produces accurate solutions, particularly in the presence of high permeability flow channels, which lead to strong restrictions on the time step selection. Numerical simulations are presented and discussed for applications in CO₂ sequestration and oil reservoir simulation.

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CP13**Testing Nonlinear Solver Techniques on Difficult Finite Element Problems in Unsaturated Flow in Porous Media**

Discretizations of unsaturated flow in porous media create extremely difficult nonlinear systems of equations to solve. This presentation will show results of testing combinations of Newton only and Newton with Picard nonlinear iterations with bisection, quadratic, and forcing function only line searches. A three-dimensional research groundwater finite element computer program written for the parallel environment was used for the testing. Results for both an analytical solution and a laboratory test problem will be presented.

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CP14**Finite Volume Approximation of a Multi-Component Multi-Phase Reservoir Model with Heat Transfer**

In order to interpret recorded temperatures, we are interested in the thermal simulation of a multi-component, multi-phase (oil, gas and water) flow in petroleum reservoirs. To do, we have extended an existing isothermal simulator (GPRS : General Purpose Reservoir Simulator) by adding an exhaustive energy equation and corresponding thermodynamics. Finite volumes are employed for the space discretization and the nonlinear system obtained is solved by Newton-Raphson's method. Numerical tests including real test-cases will be presented.

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CP14**Analysis of Spontaneous Ignition in Porous Media**

Stability of combustion in a porous medium is studied in a simplified model that takes into account the balance between heat generation with temperature dependence given by Arrhenius law and heat losses due to conduction to the rock formation. The system evolution is described by infinitely many nonlinear modes. Its long time behavior is dictated by the two dominant modes, whose phase diagram contains two attractors and a saddle, as in classical chemical engineering.

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CP14**Rarefaction Waves for Flow in Porous Media with Mass Transfer Between Phases**

Using singular perturbation methods, we study the long time behavior of rarefaction waves appearing in stiff non-hyperbolic system of balance laws modelling thermal flow in porous media for several chemical species and phases. By enforcing thermodynamical equilibrium laws, they reduce to systems of conservation laws, where non-isothermal evaporation or condensation rarefactions appear. However under thermodynamical equilibrium there should be no mass transfer between phases: we discuss here the contradictory existence of these mass transfer rarefaction waves.

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CP14**Mathematical Modelling of Crown Forest Fire Initiation**

Mathematical model of forest fire was based on an analysis of known experimental data and using concept and methods from reactive media mechanics. The forest and combustion products are considered as a homogeneous two temperatures, reacting, non - deformed medium. The research is done by means of mathematical modeling of physical processes. It is based on numerical solution of Reynolds equations for chemical components and equations of energy conservation for gaseous and condensed phases. The boundary-value problem is solved numerically. As a result of mathematical modeling the fields of temperatures, mass concentrations of components of gaseous phase, volume fractions of components of solid phase, as well as vectorial fields of velocity at different instants of time with taking into account mutual influence of the layer of atmosphere and a crown fire on each other was obtained.

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CP14**Nonlinear Operator Splitting for Thermal Multi-**

Phase Multi-Component Displacements

The characteristics associated with temperature and compositions are closely related in thermal-compositional flow problems. However, use of a tie-line based Compositional Space Parameterization (CSP) approach, these characteristics can be separated at the nonlinear level with appropriate assumptions. For more than two phases, tie-simplexes (tie-triangles for three-phase) can be used for the parameterization. We demonstrate that for thermal-compositional simulations, we can employ an efficient sequential coupling scheme, thus avoiding a fully coupled strategy.

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CP15

A Numerical Method for System of Wave, Current, and Seabed Morphology in Coastal Processes

In order to accurately simulate multi-physics coastal ocean processes, the wave action equation, the shallow-water equations, and the Exner equation are coupled in a simultaneous manner. A flux-limited version of the Roe scheme is derived to discretize the coupled system for high-resolution solutions. Numerical examples and prediction of actual problems will also be presented to demonstrate the performance in comparison with conventional approaches and interaction among wave, current, and seabed morphology.

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CP15

Morphodynamics Discontinuous Galerkin Modelling with Applications to Stratigraphy

Morphodynamics is the study of the time-dependent interaction and adjustment of the seafloor (or riverbed) topography and hydrodynamic processes. To deal with problems in which complex domains and a range of scales between the physical processes are involved, the application of robust numerical methods is of paramount importance. In this work, we introduce a discontinuous Galerkin method to solve the hydrodynamics and the seafloor evolution and apply it to stratigraphy modelling.

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CP17

Maximum Likelihood Parameter Estimation by Ensemble-Based Filters

The maximum likelihood (MLE) parameter estimation is a mathematically rigorous and practically robust method, and ensemble-based filters can be an efficient tool for MLE parameter estimation. These filters calculate the likelihood function of the observations. I will discuss the MLE method, its implementation for ensemble-based filters, and advantages and disadvantages. I will also present the results of estimating the noise strength of a stochastic PDE model that conceptually represents an Atlantic Ocean Thermohaline Circulation.

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CP17

Estimation of Non-Gaussian Random Fields with the Ensemble Kalman Filter and Kernel Principal Component Analysis

Because history matching is an ill-posed problem with non-unique solutions, additional prior information, usually in the form of geological constraints on the history matching problem, is generally required to obtain geologically realistic history matched models that have good predictive capability. However, history matching is a computationally intensive process, especially for large scale simulation models, as it usually requires numerous simulations to obtain a history matched solution. Towards this end, the ensemble Kalman filter (EnKF) has recently generated significant attention as an efficient approach for assimilating dynamic data. Although the EnKF has many advantages such as ease of implementation and efficient uncertainty quantification, it is technically appropriate only for random fields (e.g., permeability) characterized by two-point geostatistics (multi-Gaussian random fields). Realistic systems however are much better described by non-Gaussian random fields characterized by multipoint geostatistics, which is capable of representing key geological structures such as channels. History matching algorithms that are able to reproduce realistic geology provide enhanced predictive capacity and can therefore lead to better reservoir management. In this work, we apply kernel principal component analysis (KPCA) to parameterize non-Gaussian random fields characterized by multipoint geostatistics. By using high order polynomial kernels, kernel PCA enables preserving arbitrarily high-order statistics of non-Gaussian random fields, thereby providing the capability to reproduce complex geology. The KPCA parameterization is then applied in conjunction with EnKF, which allows dynamic data assimilation while ensuring that the prior geological characteristics of the updated random fields (such as channels) are retained during the Kalman update. Furthermore, the KPCA parameterization dramatically reduces the number of state variables on which the EnKF is applied, thereby improving the efficiency of the EnKF. The overall procedure is then applied to several synthetic examples. The approach is shown to better reproduce complex geology, which leads to improved history matches and better predictions, while retaining reasonable computational requirements.

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CP17

Wavelet Kernel Anova

A new response surface method called Wavelet Kernel ANOVA, is proposed for uncertainty propagation and sensitivity analysis of an expensive multiphase flow reservoir simulator. The method is based on a wavelet Reproducing Kernel Hilbert Space (RKHS) technique. An adaptive experimental design method is also proposed to iteratively improve the accuracy of the response surface. The performance of the method are compared with a similar approach based on kriging on a realistic reservoir model.

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CP18

THEREDA A Thermodynamic Reference Database for Nuclear Waste Disposal in Germany

THEREDA provides consistent thermodynamic datasets to assist the long-term safety assessment of nuclear waste repositories. It meets specific German requirements (high salinities and temperatures). THEREDA is build on a relational SQL-database. The application of referential integrity, thermodynamic dependencies, alternative datasets and uncertainty estimates allows to deliver tailor-made parameter files for use in geochemical modelling software like EQ3/6, GWB and ChemApp covering law-of-mass-action and Gibbs-energy-minimization codes.

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CP18

Mathematical Issues in Subsoil Bioventing Modelling and Optimal Design

Oxygen is required in bioventing to improve the activity of bacteria to biodegrade contaminants in the subsoil and thus air is inflated through wells. The mathematical model describes the bacteria population dynamics and the dynamics of a multiphase, multicomponent fluid in porous media. A critical point of the design problem is to choose well positions and air flow rates to optimise the biodegradation process. Several approaches are possible: minimising the costs, maximising the instantaneous biodegradation rate, maximising oxygen concentration, subsoil air flow evaluation and so on.

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CP19

Application of a Coupled VF/EF Multi-Scale Method to Cement Media Homogenization

We present here the results of a work on a multiscale resolution method using both Finite Volumes and Elements in the field of numerical homogenization. Our method rely upon the coupling of two grid scales: a coarse one and a fine one. The trick is to build a Finite Element basis on the coarse grid from problems solved on the fine one. In previous work on this subject, the Finite Element method was used in both the fine and coarse scales, whereas, in our approach, the fine scale simulations are made via Finite Volumes. This way, we hope to increase the stability of the method in view of strong discontinuities and anisotropy of the studied media. Our application exemple is a model of cement media, where very important variations of diffusivity occur.

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CP19 Subdomain Time Stepping for Transport in Porous Media

In many problems concerning transport in heterogeneous porous media the simulation domain can be divided into several subdomains with different hydrogeological properties. These different properties imply different time scales that we would like to take into account by using different time steps in the different subdomains. This leads to space time domain decomposition. We discuss various formulations of this domain decomposition method using the Schur complement formulation or the Schwarz waveform relaxation method.

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CP19 Upscaling Fast Reaction in Stratified Aquifers

We analyze the irreversible bimolecular reaction $A+B \rightarrow C$ in a stratified random porous medium. In case of fast reaction, the problem can be solved in terms of a single advection-dispersion equation for the mixing ratio (Z). We compute the reactants concentrations expected values by using the probability density function (pdf) of Z . We assume the pdf of Z to be beta-distributed with mean and variance computed by semi-analytical solutions

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CP20 Modern Techniques of Software Development for Simulation of Complex Applications – A Selection of Recent Development in the Context of the Dune Framework

In this paper we present software techniques as well as recent development of the software package DUNE [1], [2] and in particular of the module DUNE-FEM [3]. For several test problems as well as for more complex applications, such as the simulation of fuel cells, we present numerical results. These results have been obtained using modern simulation techniques such as higher order continuous and discontinuous Galerkin methods (also in a stabilized version [4]) in combination with local grid adaptivity. The parallelization of the code has been taken into account which is in combination with local grid adaptivity a non-trivial part since dynamic load balancing has to be done.

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CP20 Nonlinear Solution Strategies for Compositional Simulation

We present a simulation framework based on automatic differentiation that provides wide flexibility in choosing the nonlinear formulation and selecting primary and secondary variables. The behavior of new and existing nonlinear formulations for compositional simulation is analyzed. Fully implicit formulations are considered, where the full Jacobian in terms of both the primary and secondary variables is constructed. The behaviors of the Newton iterations are analyzed for different variable sets, equation alignment, and nonlinear updating strategies.

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MS1**Model Reduction of Oceanic Flows**

Both accurate and computationally efficient simulations of turbulent flows are needed to understand and predict oceanic flows. Reduced-order models represent natural choices in these applications. The fundamental challenge is to retain the physics of the underlying turbulent flow while keeping the computational cost at a minimum. In this talk, we will present reduced-order modeling strategies synthesizing ideas originating from proper orthogonal decomposition and large eddy simulation of turbulent flows. In particular, we will present approaches based on the variational multiscale and dynamic subgrid-scale methods. Analysis and numerical illustrations of our methodology will also be presented.

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MS1**Numerical Simulation of Population Balance Systems**

The talk will describe a numerical approach for simulating population balance systems which is mainly based on finite element methods. It will address the following topics:

- the simulation of the turbulent background flow,
- the simulation of transport-dominated equations without spurious oscillations in the computed solutions,
- the impact of using different schemes for solving the higher-dimensional equation for the population balance.

The numerical simulations will consider a precipitation process.

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MS1**Large Eddy Simulation of Mixing in the Lock-exchange Problem**

LES of a 3D lock-exchange problem are presented, which contains shear-driven mixing, internal waves, interactions with boundaries and convective motions, while having a simple domain, initial and boundary conditions, and forcing. Two general classes of LES models are tested, namely eddy viscosity models based on constant-coefficient and dynamic Smagorinsky models, and an approximate deconvolution (AD) model. It is found that constant-coefficient

Smagorinsky models can only provide a marginal improvement over under-resolved simulations, while both dynamic Smagorinsky and AD models lead to significant improvements in mixing accuracy. The primary accomplishment of this study is that it is shown that the hybrid approach attains the best agreement with the mixing curve from DNS, while being computationally approximately a thousand times faster.

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MS1**Resolution and Scale Dependence of Relative Dispersion in a Hierarchy of Ocean Models**

We examine a hierarchy of ocean models, ranging from simple 2D turbulence simulations to North Atlantic HYCOM output, to determine the effect of Eulerian spatial model resolution on the two particle statistics of synthetic drifter trajectories. In each case, particle dispersion at large time and space scales is found to be controlled by hyperbolic structures produced by identifiable meso-scale features of the flow. In all cases, time-distance graphs given in terms of computed Finite Size Lyapunov Exponents show an increase in the extent of exponential scaling with increasing spatial smoothing of the velocity field and scaling of the limiting exponent with resolved hyperbolicity.

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MS2**Modeling of Multi-Phase Flow Processes in Heated Fracture-Matrix Systems**

Analysis of the proposed underground repository for radioactive waste at Yucca Mountain, Nevada, requires prediction of water-vapor flow processes in unsaturated fractured rock at elevated temperatures near and above the boiling temperature of water. This constitutes a challenging modeling problem. We elaborate on these challenges and present possible conceptual and solution approaches, with specific focus on the respective roles of fractures and matrix and their interaction.

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MS2

Massively Parallel Discrete Fracture and Matrix Simulations - A Route to Faster and More Realistic Predictions

We present a new massively parallel algorithm for discrete fracture and matrix simulations which is based on finite element finite volume discretisations and hierarchical solvers. We observe linear scaling for up to 64 processors on models containing several million degrees of freedom. This now allows us to resolve the non-linear coupling of small scale capillary – viscous and large scale gravitational – viscous processes adequately for realistic high-resolution representations of fractured reservoirs.

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MS2

Complex Gas–Water Processes in Discrete Fracture–Matrix Systems

Degassing effects may occur in fractures in the vicinity of deep radioactive-waste-disposal sites as a result of a pressure drop. These effects play an important role e.g. in the investigation of the hydraulic conditions in the near field of the disposal sites. The aim of this presentation is to contribute to the understanding of non-isothermal behavior of water–gas systems in the near field of atomic waste disposal sites in fractured porous media. For the simulation on the laboratory scale we use a percolation model. To transfer the information from the laboratory scale to the field scale we use a renormalization scheme.

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MS2

An Interfacial-area Based Approach for Modeling Degassing Processes in Fractured Porous Media

In the vicinity of radioactive waste disposal sites, degassing might occur in fractures which is to be avoided as it allows radioactive substances to reach the ground surface relatively quickly. The degassing in the fracture is highly dependent on the interfacial area separating the fluid phases which cannot be taken into account by classical models. Therefore, we present a new approach based on interfacial areas and derive constitutive equations for fractures from a micro-scale model for single fractures.

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MS3

Production Optimization and Reservoir Inverse Modeling Using Principal Component Analysis

Principal Component Analysis (PCA) is the basis of powerful model order reduction procedures for optimization within the oil industry. By PCA a high-dimensional linear space is optimally projected onto another space of much lower dimension. These spaces can represent state variables (pressure and saturation) and reservoir properties (permeability and porosity). In this talk I will explain the fundamentals of PCA and illustrate its use in optimization by examples from production optimization and reservoir model inversion.

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MS3

Identifiability, Controllability and Observability in Hydrocarbon Reservoir Models

Over the past few years systems and control concepts have been applied in reservoir engineering, e.g. optimal control, Kalman filtering, model reduction. The success of these applications is determined by the identifiability, controllability

bility and observability properties of the reservoir model at hand. In this presentation the controllability and observability properties of single-phase and multi-phase flow reservoir models are analyzed and interpreted. Additionally, it is shown how to determine and use approximate model structures with identifiable parameterizations.

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MS3

Model Reduction via Multiscale Methods: Application to Water Flooding Optimization

In this talk we discuss the use of a multiscale mixed finite element method (MsMFEM) for model order reduction in reservoir engineering optimization problems. We illustrate the use of the methodology for finding optimal rates and well-placement in water-flooding examples. We also discuss pros and cons for the MsMFEM approach compared to e.g., PCA (principal component analysis)-based techniques.

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MS3

Reducing Model Order by the Definition of a Random Function From a Given Set of Model Realizations

In this talk we provide a novel framework for geostatistics/spatial modeling. We establish a method for defining a random function from a set of generated/measured realizations, typically associated with uncertainty analysis processes. This function reduces drastically the order of the model. Once the random function is available, we show how consistent sets of new realizations, with structural properties similar to the initial set, can be generated without re-running the algorithm or consulting the generating source.

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MS4

Gas Migration in a Nuclear Waste Repository; a Unified Modelling of Fully and Partially Saturated Porous Materials

Motivated by modelling the gas migration in an under-

ground nuclear waste repository, we derive a new compositional model of compressible multiphase flow and transport in porous media, with interphase mass transfer. This new unified modeling of fully and partially water saturated porous materials makes possible a unified numerical treatment of both fully and partially water saturated situations. Existence of solutions, is proved under adequate assumptions, and numerical simulations showing the efficiency of this modeling are presented.

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MS4

Phase Exchange in Two-phase Flow in Porous Media and Complementary Problems

Two-phase flow with phase exchange is modeled as a set of time dependant nonlinear partial differential equations with nonlinear complementary conditions. Such a formulation allows appearance and disappearance of a phase as well as the use of some laws which are widely used as Henry's law. We discretize the problem with cell-centered finite volumes method or mixed finite elements and discuss appropriate solvers for the solution of the resulting nonlinear complementary problems.

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MS4

Fully Coupled HMFE Approximation for Two-phase Flows in Porous Media

For modeling CO₂ underground storage, two-phase, two-component flow with possible disappearance of each phase and phase-exchange is considered. By neglecting temperature variations the model is reduced to a system of two time-dependent partial differential equations. The unknowns are quantities derived from saturations, compositions and pressures, with relations independent of time and space. The discretization ansatz is a mixed finite element method, not necessarily of lowest order. For the chosen discretization fluxes are explicitly eliminated and condensation leads to a nonlinear equation in terms of Lagrange multipliers at each time step.

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MS4**Principle of Equivalence and Method of Negative Saturations for Multicomponent Flow with Phase Transitions Through Porous Media**

We analyse the flow with phase transitions when the two-phase fluid can be alternated with the zones occupied by single-phase non-equilibrium fluid. The principle of equivalence is proved which says that a non-equilibrium single-phase fluid is hydrodynamically equivalent to an imaginary two-phase equilibrium fluid having specific physical properties called the equivalence conditions. One of these conditions necessarily implies that the saturation of one imaginary phase is negative. We prove the consistence theorem which shows that such equivalence conditions do not contradict to fundamental thermodynamic principles. The equivalence theorem allows for developing an efficient numerical method of modeling these processes, by applying the uniform two-phase flow equations for all the flow domain, but different thermodynamic constitutive conditions for single-phase and two-phase zones. The moving interface between these zones is detected automatically once the saturation becomes negative. The method is tested on one-dimensional analytical solutions. The numerical example of solving two-dimensional flow problems with irregular shape of the interface are obtained. The advanced version of the method is developed for the cases of diffusion, adsorption and chemical reactions, when the interface between zones is detected as the surface of the weak discontinuity of the saturation field. The simulated examples concerns oil displacement by partially miscible gas and CO₂ injection in an aquifer.

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MS5**Gaussian Process Emulators for Groundwater Flow**

We explore the application of Gaussian process emulators to uncertainty analysis of groundwater flow models. Emulators statistically approximate the output of computer models and can be used as cheap substitutes for the model. A model of groundwater flow through the Culebra Dolomite at the Waste Isolation Pilot Plant site is chosen as a test case to illustrate the methods. The uncertainty in the output of the model given the uncertainty in the inputs is quantified.

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MS5**Generalized Spectral Decomposition for Uncer-****tainty Quantification in Elliptic Equations**

In this talk, we present a Generalized Spectral Decomposition method for probabilistic uncertainty quantification in elliptic equations. The decomposition aims at approaching the stochastic solution on reduced bases (stochastic and deterministic), similar to the Polynomial Chaos expansions, except that the expansion bases are not selected a priori but constructed and adapted to the problem equations and parameters uncertainty. Different algorithms are considered for the construction of the reduced bases (Power-type and Arnoldi-type iterations), and compared on a test problem related to steady linear and non-linear ground water flow simulations (Darcy equations). Performance and implementation aspects are discussed with regard to the classical stochastic finite element method, and we discuss the extension of the Generalized Spectral Decomposition method to large unsteady problems arising in nuclear waste disposal simulations.

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MS5**Efficient Iterative Solvers for Stochastic Groundwater Flow Problems**

We consider finite element discretizations of PDEs with a stochastic differential operator arising in groundwater flow simulations. We report on the design of efficient iterative solvers for the resulting large coupled linear system of equations. In particular we present a new approach for preconditioning such linear systems which takes advantage of the special Kronecker product structure of the Galerkin matrix. We demonstrate the efficiency of our techniques on selected model problems.

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MS5**Efficient Numerical Methods for Stochastic Computations**

Numerical algorithms for effective incorporation of uncertainty into differential equations are discussed. The uncertainty is modeled as functions of random variables, and the governing equations are treated as stochastic. By using generalized polynomial chaos (gPC) expansion, the solu-

tions are expressed as convergent series of orthogonal polynomials in terms of the random variables. Based on gPC, various numerical schemes can be designed, via either a stochastic Galerkin (SG) approach or a stochastic collocation (SC) approach. In this talk we discuss and compare the strength and weakness of gPC based SG and SC methods. The focus is on their accuracy and efficiency. We will also demonstrate the clear connection between these methods and the classical deterministic spectral methods and their applications to inverse problems such as parameter estimation.

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MS6
Interfacial Momentum Balance Between Non-equilibrium Phases

The net stress on a flat interface is not zero during a phase change. A net stress is needed to balance the jump in momentum experienced by the molecules as they cross the interface; a stress-free interface introduces an error in the solution for the velocity field. This work presents an expression for interfacial momentum balance between non-equilibrium phases and investigates the equilibration process in the presence of natural convection.

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MS6
Numerical and Mathematical Aspects of Multi-phase/Component Solubility in Water

The numerical and mathematical aspects of multi-phase/component solubility in water are considered where thermodynamically consistent three-phase behavior is coupled with nonlinear transport in porous media. In this model, several hydrocarbons are allowed to dissolve in the aqueous phase while all other components expect water exist in the oil and gas phases. The proposed computation of any gas solubility in the aqueous phase is based on EOS framework. The numerical simulation results are presented and discussed.

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MS6
Front Tracking Technique for Three Component Two Phase Incompressible Flows

Abstract not available at time of publication.

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MS6
Tie-simplex Based Parameterization for Thermodynamical Equilibrium Computations of Multi-component Systems with Arbitrary Number of Phases

We present a general framework for the computation of thermodynamic equilibrium of multi-component systems that form an arbitrary number of phase. We parameterize the high-dimensional compositional space using tie-simplexes (tie-triangles for three-phase) to represent the multi-phase regions. The tie-simplex computation and interpolation procedure complement the parameterization and form a complete mathematical framework. We demonstrate the efficiency of the method for several multi-phase equilibrium problems of practical interest that include both equilibrium flash calculations and multi-phase, multi-component flow problems.

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MS7
Geological Storage as a Carbon Mitigation Option

Abstract not available at time of publication.

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MS7
On the Use of Streamlines and Front Tracking for Compressible Flow

We investigate the use of streamline methods and front tracking for compressible flow. Operator splitting is used to incorporate gravity effects. We apply this method for the injection phase of CO₂ storage and point out in which situations the method has advantages and when other approaches should be considered.

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MS7
An Efficient Upscaling Based on a Unified Fine-

scale Multi-physics Model

The main challenge in modeling fluid flow through naturally-fractured carbonate karst formation is how to address various flow physics in complex geological architectures due to the presence of caves which are connected via fracture networks at multiple scales. In this paper, we present an efficient upscaling process that is based on a unified fine-scale multi-physics model which adaptively couples Stokes-Brinkman with discrete fracture network models. The underlying idea is to use Stokes-Brinkman model to represent flow through rock matrix, void caves and intermediate flows in high permeability regions and to use discrete fracture network model to represent flow in fracture network. This unified approach adaptively treats fractures as lower dimensional geometries with permeabilities assigned according to their apertures. Consequently, various numerical solution strategies can be efficiently applied to greatly improve the computational efficiency in flow simulations.

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MS7

On Eulerian-Lagrangian Formulations and Their Analyses

We present optimal-order error estimates for a class of Eulerian-Lagrangian methods for advection-diffusion equations, which are uniform with respect to the vanishing parameter ϵ . The estimates depend on the given initial, boundary, and right side data but not on the true solution. We also discuss optimal-order error estimates for Eulerian-Lagrangian methods for the coupled system in porous medium flow. These results justify the strength of Eulerian-Lagrangian methods. Numerical results are presented to verify the analysis.

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MS8

Analysis of a Scale Similarity LES Model Designed for Certain Stratified Flows

We propose and give some mathematical analysis results for a Large Eddy Simulation model which involves regularization only in the horizontal variables. The method we consider, which fits into the class of *scale similarity models*, is similar to the ‘‘Simplified Bardina model’’ introduced by Layton and Lewandowski (2006). We are able to prove that our new model has good mathematical properties (existence and uniqueness in appropriate Sobolev space). The mathematical foundation is one of the first steps for the validation, even if numerical experiments on realistic problems will be the necessary further step.

The idea of considering extra-viscosity (sub-grid-scale terms) acting only in the horizontal variables is well diffused in the community, especially for the mixing dam

breaking problem in the context of Boussinesq approximation, see Özgökmen *et al.* (2007) and this is one of the motivations for our work. Moreover, the analysis of fluids with very different viscosity coefficients in the horizontal and vertical direction is motivated also by the study of Ekman layers, see for instance the introduction of Chemin *et al.* (2000), Desjardins and Grenier (2000) and Pedlosky (1979).

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MS8

A Goal-Oriented Mesh Adaptive and Dual-Weighted Pod for Data Assimilation into Ocean Modelling

A novel dual weighted POD method for adapting mesh, order reduction and 4D-Var data assimilation is presented here. The aim is to (1) optimise the reduced bases, thus improving the quality of reduced ocean models representation of the goal; (2) design an error measure to guide an adaptive meshing algorithm. The goal functional for optimising reduced bases and meshes has been designed to be consistent with that for 4-D Var data assimilation.

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MS8

On a LES-deconvolution Model for the Ocean with a Fixed Wind

We model the oceanic flow by using the Navier-Stokes equations together with the rigid lid assumption, which yields flux conditions for the velocity at the surface, that couple the ocean to the atmosphere. We stay here in the case of a fixed atmospheric wind. We start by showing how to adapt the periodic Leray-Alpha model to the case of those realistic boundary conditions. We next turn to the Layton-Lewandowski deconvolution model, based on the Van Cittert algorithm. This model cannot be adapted like this to the case of the ocean. We observe that the Van Cittert algorithm is in fact nothing but a finite difference scheme of a certain evolution equation. This yields a new LES deconvolution model adjusted to the ocean, for which we prove the existence and the uniqueness of a smooth solution. We also prove the convergence of those solutions to a dissipative solution to the Navier-Stokes equations when the deconvolution parameter goes to infinity. This research work has been initially performed by A.-C. Bennis, R. Lewandowski and E.-S. Titi. R. Lewandowski is supported by the ANR project 08FA300-01.

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MS8**Three-Dimensional Dynamics in Non-Parallel Shear Stratified Flows**

The instabilities of non-parallel flows such as those induced by polarized inertia-gravity waves embedded in a stably stratified environment are analyzed in the context of the 3D Euler-Boussinesq equations. We derive a sufficient condition for shear stability and a necessary condition for instability in the case of non-parallel velocity fields. Three dimensional numerical simulations of the full nonlinear equations are conducted to characterize the respective modes of instability, their topology and dynamics, and subsequent breakdown into turbulence. We investigate three-dimensional characteristics and present computational results on Lagrangian particle dynamics.

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MS9**Asymptotic and Numerical Modelling of Flows in Fractured Porous Media with Finite Volume Methods**

We study some asymptotic models used to compute the flow outside and inside fractures in 2-D heterogeneous porous media. The flow is governed by the Darcy law with large discontinuities in the permeability tensor. The fractures, supposed to have a small aperture with respect to the macroscopic length scale, are then asymptotically reduced to immersed fault interfaces. A cell-centered finite volume scheme on general polygonal meshes fitting the interfaces is derived to solve the set of 2-D/1-D equations with the additional differential transmission conditions linking both pressure and normal velocity jumps through the interfaces. We prove the convergence of the FV scheme and derive existence and uniqueness of the solution to the asymptotic models proposed. Various numerical results are reported showing different kinds of flows in the case of impermeable or partially/highly permeable immersed fractures. These numerical solutions of the asymptotic models are validated by comparing them to the solutions of the global Darcy model or to some analytic solutions.

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MS9**Development of Model Concepts for Flow in Macro-porous Media on Different Scales**

The fast infiltration of heavy rainfalls in macro-porous hillslopes is one of the key processes which triggers fast infiltration, saturation and pressure increase and thus deformation processes. A so-called cascade model concept has been developed for macropore infiltration based on controlled laboratory experiments and it is implemented in the framework of a two-phase flow model concept for porous media. The exchange parameters which are determined by this tool will be transferred to a double continuum model concept which is then applied on the field scale.

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MS9**Deformation Band Populations in Fault Damage Zones - Impact on Fluid Flow**

Fault damage zones in highly porous reservoirs are dominated by deformation bands that generally have permeability-reducing properties. Due to an absence of sufficiently detailed measurements and the irregular distribution of deformation bands, a statistical approach is applied to study their influence on flow. A stochastic model of their distribution is constructed, and band density, distribution, orientation and flow properties are chosen based on available field observations. The sensitivity of these different parameters on the upscaled flow is analyzed. The influence of a heterogeneous permeability distribution was also studied by assuming the presence of high permeability holes within bands. The fragmentation and position of these holes affects significantly the block effective permeability. Results of 1D and 2D local upscaling are compared and qualitatively similar results for the flow characteristics are obtained. Further, the procedure of iterative local-global up scaling is applied to the problem.

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MS9

Preferential Flow in Fissure Systems

The asymptotic analysis of Darcy flow near a very thin highly-permeable fissure is revisited. The limiting problem is Darcy flow in the region coupled to tangential Darcy flow through the lower-dimensional interface approximation of the fissure. Stokes flow in the fissure leads to Brinkmann flow in the interface model. For a fine-scale periodic structure of highly-permeable fissures of width decreasing at twice the rate of the periodic scale, we obtain the homogenized limit and establish the two-scale convergence. (preliminary report)

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MS10

Particle Swarm Optimization with Surrogate Functions for Water Management Problems

We provide a framework to improve the efficiency of the particle swarm optimization method by using surrogate functions. For water resources management problems, this helps alleviate the burden of costly simulation calls required to model groundwater flow and transport that are embedded in the objective function. We present results on a hydraulic capture problem posed as a mixed-integer nonlinear problem in determining the number of wells, well rates, and locations to minimize clean up costs.

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MS10

Tailoring Hybrid Optimization Methods for Water Resources Management

Hybridizing optimization methods has emerged as highly promising. However, the effectiveness of this approach may be compromised if the methods combined are not suited to one other or to the application of interest. In this talk, we will discuss hybrid optimization in the context of water resources management. We will focus on the characteristics of the problem domain and of some optimization techniques and present numerical results demonstrating the efficacy of tailoring hybrids.

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MS10

Hybrid Optimization Methods for Simulation Based Problems

Simulation based optimization is increasingly important for hydraulic application problems, especially the need to handle real-valued as well as integer-valued variables is emerging. Hybrid optimization methods applied in a well suited framework can help to solve arising problems with less simulations calls if they are well adapted for the underlying problems. In this talk we will discuss mixed-integer nonlinear simulation based optimization using surrogate functions for efficient derivative free optimization.

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MS10

Groundwater Calibration with POD

We demonstrate a POD (proper orthogonal decomposition) tool for calibration of models for saturated flow in porous media. POD was developed for flow control and builds a global basis from “snapshots” taken from a dynamic simulation. In our steady-state context we build the basis from the sensitivities. The advantages of POD are that matrix assembly and factorization for the finite element simulation are moved out of the optimization loop. We show three-dimensional results that indicate that the performance of the optimization using POD is essentially the same as that for the much more expensive optimization using the full finite element simulator. We may also show results for global optimization using POD as the surrogate model.

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MS11

Coupling Discontinuous Galerkin Discretizations Using Mortar Finite Elements for Advection-Diffusion-Reaction Problems

We investigate DG-DG domain decomposition coupling using mortar finite elements to approximate the solution to general second-order partial differential equations. This class of equation includes second-order elliptic and parabolic equations, advection-reaction equations, as well as problems of (mixed) hyperbolic-elliptic-parabolic type. In the formulation, we consider the upwinded flux for the advective flux and provide the matching condition by weakly imposing continuity of the total flux on the *inflow* boundary part of the interface and continuity of the total

flux and the solution on the *characteristic* boundary part of the interface via mortar finite elements. The subdomain grids need not match and the mortar grid may be much coarser, giving a two-scale method. The diffusion coefficient is allowed to be degenerate. Convergence results in terms of the fine subdomain scale h and the coarse mortar scale H are then established. If the interface lies in the advection-reaction regime, with proper choice of h and H , optimal convergence rates are achieved. A non-overlapping parallel domain decomposition algorithm reduces the coupled system to an interface mortar problem. The properties of the interface operator are discussed.

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MS11

Analysis of MPFA Convergence on General Geometries

The similarities between the multi-point flux approximation (MPFA) methods and the mimetic finite difference method can be used to prove convergence of the MPFA methods on general grids in 2D and 3D. We examine the assumptions needed for convergence of the MPFA methods, with particular attention to the limitations posed by the analysis and how the theory compares to the numerical convergence results.

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MS11

Modeling Multiphase Flow Coupled with Biogeochemistry in Porous Media

Abstract not available at time of publication.

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MS11

A Multipoint Flux Mixed Finite Element Method on Hexahedra

We present a mixed finite element (MFE) method for Darcy flow on hexahedral elements, which reduces to cell-centered finite differences and performs well for discontinuous full tensor coefficients. Motivated by the multipoint flux approximation (MPFA) method where sub-face fluxes are introduced, we introduce an enhanced version of the lowest order Brezzi-Douglas-Marini (BDM) MFE space involving four velocity degrees of freedom per face. A special quadrature rule is employed that allows for local velocity elimination and leads to a symmetric and positive definite cell-centered system for the pressures. Theoretical and nu-

merical results indicate second-order convergence for pressures at the cell centers and first-order convergence for sub-face fluxes if the grids are sufficiently regular. Second-order convergence for face fluxes is also observed numerically.

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MS12

Homogenization of Porous Media by the Periodic Unfolding Method

We consider the Stokes and the Navier-Stokes problems in a perforated domain. The holes are periodically distributed with a period e , their size is of the order d . Both d and e are small parameters. Our aim is to give the asymptotic behavior of the velocity and of the pressure of the fluid, as these two parameters go to zero. We first discuss the case $d = 1$ corresponding to the classical homogenization (cf. [3] and [4]). For the general case $d = ea$ (i.e., the case of small holes), we derive several limit problems, corresponding to different values of a . These limit problems are either the Darcys law, or a Stokes problem or the Brinkman law. Finally, we study the case of partially perforated domains. The proofs use the periodic unfolding method (see, for instance [1] and [2]) which avoiding the introduction of extension operators, allows us to treat complex geometries of domains. References [1] D. Cioranescu, A. Damlamian, G. Griso, Periodic unfolding and homogenization, C. R. Acad. Sci. Paris S er. I Math. 335 (2002), 99-104. [2] A. Damlamian, An Elementary Introduction to Periodic Unfolding, GAKUTO International Series Math. Sci. Appl. 24 (2005), 119-136. [3] E. Sanchez - Palencia, Non homogeneous Media and Vibration Theory, Lecture Notes in Physics 127, Springer Verlag (1980). [4] L. Tartar, Incompressible fluid flow in a porous medium- convergence of the homogenization process. Appendix in [3].

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MS12

Multiscale Models for Processes with Evolution of Microstructures

Many problems in science and engineering involve time-varying microstructures. Important examples are phase transitions with microstructures of dendritic or eutectic type, or processes in porous media, where deposition/resolution may change the geometry of pores. In such cases the application of standard homogenization does not lead to a purely macroscopic model as in more traditional examples, but to multiscale models. We address the derivation and analysis of such models and their use in simula-

tions.

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MS12

Upscaling of Differential Equations Modelling the Reactive Flow Through a Deformable System of Biological Cells

We consider a system of model equations coupling fluid flow, deformation of solid structure and chemical reactions in biological tissue. Our goal is to obtain the upscaled system modeling reactive flow through biological tissue on the macroscopic scale, starting from a system on the cell level. The novelty of the upscaled model is that it includes Biot's equations from the soil consolidation theory, coupled with reactive transport. (Joint work with W. Jaeger and M. Neuss-Radu)

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MS12

Crystal Dissolution and Precipitation in Porous Media

We propose a pore scale model for crystal dissolution and precipitation in a porous medium. As a result of the precipitation and dissolution the pore geometry may change. Using the proposed model we derive upscaled effective equations on the Darcy scale via a formal homogenization procedure. Numerical simulations show that solutions of the upscaled model match the averaged solutions of the pore-scale model very well.

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MS13

Osmotic, Swelling, and Disjoining Pressures at Multiple Scales

In swelling porous media, pressures commonly used include disjoining pressure, osmotic pressure, and swelling pressure. These are attributed to microscopic forces such as electrostatic forces, Van der Waals forces, and surface hydration. Here we discuss the definitions of these different pressures and examine the relationship between them and microscale forces within the framework of two upscaling approaches for swelling porous materials: hybrid mixture theory and homogenization.

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MS13

Electro-chemical and Swelling Behaviour of Active

Hydrated Materials

Charged hydrated materials exhibit internal coupling mechanisms stemming from the intrinsic characteristics of the constituents. In this content, the model under consideration consists of a fluid-saturated solid matrix carrying volume-free fixed negative charges, while the pore fluid is given by a mixture of a liquid solvent and the cations and anions of a dissolved salt. Based on the well-founded Theory of Porous Media (TPM), use is made of the assumption of quasi-static processes. The governing equations are given by the volume balance of the fluid mixture governed by the hydraulic pressure, the concentration balance governed by the cation concentration, the overall momentum balance governed by the solid displacement and the electrical continuity equation governed by the electrostatic force. Furthermore, the mechanical solid extra stress is described by an extended neo-Hookean material law, while the viscous fluid flow follows an extended Darcy's law, which includes the gradients of the ion concentrations and the electrical potential. Furthermore, the ion diffusion is described by an extended Nernst-Planck equation. Finally, the model is implemented into the FE tool PANDAS by use of a mixed finite element scheme. The presented examples proceed from boundary conditions depending on internal variables such that certain stabilisation techniques are needed.

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MS13

Ionic Multi-Species Transport in Porous Materials with Account to Surface Charge Phenomena

A set of macro level Nernst-Planck-Poisson type of equations are derived, describing the diffusion of ionic species in the pore water of a porous material with charged pore walls, using the electroquasistatic hybrid mixture theory. The effect of the surface charge on the global ionic diffusion is studied by a separate microscopic tentative approach based on ionic double layer formations. A numerical solution technique based on the finite element approach is formulated.

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MS13

Passive Measurements of Electrical Potential as a Non-intrusive Method to Determine and Locate Hydromechanical Disturbances

A pore scale model of transport of ions in a charged porous material is developed using a volume averaging operator applied to the Nernst-Planck and Stokes equations that couple Maxwell and Biot equations. The macroscopic equations are solved with a finite element method. We present results of the forward and inverse modeling. The inverse modeling is developed inside a Bayesian framework using MCMC samplers. Different applications are shown in hydrogeophysics and volcanology.

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MS14**Corrected Operator Splitting for Two-phase Flow with Gravity Forces in Porous Media**

In this talk, we apply the corrected operator splitting (COS) algorithm for two-phase flow including gravity in porous media, combining the characteristics method with the finite volume method. The motivation is to gain the computational efficiency from the hyperbolic solver and a good handling of the non-linear flux term with a more accurate shock width using large time step. The methodology of the COS algorithm is described and numerical results are given.

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MS14**Mixed Multiscale Finite Element Methods for Porous Media Flows Using Limited Global Information**

In this talk, I will describe multiscale methods for fluid-structure interaction. This is a highly nonlinear problem that involves coupling Stokes equations with elasticity. We propose several multiscale methods and their analysis. Numerical results are presented. This is a joint work with Peter Popov and Yuliya Gorb.

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MS14**On Taking Large Time Steps for Transport**

A major advantage of multi-scale methods compared to classical upscaling consists in their ability to reconstruct fine-scale velocity fields, which can be used to solve for phase transport. Here, the stability of an implicit fractional flow formulation is investigated and an analysis of the classical Newton-Raphson scheme explains the well known, severe time step size restriction for S-shaped flux functions. Then, a simple, unconditionally stable modification is devised.

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MS14**Multi-scale Multi-physics Models for Flow and Transport in Porous Media**

Physical processes generally take place on different temporal and spatial scales. Also, on the same scale, they may vary in space. A standard approach would solve for the most complex processes occurring in the domain of interest on the finest relevant scale. This is unnecessarily expensive. Therefore, we discuss multi-scale multi-physics approaches which allow to take the space and time dependence of processes into account, thus reducing the required amount of data and computing time.

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MS15**Reduced-Order Models for Time-Periodic Dynamics in Ocean Flows**

A number of phenomena in ocean flows exhibit time-periodic dynamics. These may arise due to diurnal forcing or are inherent flow features such as breaking waves or Langmuir cells. In this talk, we discuss the adaptation of reduced-order model development based upon proper orthogonal decomposition (also known as empirical orthogonal functions) to include sensitivity variables. The resulting dynamical systems exhibit better long time integration behavior. This improvement is preserved as parameters in the model are varied.

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MS15**Chemical Data Assimilation: Computational Tools and Applications**

The task of providing an optimal analysis of the state of the atmosphere requires the development of novel computational tools that facilitate an efficient integration of observational data into models. We discuss several new computational tools developed for the assimilation of chemical data into atmospheric models. The distinguishing feature of these models is the presence of stiff chemical interactions. The variational tools presented in this talk include automatic code generation of chemical adjoints, properties of adjoints for advection numerical schemes, calculation of energy singular vectors and their use in placing adaptive observations. Data assimilation results using the 4D-Var method are shown for several real test problems to illus-

trate the power of the proposed methods.

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MS15

Some Mathematical Problems in Geophysical Fluid Dynamics

Abstract not available at time of publication.

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MS15

Dynamic Transitions in Thermohaline Circulation

Abstract not available at time of publication.

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MS16

Simulation of Flow and Transport Processes in a Discrete Fracture Matrix System I. Geostatistical Generation of Fractures on an Aquifer Analogue Scale

The critical step for the discrete fracture model approach is the generation of a representative fracture network. In this study, we will show a geostatistical fracture generator which integrates statistical geometries and spatial characteristics in terms of a standardized variogram, neighborhoods and a fracture cell density. Later the flow and transport behavior of a fracture matrix system is investigated, where the fracture matrix system is represented by the generated fracture network embedded in a porous rock matrix.

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MS16

Automated Characterization of Fractured Reser-

voirs from Well Tests

Geologically-realistic models of fractured reservoirs are constructed via a workflow involving the integration of various data. However these data are often incomplete and uncertain, such that the model parameters cannot be fully characterized. The Covariance Matrix Adaptation-Evolution Strategy has been used to estimate identifiable fracture sets conductivities from well tests data. The global sensitivities of the conductivities are computed during optimization from a response surface methodology and the Sobol decomposition technique.

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MS16

A Linear Finite-element Node-centered Finite-volume Method Including Jump Discontinuities Applied to 2-phase Fracture / Matrix Flow

Using operator-splitting, we compute pressure / velocity with the FEM and 2-phase transport with the FVM. At material interfaces, where saturation can become discontinuous, we enrich this discretisation with as many degrees of freedom as materials are joined. Additional functionality computes sector-to-sector fluxes, retaining higher-order accuracy, and pressure on the enriched mesh. An implicit calculation of nonlinear diffusive transfer processes across fracture-matrix interfaces complements our new method.

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MS16

Flow simulation in 3D Discrete Fracture Networks

The simulation of flow in discrete fractured media leads to solve very large linear systems. Those systems are sparse and with a specific shape due to the underlying physical problem. In order to solve efficiently this type of systems, different solvers have been tested. We used both direct and iterative ones. The iterative solvers were based on a multigrid method or a conjugate gradient with various preconditionings. Sequential and parallel versions were tested on clusters.

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MS17

An Inverse Problem for Coupled Heat-Groundwater Transport in the Shallow Subsurface

In an effort to improve synthetic thermal imagery for remote sensing technologies, a suite of closely coupled numerical simulators has been developed. This computational testbed includes thermal and moisture transport finite element models, coupled with solar and vegetation models. It is well suited for simulations of specific scenarios, which otherwise might be difficult and time consuming to reproduce in the field. This talk will focus on the inverse problem related to determining material properties.

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MS17

Forecasting Subsurface Model Performance During Simulation-based Optimization

In subsurface transport models, constraint violations may occur before complete simulation of the remediation time-frame. A new approach exploits this behaviour by monitoring remediation constraints during simulation. For a given function evaluation, simulation is pre-empted (terminated early) if infeasible results are forecasted. A demonstration problem is presented involving the design of a barrier system constructed from sorptive materials. Results suggest that model pre-emption can significantly reduce computational cost without affecting solution quality.

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MS17

Inverse Modeling for Non Linear Groundwater Systems with Local RBF and Global Optimization Algorithms with Application to a Large Chinese Aquifer

We present new optimization algorithms for identifying parameters in nonlinear partial differential equation models of groundwater aquifers. The approach incorporates both local and global optimization methods. It includes the use of response surfaces of the objective function in order to reduce the number of times the computationally expensive PDE model must be computed. The method is applied to data from a large (456 sq km) aquifer that supplies water to Beijing, China.

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MS17

Simulation-based Nonlinear Least Squares Fitting

In this talk we will discuss the development of a trust region-based derivative-free optimization solver for nonlinear least squares problems. Our emphasis is on achieving rapid decrease of the residuals since the simulation-based objectives of interest to us are computationally expensive and rarely allow for many evaluations. The central issue is managing the set of models as the evaluation history grows. We will illustrate the algorithm on a variety of scientific applications.

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MS18

Quasi-Positive Families of Continuous Darcy-Flux Finite Volume Schemes

Families of continuous Darcy-flux control-volume distributed (Multi-point flux Approximations) CVD(MPFA) finite volume schemes are presented for the general full-tensor porous media pressure equation. These schemes maintain flux and pressure continuity while only depending on a single degree of freedom per control-volume. The new families of schemes are compared with earlier formulations in terms of quadrature range, numerical convergence and stability for challenging problems involving high full-tensor anisotropy.

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MS18

Fully Conservative Streamline Methods for Two-phase Flow

Linear transport of a tracer in an ambient fluid can be approximated by a fully conservative characteristic or Lagrangian method in which both fluids are conserved locally. Nonlinear two-phase flow is a similar transport problem, except that streamlines and characteristics no longer coincide. We extend linear characteristic methods to two-phase streamline methods in one space dimension, preserving the masses of both fluids. Our method is effective with time-steps that are several times the CFL step.

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MS18**Control Volume Mixed Methods and Relationships to MPFA**

The control volume mixed finite element method (CVM-FEM), applied to flow equations in porous media, is a variant of the RT₀ mixed method in which finite-volume vector velocity test functions yield a discrete Darcy law on control volumes, in addition to the usual cell-by-cell conservation. The talk will discuss new results on superconvergence for CVMFEM on distorted quadrilaterals, analysis of CVMFEM with mortar couplings, and schemes that combine features of CVMFEM and multipoint flux approximation (MPFA).

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MS18**A Mortar Multiscale Solver for Stochastic Approximations of Flow in Random Porous Media**

Recent work has shown that the construction of a multi-scale basis for the mortar mixed finite element method can greatly reduce the computational cost in solving the coarse scale interface problem. We show that this multiscale basis only needs to be computed for the mean of the random field and can be reused as an efficient preconditioner for each of the subsequent stochastic realizations.

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MS19**Modeling the Pore Space in Carbonate Reservoirs by Using Acids**

Carbonate reservoirs can contain large fractures that can cause short circuit flows leaving much oil unproduced. This paper investigates the idea of permeability reduction in the fracture by injection of a mixture of acids. A 1-D simulation shows that upstream dissolution and downstream precipitation of CaSO₄ are the dominant processes. A 2-D simulation shows that downstream fractures are clogged, whereas continuously wormholes are created upstream. A

comparison to experimental results is made.

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MS19**Modelling Microbial Clogging in Porous Media on the Darcy Scale**

A concept is presented to model biomass accumulation in the subsurface on the Darcy scale. It accounts for bacterial growth, deposition of bacteria on the porous medium, detachment, decay, and the effects of biofilm growth on the hydraulic properties of the porous medium. The intended application is the simulation of the plugging of damaged or fractured cap-rock in injection well vicinity in a CO₂ storage reservoir and the protection of well cement against corrosion using biofilms.

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MS19**Fast-reaction Asymptotics for a Reaction-diffusion System with Distributed Microstructure**

We investigate a reaction-diffusion process in a two-phase medium with microscopic length scale ϵ . The diffusion coefficients in the two phases are highly different ($d_1/D = \epsilon^2$) and the reaction constant k is large. First, the homogenisation limit $\epsilon \rightarrow 0$ is taken, which leads to a two-scale model. Afterwards, we pass to the fast-reaction limit $k \rightarrow \infty$ and obtain a two-scale reaction-diffusion system with a moving boundary traveling within the microstructure. This results are the outcome of a joint work with Sebastian A. Meier (Bremen, Germany).

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MS19**Biofilms in Porous Media: Theoretical and Exper-**

imental Advances

I will discuss efforts, developed over the last 10 years, to formally upscale the transport and reaction processes associated with biofilms in porous media. Our results to date are *multi-scale*, starting from the cell scale, and currently ending (after a sequence of upscaling efforts) at the Darcy scale. Both local mass equilibrium and non-equilibrium models have been examined. I will also discuss recent successes in imaging biofilms in porous media using x-ray tomography.

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MS20

Coupled Hydro-Geomechanical Analysis of Fault Reactivation and Water Induced Compaction

Injection and production of fluids cause changes of pressure, temperature and saturation that affect the state of stress in oil reservoirs, resulting in porosity and permeability variations. It is therefore a coupled hydro-geomechanical problem. Reservoir simulation with geomechanical coupling, considering the appropriate constitutive behavior of the materials, allows realistic modeling of water induced compaction and fault reactivation, that can influence in the production of oil due to pressure and fluid loss in the reservoir.

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MS20

Macroscopic Effects of Dissolution of Intergranular Contacts: A Multi-scale Analysis

The paper investigates dissolution/diffusion phenomena that occur within the intergranular contact and their influence on macroscopic behavior of chalk rocks. The intergranular interface is modelled as an evolving structure in which the contact between grains takes place along a set of isolated islands surrounded by fluid. The mathematical description of dissolution and diffusion processes is obtained by incorporating molecular and volume averaging. Extensive numerical studies of interface structure evolution are carried out. The macroscopic description of chemo-mechanical coupling is formulated by invoking an evolution law that employed the notion of a dual time scale associated with the intergranular contact evolution.

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MS20

Reactive Transport in Porous Media: Multiple-Scale Analysis, Instability Phenomena

Reactive transport in porous media is of paramount importance in many applications. Finding the correct chemical reaction scheme is one of the major modelling complexity. However, coupling with transport brings additional difficulties. Two-types of difficulties are considered in this review of recent results: (i) multiple-scale problems, with the development of effective surface properties and "homogenized" models taking into account the various scales of the pore and media geometry, as well as surface roughness and heterogeneity, (ii) hydrodynamics instabilities during dissolution processes.

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MS20

Numerical Solution to an Integro-differential Equation Modeling Swelling Porous Materials

We demonstrate the results of a discrete scheme used to solve a nonlinear model of a swelling porous material. The model is cast as a Volterra partial integrodifferential equation (VPIDE) of the second kind where the dependent variable is the liquid phase volume fraction. A pseudospectral differentiation matrix is constructed to compute the spatial derivatives and a Volterra Runge-Kutta scheme is used to solve the VPIDE at each time step.

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MS21

Setup of the MoMaS Reactive Transport Benchmark

We will present here the definition of the reactive transport benchmark of MoMaS. According to the interests of MoMaS, the reactive transport problem should be representative of the problems encountered in nuclear waste disposal simulations. Moreover, we want to interest a community as large as possible: geochemistry, hydro geology, numerical methods, applied mathematics... Nevertheless, the high complexity of both transport and chemical phenomena occurring in such a system may be an obstacle for some researcher who may not be familiar with hydrogeological and geochemical concepts. The problems proposed here are built on the same mathematical concepts as real hydro-geochemical problems, but their description has been simplified. The difficulty for building this benchmark was also to provide a sufficient simple problem without loss of mathematical and numerical difficulties. The objectives of this benchmark are to propose a challenging test for numerical methods used on reactive transport modelling in porous media. In order to focus on numerical methods, the problem presented here is on quite small size, from hydrodynamic and from geochemical point of view. To obtain a really challenging test, the chemical coefficients presented in this benchmark are not real one; but they are still realistic. This benchmark consists in three independent parts, ranked by complexity: Easy, Medium, Hard. Each part consists of a 1D and a 2D reactive transport problem. The flow and transport phenomena are the same for the

three parts. From one part to the other, some chemical phenomena are added increasing the difficulties.

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MS21

Results of the GdR MoMaS Reactive Transport Benchmark with RICHY2D

In this talk the software RICHY2D for the simulation of reactive transport in porous media and computational results for nine of the twelve MoMaS benchmark problems are presented. The software is based on the one-step method. In order to reduce the size of the resulting discrete problems, it uses a reformulation of the system. RICHY2D is based on M++ a platform for solving systems of nonlinear partial differential equations with Finite Elements in parallel.

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MS21

Coupling Transport and Chemistry in Porous Media with a Newton-Krylov Method: Application to the MoMaS Benchmark

Reactive transport modelling leads to the coupling between a set of advection-diffusion PDE's, and a set of algebraic equations. The resulting nonlinear system is solved by a Newton-Krylov method (which does not require storing the jacobian matrix), using as main unknowns the total mobile and total immobile concentrations. The main advantage is to keep chemistry distinct from transport, while still providing a globally coupled algorithm. We validate the method on the 1D and 2D MoMaS benchmark.

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MS21

Numerical Results with a Global Method for 2D

Reactive Transport Problems

We have developed a global numerical method for reactive transport problems based on a robust and efficient Differential Algebraic Equations (DAE) solver. The coupled Partial Differential Algebraic Equations (PDAE) are first discretised in space by a finite difference method. The resulting DAE are then discretised in time by a BDF method in association with a modified Newton-LU method. We have used our method to simulate 2D problems, in particular some of the Geochemistry MoMaS benchmarks.

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MS22

Data Assimilation for a Viscous Incompressible Fluid

We study the inverse problem of determining the initial state, and possibly the forcing, of a viscous incompressible fluid observed directly or indirectly over a period of time. We will formulate this as a Bayesian inverse problem, giving rise to a probability measure on function space for the initial vector field, and the forcing (or model error). We will describe effective MCMC methods that allow us to sample from such a distribution, and present some numerical results.

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MS22

Quantifying Robustness of Mixing Diagnostics Inferred from Satellite Altimetry

Several recent studies make use of satellite altimetry data to infer mixing diagnostics in the global surface ocean. The reliability of these diagnostics is unclear, however: in particular, the effect of unresolved scales on turbulent transport cannot be quantified. We examine a range of mixing diagnostics in simulations of quasigeostrophic and surface quasigeostrophic turbulence and directly probe their dependence on sampling resolution. In this way, we aim to quantify the robustness of altimetry-inferred mixing diagnostics.

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MS22**Relative Dispersion in the Atmosphere and Ocean**

A signature of Lagrangian chaos is that the separation between two particles deployed at slightly different positions in a flow will grow exponentially in time. In this talk we examine the statistics of particle pairs from in situ experiments in the atmosphere and ocean. There are indeed indications of exponential growth at smaller spatial scales, but the behavior at larger scales differs, apparently due to the large scale circulation.

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MS22**Effective Diffusivity: A Tool to Quantify Inhomogeneous, Instantaneous, and Irreversible Transport**

When advection-diffusion of a passive tracer is described with respect to the level set of the tracer itself, it becomes pure diffusion with a spatially and temporally varying diffusion coefficient. I will review this effective diffusivity formalism, its relationship to other metrics of statistical mechanics, its applications to quantify inhomogeneous mixing in the ocean and atmosphere, and some ideas for parameterization.

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MS23**An Experimental Setup of Ground-based and Airborne Systems to Study Spatio-temporal Structures in Atmosphere-Land Surface Energy, Water and CO₂ Exchange**

Exchange processes between land surface, vegetation and atmosphere over structured, inhomogeneous regions are investigated in an experimental approach. For that purpose ground-based long-term monitoring and dedicated campaigns are combined within the Rur catchment, Germany. Four campaigns covering different vegetation periods have been performed with instrumentation ranging from leaf level gas exchange, eddy correlation stations, scanning remote sensors to aircraft observations. Synergistic data analysis shall reveal spatio-temporal structures in the exchange processes and their relation to external parameters.

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MS23**Patterns in Soil-Vegetation-Atmosphere Systems: Theory, Modeling and Data Assimilation**

The Transregio 32 is an interdisciplinary project based on the hypothesis that explicit representation of patterns in the soil-vegetation-atmosphere system in experimental and theoretical studies will improve our understanding and predictions of the pertinent mass, energy, and momentum fluxes and their interactions. We will provide an overview of the research activities at the Universities of Bonn, Cologne and Aachen and the Research Center Jlich including the application of coupled simulation tools in conjunction with measured data and data assimilation techniques

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MS23**Non-invasive Methods and Modelling Approaches to Study the Impact of Subsurface Structures on Flow and Transport**

Geophysical methods may play an important role in managing our terrestrial environment and in maintaining ecosystem functioning and services. Especially, the application and further development of hydrogeophysical methods combined with mathematical models seem very promising to maintain and protect soil and groundwater quality. Hydrogeophysical methods may help to improve our control on storage, filter and buffer functions of soils and groundwater systems. Moreover, methods are needed that will help us to bridge the gap between the scale of measurements and observations and the scale at which management of terrestrial systems takes place. In this presentation several examples will be presented showing how hydrogeophysical research can contribute in meeting these challenges and may be used to characterize subsurface water flow and transport.

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MS23**Atmospheric-land Feedbacks in Clear and Cloudy Boundary Layers**

We investigated the effect of land surface heterogeneity on cloud formation using a large eddy simulation model. Our study showed that by altering the turbulent structure of the atmospheric boundary layer, heterogeneity may create conditions that are favourable for cloud formation. However, the results of the model are sensitive to the numerics. The choice of the advection scheme has significant influence on the transport over the interface between the turbulent boundary layer and the laminar free atmosphere, which is at the height at which clouds form.

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MS24

Analysis and Algorithms for a Regularized Cauchy Problem arising from a Non-Linear Elliptic PDE for Seismic Velocity Estimation

We derive and study nonlinear elliptic PDE's in 2D and 3D connecting the Dix velocity and geometrical spreading of the image rays, and hence the true seismic velocity which is a product of the Dix velocity and the geometrical spreading. The physical setting allows us to pose only a Cauchy problem, and hence is ill-posed. However we are still able to solve it numerically on a long enough interval of time to be of practical use.

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MS24

Review of Recent Advances in Time-domain Seismic Imaging

Abstract not available at time of publication.

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MS24

Ray-theoretical Aspects of Seismic Time Migration and Demigration

This work is devoted to a ray-theoretical analysis of elementary wavefields inherent to time migration and demigration of seismic data. For such processes we base ourselves on the standard hyperbolic traveltimes approximation with respect to source-receiver offset and migration aperture. Essential is also the construction of two-way surface-to-surface ray propagator matrices corresponding to normal rays, for which the slowness vector is normal to the subsurface reflector, and image rays, for which the slowness vector is normal to the measurement surface in the time-migration domain. The combination of such matrices provides useful insight into the processes of seismic migration and demigration.

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MS24

Time Migration Velocity Analysis by Image-wave Propagation in the Common-image Gatherers

Image-wave propagation or velocity continuation describes the repositioning of a migrated seismic event as a function of migration velocity. In the common-image gather (CIG) domain, it can be used for iterative migration velocity analysis. Continuation of CIGs allows to detect those velocities at which events flatten. A correction formula translates constant flattening velocities into varying time-migration velocities. Thus, the migration velocity model can be improved iteratively until a satisfactory result is reached.

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MS25

An Hybrid Finite Volume Method for Two Phase Flow Problems: Formulation, and Numerical Results

We will present extension of Sushi finite volume method in the case of two phase flow in porous media. The scheme uses unknowns at the centre of the cells and unknowns on the interfaces. In relation with these last unknowns, we have to ensure continuity of some fluxes : different choices can be retained and we will discuss this point. We will compare our results with results obtained by other methods as mixed finite elements.

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MS25

Cell Centered Finite Volume Schemes for CO2 Ge-

ological Storage Simulations

In this talk, we study the near well discretization of CO₂ storage models using cell centered multipoint flux approximation schemes for the Darcy fluxes. The finite volume discretization uses an hybrid mesh connecting a near well radial mesh to the reservoir mesh for a deviated well. The system of equations is a two phase two components Darcy flow model with dissolution of the CO₂ component into the aqueous phase.

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MS25

Discretisation Schemes for Anisotropic Heterogeneous Problems on Near-Well Grids

In this work, we construct analytical solutions for near-well flow which is not aligned with a radial inflow pattern. These solutions resemble strongly heterogeneous, possible anisotropic media, which is less accounted for in existing near-well models. We compare different control volume discretisation schemes and radial-type grids for such cases, and give their convergence behavior. The results of these singlephase flow test cases are supported by multiphase flow simulations.

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MS26

Local-global Two-phase Upscaling of Flow and Transport in Heterogeneous Formations

We present a local-global two-phase (LG2P) upscaling approach to generate upscaled transport functions. The LG2P upscaling directly incorporates global coarse-scale two-phase solutions into local upscaling. It effectively captures the impact of global flow, while avoiding global two-phase fine-scale simulations. Local boundary conditions are updated with time-dependent coarse solutions, therefore capturing the global flow both spatially and temporally. Through various examples, we show that the method consistently provides accurate coarse models for both flow and transport predictions.

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MS26

Dynamic Upscaling of Multiphase Flow in Porous Media Via Adaptive Reconstruction of Fine Scale Variables

We propose an upscaling method that is based on dynamic simulation of a given model in which the accuracy of the upscaled model is continuously monitored via indirect error-measures. If the indirect error measures are bigger than a specified tolerance, the upscaled model is dynamically updated with approximate fine scale information that is reconstructed by a multi-scale finite volume method. The new upscaling algorithm is validated for two-phase, incompressible flow in heterogeneous porous media.

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MS26

Generic Global Scale-up: Advantages and Challenges

Generic global scale-up is based on global flow solutions obtained using generic boundary conditions as opposed to well-driven boundary conditions tailored to specific flow scenarios as in other global scale-up methods. This paper review some of the advantages of generic global scale-up, its relation with global multiscale finite element methods, and the challenges in its practical applications. Some practical resolutions to address the challenges are also discussed.

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MS26

Numerical Upscaled Model of Transport with Non-separated Scales

We show numerical results for a new model for advection-diffusion-dispersion in porous media in the presence of multiple scales which are not necessarily well separated. The model, developed theoretically in prior work and motivated by experiments of Haggerty et. al., includes as special cases the classical homogenized model as well as the double porosity models, but is characterized by presence of additional memory terms. We discuss various discretizations for the model with special attention paid to handling the new memory terms. Most significant issue is how to detect which terms are important in what regimes of flow and transport and how the model compares with experimental

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MS27

A Unified Mixed Formulation Naturally Coupling Stokes and Darcy Flows

Solving Stokes-Darcy coupled flow using stable Galerkin formulations for both subproblems usually leads to unbalanced rates of convergence. We present a stabilized mixed FEM for Darcy flow, compatible with Galerkin stable elements for Stokes, with balanced rates of convergence for velocity and pressure. The discontinuities of the solutions on the interface of the free fluid and the porous medium are incorporated in the finite element approximation by linear transformations derived from the interface conditions.

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MS27

The Chaotic Dynamics of Anomalous Dispersion as Models by a Nonstationary extension of Brownian Motion

Given an arbitrary mean square displacement, we show how to construct a family of stochastic processes with this displacement and with independent, nonstationary increments. The resultant process is used to model anomalous and classical diffusion. By computing the fractal dimension it is shown that the complexity of the family of processes is the same as that of Brownian motion. An analytical expression is developed for the finite-size Lyapunov exponent and numerical examples presented.

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MS27

Domain Decomposition for Poroelasticity and Elasticity with DG Jumps and Mortars

We couple a time-dependent poroelastic model in a region with an elastic model in adjacent regions. We discretize each model independently on non-matching grids and we realize a domain decomposition on the interface by introducing DG jumps and mortars. The unknowns are condensed on the interface allowing the computation in each subdomain to be performed in parallel. We establish error estimates for an algorithm where the computation of the

displacement is time-lagged.

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MS27

Preferential Flow and Geomechanics

Dynamic capillary pressure effects alter classical parabolic models of filtration flow to those of pseudoparabolic type. These effects become substantial in fast processes or at small scales. We consider these issues in the filtration through elastic porous media with such pressure-saturation relationships.

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MS28

Multi-D Upwinding for Multi-Phase Transport in Porous Media

Multidimensional methods for hyperbolic equations can lessen the correlation of numerical errors with the computational grid reducing bias in inherently unstable flow problems. We present a family of monotone multidimensional methods for two-phase flow with gravity, which is extendable to more general scalar hyperbolic equations. A local coupling in the flux calculation is introduced through the use of interaction regions resulting in a compact stencil and extension to any grid topology.

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MS28

Multidimensional Upwind Schemes for Flow in Porous Media on General Quadrilateral and Triangular Grids

Standard reservoir simulation schemes employ single-point

upstream weighting for convective flux approximation. These schemes introduce both coordinate-line numerical diffusion and cross-wind diffusion into the solution that is grid and geometry dependent. New locally conservative higher-order multi-dimensional upwind schemes that minimize both directional and cross-wind diffusion are presented for convective flow approximation. The schemes are coupled with full-tensor Darcy flux approximations. The new schemes are comprised of two steps; (a) Truly multi-dimensional upwind approximation, which involves flux approximation using upwind information obtained by upstream tracing along wave-vector paths where wave information travels in multiple dimensions. Multi-dimensional formulations using edge-based and cell-based approximations that reduce cross-wind diffusion are presented. Conditions on tracing direction and CFL number lead to a local maximum principle that ensures stable solutions free of spurious oscillations. (b) Higher-order approximation that corrects the directional diffusion of the approximation. Benefits of the resulting schemes are demonstrated for convective reservoir simulation test cases involving a range of unstructured grids and permeability fields. While standard simulation methods yield relatively poor results for such cases, the new methods prove to be particularly effective.

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MS28

Eulerian-Lagrangian Methods for Multiphase Multicomponent Transport

Transport in porous media is often advection-dominated. This leads to efforts to incorporate Lagrangian techniques into numerical schemes, in order to overcome CFL limitations, numerical dispersion, and non-physical oscillations. In multiphase transport, these efforts are made easier by working with an adjoint system, whose natural interpretation is in terms of mass movement rather than wave propagation. The talk will explain this in the context of Eulerian-Lagrangian methods for multiphase multicomponent transport and will outline some recent developments.

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MS28

Discontinuous Galerkin Methods for Transport in Porous Media

Two-phase flow in porous media has important applications for petroleum reservoir engineering and groundwater processes. Both applications may involve multiple time and spatial scales, long simulation time periods, and many coupled nonlinear components. In particular, the advection-dominated component and the nonlinear coupling of compressibility, capillary pressure and relative permeabilities often result in sharp saturation fronts, which demands steep gradients to be preserved with minimal oscillation and numerical diffusion. In this talk, we consider the combined method of discontinuous Galerkin (DG) and mixed finite element (MFE) for simulating two-phase flow

in porous media. A number of numerical examples are presented to illustrate computational advantages of DG methods for porous media flow, with emphasis on the treatment of capillary pressure heterogeneity and the dynamic mesh modification.

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MS29

Stochastic Velocity Field Models for Eddy-Rich Flows

Recent high-resolution radar observations of surface velocity have revealed submesoscale eddies in the coastal areas. By an objective estimation method, eddies are detected and their parameters such as center coordinates, size, and intensity are estimated. The obtained statistics are used to parametrically represent the birth-death process of eddies via a model stochastic velocity field known as inlar flow. The model is developed further to represent the eddy amplitude decay more accurately.

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MS29

Solving the Pressure Poisson Equation in Large-aspect Ratio Ocean-shaped Domains

A key challenge in the development of non-hydrostatic ocean models is that the Poisson equation for pressure must be solved in a domain with extremely large aspect ratio ϵ . This leads to a matrix with a condition number which is bounded from below by $c\epsilon^{-2}$ for some positive constant c as $\epsilon \rightarrow 0$, in the case in which Neumann boundary conditions are applied everywhere. Since the convergence rate (required number of iterations for a given tolerance) for iterative solvers scales with condition number, this makes standard iterative solvers extremely slow. However, in the case in which Dirichlet boundary conditions are specified, the condition number is bounded from above by the condition number of the matrix which one must solve for a hydrostatic model. This motivates the preconditioner approach used by the MITgcm ocean model. However, as formulated, that approach can not easily be extended to fully unstructured meshes such as those used by the Imperial College Ocean Model (ICOM). In this talk, we prove some estimates on the condition number for finite element discretisations of the Poisson equation in the large aspect ratio limit, and suggest a new approach for preconditioning the matrix system based integrating an approximated reduced system for the top surface boundary condition in a multi-grid solver. These solvers enable previously unachievable simulations in large aspect ratio domains (such as three-dimensional gyres) and we will present some of our latest results from these simulations.

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MS29**CABARET in the Ocean Gyres**

A new high-resolution numerical method is proposed for modelling quasigeostrophic mesoscale ocean dynamics in eddying regimes. The method is based on a novel, second-order non-dissipative and low-dispersive conservative advection CABARET scheme. The properties of the new method are applied to the classical model of the double-gyre ocean circulation. It is demonstrated that, in turbulent regimes, the new method leads to a significant acceleration of the numerical solution convergence, in comparison to the conventional second-order method.

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MS29**Large Eddy Simulation of Sub-mesoscale Motion Due to Surface Frontal Instability**

The behavior of ocean flows at the sub-mesoscale range is poorly understood despite its importance for many practical problems, such as the short-term dispersion of pollutants and oils spills. Most ocean models rely on hydrostatic dynamics, mixed-layer and subgrid-scale parameterizations to represent these processes. In this study, large eddy simulations of frontal instability are carried out and mixing across the front is quantified using background potential energy, drifter releases to compute finite-scale Lyapunov exponents and relative dispersion.

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MS30**Improving Time Integration by Conservative Regularization of Atmospheric Equations**

We present a conservative regularization approach to the compressible Euler equations that replaces the pressure gradient in the momentum equations by the gradient of a smoothed pressure field. The smoothing selectively slows down the fastest sound wave components only, without altering the slow dynamics and does not introduce additional viscosity. We will present numerical results from a 2D ver-

tical slice model.

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MS30**Peer Methods for the Compressible Euler Equations.**

A new time-splitting method for the integration of the compressible Euler equations is presented. It is based on a two-step peer method which is a general linear method with second-order accuracy in every stage. The scheme uses a computationally very efficient forward-backward scheme for the integration of the high-frequency acoustic modes. With this splitting approach it is possible to integrate stably the compressible Euler equations without any artificial damping. The peer method is tested with the dry Euler equations and a comparison with the common split-explicit second-order three-stage Runge-Kutta method by Wicker and Skamarock shows the potential of the class of peer methods with respect to computational efficiency, stability and accuracy.

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MS30**Auxiliary Variables and Deferred Corrections for Divergence Constrained Flows**

A class of methods for the numerical solution of incompressible and low-Mach number flows based on a novel combination of deferred corrections and auxiliary variables is presented. Temporal integration is done using spectral deferred corrections which allow multiple terms in an equation to be treated either implicitly or explicitly and with different time steps and can easily be constructed to attain high formal order of accuracy. These methods are combined with a finite volume discretization of an auxiliary variable formulation of the equations of motion to produce higher-order accurate flow solvers. The key idea in auxiliary variable methods is to formulate an equation for a variable which does not have an explicit divergence constraint but from which the desired constrained velocity can be numerically extracted by the analog to the procedure used in projection methods. Examples from incompressible, 0-Mach, and low-Mach number flows will be presented.

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MS30**A Discontinuous Galerkin Hp-Adaptive and Time Implicit Mesoscale Model**

Moore's law predicts a doubling in available computing power every 18 months: at this rate a $O(1km^2)$ global

climate simulation will only be achievable 30 years from now with the numerical methods currently employed in atmospheric models. We explore a class of linearly implicit time-stepping methods: Rosenbrock W-methods. With preconditioning techniques, they offer an efficient way of integrating the compressible Euler equations. We also discuss a new way to reduce the cost of evaluating Jacobians.

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MS31

Velocity Model Determination by Double Path-integral Imaging

Path-integral imaging sums over the migrated images for a set of migration velocity models. Those velocities where common-image gathers align horizontally are stationary, thus favoring these images in the sum. Thus, the image forms without knowledge of the velocity model. By executing the path-integral imaging a second time using the velocity as a weight factor in the sum, the stationary velocities can be extracted by a division of the two images.

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MS31

Unconventional Methods for Seismic Imaging

Abstract not available at time of publication.

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MS31

Generalized Moveout Approximation for Anisotropic Waves

In this paper, we consider the hyperbolic, the shifted hyperbola, the rational and the generalized traveltime approximation for the qP- and qSV-waves in a homogeneous VTI medium. We also consider the qP-wave in acoustic approximation. Fomel and Stovas (2009) proposed the generalized moveout approximation with other approximations being the special cases. Being compared with the hyperbolic, shifted hyperbola and rational approximations in few examples, the generalized approximation gives the best results.

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MS31

Fourth-order Statistics for Seismic Parameter Es-

timation

In statistics, semblance is related to the second moment and in optimization, to the least-squares solution of maximum signal energy as a characterization of reflection events. We define extensions of semblance by replacing second-order by higher-order quantities. These semblance measures behave differently in the estimation of Common-Reflection-Surface parameters by means of the hyperbolic traveltime approximation applied to multicoverage data. We find improved parameter estimates using a fourth-order semblance.

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MS32

Commercial Simulation Software for Porous Media: Capabilities and Developments

In structural engineering, automotive, oil-gas or aircraft industries the commercialization of computational mechanics software is fairly advanced. Today, a powerful finite element/finite volume technology has been established there in hands of only a few big players worldwide. In contrast, however, looking to porous media, where we mainly focus on subsurface water resources, environmental, geothermal and industrial porous material problems, the situation is rather different. Surprisingly, the water resources market is still widely dominated by a classic finite difference program, the USGS code MODFLOW, available for free (except GUI), which stems from the eighties and possesses in the meantime a number of extensions and adaptations. It has similarities to an open-source development project. On the other hand, there is an increasing number of research codes at universities funded by public authorities, which cover a large disciplinary spectrum ranging from multi-phase flow via chemical reaction systems, fracture flow modeling, deformation processes to different numerical approaches. It suggests that most of the problems seem now solvable and those software products could satisfy most desires in research and practice. Nevertheless, there are also commercial simulation software systems, for example FEFLOW, which has shown a further growing potential in the porous media market. In the present paper we will discuss the scope and requirements for such a commercial porous media modeling system. We critically ask: who needs commercial software, for what and what are the basic requirements, advantages and challenges? Where are the deficiencies and technological constraints? We characterize the status quo regarding the capabilities available, numerical features and inherent software technology. In developing innovative and globally competitive software products the following guiding principles become more important: depth and breath of capabilities, completeness (modeling

that works), availability and usefulness (GUI, interfaces, service, teaching), scalability as well as adaptive architecture. From the current stage we give an outlook to future needs and progressing software developments. Examples are given for geothermal applications and large-swelling absorbing porous materials.

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MS32

Applications of Software Tools D3F and R3T for Coupled Problems of Variable Density Flow and Transport in Porous Media

The software tools D3F and R3T can solve numerically several complex applications of subsurface flow and transport problems. The tools are based on library UG (Unstructured Grids) that enables the computations on complex geological domains discretized by an unstructured, locally adapted, multilevel grid that can be redistributed on processors of parallel computer. The tool D3F (Distributed Density Driven Flow) solves nonlinear flow and transport equation that are fully coupled due to the dependence of fluid density on transported concentration. The tool R3T (Retardation, Reaction, Radionuclides, Transport) solves many nonlinear transport equations that are coupled due to reactions (e.g., decay, slow and fast sorption, etc.) and where the transport is dominated by the advection determined from the D3F velocity field. In this talk we introduce not only the most interesting features of these software tools (implicit/explicit in time discretizations, Newton solvers with analytic linearization, level set methods, etc.), but also the experiences of a general interest concerning the development and the usage of complex software tools for this type of problems.

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MS32

Discontinuous Galerkin Method for Convection Dominated Transport in Porous Media Using DUNE

In this paper we present software techniques as well as recent development of the software package DUNE and in particular of the module DUNE-FEM. For several test problems as well as for more complex applications, such as the simulation of fuel cells, we present numerical results. These results have been obtained using modern simulation techniques such as higher order continuous and discontinuous Galerkin methods (also in a stabilized version) in combination with local grid adaptivity. Since we are interested in the simulation of complex problems the parallelization of the code has been taken into account. In adaptive simulations this becomes a non-trivial part since dynamic load balancing needs to be done. Applied to different problems the code shows a very good scalability even on a high number of processors.

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MS32

Simulation of Density and Temperature Driven Flow and Contaminant Transport in Fractured Porous Media Using d3f and r3t

In this talk, we discuss the mathematical models and the numerical methods for the simulation of the density and temperature driven flow and the contaminant transport in fractured porous media. The fractures are represented by manifolds with the reduced dimensionality. In the fractures, we consider the same phenomena as in the bulk medium. The discretized PDEs for the bulk medium and the fractures are solved as a coupled system by the Newton method with the multigrid linear solver. We present numerical results obtained using the simulation programmes d3f and r3t extended to the case of the fractured media.

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MS33

Mixed Multiscale Finite Element Methods using Limited Global Information

I will describe mixed multiscale finite element methods using limited global information. In particular, I will stress how multiple global information can be incorporated into multiscale basis functions. This is a joint work with J. Aarnes and L. Jiang.

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MS33

A Loosely Coupled Hierarchical Fracture Model for the Iterative Multi-Scale Finite-Volume Method

Recently, the multi-scale finite volume (MSFV) method for flow in heterogeneous porous media was combined with an efficient iterative procedure, which allows to converge solutions to the corresponding fine-scale references. Here, this iterative MSFV (iMSFV) method is extended by a hierarchical fracture model, where the flow in the resolved fracture network is represented on lower dimensional manifolds. Therefore, a similar datastructure as for the well

treatment in the MSFV context is employed.

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MS33 Multiscale Simulation of Fractured Reservoirs

In recent years, many different (but related) methods that attempt to capture the multiscale behavior of flow in heterogeneous reservoirs have been developed. Here, we extend our own previous models (variational multiscale mixed methods) for the simulation of flow in fractured reservoirs, in which fractures are viewed as entities of lower dimensionality than the domain. We will conclude the presentation with results for realistic problems.

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MS33 A General Iterative Scheme for the Multiscale Finite Volume Method

In the Multiscale Finite-Volume (MSFV) method a conservative velocity field is constructed from an approximate pressure field, which is obtained by superimposition of local solutions coupled by a global problem. Due to the localization assumption, the MSFV solution differs from the exact solution of the problem. By estimating the localization error, an iterative algorithm can be constructed that converges to the exact solution and conserves mass at any iteration.

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MS34 Deformation of Porous Media on the Pore Scale and Induced Variations

The deformation of porous media is calculated by solving the elastostatic equations discretized on unstructured meshes made of irregular tetrahedra. The macroscopic conductivity and permeability necessitate the resolution of the Laplace and the Stokes equations on the initial and deformed meshes. Applications will be provided for a number of media either reconstructed or measured by microtomography. Results relative to the evolution of the media and of the macroscopic properties of the media will be presented.

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MS34 Bounds of Dynamic Permeability and Related Problems

Transfer coefficients within porous media are assessed by combining the physical principles of the homogenization of periodic media and the geometrical simplifications of the self-consistent method. This approach provides two static and dynamic permeability assessments that enable to build bounds for a wide class of media. Similarly the Klinkenberg effect for rarefied fluids is estimated. As for diffusion problems, estimates of trapping coefficient and of thermal permeability involved in the dynamic gas compressibility are given.

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MS34 How to Model Dispersion in Unsaturated Double Porosity Medium? An Integrated Approach

Multi-scale, multi-components, multi-phases are the key words that characterize the double porosity media subject to geo-environmental conditions. In relation to this context we present an integrated upscaling approach which combines three issues: theoretical, numerical and experimental. A physical model was designed to imitate the double-porosity media and to enable performing the dispersion experiments in fully controlled conditions. The modelling is based on the observations and follows the logic: from micro towards macro.

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MS34 A Three-Scale Model of pH-Dependent Flows Including Ion Adsorption in Kaolinite Clays

A new three-scale model to describe the coupling between pH-dependent flows and ion transport in kaolinite clays is proposed. The porous medium is characterized by three separate nano-micro and macroscopic length scales. The pore (micro)-scale is characterized by micro-pores saturated by an aqueous solution containing four monovalent ionic species and charged solid particles surrounded by thin electrical double layers. The two-scale nano/micro model is homogenized to the macroscale leading to the derivation of effective equations.

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MS35

Statistical Distributions of Conservative and Reactive Species Concentrations in Heterogeneous Porous Media

We present a semi-analytical method of deriving the full probability distribution of concentration at observation points or volumes, which is based on first-order approximations of one- and two-particle displacements. The resulting concentration *pdf* approximately follows a beta distribution. This *pdf* can be mapped to the concentration *pdfs* of species that react upon mixing. Estimates of mean values and standard deviations based on second-order perturbation analysis rather than mapping entire *pdfs* are biased.

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MS35

Combined Deterministic and Stochastic Sensitivity Analysis - Application to Uncertainty Analysis

For a model $y=f(x)$, x uncertain vector, we want to 1) resume the influence of components of x on components of y , 2) use it for uncertainty analysis. We first choose simple o,p so, that the singular value decomposition (SVD) of $(p(F(o)))'(x)$ is almost independent of x (deterministic analysis). The SVD of $[\text{cov}(p(y),o(x))] \text{inv}([\text{cov}(o(x),o(x))])$ fairly solves 1). We can precede the analysis with a proper orthogonal decomposition of $o(x)$ to deal with correlated input components.

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MS35

Movement of Fluid Interfaces and Their Averaged Properties During Two-phase Flow in Heteroge-

neous Porous Media

The fluid-fluid interface during immiscible displacement has a strong influence on mass transfer during the flow process in heterogeneous porous media. Important criteria are the front roughness and the averaged saturation at the front. Similar to the concept of dilution and dispersion in solute transport theory, these two measures differ in their relation to processes at the fluid interfaces. This presentation discusses predictions of large scale front behavior obtained theoretical methods and experimental observations.

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MS35

Global Random Walk Simulations for Sensitivity and Uncertainty Analysis of Transport Models

The global random walk algorithm (GRW) performs the simultaneous tracking on a fixed grid of huge numbers of particles at costs comparable to those of a single-trajectory simulation by the traditional particle tracking approach. Ensembles of GRW simulations of a typical advection-dispersion process in aquifers are used to obtain reliable estimations of the input parameters for the upscaled transport model and of their correlations, input-output correlations, probability distributions, and relations between input and output uncertainty.

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MS36

Finite Volume Schemes for Simulating Meso- and Micro-scale Atmospheric Flows

Two different finite volume schemes for simulating meso- and micro-scale atmospheric flows are discussed in detail. First an adaptation of Smolarkiewicz's MPDATA scheme on unstructured grids is presented. The second finite volume scheme is based on flux-based wave decomposition suggested by LeVeque. The f-waves scheme is described in detail and Euler solutions for different benchmark problems are presented. The scheme is also compared with the National Center for Atmospheric Research's state-of-the-art WRF model.

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MS36

A Runge-Kutta Discontinuous Galerkin Method with Time Accurate Local Time Stepping

Our research objectives are the construction and application of accurate and efficient schemes for unsteady flow

problems. In this talk, a recently developed explicit Runge-Kutta based discontinuous Galerkin discretization is presented. The focus is set on the time accurate local time stepping algorithm and an efficient implementation using a mixed modal/nodal approach. To demonstrate the accuracy and efficiency of the method, several test problems for the compressible Navier-Stokes equations are shown.

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MS36

Theory and Numerics of Sound-proof Models for Atmospheric Motions

The classical Ogura and Phillips' (1962) anelastic model, subsequent extensions by Dutton and Fichtl (1969), Lipps and Hemler (1982), or Bannon (1995/96), and the pseudo-incompressible model by Durran (1988) will be revisited. We demonstrate that only the Ogura-Phillips model has a systematic single-scale asymptotic derivation, but that even multiple scales asymptotic techniques are incapable of yielding the extended anelastic or pseudo-incompressible models. In turn, we demonstrate that these models reduce, at small scales, to the incompressible Boussinesq approximation (anelastic) and to the zero Mach number, variable density flow equations (pseudo-incompressible), respectively. Thus these models are compatible with particular low Mach number limits of the compressible Euler equations at least on small scales. To show that these models do provide valid approximations to low Mach number flows in the atmosphere, more advance techniques of mathematical analysis are needed. The outline of a proof that is work in progress at the time of submission of this abstract will be provided. A Godunov-type projection method that was motivated by these considerations will be summarized and tests involving small-scale flow with large density variation as well as breaking topographic internal waves will be presented.

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MS36

Implementation of Pressure and Velocity Regularized Equations

Numerical modeling of atmospheric flows is a multiscale problem for which the treatment of turbulence and scale separated phenomena is essential. Our approach consists in studying both phenomena by means of regularizations of the underlying model equations. We have in particular studied velocity (α -Euler models) and pressure regularizations. While the concept of velocity regularization is well-known from incompressible Navier-Stokes equations, the extension of velocity regularizations to compressible flows is non-trivial. Pressure regularizations arise naturally

from semi-implicit time-stepping methods as well as from Lagrangian particle methods. We have implemented and studied both types of regularizations for the shallow-water equations and the ICON spherical spatial discretization approach. After a survey of the basic regularization concepts we will present numerical results. This is joint work with Marco Restelli, Marco Giorgetta, Tobias Hundertmark and Peter Korn. The work has been funded by the German Science Foundation (DFG) under the SPP Metstroem.

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MS37

A Multilayer Saint-Venant System : Derivation and Numerical Validation

We are interested in this talk in the derivation and analysis of a multilayer model for shallow flows. The model allows the fluid to circulate from one layer to the connected ones. The main properties (energy, hyperbolicity) of the model are exhibited. A kinetic interpretation and some numerical simulations including a recirculation case with wind forcing are also given.

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MS37

Finite Volume Simulation of the Geostrophic Adjustment in a Rotating Shallow Water System

We focus on the simulation of the geostrophic adjustment phenomenon for rotating shallow water models by means of finite volume methods. The well-balanced properties and the discrete dispersion laws of the numerical schemes play a fundamental role. Here we consider spatial discretization based on a first order Roe-type method and some higher order extensions based on WENO reconstructions. The time discretization is designed in order to provide suitable approximations of inertial oscillations, taking into account the Hamiltonian structure of the system for these solutions. Some numerical experiments for 1d and 2d problems will be shown.

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MS37

A Roe-type Scheme for Two-phase Shallow Granular Flows over Variable Topography

We consider a depth-averaged two-phase model for gravity-driven flows made of solid grains and fluid, moving over variable basal surface. In particular, we are interested in applications to geophysical flows such as avalanches and debris flows. We numerically solve the model equations by a high-resolution finite volume scheme based on a Roe-type Riemann solver. Well-balancing of topography terms is obtained via a technique that includes these contributions into the wave structure of the Riemann solution.

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MS37

High Order Well-balanced Finite Volume Schemes for Systems of Balance Laws

A new family of high-order well-balanced schemes for the numerical solution of hyperbolic systems of balance laws is proposed. The schemes are designed with use of two sets of variables, conservative and equilibrium ones. We discretize the equations in the conservative variables, while for reconstruction we use the equilibrium ones. We construct well-balanced schemes up to the fourth order and apply our technique to the shallow water equation and nozzle flow.

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MS38

The Solidification of An Ideal Ternary Alloy in a Mushy Layer

We examine a model for the solidification of a ternary alloy in a mushy layer. The effects of species diffusion are included along with heat diffusion in order to investigate the possibility of double-diffusive and other modes of convection in this system common in many geophysical systems. We investigate the properties of non-convecting base state solutions for this ternary system and then present linear stability results that reveal convective modes of instability.

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MS38

Stability of Upwelling Mantle in a Solubility Gra-

dient

Channelized melt flow due to reactive infiltration in a porous medium has been proposed as a mechanism for melt extraction in the Earth's mantle. We present analytical and numerical results from an extended mathematical formulation for melt migration in a deforming mantle column that undergoes steady upwelling. To study the spatial distribution of the channels, we explicitly track the abundance of a dissolving mineral in the otherwise nonreactive solid. We present approximate analytic solutions for steady upwelling columns, and study their stability to small perturbations using linear stability analysis. The height of the upwelling column is larger than the compaction length of the system, and therefore compaction is stabilizing the system more than previously acknowledged. Upwelling, porosity dependence of the bulk porosity, and increasing disequilibrium also stabilize the system. These linear results are in good agreement with high-resolution numerical simulations at early times. Although the system studied is stable to initial perturbations in the range of parameters of geological interest, sustained perturbations of the porosity at the inflow boundary lead to localization. Melt flow into the channel is limited by the formation of a compacting boundary layer, not previously observed. If boundary perturbations are sustained long enough the dissolving mineral is exhausted in regions of high melt flow and the channel splits due to compaction. Upward branching of channels is expected in the upper part of the upwelling column, in contrast to the inverted cascade obtained in previous studies. In summary, it is more difficult to localize melt flow than previously thought and sustained perturbations are necessary to force melt localization. The presence of mantle heterogeneity in the upwelling mantle might provide such sustained perturbations. This may provide a link between source heterogeneity and the distribution of dunite bodies in the mantle section of ophiolites.

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MS38

Open Melt Conduits in Mantle Undergoing Decompression Melting

We examine the dominating physical processes for an open channel of melt within a partially molten viscous matrix. Melting of the residual rock is fundamentally driven by the rate that heat is transported from the hotter mantle beneath; in an open conduit this is mostly provided by the motion of melt rather than matrix. Large melting rates keep channel walls open against viscous closure due to the reduced channel pressure, which is essentially magmomatic.

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MS38**Reactive Channelization in Mushy Layers and the Mantle**

The formation of chimneys in a mushy layer and the formation of dunite channels in the mantle both occur by the reactive infiltration instability. In both cases, fluid flow is driven by buoyancy through a permeable, reactive matrix up a solubility gradient, leading to matrix dissolution and channelization of flux. The theory and experiments used to study these two systems have been developed independently and yet much can be learned by a comparative study. For example, theory for the reactive-convective instability in a mushy layer assumes chemical equilibrium between crystals and brine, while the theory for magmatic systems is based on disequilibrium and linear reaction kinetics. New simulations of magmatic flow beneath a mid-ocean ridge demonstrate the power of a computational implementation based on equilibrium thermodynamics and the Enthalpy Method. New experiments on mushy layers suggest that disequilibrium and kinetics are important in explaining new phenomena. This talk will examine similarities and differences between reactive channelization in mushy layers and the mantle. It will weigh the motivations and benefits of assuming thermodynamic (dis)equilibrium in theoretical descriptions of the two systems.

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MS39**Simulation of a Benchmark - Solutions and Error Estimates**

Geological storage of carbon dioxide in deep saline aquifers is considered as a means to reduce greenhouse gas emissions. Different storage mechanisms play a role in this context. In our contribution, we are concerned with the mechanisms of residual- and dissolution trapping. We present 2D- and 3D numerical results related to a model of an extended sloping aquifer and investigate the effect of the mentioned trapping mechanisms and their proper time scales. The results of the 2D- and the 3D simulations are compared, as well as various types of boundary conditions. The results are also compared to semi-analytical solutions by Hesse et al (2008) where a sharp interface and no dissolution is assumed.

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MS39**Vertically Integrated Approaches to Large Scale CO₂ Storage**

Models of CO₂ injection into geological formations must capture both the large-scale plume and small-scale leakage

along wells. Traditional numerical methods are computationally expensive for large complex geological systems and with large numbers of wells. The VESA model combines vertically-averaged governing equations with a subscale analytical model for wellbore flow. CO₂ injection is solved numerically on a coarse grid, capturing the large-scale injection problem, while the embedded analytical model eliminates expensive grid refinement around wells.

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MS39**Investigation of Numerical Methods for CO₂ Injection**

This talk will focus on numerical methods for the benchmark problem. We investigate methods utilizing methods specially suited for advection dominated flow and gravity segregation and use operator splitting to combine this methods. In the investigation of several methods for the given benchmark problem, we focus on methods which easily can be extended to more complicated geometry. In particular we investigate streamline methods and reordering methods.

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MS39**Overview of Modeling Choices for CO₂ Storage**

This talk will give an overview of the proposed benchmark problem for this minisymposium. Recognizing that despite the simplicity of the benchmark, it poses severe computational challenges. The talk will discuss available modeling choices that may be applied to reduce the computational load, and assess these modeling choices in the context of the benchmark.

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MS40**Homogenization-based Multiscale Finite Elements for Heterogeneous Porous Media**

Multiscale methods are used to solve flow problems with heterogeneous permeability. We show that a popular mixed multiscale finite element fails to reproduce constant flow fields, and so fails to converge in any meaningful way. The problem arises for anisotropic permeability. We expect the same for isotropic permeability when the microstructure

leads under upscaling to a tensorial homogenized permeability. A modified method based on homogenization is shown to converge with respect to this microstructure.

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MS40

Sparse Finite Element Method for Periodic Multiscale Nonlinear Monotone Problems

In this talk, I will present a sparse tensor product Finite Element (FE) method for the high-dimensional limiting problem obtained by applying the multiscale convergence to a multiscale nonlinear monotone problem in \mathbf{R}^d . The limiting problem is posed in a product space, so tensor product FE spaces are used for discretization. This sparse FE method requires essentially the same number of degrees of freedom to achieve essentially equal accuracy to that of a standard FE scheme for a partial differential equation in \mathbf{R}^d . It is proved that for the Euler-Lagrange equation of a two scale convex variational problem in a smooth and convex domain, the solution to the high-dimensional limiting equation is smooth. An analytic homogenization error is then established, which together with the FE error provides an explicit error estimate for an approximation to the solution of the original multiscale problem. Without this regularity, such an approximation always exists when the meshsize and the micro scale converge to 0, but without a rate of convergence.

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MS40

A Multiscale Mixed Finite-element Method for the Stokes-Brinkman Equations

We present a multiscale mixed finite-element method for detailed modeling of free-flow and porous regions in vuggy and naturally-fractured reservoirs. The method uses a standard Darcy model to approximate flow on a coarse grid and captures fine-scale effects through basis functions computed numerically by solving local Stokes-Brinkman flow problems on the underlying fine-scale grid.

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MS40

Upscaling Inertia Effects in Flow

We discuss upscaling of inertia effects in heterogeneous porous media. From lab scale to reservoir scale we consider non-Darcy flow model; we present recent analytical and numerical results extending work with C. Garibotti. A separate project with Trykozko is on upscaling from porescale to lab scale. Connecting these scales, explain-

ing why heterogeneity and inertia seem to diminish each other's impact, as well as handling anisotropy emerging from upscaling are the main issues of this talk.

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MS41

Analysis of Immiscible Two-phase Flows in Porous Media with Discontinuous Capillarities

We consider a simplified model for two-phase flows in porous media made of different rocks. We focus on the effects of the discontinuity of the capillarity field. We first consider a model with capillarity within the rocks. Then we look for the asymptotic problem for capillarity forces remaining only at the interface. We propose a simple modeling of oil-trapping by the mean of non-classical shocks at the interface.

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MS41

A Phase-field Model of Unsaturated Flow – Stability Analysis and the Development of Gravity Fingers

Infiltration of water into homogeneous dry soil often leads to preferential flow in the form of fingers. The canonical model for unsaturated flow, known as Richards equation, is totally stable and therefore unable to reproduce this behavior. We use this physical problem to introduce a new class of models of multiphase flow in porous media, which account for the presence of a macroscopic interface (the wetting front), and explain why and how fingering occurs.

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MS41

Outflow Boundary Conditions in Porous Media Flow Equations

To model the flow in porous media one typically uses either the Richards equation if the flow can be described effectively by one phase, or the two-phase flow equations if two phases must be modeled. Due to the wide range of applications, the interest in these two systems is enormous. Rigorous analytical results became available in the 80ies, when strong nonlinearities in time-dependent problems were treated systematically. In most contributions on the subject, the analysis is simplified by restricting to Dirichlet boundary conditions, even though a physically more appropriate boundary condition is the outflow condition. After motivating and explaining this condition we present the corresponding qualitative analytical problems, a regularization technique and existence results.

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MS41

Non-linear Interface Models for Multi-phase Flow Problems in Heterogeneous Media

We consider two extensions to standard capillary pressure relationships for two phase problems. Firstly, to correct the non-physical behavior, we use a recently established saturation-dependent retardation term. Secondly, in the case of heterogeneous porous media, we apply a model with a capillary threshold pressure that controls the penetration process. Mathematically, we rewrite this model as inequality with possible discontinuities in the saturation and pressure at the interfaces. Numerical examples in 2D and 3D show the influence of the modifications.

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MS42

Monotonicity for Multi Point Flux Approximation Methods on Triangular Grids

We study the monotonicity behaviour of MPFA methods on triangular grid. For single phase flow, we find sufficient conditions for the MPFA O- and L-methods. The found monotonicity regions for the methods are also tested numerically. The tests are done for cases corresponding to both homogeneous and heterogeneous media. We also investigate the robustness of the methods with respect to monotonicity for two-phase flow. The results obtained in this work may be utilised in grid generation.

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MS42

A Finite Volume Method for Solving the Steady Convection-Diffusion Equation

We discuss a cell-centered finite volume method to approximate the steady convection-diffusion equation on meshes of triangles and tetrahedra. The method is second-order accurate through a piecewise linear reconstruction within each cell and at mesh vertices. A non-linear definition of the face gradients for the numerical diffusive fluxes allows us to demonstrate the existence of a Maximum Principle. We also consider a reformulation for meshes of convex polygons of any shape, and the connection with the DDFV method and the MFD method.

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MS42

Monotone Finite Volume Discretization of the Convection-Diffusion Equation on Polyhedral Meshes

We consider the cell-centered finite volume discretization of the steady convection-diffusion equation. The diffusion tensor may be full and anisotropic and the operator may have the dominated convection part. The computational mesh (conformal or non-conformal) is assumed to consist of convex polyhedral cells. The proposed finite volume method is monotone, i.e. it preserves non-negativity of the differential solution. Monotonicity of the method is provided by nonlinear two-point diffusion and advection fluxes derived on faces of mesh cells. The method is the 3D extension of the 2D finite volume discretization [1]. 1.Lipnikov K., Svyatskiy D., Vassilevski Yu. Interpolation-free monotone finite volume method for diffusion equations on polygonal meshes.J.Comp.Phys., 2008

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MS42

Nonlinear Finite Volume Methods for Convection-Diffusion Problems on Unstructured Polygonal Meshes

Predictive numerical simulations of subsurface processes require not only more sophisticated physical models but also more accurate and reliable discretization methods. The discretization methods used in existing simulations fail to preserve positivity of a continuum solution of the elliptic equation when the media is anisotropic and heterogeneous and/or the mesh is strongly perturbed. We present the nonlinear finite volume approach that guarantees positivity of the discrete solution on unstructured meshes and for strongly anisotropic diffusion tensors. Recently several variations of this approach have been proposed. We compare their numerical and computational properties.

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MS43

Atmospheric Simulation Using High Order Methods on Locally Adapted Unstructured Parallel Grids

We address the issue of simulating atmospheric motion in 2d using a high order conservative scheme (DG) on unstructured, locally adaptive grids. Testcases include classical mountain overflow problems and warm non-

precipitating cloud model with 3 components of air. The latter being an intermediate step towards an implementation of a simplified COSMO model using high order, conservative scheme. The advantage of such an approach is in effectively resolving of the impact of orography and dealing with boundary problems in more natural manner.

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MS43

High-Order Semi-implicit Time-integrators for the Euler and Navier-Stokes Equations

In this work, we describe the construction of high-order accurate in time semi-implicit methods for the Euler and Navier-Stokes equations used in mesoscale nonhydrostatic atmospheric modeling. The goal of this research is to compare and contrast various forms of the governing equations (e.g., should one use Exner or density for the mass and should one choose potential temperature, density potential temperature, or total energy). The form of the continuous governing equations used in the models can restrict one to only certain classes of time-integration methods (e.g., if the equations are in flux form, then it is not possible to use classical semi-Lagrangian methods). In addition, some forms of the governing equations can be more expensive to solve computationally than other forms. Another topic of discussion concerns the inclusion of adaptive time-stepping machinery into these models. While not important to the outline of the talk, for the moment we are assuming that an element-based continuous Galerkin method is used for approximating the spatial derivatives. In the future, discontinuous Galerkin methods will be included into this generalized approach. We will describe the challenges facing us with discontinuous Galerkin methods and how to implement them in conjunction with semi-implicit time-integrators.

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MS43

A 2d Discontinuous Galerkin Model for the (Non)-hydrostatic Atmosphere

The vertical structure of the averaged free atmosphere is dominated by the hydrostatic balance. Large scale waves, with horizontal spatial scales larger than 10km, are present in a non-hydrostatic model and develop similar for hydrostatic equations. In the hydrostatic case, phenomena of smaller scales either destroy the balance or do not give correct wave speeds and dispersion properties. Wave propagation will be studied within a hydrostatic and a non-hydrostatic 2-dimensional model. Both models are discretized with a high order discontinuous Galerkin method and a semi-implicit time stepping.

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MS43

New Grids for Flow on the Sphere

The logically rectangular finite volume grids for two-dimensional PDEs on the sphere and for three-dimensional problems in a spherical shell introduced in [SIAM Review 50(2008) pp. 723-752] have nearly uniform cell size, avoiding severe Courant number restrictions. We present recent results with adaptive mesh refinement using the GeoClaw software and demonstrate well-balanced methods that exactly maintain equilibrium solutions, such as shallow water equations for an ocean at rest over arbitrary bathymetry or a stratified atmosphere in three dimensions.

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MS44**Approaches to Coupled Land-energy Flux Modeling**

We will discuss benefits and associated difficulties of constructing coupled models to simulate interactions of the groundwater-landsurface-atmosphere system. These models potentially provide understanding of two-way feedbacks and are, thus, a promising tool for process understanding and prognosis. However, related physical processes cannot be described fully using first-principles approaches leading to parameterizations that are intrinsically tied to particular spatiotemporal scales. Therefore, understanding of process scalability is an important component in coupled model construction requiring careful consideration.

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MS44**Introduction to the Minisymposium: Coupled Approaches to Groundwater-atmospheric Modeling**

The linkage between groundwater and the lower atmosphere occurs via shallow soil moisture and energy transport processes. Complex, coupled nonlinear physiochemical processes and a wide range of spatiotemporal scales necessitates numerical simulation of these interactions. These computationally challenging solutions must utilize efficient algorithms and preconditioners resulting in a balance of stability, efficiency and accuracy. This talk will introduce these issues and demonstrate some numerical approaches to bridging these two systems.

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MS44**Surface-groundwater Flow Coupling Based on Boundary Condition Switching**

We develop a model of surface-groundwater flow based on boundary condition switching between surface-subsurface domains. The model is shown to be able to reproduce relevant processes at different spatial and temporal scales. Explicit finite differences for surface routing and implicit finite elements for Richards equation allow for different time-stepping strategies to capture different time scales. Model performance is analyzed numerically on sample and real-world test cases and theoretically within the context of domain decomposition methods.

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MS44**Strategies for Coupling Subsurface Flow, Land Surface, and Atmospheric Models**

Fully coupled bedrock to atmosphere models require a strategy for time stepping and passing information between the subsurface, land surface, and atmospheric mod-

els. We will present results of investigations into time cycling and operator splitting methods for a coupled model including the ParFlow variably saturated subsurface flow code, the CLM land surface flow code, and the WRF atmospheric simulation code. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was supported by the LLNL Climate Change Initiative. LLNL-ABS-409527.

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MS45**Initiating Large Slope Movements by Rain-induced Shear Bands**

Against the background of the global climate change, the computer aided prediction of landslides induced by heavy rain events is of increasing importance in order to protect life and property in alpine regions. This makes it necessary to accurately model the complex inelastic deformation behaviour of partially or fully saturated soil on the basis of sophisticated multi-phase continuum theories. In this regard, we present a triphasic porous media model capable of describing all prominent hydraulic and solid mechanical effects triggering the evolution of shear zones towards complete slope failure.

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MS45**A Double Continuum Approach for Two-phase Flow Simulation in Natural Slopes**

The fast infiltration of heavy rainfalls in macro-porous soils is one of the key processes which triggers the movement of natural slopes as it leads to a 'fast' pressure increase as well as to a fast saturation of a hillslope. The macro-porous medium is characterized by a complex channel-like network which cannot be discretely taken into account. To simulate flow processes in such media, a double-continuum model concept for two-phase flow has been developed and should be presented showing results of plausibility tests as well as of a field experiment. Special emphasis is put on the exchange parameters which are determined from laboratory experiments.

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MS45

Theoretical and Experimental Aspects on Triggering Rapid Mass Movements of the Flow-Type

Many of the world's most devastating landslide disasters can be attributed to landslides of flow type involving non cohesive soils. The flow-type characteristics of the post-failure stage are linked to the initial acceleration of the failed mass, determined by the soils' mechanical instability. In the presentation, experimental evidences of partially saturated non cohesive soils leading to flow-type behaviour are illustrated and interpreted within a geomechanical conceptual framework.

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MS45

Internal Erosion in Soils: A Multi-phase Model on Multiple Scales

Internal erosion, i.e. the debonding and movement of fines through the porous soil by hydraulic forces, could affect the mechanical and hydraulic stability of geostructures dramatically. Internal erosion is causative for many natural and technical disasters in connection with flood events and collapse-like slope failures where small triggers lead to a liquefaction of the soil. To simulate internal erosion processes, we propose a mixture theory-based multi-phase model which we compare with laboratory experiments.

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MS46

Computing Geological Storage of CO₂: A Grid Environment for Massively Parallel Simulation, Storage and Statistics

In this presentation we describe a grid environment (GE) for massively parallel simulations related CO₂-sequestration in deep aquifers. In addition to the compute functionality, the environment provides data-storage facilities and tools for statistical data-exploration. The compute

part of the GE has access to a number of supercomputers located in the Nordic countries Denmark, Finland and Norway. Storage and data-evaluation is provided by the Norway and partners in UK and Ireland. The infrastructure is based on the middlewares ARC (Nordugrid) and DiGS (EPCC). It supports the simultaneous execution of various instances of massively parallel simulations and the subsequent evaluation of the generated data. The currently supported software is MUFTE-UG, a simulation platform for Multi-Phase-Multi-Component flow simulations. Simulated time-series are stored in XML-annotated sets of files and statistical investigations can be carried out on the base of the complex meta-data. The capability of the environment will be illustrated by selected models.

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MS46

Numerical Schemes with Low Dissipation for Modelling Contaminant Transport in Porous Media on Simplicial Meshes

We present two numerical schemes with low dissipation for modeling contaminant transport in porous media. Both schemes use operator splitting and cell-centered finite volume paradigm. However, the schemes differ in the construction of the diffusive flux and the advection substeps. Also, the schemes are derived for different classes of 3D dynamic meshes, i.e. conformal tetrahedral and non-conformal hexahedral (octrees). We present the basic properties of the schemes such as order of convergence, monotonicity, computational efficiency, and compare them on the solution of several test problems.

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MS46

High Performance Simulation of CO₂ Geological Storage

The objective of the French ANR project SHPCO₂ is to develop and study advanced numerical methods for the simulation of CO₂ reactive transport on massively parallel computers. We have identified four challenging subjects that we will discuss during the session. 1. Coupling multiphase flow and reactive transport models. 2. Reactive transport nonlinear solvers. 3. Time space domain decomposition and local time stepping. 4. Dynamic load balancing for a multi-physics and multi-domain application.

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MS46

Modelling the Transport of Particulate Suspensions and Formation Damage During the Deep Injection of Supercritical Carbon Dioxide in Sandstone Formations

Prediction of CO₂ injection performance in deep subsurface aquifers and reservoirs rely on the well ability to maintain high flow rates of carbon dioxide during several decades without significantly impairing the host formation. Dynamics of solid particulate suspensions in permeable media are recognized as one major factor leading to injection well plugging in sandstones. The invading supercritical liquid-like fluid can contain variable concentrations of exogenous fine suspensions or endogenous particles generated in situ by colloidal or hydrodynamic release mechanisms. Suspended solids can plug the pores leading to possible formation damage and permeability reduction in the vicinity of the injector. As such, models which can predict well injectivity decline, are useful in the operations of planning, design, and maintenance, related to carbon dioxide injection. In this study we developed a finite element based simulator to predict the injectivity decline nearby CO₂ injection wells and also for production wells in the context of EOR. The numerical model solves implicitly a system of two coupled sets of finite element equations corresponding to the pressure-saturation two-phase flow, then a system of solute and particles convection-diffusion equations. Particle equations are subject to mechanistic rate laws of colloidal, hydrodynamic release from pores bodies, blocking in pores bodies and pores throats, and interphase particles transfer. The model was validated against available laboratory experiments at the core scale. At the field scale, challenges still exist for an accurate assessment of the permeability change due to limited current knowledge of Supercritical CO₂ and water phases micro-interactions at pore surfaces, but also to the multiscale nature of the numerical problem. Numerical demonstration examples in a saline sandstone aquifer reveal that formation damage during CO₂ injection will primarily depend on the injected particles wettability, the injection flow rate, and the medium tortuosity. Other simulation examples are provided for a CO₂ injection in a five spots pattern EOR oil field for performance assessment of the production with occurrence of in-situ sanding in a poorly consolidated sandstone reservoir.

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MS47

Using Energy Minimizing Basis Functions as a Multiscale Method, With Applications to Multigrid and Domain Decomposition Solvers

We demonstrate the applicability of energy minimizing basis functions for two-phase flow simulations, and we highlight their numerous benefits. We show how they can be implemented to obtain efficient serial (algebraic multigrid)

and parallel (Additive Schwarz with coarse space correction) linear solvers for large-scale heterogeneous problems. Moreover, they possess the same advantages of other multiscale techniques, but without the need of constructing a coarse mesh, and they are well-suited for adaptive algebraic coarsening.

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MS47

A Multiscale Finite Volume Method for Unsteady Stokes-Darcy Equations

The talk focuses on the application of the iterative-multiscale-finite-volume (IMSFV) procedure to the Stokes-Darcy system, describing flow in porous media. The standard IMSFV method is extended for solving the momentum and pressure correction equations in a fractional time stepping algorithm framework. The multiscale method allows to simulate flow and transport in porous media with geometries that can be too complicated to be resolved by a feasible computational grid. The coarse scale ensures global coupling and the fine scale ensures appropriate resolution. The method is illustrated with examples and is compared with fine scale solutions.

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MS47

A Multilevel Multiscale Mimetic (M^3) Method for Two-Phase Flows in Porous Media

The M^3 method builds recursively a problem-dependent multilevel hierarchy of models for flow in porous media. Each model is locally mass conservative. The method supports full diffusion tensors on unstructured polyhedral meshes and accommodates general coarsening strategies. We describe well modeling and adaptive strategies for updating the multilevel hierarchy. Numerical simulations for permeability fields with long correlation lengths show that even with large coarsening factors, 50 and more in each coordinate direction, the multiscale solution remains within

5% of the fine-scale solution.

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MS47

Multilevel Solvers and Upscaling Via Explicit Energy Minimisation

In this talk we highlight the strong link between robust multilevel iterative solvers and upscaling/multiscale techniques for subsurface flow. Motivated by recent theoretical results for two-level overlapping Schwarz domain decomposition methods, we investigate the construction of upscaling techniques based on energy minimisation. These include the Multiscale Finite Element Method as a special case, but in contrast to MsFEs do not require any artificial boundary conditions on coarse elements. We present and analyse a preconditioner for the arising constrained minimisation problem, that is robust to mesh refinement and arbitrary coefficient variation (requiring no scale separation). The resulting method is $O(h^{-d})$ where h is the subgrid size.

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MS48

Generalized Forchheimer Equation for Two-phase Flow Based on Hybrid Mixture Theory

We discuss the derivation of a Forchheimer-type equation for two-phase flow through an isotropic porous medium using hybrid mixture theory. Hybrid mixture theory consists of upscaling field (conservation) equations by averaging, and then exploiting the entropy inequality to obtain constitutive equations. Isotropic function theory is then used to simplify the equation for application to an isotropic porous medium. As time permits, we will discuss the extension of this theory to multiphase swelling materials.

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MS48

Multiscale Adaptive Modeling of Inertia and Non-equilibrium Processes

New experimental and modeling techniques make possible to identify and quantify inertia, dynamic effects, and non-equilibrium processes that until recently by necessity were deemed next-order or lower-scale only. The new terms and couplings that arise bring challenges for analysis and numerical modeling. We are concerned with how to determine their significance adaptively the way one handles grid adaptivity. The talk will be partly based on joint research with Showalter and Klein.

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MS48

Two-scale Pore Network Modeling for Multiphase Flow in Heterogeneous Geometries

Most of the transport phenomena of interest in subsurface flow modeling occur on multiple scales, and the complex subsurface pore spaces geometry on micro scale is notorious for dictating macroscopic flow of interest. We present an algorithm to geometrically match pore throat networks from two separate scales (that can either originate from available measurements or be constructed according to generally accepted knowledge) and show preliminary results for flow in networks based on realistic carbonate geometry.

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MS48

Experimental Analysis of Non-equilibrium Processes for Multiphase Flow in Porous Media

The effect of flow rate on interfacial configurations in porous media was investigated using computed x-ray microtomography and image analysis. One full drainage/imbibition cycle was measured and subsequently residual configurations were assessed following drainage/imbibition at flow rates varying over an order of magnitude. Results indicate that both flow rate and system history are important, especially for the imbibition process.

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MS49**Analysis of Numerical Methods for Coupling Transport and Geochemistry Equations**

Reactive transport equations involve PDE for advection-diffusion, algebraic equations for chemistry at equilibrium and ODE for kinetic chemistry. Classical methods are based on a method of lines where spatial discretization is followed by temporal discretization. We analyze here the numerical properties and convergence of four such methods, namely SNIA, SIA, DSA and DAE. We illustrate the comparison by some numerical examples.

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MS49**Efficient Solution of Large Reactive-Transport Problems Including Mineral Reactions**

The global-implicit approach applied to large multicomponent reactive transport problems in general leads to large nonlinear systems. A method is proposed to reduce the size of the system using equivalence reformulations, leading to an elimination or a decoupling of many of the unknowns. If precipitations/dissolution reactions are involved, a formulation is given which can be solved by the semismooth Newton method. Numerical results of the proposed algorithms are presented.

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MS49**Adaptive, Selective Coupling of Multicomponent Transport and Kinetic Reactions**

The efficiency of the process-preserving, globally implicit approach to solve reactive multicomponent transport problems with Newton's method can be enhanced by modifying the Jacobian. Therefore the reaction network, which defines the connectivity pattern of the system matrix, is analysed to neglect terms with the aim to decouple species equations on the level of the linear solver without deteriorating the quadratic performance of the global, process-preserving iteration. The fully adaptive algorithm can be used potentially in every time step, and works with direct as well as iterative linear solvers for reactions of kinetic type in arbitrary dimensions.

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MS49**Mixed Finite Elements and Newton Method for Reactive Solute Transport in Porous Media**

We present a mass conservative finite element scheme for

reactive solute transport in porous media. The transport is modelled by a convection-diffusion-reaction equation, including equilibrium sorption. We especially considered the case of a Freundlich type isotherm, when the equation becomes degenerate. The algorithmic aspects of our scheme are presented in [F. A. Radu, M. Bause, A. Prechtel and S. Attinger, Analysis of an Euler implicit - mixed finite element scheme for reactive solute transport in porous media, Numerical Mathematics and Advanced Applications, K. Kunisch, G. Of and O. Steinbach (editors), Springer Verlag, 2008, pp. 513-520.] and the analysis of the discretization error in [F. A. Radu, I. S. Pop and S. Attinger, Analysis of an Euler implicit - mixed finite element scheme for reactive solute transport in porous media, Numerical methods for partial differential equations, 2008, to appear.]. We focus here on the applicability of the Newton method on solving the nonlinear problems arising at each time step. For the degenerate case a regularization step is necessary. An explicit condition for the quadratic convergence of the Newton method in terms of the discretization parameters and the regularization number is derived.

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MS50**Balance-Preserving Finite Element Methods on Unstructured Meshes**

The dynamical equations of motion for the atmosphere and ocean support oscillations a vast range of spatial and temporal scales. However, large-scale flows in the atmosphere and ocean remain in a state of slow evolution called geostrophic balance in which fast oscillations are very weak; these slowly-evolving dynamical states represent our weather and the global circulation patterns. To make predictions on these timescales, special care must be taken to design numerical methods which reflect the properties of this underlying balance. Recently there has been much interest in modelling the atmosphere and ocean on adaptive unstructured meshes; this calls for new discretisation methods which reflect geostrophic balance. We introduce a new family of mixed finite element methods which provide the best possible representation of geostrophic balance on unstructured meshes. The proofs of these properties are very simple since they are based on underlying geometric structure: the discretisations have exact sequences which mimic the div-curl and curl-grad relations of vector analysis.

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MS50**Discretised Poisson and Nambu Brackets in the Context of an Atmospheric General Circulation Model**

We want to establish a coupled atmosphere and ocean model for climate simulations and numerical weather prediction. As model properties are foreseen (i) conservation of mass, (ii) conservation of tracer mass and its consistency with the continuity equation, (iii) conservation of energy and a vortex quantity; all to be achieved on triangular/hexagonal meshes. Exploring the algebraic structure of fluid equations in Poisson/Nambu bracket form facilitates to obey these properties in the numerical realization.

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MS50**Hamiltonian Particle-mesh Simulations for a Non-hydrostatic Vertical Slice Model**

We develop a non-hydrostatic vertical slice model in the context of the Hamiltonian Particle-Mesh Method (HPM) for the dry adiabatic atmosphere. The slice model is tested with the bubble-experiments described in Rob rt (1992) and the gravity wave experiment in Skamarock and Klemp (1994). The solutions are maintained smooth largely due to a "regularization" in the absence of the artificial diffusion. The regularization is implemented in harmony with a conservative force field and does not interfere with the hydrostatically balanced reference state. The accuracy of the HPM simulation is comparable to those in these references and the model performances show that the HPM method is potentially applicable to non-hydrostatic atmospheric flow regimes.

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MS50**Conservation and Wave Propagation on Hexagonal and Geodesic C-grids**

A 'geodesic' grid, comprising hexagonal and pentagonal cells, is attractive for global atmospheric modelling because it gives a nearly uniform and isotropic coverage of the sphere, avoiding the pole problems of a latitude-longitude grid. A C-grid staggering, in which the mass variable is stored in cells and normal velocity components are stored at cell edges, is also considered attractive because it gives a relatively good representation of fast waves and hence the geostrophic adjustment process. However, early studies of wave propagation for the shallow water equations on a regular hexagonal C-grid showed spurious large frequencies for near-grid-scale Rossby waves - a serious obstacle to the use of such a scheme for global atmospheric modelling. We show here that these spurious large frequencies can be avoided by a suitable discretization of the Coriolis terms. A geodesic grid comprises somewhat distorted hexagons and also pentagons. By careful consideration of the discrete vorticity budget, the regular hexagonal grid scheme is ex-

tended to the case of distorted hexagons and pentagons (indeed, any polygonal voronoi grid), ensuring both satisfactory Rossby wave propagation and energy conservation. Some sample numerical results will be shown.

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MS51**Coupling of Ground and Surface Water**

We solve the coupling of Richards equation in heterogeneous soil with non-moving surface water or depth-averaged shallow water equations. The Richards equation is treated without linearization by Kirchhoff transformation, convex minimization and monotone multigrid methods in homogeneous soil and non-overlapping domain decomposition methods to address heterogeneity. Gravity is included by upwinding. The coupling is provided by hydrostatic pressure and mass conservation leading to fixed point problems by different time scales for ground and surface water.

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MS51**Discontinuous Galerkin Methods for Coupling Depth-integrated Shallow Water Models with Richards Equation**

We describe a discontinuous Galerkin method for coupling shallow water flow and unsaturated ground water flow. The local discontinuous Galerkin method is used to approximate both the shallow water equations and Richards' equation describing flow in the vadose zone. Coupling between the two models is done weakly. Error estimates and numerical results are presented.

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MS51**Hierarchic Modelling of Free Surface Shallow Water Flow**

Abstract not available at time of publication.

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MS51**Mass Conservative DG/FV Schemes for Coupling the Richards Equation with Surface Flows**

We propose and analyze numerical schemes to couple subsurface and overland flows. The governing equations are Richards's equation in the subsurface, the kinematic wave equation on the surface, and the matching of pressure and normal velocity at the interface. Space-time discretization uses Discontinuous Galerkin/Finite Volume schemes combined with a multi-step implicit scheme in the subsurface. Multi-step coupling algorithms are proposed to ensure overall mass conservation. Numerical results illustrate the performances of the proposed algorithms.

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MS52**Tomographic Analysis of Reactive Fluid Induced Pore Structure Changes**

We have employed synchrotron microtomography with flow-column experiments to capture and quantify snapshots in time of dissolution and secondary precipitation changes in the microstructure of sediments exposed to simulated caustic waste. Dissolution induced changes included an increase in the number of larger pores. Precipitation induced changes included reduction in the number of small pores and closure of small throats, with accompanying reduction in pore coordination numbers and reduction in the number of pore pathways.

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MS52**Interfacial Energy, Surface Tension and Contact Angle**

Capillary phenomena can be equivalently described in terms of surface energies necessary to create the interfaces, or in terms of surface tensions that tend to contract the interfaces. We discuss the issues arising in presence of a solid phase and the tension balance at the triple contact line, including the component perpendicular to the solid when Young's law applies. Also implications for porous

media are discussed.

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MS52**Detailed Pore Scale Fluid Displacement Modeling Via the Level Set Method**

An accurate description of pore level immiscible fluid displacement could significantly improve macroscopic parameter predictions in real porous media. We present a simple but robust quasi-static displacement model for drainage and imbibition based on the level set method that results in geometrically and topologically correct interfaces, and is independent of the pore space complexity. Many applications include investigating fracture matrix transfer, and coupling with sediment mechanics. The code, LSMPQS, is publicly available.

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MS52**Pore Scale Modeling of Moving Crystal-fluid Interfaces Using Level Sets and Phase Field Models**

We present level-set and phase-field formulations of crystal dissolution/precipitation processes on the pore scale. These formulations are then compared to each other and used to simulate the evolution of crystalline solid-fluid interfaces inside a pore. Furthermore we will briefly discuss how these formulations can be used to upscale dissolution/precipitation processes to the Darcy scale.

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MS53**Simulation of Core-Scale Multiphase Flow Experiments with CO₂ and Brine**

Abstract not available at time of publication.

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MS53**Numerical Simulation of Key Mechanisms of CO₂ Sequestration in Stanford General Purpose Research Simulator**

We present the capabilities of Stanford's General Purpose Research Simulator (GPRS) to simulate CO₂ sequestration problems. The key known mechanisms, including hysteresis, diffusion and dispersion, and chemical equilibria have

been incorporated in GPRS. Comparison between GPRS and other simulators show close agreement and competitive efficiency for non-mineralization cases. A CO₂ mineralization case in the Johansen formation is presented, where we demonstrate that the amount of mineralized CO₂ depends strongly on the in-situ mineral composition.

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MS53

Two-phase Flow in Deformable Porous Media: Application to CO₂ Storage

Recently, CO₂ sequestration as concluding long-term stage of closed Carbon Dioxide Capture and Storage (CCS) processes considered for reducing carbon dioxide emissions into the atmosphere is subject of worldwide intensive investigations. To take into account all the relevant phenomena during spreading and storage of the injected CO₂ in the subsurface (flow and transport of multiple phases, rock deformation, non-isothermal conditions, geochemical reactions) physically founded complex mathematical models are required. The multiple coupled problems cannot be solved analytically. Rather, sophisticated numerical methods have to be applied.

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MS53

Modelling Physical Processes in CO₂ Sequestration

In this presentation, a series of models will be developed to describe the dispersal of CO₂ plumes through a subsurface aquifer, including the effects of capillary retention, drainage through fault zones or leakage into a lower permeability overlying seal rock. The models will be analysed to develop approximate similarity solutions to describe the dispersal of the plume with time, and the ensuing shape of the residual trapped CO₂ as the continuing current migrates through the stata.

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MS54

Constrained Adaptive Voronoi Gridding for Reservoir Modeling

We present our recently developed techniques for adaptive constrained 2.5D Voronoi grid generation based on a rigorous procedure of constructing Voronoi grid conforming to

piecewise linear constraints. Our approach addresses reservoir modeling challenges associated with accurate modeling of complex reservoir geometry and heterogeneous reservoir properties. Together with an accurate scale-up of fine-scale geologic properties, our gridding approach improves the consistency between geologic descriptions and reservoir simulation models, leading to more accurate simulation results.

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MS54

A New Multiscale Approach for the Simulation of Multiphase Flow Processes in Porous Media

The contamination of the unsaturated zone with a light non-aqueous phase liquid is studied, corresponding to a domain with randomly distributed heterogeneities where complex three-phasethree-component processes are relevant only in a small(local) subdomain. This subdomain needs fine resolution as the complex processes are governed by small-scale effects. For a comprehensive fine-scale model taking into account three-phasethree-component processes as well as heterogeneities in the whole (global) model domain, data collection is expensive and computational time is long. Therefore, we developed a general multi-scale concept where on the one hand, the global flow field influences the local three-phasethree-component processes on the fine-scale. On the other hand, a coarse-scale saturation equation is solved where the effects of the fine-scale multi-phasesmulti-component processes in the subdomain are captured by source/sink terms and the effects of fine-scale heterogeneities by a macrodispersion term.

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MS54**Upscaling for Multiphase Flow on 3-D Adapted Grids**

In this talk we present a methodology for coarse-scale modeling of multiphase flow in 3-D channelized domains such as those encountered when simulating gas injection processes. It integrates techniques for transmissibility upscaling, adaptive mesh refinement, and MPFA finite-volume discretization in order to balance accuracy, efficiency, and robustness. We focus on aspects that are specific to multiphase flow, including saturation-based adaptivity criteria, dynamic adaptation during transport, and streamline tracing.

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MS54**Downscaling: the Inverse to Upscaling**

Determination of conductivities from measured head-flow rate pairs is generally called inverse modelling. We present two inversion methods: the Double Constraint method and Constrained Back Projection. We do so for two discretization methods: node-based finite elements and block-centered finite differences. Downscaling is inverse modelling to determine fine-scale conductivities in coarse-scale grid blocks. The examples show that downscaling is a practical complement to homogenization if the porous medium is not periodic.

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MS55**Pore-network Modelling of Non-equilibrium Capillary Pressure Effect**

Traditional two-phase flow models assume that macroscopic phase pressures difference is a function of macroscopic saturation. However, under dynamic conditions, the difference of macroscopic phase pressures is known to be a function of time rate of saturation change. We have developed a three-dimensional regular lattice dynamic pore-network model in which we solve for the two fluid pressure fields separately. We have simulated both drainage and imbibitions processes for different viscosity ratios.

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MS55**Long Time Behavior for Dynamic Capillarity Models and Relation to Hyperbolic Conservation Laws**

We discuss an extended Buckley-Leverett (BL) equation describing two-phase flow in porous media, including a third order mixed derivatives term modeling dynamic effects in the capillary pressure. We derive existence conditions for traveling wave solutions, leading to admissible shocks for the original BL equation violating the Oleinik entropy condition. This provides nonmonotone weak solutions of the initial-boundary value problem for the BL equation consisting of constant states separated by shocks, confirming results obtained experimentally.

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MS55**Lattice Boltzmann Modeling of Macro-Porous Flow: Effects of Image Segmentation Algorithms and Comparisons with Observed Data**

In this presentation we simulate saturated flow through macroporous soil columns (7.62x18 cm) with a lattice Boltzmann model and compare results with measured saturated hydraulic conductivities. Porous geometry was obtained with an industrial CT scanner yielding a resolution of 119 microns (656x656x1482 voxels) and processed with several segmentation algorithms to generate pore solid classifications from gray-scale data. In this presentation we will define the optimal resolution and discuss the merits of selected segmentation algorithms.

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MS55**Upscaling Density-dependent Flow and the Role of Gravity Forces in Case of Transversal Dispersion**

In the talk we will discuss upscaling density-dependent flow, in particular the role gravity forces in case of transversal dispersion. We did some lab experiments, mathematical analysis and numerical computations. This is a highly interesting topic, with many details not yet fully understood.

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MS56**Solute Transport in Heterogeneous Porous Media**

Although being linear advection-dominated transport is a notoriously difficult problem. In strongly variable flow fields even high resolution finite volume methods may exhibit a high degree of numerical diffusion. We present an Eulerian-Lagrangian Localized Adjoint method on unstructured grids in two space dimensions that is locally conservative and monotone. The scheme is compared to a high-resolution discontinuous Galerkin scheme.

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MS56**Convergent Numerical Schemes for Reactive Flow in Unsaturated Porous Media**

Reactive porous media flow models are coupled systems of nonlinear degenerate parabolic equations. Due to the degeneracy, solutions of such models are lacking regularity, and an efficient numerical simulation needs requires appropriate discretization schemes. In this talk we consider In this talk we analyze the convergence of a mixed finite element scheme for reactive porous media flows. We focus on the coupling between the unsaturated flow component and the reactive component of the model.

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MS56**Numerical Solution of the Transport of Contaminants in Surface and Subsurface Flows**

This work models groundwater contamination through rivers and lakes. The resulting multiphysics problem couples the Navier-Stokes equations, the Darcy equations and

the transport equation. The flow is numerically solved by the finite element method in the surface region whereas it is approximated by the primal discontinuous Galerkin method of any order in the subsurface. The transport equation is solved with an improved discontinuous Galerkin method that minimizes the amount of overshoot and undershoot in the convection dominated regions. Convergence of the scheme and numerical simulations are shown.

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MS56**Guaranteed and Robust Discontinuous Galerkin a Posteriori Error Estimates for Convection-diffusion-reaction Problems**

We derive robust a posteriori error estimates for discontinuous Galerkin discretizations of stationary convection-diffusion-reaction problems. The estimates do not involve any undetermined constants and can be used for actual error control. They are based on $H(\text{div})$ -conforming diffusive and convective flux reconstructions. They are also locally efficient and hence suitable for adaptive mesh refinement. Numerical experiments illustrate their performance.

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MS57**Linear Fluctuation-dissipation for Low Frequency Climate Response**

Recently, we developed and tested novel computational algorithms for predicting the mean linear response of a chaotic dynamical system to small changes in external forcing via the fluctuation-dissipation theorem (FDT). The new linear response algorithms are tested on the T21 truncation of the barotropic climate with realistic Earth-like topography and two types of forcing which mimic behaviour of the atmosphere at 300 and 500 hPa geopotential height. The new methods yield greater accuracy than classical FDT methods for the linear response of both mean state and variance for both dynamical regimes.

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MS57**Statistical Model for an Incompressible Particle-**

mesh Method

In long time simulations with numerical methods, statistical averages converge - under ergodicity assumptions - to ensemble averages in an equilibrium measure. Which equilibrium measure depends on the numerical method used. In this talk we describe a model of the dynamics of the Hamiltonian particle-mesh method as adapted for quasi-geostrophic potential vorticity flow. The HPM method preserves potential vorticity pointwise, and the motion of discrete particles can be embedded in an area-preserving continuum flow. Using this knowledge, we propose a model based on random permutations of the initial PV distribution on a uniform particle arrangement. This model is validated using Monte-Carlo simulations. Next we construct a statistical mechanics theory for the model. Finally, the mean field predictions of the statistical mechanics theory are compared with long time simulations with HPM. A nonlinear stream function-PV profile is observed for both skewed and flattened distributions.

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MS57**On Stochastic Model Reduction Techniques**

We will explore the connection between several stochastic model reduction techniques in dynamical systems with time scale separation. In particular, we will explore how the approach of stochastic centre manifold reduction is linked to the homogenization approach valid on long time scales. In an application we will then use both reduction techniques for data assimilation taking into account their validity on different temporal scales.

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MS57**Parametric Estimation of Effective Stochastic Models from Discrete Data**

It is often desirable to derive an effective stochastic model for the physical process from observational and/or numerical data. Various techniques exist for performing estimation of drift and diffusion in stochastic differential equations from discrete datasets. In this talk we discuss the question of sub-sampling of the data when it is desirable to approximate statistical features of a smooth chaotic trajectory by a stochastic differential equation. In this case estimation of stochastic differential equations would yield incorrect results if the dataset is too dense in time. Therefore, the dataset has to sub-sampled (i.e. rarefied).

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MS58**Numerical Analysis of the Navier-Stokes/Darcy Coupling**

We present mathematical and numerical models for simulating incompressible fluid flows through porous media. The main applications of our interest are the hydrological environmental ones and mass transfer in biomechanics. We outline the analysis of a coupled Navier-Stokes/Darcy problem. After proving its well-posedness using the Beavers and Joseph interface conditions, we introduce a stable Galerkin finite element approximation and we study effective iterative schemes based on domain decomposition theory to compute its solution.

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MS58**A Fully Mixed Finite Element Method for the Coupling of Stokes and Darcy Flows**

In this paper we analyze a fully mixed finite element method for the coupling of fluid flow with porous media flow. Flows are governed by the Stokes and Darcy equations, respectively, and the corresponding transmission conditions are given by mass conservation, balance of normal forces, and the Beavers-Joseph-Saffman law. We consider dual-mixed formulations in both the Stokes domain and the Darcy region, which yields the introduction of the traces of the porous media pressure and the fluid velocity as suitable Lagrange multipliers. The finite element subspaces defining the discrete formulation employ Raviart-Thomas elements for the velocities, piecewise constants for the pressures, and continuous piecewise linear elements for the Lagrange multipliers. We apply the Babuska-Brezzi theory together with a classical result on projection methods for Fredholm operators of index zero, to show stability, convergence, and a priori error estimates for the associated Galerkin scheme. In addition, we provide a residual-based a posteriori error estimator for this coupled problem. Finally, some numerical results are reported.

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MS58

Optimal Neumann-Neumann Solvers for Mortar Coupling of Stokes-Darcy

We consider the coupling across an interface of a fluid flow and a porous media flow. The differential equations involve Stokes equations in the fluid region and Darcy equations in the porous region, and coupled through an interface with Beaver-Joseph transmission conditions. The discretization consists of Stokes finite elements in the fluid region, Raviart-Thomas finite elements in the porous region, and the mortar Lagrange multipliers on the interface. We allow nonmatching meshes across the interface. Due to the small values of the permeability parameter of the porous medium and the nonmatching nature of the problem and the discretization, the resulting symmetric indefinite discrete system is ill conditioned and has a nontrivial saddle point problem structure. In this talk we discuss these issues and show that preconditioners based on the Finite Element by Tearing and Interconnecting (FETI) method are more suitable than preconditioners based on the Balancing Domain Decomposition (BDD) method. We discuss condition number estimates for the preconditioners and their dependence on the permeability and mesh size ratio across the interface. Numerical experiments will be presented to confirm the sharpness of the theoretical estimates.

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MS58

Multiscale Mortar Methods for Coupling of Stokes and Darcy Flows

We discuss numerical modeling of coupled ground water and surface water flows, based on Beavers-Joseph-Saffman interface conditions. The domain is decomposed into a series of small subdomains (coarse grid) of either Stokes or Darcy type. The solution is resolved locally (on each coarse element) on a fine grid, allowing for non-matching grids across subdomain interfaces. Coarse scale mortar finite elements are introduced on the interfaces to impose weakly certain continuity conditions. By eliminating the subdomain unknowns the global fine scale problem is reduced to a coarse scale interface problem, which is solved using an iterative method. We precompute a multiscale flux basis, solving a fixed number of fine scale subdomain problems for each coarse scale mortar degree of freedom, on each subdomain independently. Taking linear combinations of the multiscale flux basis functions replaces the need to solve any subdomain problems during the interface iteration. We present theoretical and numerical results for local discretizations based on conforming or discontinuous elements for Stokes flow and mixed finite elements for

Darcy flow.

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MS59

Experimental Measurement and Modeling of the Oscillation of Oil-water Interface Lined with Paramagnetic Nanoparticles

We present multidisciplinary effort in developing techniques for determination of oil saturation in reservoir rocks using paramagnetic nanoparticles. The efforts include pore-scale experiments with nanoparticles designed to preferentially absorb to the oil/water interface and that can be detected remotely as well as numerical modeling. The modeling assumes capillarity to be a dominant restoring force when the oil-water interface is exposed to an oscillating external magnetic field, resulting in a pressure wave from the interface movement.

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MS59

Macroscale Modeling of Porous Media Systems: The Devil is in the Deviations

When applying averaging theory to obtain equations for porous media flows, it is well known that deviation terms related to the difference between products of averages and averages of products require careful attention. When using the thermodynamically constrained averaging theory (TCAT), one is also able to show that differences between averages of quantities calculated over different domains can be important. Here, we illustrate this effect and provide some examples where this issue impacts the equation forms.

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MS59

Interfacial Area, Capillary Pressure and Saturation at the Pore-scale: Observations and Lattice Boltzmann Simulations

We present a comparison between interfacial areas obtained from microtomographic images of glass bead porous media and lattice-Boltzmann simulations for drainage and imbibition processes. There is good agreement between the measured and simulated capillary pressure curves and interfacial areas and we find a unique capillary pressure-saturation-interfacial area relationship that is useful in describing hysteretic phenomena. Interfacial area per volume appears to be dependent upon the dominant flow mechanism and pore connectedness.

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MS59

Effect of Pore Space Morphology on Interfacial Configurations in Porous Media

Fluid configurations in porous media can vary significantly between drainage and imbibition. Using computed x-ray microtomography, we measure significant differences in wetting-nonwetting interfacial area for different pore space morphology, and for drainage and imbibition. The data is analyzed using pore network characterization and expressions based on energy dissipation.

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MS60

High Resolution Parallel Simulations of CO₂ Storage in Saline Aquifers

Modeling long-term movement and risk of escape of vast amounts of CO₂ will require coupled models that capture the physical and chemical evolution of the system at the appropriate scale. The geological models are often up-scaled for numerical models to reduce the computational times. However, upscaling causes loss of fine grid information and introduces numerical dispersion. Long term, high-resolution, and large-scale modeling of flow and transport of CO₂ will be presented using an in-house simulator with distributed computing and efficient numerical algorithms

and solver.

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MS60

Balance of Forces During CO₂ Injection in Geological Formations

The CO₂ storage capacity of geological formations is of great interest for the selection of potential storage sites in carbon capture and storage (CCS) projects. A detailed analysis essentially requires a thorough understanding of the interaction of forces acting within the system. By defining characteristic quantities for length, time, pressure and velocity, the governing multiphase flow equations can be non-dimensionalised. This allows for the definition of physically sound dimensionless numbers in conformity with the multiphase flow equations. The dimensionless numbers resemble the ratios of acting forces like viscous, capillary and gravitational forces. An analysis of the relation of forces in reservoirs with different parameter setups allows their intercomparison with respect to their CO₂ storage capacity potential. To back up the analysis, a comprehensive reservoir parameter database with more than 1200 reservoirs is analysed and statistical characteristics are derived. Effects of reservoir parameters like depth, temperature, absolute and relative permeability, as well as capillary pressure are investigated by analytical and numerical 1D and 3D experiments. It is shown that dimensionless numbers can be used to qualitatively order reservoirs by their CO₂ storage capacity with respect to the forces acting in the reservoir. Moreover, it is shown that the relative permeability relations together with the residual saturations have a great influence on the balance of forces.

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MS60

Analytical Models of CO₂ Storage at the Basin Scale Including Residual Trapping and Dissolution

Carbon capture and storage will be a viable climate change mitigation technology only if several gigatonnes of carbon dioxide are injected every year. In this talk, we will present

mathematical models of CO₂ migration at the scale of a geologic basin that, despite their simplicity, account for the essential flow physics during the injection and post-injection periods. In particular, we present new analytical results that include the combined effect of residual trapping and dissolution into the brine.

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MS60

Probability Density Function Approach for Modeling Complex Multi-phase Flow in Porous Media

We present a new methodology, which provides a link between Lagrangian statistics of phase particle evolution and Darcy scale dynamics. Each particle has a state vector consisting of its position, velocity, fluid phase information and possibly other properties like phase composition. The approach is applied for modeling CO₂ dissolution into brine and resulting non-equilibrium multiphase dynamics. It is shown that opposed to the stochastic formulation, the corresponding Darcy based deterministic formulation is unclosed.

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MS61

Darcy-Forchheimer Upscaling for Near-well Flow Modeling

The objective of this work is to provide a methodology to upscale the Darcy-Forchheimer flow equation which accounts for non-Darcy effects. These effects are important in high velocity regions (near-well). Unlike Darcy transmissibility, the upscaled Darcy-Forchheimer transmissibility depends on flow rate. To overcome this difficulty an iterative local-global upscaling technique is proposed. The main idea is to use the rate information from global coarse model as target rate when performing the local upscaling.

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MS61

Efficient Coarsening of Fluid Transport Problems

We propose a new method for flow-based coarsening that adapts to varying requirements with respect to accuracy and simulation time. By adapting the coarse grid to high-flow regions and retaining fine-grid fluxes along each coarse edge, we achieve good accuracy of production curves and saturation profiles. Incorporating causality of the discrete fluxes as an additional measure enables the use of highly efficient nonlinear block solvers.

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MS61

Multi-scale Algorithm of Support Operator Method

The multiscale method is based on using the coarse grid for pressure equation and fine grid for saturation equations. The essential feature of the method is construction of the basis functions by solving the one-phase stationary equations. These basis functions take account of fine grid structure. It is possible to construct total permeability tensor and to up-scale the relative permeability using the dissipative energy integral approximation. The coarse grid equation is solved using support operator method. Some results of modeling are represented.

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MS61

MPFA Mortar Multiscale Method for Multiphase Flow in Porous Media

An iterative coupling method employing a mortar MPFA method and a discontinuous Galerkin method for the pressure and saturation equations respectively is formulated for multiphase flow. This approach can be viewed as a multiscale scheme for the coupled multiphysics problem.

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MS62**Stochastic Galerkin Method for Transport Equation**

In this work we consider a transport equation with stochastic coefficients which model pollution concentration

$$\begin{aligned} -\operatorname{div}(\varrho(x, \omega)) &= f(x, \omega) && \text{in } \mathcal{G} \times \otimes, \mathcal{G} \subset \mathbf{R}^3 \\ \varrho(x, \omega) &= a(x, \omega) \nabla c(x, \omega) - \vec{q}(x, \omega) c(x, \omega), && \\ c &= 0 && \text{on } \partial \mathcal{G}, \end{aligned}$$

where ω is a random variable, $a(x, \omega)$ a diffusion coefficient, modelled by a random field, $c(x, \omega)$ is the concentration of one substance in another substance and the source term is modelled by $f(x, \omega)$. The flow $\vec{q}(x, \omega)$ can be computed from the equation predicting the groundwater flow through the aquifer \mathcal{G} . The governing equations are

$$\begin{aligned} -\operatorname{div}(\vec{q}(x, \omega)) &= p(x, \omega) && \text{in } \mathcal{G} \times \otimes, \mathcal{G} \subset \mathbf{R}^3, \\ u &= g(x) && \text{on } \partial \mathcal{G}, \end{aligned}$$

where $\vec{q}(x, \omega) := \kappa(x, \omega) \nabla u(x, \omega)$, the conductivity coefficient $\kappa(x, \omega)$, the right-hand side $p(x, \omega)$ and the solution $u(x, \omega)$ are random fields. The term ∇u models the pressure gradient. The initial domain \mathcal{G} is occupied by the aquifer. After discretisation of the deterministic and stochastic operators we apply the stochastic Galerkin method to solve this equation. In the conclusion we give a numerical example.

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MS62**Computational Modeling of Inertia Effects at Porescale**

We propose algorithms for computational upscaling of flow from porescale (microscale) to lab scale (mesoscale). We use traditional continuum Navier-Stokes solvers at porescale. Properties of flow in complex pore geometries are averaged to derive permeability and inertia coefficients. Convergence of solutions and averaging techniques are major concerns but these can be relaxed if only mesoscopic parameters are needed. For media which are heterogeneous and anisotropic at mesoscale we discuss appropriate non-Darcy models extending Forchheimer model.

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MS62**Numerical Methods for Unsaturated Flow with Dynamic Capillary Pressure**

Traditional unsaturated flow models use a capillary pressure-saturation relationship determined under static conditions. Recently it was proposed to extend this relationship to include dynamic effects and in particular flow rates, which results in model equations of nonlinear, degenerate pseudo-parabolic type. We study numerical discretizations of such models; we discuss the difficulties associated with the degenerate pseudo-parabolic character of

the equations and multiscale heterogeneity of the medium, and the convergence of schemes.

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MS63**Multi Point Flux and Mixed Finite Element Approximation in Porous Media: Error Analysis and Numerical Studies**

Here, in particular multi point flux and mixed finite element approximations of flow and transport processes in porous media are considered. A new proof of convergence for a multi point flux approximation scheme on triangular meshes is presented. Multi point flux approximation control volume methods are discretization techniques developed for an accurate and reliable reservoir simulation. They offer explicit discrete fluxes, which allows a wide class of applications. Various aspects of a reliable simulation of simultaneous reactive transport processes are also addressed.

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MS63**A Stability Criterion for Heterogeneous Density Driven Flows**

Variable density flows can occur due to temperature differences in deep aquifers and due to salinity differences in coastal aquifers and refuse dumps. Therefore, their relevance cuts across many practical applications like exploitation of geothermal energy resources, oil recovery from aquifers and remediation of contaminated sites. A typical feature of density dependent flow problems is that they can become unstable (physically or numerically). Variable density flow problems are difficult to solve due to the nonlinearities and coupling between fluid flow and solute transport processes. A big challenge to-date is to derive a general criterion that states whether flow is physically stable or unstable; and the optimum computational grid resolution required to solve the problem without creating numerical (artificial) instabilities. We present a new stability criterion for heterogeneous flow based on the homogenization theory. Relevant numerical simulations are presented to sustain our theoretical results.

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MS63

Error Estimates for the Finite Volume Method for a Copper Heap Leaching Model

This work is motivated by a combined mixed finite element (MFE) - finite volume (FV) scheme of a two phase flow model for the heap leaching of copper ores modeled by a degenerate parabolic equation

$$\partial_t u - \nabla \cdot (\nabla \beta(u) + F(u)) = r(u), \quad \text{in } Q_T \equiv (0, T) \times \Omega. \quad (1)$$

Initially we have $u(0) = u^0$ in Ω , whereas $u = 0$ on $\partial\Omega$. In the above $0 < T < \infty$ is fixed, Ω is a bounded domain in \mathbf{R}^d ($d \geq 1$) with a Lipschitz continuous boundary. The function $\beta : \mathbf{R} \rightarrow \mathbf{R}$ is non-decreasing and differentiable. By degeneracy we mean a vanishing diffusion, namely $\beta'(u) = 0$ for some u . We prove error estimates for the finite volume discretization for this model. Several numerical results illustrating the performance of the algorithm are provided.

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MS63

A Multiscale Preconditioner with Applications to Solute Transport in Porous Media

The mortar mixed finite element method can be viewed as a multiscale method for the pressure equation, with recent developments showing that the construction of a multiscale basis can greatly reduce the computational cost. We show that this multiscale basis does not need to be recomputed if used as a preconditioner for a Krylov method. We apply this preconditioner to an IMPEC formulation for the transport of a solute.

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PP0

2.5D Finite-Difference Solution of the VTI Acoustic Wave Equation

2.5D processing is a mathematical formalism of a 3D wave propagation in a 2D model. Assuming that there is no variation in the earth model in the transverse direction of the acquisition line. Using this symmetry, the 3D problem can be reduced to a repeated 2D problem. In this work, we apply the 2.5D formalism to describe a VTI wave propagation in a 2D model that preserves 3D geometrical

spreading effects. This propagation is cheaper than the 3D wave propagation.

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PP0

An Application of Fuzzy Transform in Geophysics

Fuzzy Transform (F-transform) have been introduced as an approximation method which encompasses both classical transforms as well as approximation methods studied in fuzzy modelling and fuzzy control. It has been proved that, under some conditions, F-transform can remove a periodical noise and reduce random noise significantly. In this work, we show how to use F-transform in order to solve wave equation with noise and how to use this theory in geophysics.

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Paraxial Approximations for the VTI Acoustic Wave Equation

In vertical transversally isotropic (VTI) media the acoustic wave equation is

$$\frac{\partial^4 u}{\partial t^4} - (1 + 2\eta)v^2 \frac{\partial^4 u}{\partial x^2 \partial t^2} = v_v^2 \frac{\partial^4 u}{\partial z^2 \partial t^2} - 2\eta v^2 v_v^2 \frac{\partial^4 u}{\partial x^2 \partial z^2} \quad (2)$$

where, $u(x, z, t)$ is the pressure field, η is a anisotropy parameter, and v_v and v are, respectively, the vertical qP-wave velocity and NMO velocity. Paraxial wave-equation approximations are used to describe wave propagation with a preferred direction. In this work, we derive paraxial approximations for equation (1), using higher order Padé approximations, in order to reduce computation cost in migration algorithms with a good accuracy.

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PP0

Anisotropic Complex-Padé Finite-Difference Depth Migration

Standard real-valued finite-difference (FD) migration cannot handle evanescent waves correctly, which can lead to numerical instabilities in the presence of strong velocity variations. A possible solution to these problems is the complex Padé approximation, which avoids problems with evanescent waves by a rotation of the branch cut of the complex square root. In this work, we apply this approximation to the acoustic wave equation for vertical transversely anisotropic media to derive more stable FD migration for such media.

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PP0

Fluid Flow, Transport and Reaction Processes, Monod and Van Genuchten Parametrization, Parameter Identification, Output Least Squares Method, Formfree Identification, Adaptive Sqp Method

Recent challenges like bioremediation, longterm underground storage of reactive waste or underground carbon-dioxide sequestration require more and more complex multicomponent reactive transport and fluid flow models. Although being demanding concerning their efficient numerical approximation, the decisive bottleneck in using such models seems to lie in the availability of the increasing range of reaction and hydraulic flow parameters entering such a model (Monod parameters in multiplicative Monod models in conjunction with bioremediation and rate parameters in kinetic mass action law models as well as van Genuchten parameters for the modelling of hydraulic properties ...). We address the reliable and accurate identification of such parameters from one of most controlled experimental set ups, namely from soil column breakthrough curves (letting the upscaling issue aside), but the following methodology can also applied to field experiments. It is well-known that the (missing) sensitivity and the correlation of parameters prevent a reliable reconstruction from naive history matching (output least squares minimization). For a fixed experimental setup we propose a systematic use of the singular values of the sensitivity matrix in the definition of the error functional to design an adaptive approach

in which after each termination in a (local) minimum the error functional is changed. Applications to the identification of Monod and van Genuchten parameters show significant improvements in possible accuracy. Furthermore, a favourable form free approach with hierarchical treatment for the global parametrization of one- or multidimensional nonlinearities are used. Thereby, because of the so called *curse of dimensionality* sparse grids are applied in case of higher dimensional problems to decrease the degree of freedom significantly. In addition the presented methods can also be combined with a hierarchical concept to filter out the most sensitive parameters and identify them first. In a further step these approaches can be used also within experimental design to find more appropriate sequences of experiments which can be taken into account into a multiexperiment identification approach.

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PP0

Detection and Approximation of Fault Lines from Scattered Data

We propose a method for the detection and accurate approximation of surface fault lines. First, to locate all the data points close to fault lines, we consider a procedure based on a local interpolation scheme involving a IDW formula. Then, we find further sets of points generally closer to the faults than the fault points. Finally, after applying a nearest-neighbour searching procedure and a refinement technique, we outline some approximation methods for the fault lines.

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PP0

A Method for Conditioning Stochastic Groundwater Flow Fracture Network Models.

Calculations of groundwater flow through fracture networks are of great importance for performance assessments of potential radioactive waste repositories located in hard rocks. We present a method for conditioning the transmissivities in a fracture network model on observed measurements of groundwater heads and flows to boreholes. The method is illustrated by application to a number of simple test cases and to a model of a site for which field data are available.

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PP0

A Modified Idw Algorithm for Scattered and Track Data Interpolation

We propose an accurate and efficient interpolation method, and the relative algorithm, for modelling unknown surfaces. It is based on a modified IDW formula (with least square or radial basis function approximants as nodal functions) and exploits the particular strip structure to optimize the searching procedure of the nearby data points. The method works well from both scattered data and track data, and guarantees a high parallelism.

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PP0

Soil Reaction Estimates for Laterally Loaded Piles Using Euler-Bernoulli Beam Theory and a Simple Polynomial Curve Fitting Algorithm on Lateral Deflection Measurements

A simple numerical procedure is proposed to estimate soil reactions along laterally loaded piles. The technique involves using lateral deflection measurements of the pile obtained from slope inclinometer measurements. The deflected shape of the laterally loaded pile is estimated using a simple polynomial curve fitting algorithm that is applied sequentially to the slope inclinometer data with depth. The procedure is used to derive curvature versus depth and moment versus depth. The procedure is calibrated with a full-scale experimental program involving lateral load test to three well-characterized piles where slope inclinometer data was available as well as curvature and moment data along the pile depth. The proposed procedure provides very good estimates of the measured bending moments and the soil reactions back-calculated using more conventional methods such as the use of a finite difference discretization of the pile with the soil reaction modeled with p-y curves.

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PP0

Evolution of the Uralide Orogenic Wedge - a Numerical Simulation

The Uralide orogen exhibits a bivergent orogenic wedge with a foreland thrust belt at the pro-wedge side and

lower crustal material originating from the pro-wedge in the retro-wedge. In this study a Distinct Element Method is used to investigate the tectonic evolution of the Uralide wedge and to determine the influence of the neighbourhood of strong island arc rocks and a serpentinitic melange, isostatic compensation and basal viscous flow on the structure of the orogen.

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PP0

Parameter Estimation for Water Transport in Heterogeneous Porous Media

The solution of Richards' equation requires the estimation of the parameters of a parametrisation of the hydraulic properties (capillary pressure-saturation curve, relative permeability). A typical method is multi-step outflow, where a sample is placed on a ceramic plate and desaturated by reducing the pressure stepwise at the lower boundary. Parameter estimation from multi-step outflow experiments requires usually the assumption of macroscopic homogeneity for the sample. If the structure of the sample (the arrangement of materials) can be determined independently (e.g. by geophysical measurements) it is possible to take it into account in the inversion process and estimate the hydraulic properties of the subscale materials. A very robust forward model massive parallel computing is necessary to get a fast solution of the large 3D forward problems which need to be solved.

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PP0

Information Mining Models for Interdisciplinary Research

The conference contribution describes the concept, implementation and application of an innovative information mining approach in an interdisciplinary research project. Target of the research project is to simulate the long-term deformation of large mountain sides. One key challenge in the interdisciplinary research project is to identify the interaction of the different physical processes such as meteorology, hydrology, surface flow, infiltration, sub-surface flow, soil mechanics, shear band deformations and hill slope movements with given geological and topographical heterogeneity. Key idea of this ongoing research work is to combine the different well known data mining methods to identify relationship between the different physical state variables as interdisciplinary application.

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PP0

Model Integration and Coupling in a Hydroinfor-

ematics System

The conference contribution describes the concept, implementation and application of an innovative information system to couple different simulation models. Application target is an interdisciplinary research project to simulate the long-term deformation of large mountain sides. The system supports the coupling of models from hydrology, multi-phase groundwater flow and soil mechanics as well as laboratory experiments and field measurements by generalized sets of objects to manage physical state variables including scaling, mapping and transformation. This approach allows a more flexible coupling of simulation models from different disciplines on flexible scales and approximation levels.

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PP0

Colloidal Influence on Fluid Dynamics in Porous Media

A microscopic model at the pore scale for fluid flow in porous media influenced by colloid dynamics is presented. Special attention is paid to ad-/desorption processes of colloidal particles at the solid matrix caused by the total interaction energy between particles and matrix as well as to thereby influenced evolving microstructure. In order to achieve some macroscopic description of the concerned phenomena, the derived model is homogenized with the method of asymptotic two-scale expansions.

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PP0

A New Method for Assigning ,the Eigenvalues Sign in Equation $(Ax = \lambda X)$ and $(Ax = \lambda Bx)$

The inertia of an $n \times n$ complex matrix A, is defined to be an integer triple, $In(A) = (\pi(A), \nu(A), \delta(A))$, where $\pi(A)$ is the number of eigenvalues of A with positive real parts, $\nu(A)$ is the number of eigenvalues with negative real parts and $\delta(A)$ is the number of eigenvalues with zero real parts. We are interested in computing the Inertia for large unsymmetric generalized eigenproblem (A,B) for equation $A\varphi = \lambda B\varphi$ Where A and B are $n \times n$ large matrices. For standard eigenvalues problem let $B =$ Identity matrix. An obvious approach for determine Inertia of pair(A,B), is to transform this to a standard eigenproblem by inverting either A or B. In this paper we show that the eigenvalues sign can be computed by assigning the interval that including all the eigenvalues and this method is compared by results in Matlab.

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PP0

Nonstandard FDTD Scheme for Computation of Elastic Waves

Finite-difference method in time-domain (FDTD) is one of the most popular techniques used for modeling of wave propagation in many fields. Recently, FDTD schemes called nonstandard FDTD have been developed in computational electromagnetics and acoustics to efficiently reduce the numerical dispersion and grid anisotropy. In this study we propose a nonstandard FDTD scheme for elastic wave computation, which gives highly accurate solutions both for P and S waves.

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PP0

Efficient Time-Stepping for Advection Dominated Reactive transport in Heterogeneous Porous Media

Reactive transport in heterogeneous porous media is common to many applications, including groundwater contamination and CO2 storage. Such processes are inherently multiscale in nature and highly non-linear, rendering accurate and fast numerical solutions challenging. We demonstrate that a finite volume discretization can be integrated in time with exponential integrators where a linear system is solved exactly. Using a Krylov subspace or Leja points to approximate the exponential makes these methods competitive compared to standard integrators.

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