Program for the 2008 Front Range Applied Mathematics Student Conference

Breakfast and Registration: 8:30 - 9:00

Morning Session I - Room 1312
9:00 - 11:00

9:00 - 9:20	Eugene Vecharynski *University of Colorado at Denver*	The Convergence of Restarted GMRES for Normal Matrices is Sublinear
9:25 - 9:45	Adrianna Gillman *University of Colorado at Boulder*	The Numerical Performace of a Mixed-Hybrid Type Solution Methodology for Solving High-Frequency Helmholtz Problems
9:50 - 10:10	Srihari Sritharan *University of Wyoming*	Solitons to Shockwaves: Simulation and Animation of Nonlinear Waves on Lattice
10:15 - 10:35	James Adler *University of Colorado at Boulder*	Nested Iteration First-Order Least Squares on Incompressible Resistive Magnetohydrodynamics
10:40 - 11:00	Geoffrey Sanders *University of Colorado at Boulder*	Convergence Theory for Nonsymmetric Smoothed Aggregation Multigrid

Morning Session II - Room 1315
9:00 - 11:00

9:00 - 9:20	Joseph Adams, Jonathan Olson, and Ryan Schilt *University of Colorado at Boulder*	Exemplar-Based Multiresolution, Seam Carving, and their Applications to Image Processing
9:25 - 9:45	Michael Presho *University of Wyoming*	The Effect of Uncertainty in Interface Location
9:50 - 10:10	Kirk Nichols *University of Colorado at Boulder*	Variational Integrators in Numerical Modeling of Mechanical Systems
10:15 - 10:35	Phantipa Thipwiwatpotjana *UCDHSC*	Algorithm for Solving Optimization Problems with Interval Valued Probability Measure
10:40 - 11:00	Ryan Kennedy *University of Colorado at Boulder*	Confidence Intervals for Probabilistic Pattern Matching

Break: 11:00 - 11:15

Plenary Address, Harry L. Swinney: 11:15 - 12:15 Room 1130

Emergence of Spatial Patterns in Physical, Chemical, and Biological Systems

Lunch: 12:15 - 1:00
Afternoon Session I - Room 1312
1:00 - 2:15

1:00 - 1:20	Ben Jamroz *University of Colorado at Boulder*	A Reduced PDE Model for the Magnetorotational Instability
1:25 - 1:45	Elizabeth Untiedt *University of Colorado at Denver*	Fuzzy Natural Numbers
1:50 - 2:15	Keith Wojciechowski *University of Colorado at Denver*	Using Pseudospectral Methods to Solve a Nonlinear Transport Equation

Afternoon Session II - Room 1315
1:00 - 2:15

1:00 - 1:20	Kye Taylor *University of Colorado at Boulder*	Geometric Parameterization and Denoising of Manifold-Valued Data
1:25 - 1:45	Bedrich Sousedik *University of Colorado at Denver*	A Recent View on the BDDC Method and its Parallel Implementation
1:50 - 2:15	Christian Ketelsen *University of Colorado at Boulder*	Numerical Challenges in Lattice Quantum Chromodynamics

Plenary Speaker (11:15 - 12:15)

Emergence of Spatial Patterns in Physical, Chemical, and Biological Systems

Harry L. Swinney, University of Texas at Austin

We consider macroscopic systems driven away from thermodynamic equilibrium by an imposed gradient, for example, a gradient in temperature, velocity, or concentration. The equation of motion for such systems is generally a nonlinear partial differential equation for the fields (e.g., temperature, velocity, and/or concentration field). For a sufficiently small imposed gradient, these fields will have the same symmetry as the system geometry; this solution is called the base state. We will consider the general principles for the loss of stability of the base state and the formation of ordered spatial patterns. For strong forcing, the patterns can become chaotic or even turbulent, yet some order often persists. The general principles of pattern formation will be illustrated with examples from physics, chemistry, and biology.

MORNING SESSION I

THE CONVERGENCE OF RESTARTED GMRES FOR NORMAL MATRICES IS SUBLINEAR

Eugene Vecharynski
University of Colorado at Denver

While a lot of efforts have been put in the characterization of the convergence of full GMRES, we have noticed that very few efforts have been made in characterizing the convergence of restarted GMRES despite the fact that this latter is the most practically used. Our current research aimed to better understand restarted GMRES.

Our main result proves that the convergence of restarted GMRES for normal matrices is sublinear. That is to say if after one GMRES cycle we have observed a given residual decrease, then the next GMRES cycle will necessarily have a smaller residual decrease. The proof relies on the observation that GMRES(A, m, r_0) and GMRES(A^H, m, r_0) both provide the same residual norm after one cycle. From this main theorem flows two corollaries. Firstly, we can characterize the convergence of GMRES(n-1) for normal matrices. Secondly, we can rederive a result from Baker, Jessup and Manteuffel (2005) about alternating residuals for GMRES(n-1) applied to Hermitian or Skew-Hermitian matrices.

THE NUMERICAL PERFORMACE OF A MIXED-HYBRID TYPE SOLUTION METHODOLOGY FOR SOLVING HIGH-FREQUENCY HELMHOLTZ PROBLEMS

Adrianna Gillman
University of Colorado at Boulder

The numerical solution of problems involving waves has been an area of active research for almost half of a century. This is due in part to the importance of applications that require a practical solution of wave phenomena problems such as sonar, radar, geophysical exploration, medical imaging, nondestructive testing, and more recently meteorology. Despite the tremendous progress that has been made in the recent years, this area is still regarded as one of the most challenging in scientific computation. The challenge of efficient computation at high wavenumbers, in particular, has been designated as one of the problems still unsolved by current numerical techniques. Indeed, standard computational methods such as Galerkin finite element methods (FEM) are unable to cope with wave phenomena at short wavelengths because they require a prohibitive computational effort in order to resolve the waves and control numerical dispersion errors. For example, solving an acoustic scattering problem using quadratic finite elements for $ka = 10$, where k is the wave number and a characterizes the dimension of the considered submarine-like scatterer, requires solving a system with 10 millions complex unknowns while sonar applications require solving these exterior Helmholtz problems for ka larger than 200. This simply rules out reliable solutions of the Helmholtz equation by the standard Galerkin FEM in the mid- and high-frequency regimes. Therefore, it is significant to develop discretization schemes that avoid, or at least control effectively, the error associated with solving wave equations for high frequencies (the so-called pollution error) in order to be able to address practical problems.

We proposed a mixed hybrid type formulation for solving Helmholtz problems in which the solution is approximated locally by oscillated finite element polynomials using any shaped elements. These shape functions are more suitable then those of existing approximation schemes because they take into account the frequency. In addition, the continuity across element boundaries of the solution is enforced weakly by Lagrange multipliers. The discontinuous nature of the approximation enables static condensation of primal variables prior to assembly. Consequently, the computational complexity of the proposed discretization method is determined mainly by the total number of Lagrange multiplier degrees of freedom introduced at the edges of the finite element mesh, and the sparsity pattern of the corresponding system matrix. Numerical results are reported to illustrate the potential of the proposed solution methodology for solving efficiently Helmholtz problems in the mid-and-high frequency regimes.

SOLITONS TO SHOCKWAVES: SIMULATION AND ANIMATION OF NONLINEAR WAVES ON LATTICE

Srihari Sritharan
University of Wyoming

Using MATLAB 7.1, we calculated computational solutions to a variety of nonlinear wave equations. After discretizing the partial differential equations, we got nonlinear dynamical systems on a lattice. We utilized both an ODE and Algorithm solver method to get explicit solutions with soliton and shockwave behavior. Using a 64 particle model, we plotted and animated our results in several forms, including a linear lattice, a ring lattice (when appropriate), kinetic energy animations and phase plots. Furthermore, our use of an algorithm solver yielded threedimensional plots describing shockwave evolution. Our calculations included the use of the Linear Advection Equation, the second order wave equation, the Toda Exponential Lattice, the Inviscid Burgers Equation, and the SineGordon Equation. We finished our project with the experimentation of controls on our previously calculated lattices.

NESTED ITERATION FIRST-ORDER LEAST SQUARES ON INCOMPRESSIBLE RESISTIVE MAGNETOHYDRODYNAMICS

James Adler
University of Colorado at Boulder

Magnetohydrodynamics (MHD) is a single-fluid theory that describes Plasma Physics. MHD treats the plasma as one fluid of charged particles. Hence, the equations that describe the plasma form a nonlinear system that couples Navier-Stokes with Maxwell's equations. To solve this system, a nested-iteration-Newton-FOSLS-AMG approach is taken. The system is linearized on a coarse grid using a Newton step and is then discretized in a FOSLS functional upon which several AMG V-cycles are performed. If necessary, another Newton step is taken and more V-cycles are done. When the linear functional has converged "enough," the approximation is interpolated to a finer grid where it is again linearized, FOSLized, and solved for. The goal is to determine the most efficient algorithm in this context. One would like to do as much work as possible on the coarse grid including most of the linearization. Ideally, it would be good to show that at most one Newton step and a few V-cycles are all that is needed on the finest grid. This talk will develop theory that supports this argument, as well as show experiments to confirm that the algorithm can be efficient for MHD problems. Currently, two test problems have been studied, both with the use of FOSPACK: a 3D steady state MHD test problem with a manufactured solution, and, for a more realistic problem, a reduced 2D time-dependent formulation. The latter equations can simulate a "large aspect-ratio" tokamak, with non-circular cross-sections. Here, the problem was reformulated in a way that is suitable for FOSLS and FOSPACK. This talk will discuss two stopping criteria. First, on each refinement level, when should one stop solving the linear system and re-linearize the problem. Secondly, how does one choose whether to do another Newton step or move to a finer grid. In addition, different types of h and p refinement will be tested, as well as adaptive mesh refinement. The goal is to resolve as much physics from the test problem with the least amount of work.

CONVERGENCE THEORY FOR NONSYMMETRIC SMOOTHED AGGREGATION MULTIGRID

Geoffrey Sanders
University of Colorado at Boulder

Applying smoothed aggregation multigrid (SA) to solve nonsymmetric linear systems, $A\mathbf{x} = \mathbf{b}$, can be problematic due to a lack of minimization principle in the coarse-grid corrections. We propose an approach that is based on approximately applying SA to the symmetric positive definite matrices $\sqrt{A^*A}$ or $\sqrt{AA^*}$. These matrices, however, are typically full and difficult to compute, and it is therefore not computationally efficient to use these matrices directly to form a coarse-grid correction. Our proposed approach approximates these coarse-grid corrections by using smoothed aggregation to accurately approximate the right and left singular vectors of A that correspond to the lowest singular value. These are used to construct the interpolation and restriction operators, respectively. We present some preliminary two-level convergence theory and numerical results.

MORNING SESSION II

EXEMPLAR-BASED MULTIRESOLUTION, SEAM CARVING, AND THEIR APPLICATIONS TO IMAGE PROCESSING

Joseph Adams, Jonathan Olson, and Ryan Schilt
University of Colorado at Boulder

Exemplar-Based Multiresolution is a reversible decomposition of hierarchical data into a difference tree. It is constructed at each level by finding an exemplar and storing the differences between it and all other data points at that level. Since many differences are usually small, they can be removed to compress the data. By defining a multiresolution structure for an image, we can then decompose it into a difference tree. Using the difference tree, we can quickly recover an approximation to the original image using simple arithmetic. When compared with standard wavelet image compression techniques, our algorithm yields slightly worse error. However our algorithm can be used on arbitrary hierarchical structures with user-defined difference functions to which wavelets would not apply. Seam Carving is a method used to resize images by carving out only parts of the image, instead of scaling an image. An energy is defined for each pixel, and seams are removed by finding paths through the image with the least total energy. We have implemented a fast seam searching algorithm similar to Dijkstras algorithm in which computational complexity is proportional to the number of pixels in the image.

THE EFFECT OF UNCERTAINTY IN INTERFACE LOCATION

Michael Presho
University of Wyoming

The study of reservoir fluid flow is a broad research topic with plenty of room for advancement. In our research we considered the effects of uncertainty with respect to the location of a composite reservoirs interface. In order to isolate the source of uncertainty we chose two idealized models in which analytical solutions could be found. We assume that the interface location follows certain statistical distribution from which a number of its realizations can be generated. A Monte Carlo simulation is then performed to obtain various statistical moments of the flow solution related to the nature of location uncertainty. In the future we hope to perform sensitivity analysis on the problem with adjoint (or other) methods.

VARIATIONAL INTEGRATORS IN NUMERICAL MODELING OF MECHANICAL SYSTEMS

Kirk Nichols
University of Colorado at Boulder

Variational Integrators are a relatively unexplored numerical integration tool derived from variational calculus that are efficient in modeling dynamics. The presentation would begin with a trivial example to prove the variational integrator is worth listening to and then progressively add on more theory to increase the robustness of the variational integrator.

Our trivial example is considering a one-link pendulum. Given coordinate system theta and fixed length L, we will derive the corresponding Lagrangian equation and the Euler-Lagrange Equation. Once at this ODE, we will explore the application of variational integrators modeling the system versus other numerical integration techniques, such as explicit euler integration and linearly implicit euler integration. The comparisons are best seen with animations which I have created.

Once the audience is sold that variational integrators are worth listening too, we will explore methods of representing more robust dynamical systems, first considering a multi-dimensional pendulum. With a larger configuration space, a generalized coordinate system will be used so that the pendulum doesnt disconnect, as each new link is represented directly as a result of its parent, with the root link fixed in the spatial frame.

We then need to derive methods in calculating the kinetic and potential energy of the system, of which the Lagrangian is calculated. This involves the creation of the body jacobian matrix, which maps forces from children links up to the parent. With our Lagrangian created, we then derive the continuous and discrete Euler Lagrange equations from Hamiltons Principle of Least action. With the equations derived, we then have the structure necessary to model a multi-dimensional pendulum. More animations.

We then consider elasticity in a cable. This requires use of the finite element method to model additional potential energy created by axial elongation and bending forces. We then present the continuous and discrete Euler-Lagrange equations for a constrained system, thus introducing another advantage of variational integrators in the ability to perfectly model constraints. More animations, this time of an elastic cable.

ALGORITHM FOR SOLVING OPTIMIZATION PROBLEMS WITH INTERVAL VALUED PROBABILITY MEASURE

Phantipa Thipwiwatpotjana
University of Colorado at Denver Health Sciences Campus

We are concerned with three types of uncertainties: probabilistic, possibilitistic and interval. By using possibility and necessity measures as an Interval Valued Probability Measure (IVPM), we present IVPMs interval expected values whose possibility distributions are in the form of polynomials. By working with interval expected val- ues of independent uncertainty coefficients in a linear optimization problem together with operations suggested by Lodwick and Jamison (will be explained during the talk), the problem after applying these operations becomes a linear programming problem with con stant coefficients. This is achieved by the application of two functions. The first is applied to the interval coefficients, $v : I \rightarrow R^k$, where $I = \{[a, b]|a \leq b\}$. The second is $u : R^k \rightarrow R$, applied to the product we got from a previous function. Similar concepts hold for any types of optimization problems with linear constraints. Moreover, it implied that optimization problems containing all three types of uncertainties in one problem can be solved as ordinary optimization problems.

CONFIDENCE INTERVALS FOR PROBABILISTIC PATTERN MATCHING

Ryan Kennedy
University of Colorado at Boulder

A crucial problem in computational biology is determining the probability of finding certain patterns in random RNA-sequence pools. Directly calculating these probabilities via simulation is infeasible because the probabilities are so small. Additionally, calculating the exact probabilities is computationally impractical for large motifs. Various approximation methods have been proposed, including simple information-based approaches and Poisson approximations. However, the first method is often inaccurate and the error incurred in the Poisson approximation has only been quantified for rather specific patterns in the literature. In this talk, we introduce an alternative method for estimating these probabilities. We are able to achieve a considerable complexity reduction over exact calculations and determine tight lower- and upper-bounds for confidence intervals on the actual probabilities. This research is supported by the NIH grant R01GM048080.

AFTERNOON SESSION I

A REDUCED PDE MODEL FOR THE MAGNETOROTATIONAL INSTABILITY

Ben Jamroz
University of Colorado at Boulder

Accretion disks occur widely in astrophysics, and are found in binary star systems, protoplanetary systems, as well as near black holes at the center of spiral galaxies. The accretion rates of these disks, deduced from observation, requires an efficient mechanism for angular momentum extraction. The magnetorotational instability, in magnetized accretion disks, is widely believed to be the mechanism providing the necessary angular momentum transport. Taking advantage of disparate spatio-temporal scales relevant to astrophysics and laboratory experiments, one can derive a reduced PDE model for the magnetorotational instability. These reduced equations, which are characterized by a back-reaction onto the imposed local shear, can be used to analyze the nonlinear saturation of this instability and measure local angular momentum transport.

FUZZY NATURAL NUMBERS

Elizabeth Untiedt
University of Colorado at Denver

This talk will explore the recent idea of fuzzy natural numbers, which represent the cardinality of a fuzzy set. The concept of fuzzy natural numbers will be extended to define fuzzy relative integers and fuzzy rational numbers. The speaker will define fuzzy prime numbers, and introduce and prove some original related theorems.

USING PSEUDOSPECTRAL METHODS TO SOLVE A NONLINEAR TRANSPORT EQUATION

Keith Wojciechowski
University of Colorado at Denver

Numerical methods for time-dependent linear partial differential equations (PDEs) typically discretize the spatial derivative and use any number of time-marching schemes readily available whereas numerical methods for time-dependent, nonlinear PDEs can be highly specialized. For example, in the case of linear problems, there are implicit and explicit Euler methods, alternating-direction implicit (ADI) methods, and the Crank-Nicoloson method for parabolic problems as well as the Leapfrog method, Lax-Wendroff method, and backward-difference in time method for hyperbolic problems. In the case of nonlinear problems, Runge-Kutta methods are a typical first attempt.

The accuracy with respect to the spatial derivative can be improved by either choosing high-order polynomials or finite-difference formulas or using spectral differentiation matrices. Spectral methods are implemented by approximating the spatial derivative using a global interpolant through discrete data points, then differentiating the interpolant at each point. Under favorable circumstances spectral methods boast a higher accuracy per computational cost than finite differences or finite elements (note that spectral differentiation matrices are sparsely implemented via the FFT). A nonlinear transport model for a swelling porous material is proposed and numerically solved. A pseudospectral method is implemented for the spatial derivatives while the time-stepping is executed by separating the equation into linear and nonlinear parts. The linear part is solved exactly while the nonlinear part issolved using numerical quadrature. This method is then compared to a fourth-order Runge-Kutta scheme.

AFTERNOON SESSION II

GEOMETRIC PARAMETERIZATION AND DENOISING OF MANIFOLD-VALUED DATA

Kye Taylor
University of Colorado at Boulder

Several methods for learning a datasets underlying topological structure have been proposed that typi- cally rely on the spectral properties of a similarity matrix defined on a dataset, e.g. Laplacian Eigenmaps, Diffusions Maps, Isomap, and Local Linear Embedding just to name a few. Diffusions Maps and Laplacian Eigenmaps are appealing algorithms due to convergence guarantees as well as the perspective gained by making the connection between the diffusion operators and random walks defined on the datasets. Because analysis and inference can be complicated by noisy measurements and less than optimal sampling of the feature space, I will also discuss investigations into improving the parameterization produced by these algorithms when the dataset is corrupted by noise. To remove noise, one approach uses the spectral properties of the operator defined on the dataset to build a filter to denoise a signal. I will discuss several experiments involving this algorithm including removing noise from images, time series, and other low-dimensional manifolds. In addition, I will consider the consequences of applying the filter, effects of nonuniform sampling, as well as computational costs and practical issues.

A RECENT VIEW ON THE BDDC METHOD AND ITS PARALLEL IMPLEMENTATION

Bedrich Sousedik
University of Colorado at Denver

The presentation covers an ongoing effort to efficiently implement the Balancing Domain Decomposition with Constraints method (BDDC) for solving large systems of equations arising from linear elasticity analyses. The BDDC method is seen as a preconditioner in PCG method. Within this framework, solution to an inexact problem is found by a direct solver. In our latest formulation of the method, decomposition of the domain just gives us a way to construct the inexact problem. It is done by relaxing most (but not all) the continuity requirements on the solution among subdomains and thus "inflating" the space where the problem is defined. We end up with a larger matrix than the one of the original problem, which is then solved exactly. However, the simple structure of this matrix makes the solution by a direct method easy and thus possible to use it for preconditioning. In finite element terminology, the larger problem is constructed by so called "partial assembly", a process that does not assemble the matrix at most of the interface nodes among subdomains. The current version of the implementation is based on the Multifrontal Massively Parallel Solver (MUMPS), an interesting open source package for solving linear equations that will be in short introduced.

NUMERICAL CHALLENGES IN LATTICE QUANTUM CHROMODYNAMICS

Christian Ketelsen
University of Colorado at Boulder

Quantum Chromodynamics (QCD) is the predominant theory describing the strong interactions in the standard model of particle physics. The strong force confines quarks together inside of composite particles like protons and neutrons. Unlike particles prevalent in quantum electrodynamics (QED), the forces between quarks get stronger as the distance between the particles increases. This makes the usual asymptotic techniques employed in QED inadequate as a means of characterizing the strong force. As a result, large scale numerical simulations are necessary to model these interactions for physically realistic parameters.

The large computational obstacle in such simulations is the numerical solution of a large system of partial different equations which we discretize on a four dimensional space-time lattice. For physically interesting parameters the resulting linear system is large, highly disordered, and near singular, making traditional iterative solution methods insufficient. A brief introduction will be given to popular discretizations of the governing equations and a new discretization based on a least squares finite element method will be presented. Methods based on smoothed aggregation multigrid will be explored for the solution of the resulting linear systems.