CP1

Modeling Radiative Heat Transfer in Multifilament Fiber Melt-Spinning

The overall goal of this effort is to develop an accurate model for the thermal environment downstream of dies so that local heat transfer rates can be realistically determined and included in models of fiber drawing. The goal is to assess the influence of each heat transfer mode (radiative and convective) at various locations along the spinline and possible interactions between them, under a variety of processing conditions. In the current work we focus on the development of the radiative heat transfer model and use a simple approach for the convective heat transfer contribution. The latter component is calculated as part of the flow-induced crystallization model of Doufas et al. for a single melt-spun fiber (Journal of Non-Newtonian Fluid Mechanics, 92, 27-66, 2000), extended to the multifilament setting with a technique similar to Dutta's approach (Polym. Eng. Sci., 27, 1050-1058, 1985). A Monte Carlo method is implemented for radiative heat exchange between fibers, the spinneret, and the background. Temperature variations along individual fibers and the resulting local radiative heat transfer are taken into account. This approach allows ready investigation of parametric effects related to geometry and is more realistic than methods of prior studies. Preliminary results using this model indicate that the radiative heat transfer component can have non-negligible influence on the temperature profile and on the location of the transition region where crystallization occurs in the fiber. Correct prediction of the transition region is critically important for correct modeling of resulting fiber properties. These results will be presented along with a brief discussion of continuing work.

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CP1

Active Vibration Control and Model Updating in Structural Dynamics : Linking Control To Industry

The use of active feedback control strategy is a natural way to stabilize and control dangerous vibrations in vibrating structures. The existing vibrations control techniques are fraught with numerous computational and engineering difficulties. A novel practical approach for vibration control and related model updating problem overcoming some of these difficultes has been developed by the author and his collaborators in recent years. These advances will be reviewed and a brief discussion presented on future reserach.

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CP1

Portable Performance Optimizations for Vector and Microprocessor Based Supercomputers

We will present portable performance optimizations based on a performance history of the fusion code GYRO on two diverse architectures, namely a Cray X1E and a Cray XT3 (both single- and dual-core.) The contribution of this work will be a summary of the performance enhancements that are portable to these machines. Knowing what performance optimizations are portable across a variety of machines is essential because good performance is more than finding the right compiler options.

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CP2

Toward Fast and Accurate Methods for Dose Computation in Radiotherapy

A deterministic Boltzmann transport model for dose calculation in electron radiotherapy is presented. We investigate several ways to simplify the deterministic model having two goals in mind, lower computation times on the one hand, high accuracy and model inherent incorporation of tissue inhomogeneities on the other hand. While being fast, the second property is lost in the often used pencil beam models. Several test cases, including the irradiation of a water phantom, are presented.

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CP2

Modeling Cell Aggregation in Nonlinear Shear Flow Via the Population Balance Equation

Cell aggregation and adhesion in a nonuniform shear flow is a problem of great interest in many biological studies such as the study of tumor extravasation during metastasis. We model such a process using the population balance equation. The basic mathematical properties and convergent numerical scheme are established. We also present numerical simulation results on the leukocyte (PMN)-melanoma cell emboli formation and subsequent tethering to the vascular endothelium (EC).

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CP2

An Integrative Computational Model of Multicil-

iary Beating and Its Applications

Cilia are microscopic hair-like organelles projecting from the cell surface. The study of the motility of cilia and flagella is of great importance in biology and medicine. Biologists revealed that nearly all mammalian cells form a cilium. In human body, cilia and flagella are present on almost all cells including cells in embryo, kidney and brain. Cilia perform essential motile and sensory functions and play important roles in cell motility of sperm and ovum along the respective reproductive tracts, transport of mucus across respiratory epithelia, cerebrospinal fluid movement in the brain, etc. The core of a cilium is called axoneme, in which dyneins fueled by ATP are responsible for the motility of cilia. We present an integrative computational model of multiciliary beating and its applications. The axoneme is modeled by Dillon-Fauci approach which was first used in [1] in 2000. Dillon-Fauci axoneme model is simple but very successful in modeling the cilia and sperm motility ([1] Dillon, R. H. and Fauci, L. J. (2000). An integrative model of internal axoneme mechanics and external fluid dynamics in ciliary beating. Journal of Theoretical Biology, 207:415-430. [2] Dillon, R. H., Fauci, L. J., and Omoto, C. (2003). Mathematical modeling of axoneme mechanics and fluid dynamics in ciliary and sperm motility. Dyn. Contin. Discrete Impuls. Syst. Ser. A Math. Anal., 10(5):745-757. Progress in partial differential equations (Pullman, WA, 2002). [3] Dillon, R. H., Fauci, L. J., and Yang, X.,(2006) Sperm Motility and Multiciliary Beating: an Integrative Mechanical Model, Computers and Mathematics with Applications, In press. [4] Dillon, R. H., Fauci, L. J., Omoto, C. and Yang, X. Fluid Dynamic Models of flagellar and ciliary beating, submitted to "Annals of the NY Academy of Sciences".). This model, based upon the immersed boundary method (Peskin), couples the internal force generation of the molecular motors through the passive elastic structure with the external fluid mechanics governed by the Navier-Stokes equations. In our numerical results, we show how a single cilium interacts with its neighboring cilia, how viscosity effects its beating frequency, how synchronization phenomena are generated. We also compare the total flow pumped by cilia vs. viscosity, beat frequency. We present the ATP consumed at the end of each power and recovery stroke. At last I will present the computer simulations for mucociliary transport and chlamydomonas swimming, etc. and the current progress and future directions of our work.

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CP3

Unsteady Stagnation-Point Flow with a Magnetic Field

The unsteady two-dimensional stagnation-point flow of a viscous fluid impinging on an infinite plate in the presence of a transverse magnetic field is studied. The plate is making harmonic oscillations in its own plane. A finite difference technique is employed and solutions for large frequencies of the oscillations are obtained for various values of the Hartmans number.

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CP3

Performance of Amg-Type Preconditioners for Fully-Coupled Solution of Fe Transport/Reaction Simulations

This talk will present recent results of the application of Newton-Krylov methods with coupled preconditioners that utilize algebraic multilevel methods. The preconditioners are evaluated for two different transport/reaction systems: the Navier-Stokes equations for incompressible flow with transport and reaction, and the solution of the drift-diffusion equations to model semiconductor devices. Performance and scaling results for large-scale simulations will be presented. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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CP3

Parallel Implicit Adaptive Mesh Refinement for Resistive Magnetohydrodynamics

Application of parallel implicit adaptive mesh refinement (AMR) to simulate resistive magnetohydrodynamics is described. Solving this challenging multi-scale, multi-physics problem can improve understanding of reconnection in magnetically-confined plasmas. Implicit time integration is used to step over fast Alfven time scales. At each time step, large-scale systems of nonlinear equations are solved using Jacobian-free Newton-Krylov methods together with a physics-based preconditioner on AMR grids.

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CP4

Is it Possible to Decrease the CFL-Number Dependency of Explicit Schemes?

In order to achieve an efficient discretization for LES and DNS of wall-bounded turbulent flows, we are trying to increase the stability region of one-stage explicit schemes because a one-stage explicit algorithm is considerably more efficient and easier to implement than the corresponding multi-stage scheme. First, we mathematically prove that it is possible to decrease the CFL-dependency of explicit schemes though at the first glance, it may be inferred that our conclusion is in contrast with von Neumann theorem! Then we propose a systematic procedure for stabilizing explicit schemes for larger CFL numbers. The method is based on tuning the coefficients of higher-order terms while preserving the consistency of discretization by matching the coefficients of lower-order terms. Finally, we drive several high-order CFL-independent one-stage explicit schemes. Preliminary results reveal that the current high-order schemes are efficient and bring higher rates of convergence.

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CP4

Ripple: Residual Initiated Polynomial-Time Piecewise Linear Estimation

Piecewise linear estimation algorithms are used in engineering problems, where the individual response functions can be approximated by linear local approximations. The performance of most robust estimation algorithms degrades in higher dimensions due to exponential complexity and sparse data. A robust polynomial-time piecewise linear estimation algorithm has been developed that selects minimal sets of data based on a minimal residual criterion. RIPPLE is shown to perform better than other robust estimation algorithms in high dimensions.

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CP4

Applications of New Matrix Formalism for Series Solutions to Some Physical Models

New matrix formalism for finding series solutions to differential equations is presented. The method allows to easily derive recurrence relations for Laurent coefficients of solutions to ODEs and PDEs from a broad class. In particular, the class includes nonnpolynomial ODEs with nonlinear term in the form $f(u(t))$ where f is an analytic function. We focus on applications of the method to various models in physics including integrable (Burgers, KdV) and nonintegrable (Kuramoto-Sivashinsky, Henon-Heiles) equations.

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CP5

Complex Version of High Performance Computing Linpack Benchmark (hpl)

The High Performance Linpack (HPL) Benchmark is used in benchmarking the TOP 500 computers by solving a dense double precision linear system using LU factorization. HPL can be tuned to use recursive and hybrid algorithms and is more efficient than ScaLAPACK PZGESV that uses only a right-looking algorithm. This effort uses scripts and the C99 compiler to generate a complex version of HPL to ultimately improve the performance of solvers in fusion applications.

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CP5

A New Scaling Formula for the Linpack Benchmark

Dimensional analysis predicts a simple scaling formula for the Linpack benchmark. The computational power $r(p, q)$, on a set of processors decomposed into a (p, q) grid, is determined by the computational power $r(p_0, q_0)$, on a set of processors decomposed into a (p_0, q_0) grid, and two scaling parameters α and β such that

$$r(p, q) = (p/p_0)^{\alpha}(q/q_0)^{\beta} r(p_0, q_0).$$

These scaling parameters describe the interaction between the numerical algorithm and the system architetcure. Perfect scaling corresponds to $\alpha = \beta = 1$; no scaling corresponds to $\alpha = \beta = 0$. The scaling parameters measure the symmetry of the machine with respect to the chosen algorithm and processor decomposition. We have determined these parameters by performing a sequence of fixed-time measurements where the problem size increases with the number of processors such that the execution time remains constant. Measurements on a collection of machines confirm that the conjecture implied by dimensional analysis is

in fact correct.

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CP6

Preconditioning the MLFMA Solution of EFIE with Nested Flexible Iterative Solvers

We consider ill-conditioned dense linear systems generated by the electric-field integral equation (EFIE) of computational electromagnetics. When such systems are solved with the multilevel fast multipole algorithm (MLFMA) within an iterative solver, strong preconditioners are needed. For this purpose, another (inner) iterative solver that is nested inside the main (outer) iterative solver can be used as a preconditioner, provided that a flexible outer solver is used, allowing the preconditioner change from iteration to iteration. With this mechanism, the outer solver is used to solve the EFIE system and the inner solver is used to provide the preconditioner. One of the possibilities for the outer solver is the flexible GMRES (FGMRES).

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CP6

A Parallel Implicit Overlap Method for Solving 3D Electromagnetic Wave Scattering Problems

Maxwells curl equations in the time domain are solved by combining linear finite element algorithm and the well known finite difference time domain method. Hybrid meshes are employed while a local implicit scheme is applied on those tetrahedral elements with tiny grid sizes. Boundary integral term is investigated at PEC boundaries. The complete solution procedure is parallelized. Examples are included to demonstrate the numerical performance of the techniques that are proposed.

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CP6

Parallelization of Beam Dynamic Code TRACK

In the accelerator design and beam dynamic simulations, it is very important to simulate large number of particles. Parallel computing has been applied to beam dynamic code TRACK. The space charge effect is described by the Poisson equation. In this talk we compares several different parallel models for Poisson equation and give results in the accelerator simulations. These results show that parallel computing has greatly improved the capability of accelerator design and beam dynamic simulations.

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CP7

Scalable Lasto for Electronic-Structure Calculations

We are developing the Scalable Linear Augmented Slater Type Orbital (LASTO) method for electronic-structure calculations of clusters. To solve Schrödinger equation, we use mixed basis sets which are consisted by a linear combination of numerical functions inside atom centered spheres and exponentially decaying functions (Slater-type orbital, STO) between spheres. As numerical experiments, we compute the Pd clusters and hydrogen absorption of Pd cluster.

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CP8

Computational Issues in Simulation of Gas Pipeline Networks

We are interested in computational issues arising in the context of gas flow in pipeline networks. Here, the dynamics of the flow inside the gas pipes is described by the isothermal Euler equations. In areas of the network where we expect less complex gas dynamics, we apply simplified models for predicting the flow. We discuss algorithms for the arising coupled hierarchy of gas models and present numerical results for a network similar to the Canadian Mainline Gas Network.

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CP8

Long Memory Mori-Zwanzig Models for the Euler Equations

A long memory model for dimensional reduction, known as the t-model, is derived through the Mori-Zwanzig formalism of irreversible statistical mechanics. The model is

applied to the estimation of the rate of decay of solutions of the Burgers equation and of the Euler equations in two and three space dimensions. In the Burgers case, the model captures the rate of decay exactly. For the Euler equations in two space dimensions, the model preserves energy as it should. In three dimensions, we find a power law decay in time and observe a temporal intermittency. If time permits, we will discuss briefly a hierarchy of Mori-Zwanzig models in which the t-model is the first one. This is joint work with A. Chorin, O. Hald and Y. Shvets.

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CP8

Identification of Effects of Interface Imperfections on Turbulent Fluid Flows

We address the problem of characterization of the effects of initial interface disturbances on a Rayleigh-Taylor flow. The connection between the initial imperfections and the turbulent flow is uncertain and fundamentally nonlinear. To identify the components of the imperfection field that have the greatest influence on the growth rate, we construct the Hessian matrix of the transfer function from DNS simulations, and compute the dominant eigenvectors via an adjoint-based matrix-free truncated Lanczos procedure.

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CP9

A Multiscale Total Variation Based Image Registration Method with Application to Brain Images

Recent studies in total variation models for image restoration have led to increased theoretical understanding and practical implementations of scale space methods for decomposing an image into its essential (cartoon) and spurious (noise and texture) parts. Noise and texture add irrelevant complexity to the data resulting in problems with unnecessary high dimensionality and consequently longer processing times. Image registration benefits from such decomposition methods for the essential features detectable in the cartoon image will almost exclusively drive a successful registration. We present an image registration method combining total variation based image decomposition with a multiresolution triangulation scheme that significantly reduces problem dimensionality to a few pixels. We demonstrate our method in brain images composed of small and large scale structures.

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CP9

Variational Shape Optimization for Simultaneous Segmentation and Denoising of Images

We introduce a novel computational method for the Mumford-Shah problem. We recover region boundaries in a given image and a piecewise smooth approximation. Casting this as a shape optimization problem, we adopt an inexact Newton approach and propose a finite element method for curve evolution. The method incorporates topological changes such as splitting for detection of multiple objects. We employ space adaptivity and a coarse-to-fine approach to process large images efficiently.

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CP9

Regularized 3-D Reconstructions from Spherically-Averaged Fourier Transform Magnitude and Solution X-Ray Scattering Experiments

Measuring the scattering of a beam of x-rays off a solution of identical particles gives data that is the spherically-averaged magnitude of the Fourier transform of electron number density in the particle. Since solving a nonlinear least squares problem does not incorporate all biological knowledge about the particles, regularizers are proposed based on the spherically averaged electron scattering density autocorrelation and based on 2-D and 3-D measures of curvature of the particles.

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CP10

A Boundary Integral Method and Adaptive Treecode for Poisson-Boltzmann Equation

A boundary integral method (BIM) is developed for computing the Poisson-Boltzmann equation (PBE), which is derived from a continuum model of the solvent and counterion environment surrounding a biomolecule. The BIM provides a rigorous treatment on issues of the singular charges, the solute-solvent interfaces, and the infinite domain associated with the PBE. The boundary integrals with regularized kernels are evaluated by an adaptive treecode algorithm based on Taylor approximation in Cartesian coordinates, and the necessary Taylor coefficients are computed by a recurrence relation. Numerical experiments are included to show the efficiency of the pro-

posed method.

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CP10

A Local Regularization Method for the Solution of Fredholm Integral Equation of the First Kind

The solution of many engineering problems involves the solution of Fredholm integral equation of the first kind

$$\int_0^1 K(s,t)x(t)dt = d(s) \quad , \qquad 0 \le s \le 1$$

The computational approach to the solution of this equation requires its discretization, which leads to a linear system of equations of

$$Kx + e = d$$

Since the Fredholm integral equation is ill-posed, this linear system is ill-conditioned . For its solution, we use a local regularization method, as opposed to classical regularization methods, resulting in better approximation of the exact solution.

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CP10

Numerical Analysis of An Integro-Differential Equation

Consider the integro-differential equation

$$u_t(x,t) = \epsilon \int_\Omega J(x-y)\left(u(y,t) - u(x,t)\right) dy + f(u),$$

with initial condition $u(x,t_0) = u_0(x)$, $x \in \Omega$, $t > 0$, $\Omega \subseteq \mathbf{R}^d$ with $d = \{1,2,3\}$, $\epsilon > 0$, $J(x) = J(-x)$ and $f(u)$ is a bistable function. This type of initial value problem (IVP) arises in the modelling of various physical and biological process. We study the numerical analysis of this IVP and also investigate its long time dynamics.

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CP11

A Level Set Approach to Dislocation Models of Low-Angle Grain Boundary Structure and Motion

Dislocation models are useful for gaining insight into the meso-scale structure and motion of low-angle grain boundaries. Using a level-set formalism for dislocation dynamics pioneered by our group, we examine the equilibrium structure of grain boundaries formed from straight-line dislocation networks constructed using Frank's formulas. We also investigate the dependence of grain boundary mobility on the mobility of individual dislocations and grain boundary geometry. The computational efficiency required to study these models is provided by a parallel level set method software library (LSMLIB) that we have recently developed.

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CP11

High-Order Mimetic Finite-Difference Modeling of Shear Crack Propagation

A fourth-order finite-difference traction-at-split-node implementation of faulting boundary conditions is presented in this work. Geometry of the fault and initial shear stress allow only in-plane motion which is modeled in the plane (x,z). Our two dimensional method combines a one-sided discretization of the jump conditions along the fault segment with a staggered discretization of the equations of motion within interior of the embedding medium. Fourth-order numerical differentiation of elastic fields is performed in the whole domain by using a new set of differentiators called mimetic or conservative finite differences. Convergence and accuracy of our algorithm are shown through two test cases. First, the analytical solution of a self-similar fixed-rupture velocity model is reproduced as the grid size decreases. Next, we simulate the propagation of a spontaneous rupture, governed by a linear slip-weakening friction law that defines a cohesive law. Our results are assessed using an alternative numerical solution given by a well established Dynamic Fault Model (DFM) algorithm.

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CP11

Morphology of Critical Nuclei in Solid State Phase Transformations

Predicting the shape of a critical nucleus in solids has been a long-standing problem in solid-state phase transformations. We present a diffuse-interface approach together with minimax algorithm for predicting the critical nucleus morphology in elastically anisotropic solids. It is found that strong elastic interactions may lead to critical nuclei with non-convex shapes.

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CP12

Hessian-Based Model Reduction for PDE-Constrained Optimization

We present a new methodology to create reduced-order models for large-scale, ill-posed inverse problems. The problem of determining a suitable reduced basis is formulated as a sequence of optimization problems. We show that, under certain non-restrictive assumptions, these problems have a closed-form solution that entails computation of the dominant eigenvectors of a Hessian matrix. Furthermore, the method scales well to problems with a large number of parameter inputs. The methodology is demonstrated for a large-scale contaminant transport inverse problem.

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CP12

A Two-Dimensional Arnoldi Algorithm for Model Order Reduction of Parameterized Linear Dynamical Systems

The presence of parameters and variability in the design and manufacturing process of modern microelectronics poses new challenges to existing model reduction techniques. In this talk, we present a multiparameter moment-matching reduction algorithm for the simulation and analysis of large scale parametrized linear dynamical systems. The new algorithm uses a novel two-dimensional Arnoldi process and is computationally stable and robust. In addition, it is structural preserving. Examples from parameterized integrated circuits and microelectromechanical (MEMS) devices will be used to compare the new algorithm with the existing ones.

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CP12

Reduced System Computing for Singularly Perturbed Differential Equations

Reduced System Computing (RSC) is a software system for studying singularly perturbed differential equations. It avoids the problem of numerical stiffness by concatenating solutions to the fast and slow subsystems that arise in the singular limits of the differential equations. Tools for solving initial value problems and for computing periodic orbits will be presented, along with an application of RSC to a pair of coupled relaxation oscillators.

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CP13

Direct Linear Solvers for Finite Element Modelling of Large Industrial Applications

Krylov subspace methods are widely used in simulation softwares even if they are all likely to suffer from slow convergence and divergence for problems which arise from large industrial applications. The main reason for this is that direct solvers based on matrix factorization are very memory consuming methods which may be unfeasible on large problems. We will discuss here the possibility of an efficient direct solving of large problems discretized by means of finite elements.

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CP13

Sparse Direct Factorizations Based on Unassembled Hyper-Matrices

For dynamic FEM applications, existing sparse direct solvers can be said to solve the wrong problem. They optimize the solution of a single linear system, while the real problem is to solve a series of systems that are derived from gradual h/p refinement of a FEM discretization. We show how a combination of elementary concepts gives a solver that is space and time efficient, and that is eminently suited to the dynamic case.

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CP13

Combinatorial Preconditioners for Scalar Elliptic Finite-Elements Problems

The talk will present a new preconditioner for linear systems arising from finite-elements discretizations of scalar elliptic PDE's. The algebraic equations that we solve are $Kx = b$, where $K = \sum_e K_e$ is a sum of element matrices K_e. The solver splits the collection $\{K_e\}$ of element matrices into a subset of matrices that are approximable by diagonally-dominant matrices and a subset of matrices that are not approximable. The approximable K_e's are approximated by diagonally-dominant matrices L_e that are scaled and assembled to form a global diagonally-dominant matrix L. A combinatorial graph algorithm approximates L by another diagonally-dominant matrix M that is much easier to factor. The inapproximable element matrices are added to M and the sum is factored and used as a preconditioner. When all the element matrices are approximable (in particular, when they are all well-conditioned), which is often the case, the preconditioner is provably efficient. Experimental results show that on some problems, especially problems with some ill conditioned elements, the preconditioner is more effective than an algebraic multigrid solver and than an incomplete-factorization preconditioner.

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CP14

Scalable Metadata and Algorithms for Structured AMR

Metadata for structured adaptive mesh refinement (SAMR) contains information about the grids forming the mesh. It grows with the number of grids. In parallel, where the global number of grids grows with the number of processors, metadata grows rapidly, leading to severe inefficiencies starting around 1K processors. We present new algorithms for managing SAMR meshes without global metadata. Significant parallel efficiency is obtained through not having to generate or operate on the global metadata.

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CP14

An Efficient Linearity-and-Bound-Preserving Conservative Interpolation (Remapping) Method for Meshes with Changing Connectivity

Remapping is one of the essential parts of most Arbitrary Lagrangian-Eulerian (ALE) methods. In this talk, we extend the idea of swept integration method to the grids with changing connectivity during the smoothing stage. We focus to the Voronoi meshes in 2D, which are used for real numerical simulations. We present several numerical examples to show that properties of this algorithm (conservativity, linearity and bound preservation) remain unchanged for grids with different topology.

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CP14

Multi-Material Interface Reconstruction Using Particles and Power Diagrams

We present a new method for interface reconstruction in multi-material flow simulations. The method introduces particles into mixed cells and uses an an attraction-repulsion model to draw particles of the same material type together. The interface is then reconstructed from the particles using a weighted Voronoi diagram or Power Diagram. The new method eliminates the material order dependence of the interface topology commonly seen in VOF reconstruction of three or more materials in a cell.

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CP15

Desensitization and the Ignition-And-Growth Model

Of the various macro-scale continuum models of reactive flow in high-energy explosives, the ignition-and-growth model has been the most widely used. Well-resolved computational experiments with the model demonstrate that it does not explicitly account for the desensitization of heterogeneous explosives, caused by exposure to low strength shocks. A modification to the model that accounts for the desensitization process is proposed. Numerical simulations employing adaptive mesh refinement on composite overlapping grids with the augmented model are conducted.

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CP15

Laser Generated Elastic Waves in a Semi-Infinite Solid

Analytical and numerical issues for thermoelastic waves by

a pulsed laser in a semi-inifinite solid were investigated. Analytic solutions were derived by using Laplace Transform techniques for thermal and mechanical problems. The effect of optical absortion coefficients on the thermal and displacement fields was studied. All numerical results were compared with the analytic solutions.

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CP15

Operator Splitting and Acceleration Methods for Solving the Neutron Transport Equation in 1-D Spherical Geometry

Our study concerns the iterative resolution of the neutron transport equation in 1-D spherical geometry. More precisely, we consider a splitting method for the collision operator taking into account the caracteristics of the transport operator. An infinite dimensional adaptation of SOR algorithm and Splitting-Diffusion Synthetic Acceleration (DSA) method are used to accelerate the procedure. Theoretical aspect for these methods are discussed, and numerical results are presented.

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CP16

Computable Condition Number Estimates for Large Least Squares Problems

Some parameter estimation problems lead to huge dense least squares problems that require a good knowledge of the problem conditioning. We propose computable statistical estimates for the conditioning of a linear function of the least squares solution. We present the corresponding parallel implementation in the framework of space geodesy and we study how these quantities compare with available estimates for large number of unknowns. The issues of rank deficient least squares problems are also addressed.

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CP16

A Comparison of Two Algorithms for Predicting the Condition Number

We present experimental results of comparing the Modified K-Nearest Neighbor (MkNN) algorithm with Support Vector Machine (SVM) in the prediction of condition numbers. While SVM is considered a state-of-the-art classification/ regression algorithm, kNN is usually used for collaborative filtering tasks. Since prediction can also be interpreted as a classsification/regression task, virtually any supervised learning algorithm (such as kNN) can also be applied. Experiments were performed on one publicly available dataset. We conclude that Modified kNN (MkNN) performs much better than SVM on this particular dataset.

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CP17

Finite Difference Techniques For Delay Differential Problems With Layer Behavior

This study deals with the singularly perturbed initial value problems for linear and quasilinear delay differential equations. The numerical methods are generated on a grid that is constructed adaptively from a knowledge of the exact solution, which involve appropriate piecewise-uniform meshes on each time subinterval. An error analysis shows that the discrete solutions are uniformly convergent with respect to the perturbation parameter. The parameter uniform convergence is confirmed by numerical computations.

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CP17

Higher Order Finite Difference Methods for Second Order Singularly Perturbed Delay Differential Equations

The approximation of solutions Delay differential equations(DDEs) has been a problem of great importance due to the versatility of its application in various fields. Development of numerical methods for DDEs are challenging because we have to use an appropriate approximation for the retarted arguments like $u(x \pm \delta)$ and $u^{'}(x - \delta)$ and the algorithm has to take care of the jump discontinuies due to the delay/advance. We will discuss a few higher order finite difference methods for second order singularly perturbed differential equation with delay/advance and its computational complexity.

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CP18

Sparse Computation on a P2P System

We present the 2-degree polynomial (2DP) A(Ax+x)+x

distribution on a peer-to-peer system, where A is a large sparse matrix. Such 2DP represents the kernel of many iterative methods for solving sparse linear algebra problems. We propose a distribution technique based on data fragmentation engendering a good communication pattern and show that our solutions need a pre-processing for matrix fragmentation by solving an NP-Complete problem but guarantee load balance.

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CP18

Reshape: A Framework for Dynamic Resizing and Scheduling of Homogeneous Applications in a Parallel Environment

Due to the unpredictability in job arrival times and varying resource requirements, static scheduling results in idle system resources, thereby decreasing the overall system throughput. To alleviate this drawback, we have developed a framework called ReSHAPE which supports dynamic resizing of parallel MPI applications executed on a distributed memory architecture. Our presentation describes the ReSHAPE framework architecture and presents results from testing the framework with structured applications that have two-dimensional data arrays distributed across a two-dimensional processor grid.

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CP18

Dynamic Load Balancing for Hyperthreaded and Multi-Core Cluster Nodes

There has been a significant shift by processor manufacturers from increasing clock speeds to on-chip parallelism: hyperthreaded and multi-core chips. These processors are becoming common in desktop systems and cluster nodes, but it is not clear how to use them most efficiently. This talk will give a brief overview of the technology and report experiences using the DRUM resource aware dynamic load balancing system in cluster environments that include dual core and hyperthreaded processors.

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CP19

Multiscale Simulation of Ionic Flux Through a Nanopore Under Applied Electric Potential

We present a multiscale model to simulate ionic flux through a nanopore of an electrodesalination membrane. The model relies on Brownian Dynamics simulations inside the nanopore, coupled with a Poisson-Nernst-Planck continuum model in the pore vicinity. The model is validated against measurements of current through track-etched nanoporous membranes under an applied electric potential. Simulations are performed to investigate the effects of pore size, membrane charge and applied potential on throughput and selectivity.

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CP19

Mathematical Modeling and Simulation of Texture Evolution

Preparing a texture suitable for a given purpose is a central problem in materials science, which presents many challenges for mathematical modeling, simulation, and analysis. We focus on the mesoscopic behavior of the grain boundary system and on understanding the role of topological reconfigurations during evolution. We formulate several types of evolution equations based on fractional kinetics and stochastic descriptions, compare its results with the simulations and discuss their limitations and possible extensions to higher dimensions.

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CP19

Mesoscopic Simulation of Self-Organization in Surface Processes

The self-organization of constituents in a two phase mixture through diffusion is known as Ostwald ripening. This multiscale phenomenon can be modeled using a class of mesoscopic models consisting of stochastic partial differential equations. In this talk, spectral schemes for stochastic partial differential equations are described and convergence verified using exactly solvable benchmark problems. These schemes are then applied to the mesoscopic model and the simulation results are compared with theoretical results such as the Lifshitz-Slyozov growth law; long time results are also described.

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CP20

Title: On Multi-Phase Flows

In this lecture, we will discuss some of the issues related to stability of flows involving multiple interfaces and computing of such flows efficiently. Results will be presented. This is an ongoing work.

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CP20

Compressible Multispecies Multiphase Flow Models

We develop comopressible multispecies multiphase flow models with surface tension and transport. We propose a closure model which satisfies all the conservation and boundary conditions after averaging the primitive equations of mass, momentum and energy. We derive three interfacial exact quantities $v*$, $p*$, $(pv)*$ directly from these averaged equations to validate our model with Rayleigh-Taylor instability simulation which have been validated against the real experiment. We also observe other properties of our simulation based on theories and experiments.

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CP20

A VOF-PLIC Method for Axisymmetric Multiphase Flow

A piecewise linear interface calculation in axisymmetric geometries is presented and implemented within RIPPLE, a 2D volume-of-fluid code. Analytical relations between the interface parameters and volume fractions are provided, emphasizing resolution of a numerical instability that occurs when one of the components of the normal vector at an interface approaches zero. Results are presented for the collapse of a cylindrical water column and the wake dynamics of one or two rising bubbles.

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CP21

Least Squares Finite Element Solution for Viscoelastic Flow Problems

The goal of this work is to implement a least squares finite element approach for the equations governing viscoelastic flows such as those occurring in polymer processes. The Oldroyd-B and Giesekus viscoelastic constitutive equations are considered, as well as Newtonian and non-Newtonian (Carreau model) formulations. The least squares method offers the advantage of generating a symmetric positive definite system of equations, and has also been recognized as potentially effective in addressing the high Weissenberg number problem which characterizes viscoelastic flows. We compare results of the weighted least squares approach to those using standard Galerkin techniques. An adaptive mesh technique designed for regions of high gradients in 2D is also presented.

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CP21

Derivative-Free Approaches for Maximizing the Lifetime of a Polymer Extrusion Filter

We consider an extrusion filter used to remove debris from a polymer melt before the liquid is spun into a fiber. We seek the optimal parameters to maximize the lifetime of the filter using a simulator developed at the Center for Advanced Engineering Fibers and Films (CAEFF). The

simulator must work as a black-box in conjunction with a derivative-free optimization algorithm. We present preliminary numerical results obtained with a variety of sampling methods for optimization.

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CP21

A Hard Constraint Algorithm to Model Particle Interactions in Polymeric Flows

We present a new algorithm to model short-range particle interactions in polymer-laden fluids. In this method the polymer is represented by a bead-rod model fully-coupled to a Newtonian solvent through hydrodynamic drag and Brownian motion. The central feature is a new rigid constraint algorithm whereby rods elastically bounce off one another to prevent crossing in polymer-polymer interactions, similar to our treatment of polymer-surface interactions. We apply the method to DNA-laden flows in array microchannels.

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CP22

Towards An Accurate Performance Modeling of Parallel Sparse LU Factorization

We present a performance model to analyze a parallel sparse LU factorization algorithm on modern cached-based, high-end parallel architectures. Our model characterizes the algorithmic behavior by taking account the underlying processor speed, memory system performance, and the interconnect speed. The model is validated using the SuperLU_DIST solver, sparse matrices from real application, and an IBM POWER3 parallel machine. It can be easily adapted to study performance of other sparse factorizations, such as Cholesky or QR.

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CP22

On Reducing Memory Usage of the Simulations Using Sparse Direct Solvers

Simulating LARGE multi-cavity accelerator structures with the finite element method is limited by available computer memory when the sparse direct solver is used to solve the resulting linear systems. This talk will present various ways of reducing the memory usage of the capability-computing simulations that use sparse direct solvers thereby allowing eigenvalue problems consisted of hundred million DOFs to be solved on existing computing platforms.

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CP22

Using Sparse Lu to Compute the Null Space of a Rectangular Matrix

Computing the null space of a sparse matrix is an important component of some computations, such as graph embeddings and parameterization of mesh data. We propose an efficient and reliable method to compute an orthonormal basis of the null space of a sparse square or rectangular matrix (usually with more rows than columns). The main computational component in our method is a sparse LU factorization with partial pivoting of the input matrix; this factorization is significantly cheaper than the QR factorization used in previous methods. We analyze important theoretical aspects of the new method and demonstrate experimentally that it is efficient and reliable.

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CP23

On the Design of Diffusion Constants for Random Walks of Squares, Triangles and Cubes

I show how to design the value of the diffusion constant D for both the random walks of Squares and Triangles over their respective regular lattices in two-dimensions, and for a random walk of a Cube on the three-dimensional Cartesian lattice. By allowing movements to grid locations other than nearest neighbors, I can design the value of the diffusion constant D to a value other than unity.

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CP23

Bandlimited $1/f$ Noise: a Signal for Robust Experiment Design

Experiment design aims to find a suitable input signal to

maximise the information obtained from an experiment. This input signal typically depends on the actual plant. To enhance robustness, it is important to use signals which are near optimal over a range of systems. Here we introduce "bandlimited $1/f$ noise" as an signal with such a property. We also present a simple and fast algorithm for generating binary signals with this spectrum.

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CP24

Estimation of Blood Alcohol Concentration by Inversion of a Diffusion Model

A protocol for estimating blood alcohol concentration is proposed. This methodology requires calibrating short period data coming from a skin sensor to the subject under study and then inverting the forward model for long period data. A simulation study is performed to observe the influence of parameter changes on vapor alcohol removed through the skin and blood alcohol concentration. This avoids calibrating model parameters to subjects to whom it is not ethic to offer alcohol.

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CP24

Application of the Stochastic Galerkin Method for Analysis of Human Cardiac Ion Channel Models

Based on the Weiner-Hermite polynomial chaos expansion, the stochastic Galerkin method efficiently computes numerical solutions for stochastic systems. Unlike such techniques as sensitivity analysis, perturbation methods, and second moment-analysis, this method is applicable to a large number of systems while requiring less computational effort than sampling based stochastic methods like Monte Carlo. We utilize the stochastic Galerkin method to assess the impact of stochastic rate coefficients on the predictions of Markovian cardiac ion channel models.

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CP24

A Coupled Diffusion-Elasticity PDE-Constrained Framework for Simulating Gliomas Growth: a Medical Imaging Perspective

Primary brain tumors constitute a significant health challenge, due to their grim prognosis. More than 50% of primary brain tumors are gliomas, which are seldom treatable with resection and ultimately progress to high-grade, leading to death in only 6-12 months. There is a pressing need for deepening our understanding of the characteristics of the spatio-temporal progression of brain cancer, and for determining predictive factors for cancer invasion, using phenotypic cancer profiles derived from imaging, histopathology and potential other sources. Such predictive factors would allow us to apply more aggressive treatments, yet treatments that are spatially adaptive to tissue that is highly likely to be invaded by cancer, in order to maintain patient functioning at acceptable levels. This work proposes a simple unified framework for modeling gliomas growth and the subsequent mechanical impact on the surrounding brain tissue (mass-effect), with estimation of unknown parameters via a PDE-constrained optimization method. We target a medical imaging context, where such a framework primarily aims at the following goals: (1) improving the deformable registration from the brain tumor patient image to a common stereotactic space (atlas); and (2) having, to a certain extent, predictive capabilities for glioma growth, after its parameters are estimated for a given patient. The first is important for integrative statistical analysis of tumors in groups of patients and surgical planning. The second is important for general treatment planning and prognosis. To our knowledge, this is among the first attempts in the specialty literature to introduce a PDE-constrained optimization formulation in the context of modeling tumor growth based on available patient imaging data. The present work is dedicated mostly to formulation and methods, with extensive 1D numerical experiments performed for a preliminary evaluation of the overall formulation/methodology. The 3D MRI-based simulations are work-in-progress; a simplified biomechanical version has already been implemented and reported elsewhere.

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CP24

Non-Newtonian Blood Flow in a Stenosis and Aneurysm: Transient and Steady State Simulations.

This study considers the steady state and transient simulations of blood flow through two three-dimensional models of an arterial stenosis and an abdominal aortic aneurysm. Four non-Newtonian blood models, namely the Power Law , Casson, Carreau and the Generalized Power Law, as well as the Newtonian model of blood viscosity, are used

to investigate the flow effects induced by these different blood constitutive equations. Results show significant differences between modelling blood as a Newtonian and non-Newtonian fluid. The dependence of the flow on the dimensionless parameters is examined and differences from the Newtonian case are discussed.

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CP24

Brain Surface Conformal Parameterization with Algebraic Functions

Here, we introduce a parameterization method for brain surfaces based on algebraic functions. By solving the Yamabe equation with the Ricci flow method, we can conformally map a brain surface to a multi-hole disk. The resulting parameterizations do not have any singularities and are intrinsic and stable. It also offers a method to explicitly match landmark curves between anatomical surfaces such as the cortex, and to compute conformal invariants for statistical comparisons of anatomy.

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CP25

Accurate High-Performance Multigrid Solvers in Reconfigurable Hardware

In this paper, we present a hardware implementation of the V-cycle Multigrid method for finding the solution of a 2D-Poisson equation. We use Handel-C to implement our hardware design, which we map onto available Field Programmable Gate Arrays(FPGAs). We analyze the implementation performance using the FPGA vendors' tools. We compare our findings with a C++ version of thr algorithm. The obtained results show better performance when compared to existing software versions.

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CP25

Inverse Molecular Design by Local Enumeration

In previous work we have developed a method for the inverse design of chemical structures (Chuchwell et al., 2004; Brown et al., 2006). A key step in our method involves the solution of a system of constrained linear Diophantine equations. In this work we describe a novel method for the solution of these equations using the Fincke-Pohst algorithm. This approach simultaneously controls both combinatorial explosion and extrapolation error. We benchmark our method against past results.

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CP25

Credibility: How Will Science Judge Our Mathematical Or Computerised Models?

We review the literatures of computational languages and simulation methodology so as to investigate the answer to the ultimate question asked of any of our mathematical or computerised models, particularly those in the life sciences: viz., credibility. We compare and contrast the two model-building activities, reaching thereby an understanding of the Scientific Method, itself then revealed to be a quite pre-human process: quite biological (first genes; then neurons), this model-building process has ensured biological survival.

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CP25

Formal Constraints on Memory Management in Overloaded Arithmetic

Memory management rules for overloaded arithmetic are expressed in the Object Constraint Language (OCL) and applied to an advection/diffusion model. One set of constraints eliminates memory leaks. A second set ensures economical memory recycling. It is demonstrated that runtime assertion checks inspired by the constraints exposed an exceptionally hard-to-reproduce compiler bug. Furthermore, the interplay between OCL and Fortran capabilities led to a breakthrough that improved the readability of our code by facilitating operator overloading.

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CP26

Robustness of the Multivariate Spline Method for Numerical Solution of Partial Differential Equations

Multivariate spline functions are smooth piecewise polynomial functions over triangulations consisting of n-simplices in the Euclidean space $\mathbf{R}^n$. We review how they are used with Lagrange multipliers to enforce the smoothness conditions, the boundary conditions and the constraints in numerical solution of partial differential equations. We then demonstrate the robustness of this approach on two singular perturbation problems, a fourth order problem and a Stokes-Darcy flow.

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CP26

Alternative Way to Solve Nonlinear PDEs

Generally Newton-Krylov method is the first choice in solving nonlinear problems. But it is expensive to construct Jacobian matrix at each iteration, Even the Jacobian-free one is used, information of the Jacobain matrix is still needed to form the preconditioner. The linearizing process may also generating additonal numerical errors. Here we present an alternative way called pseudo-transient continuation by adding first and second order time derivative to the equation and advancing the resulting time-dependent equation to steady state. Therefore, only the stiffness matrix itself is involved. An efficient way is developed to initialize the system and dynamically precondition the iterative solve. The solve is accurate and the symmetric structure of periodic boundary condition is well preserved.

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CP26

Title : Fast and Accurate Methods with Domain Embedding

In this lecture, we will present some fast and accurate algorithms for solving several types of partial differential equations (pdes) in simple geometries. The class of pdes involved may involve both, constant and non-constant coefficient pdes and the geometries both, two- and three-dimensional. Adaptation of these algorithms to complex geometries will be discussed and results on applications using these methods will be presented. This is an ongoing work.

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CP26

For the Inf-Sup Condition on Mesh-Dependent Norms on a Concave Polygon

In this talk I will discuss about the Babuska-Brezzi(inf-sup) condition when certain mesh-dependent norms are considered on a concave polygon in the plane. The model problem is the Laplace problem with zero boundary condition on a polygon.

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CP26

An h-p Adaptive Strategy for Wave-Like Functions

The hp version of the finite element method is an adaptive finite element approach in which adaptivity occurs in both the size, h, of the elements and in the order, p, of the approximating piecewise polynomials. The objective is to determine a distribution of h and p that minimizes the error using the least amount of work in some measure. We present a strategy for selecting between h and p refinement for functions exhibiting wave-like behaviour.

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CP27

New Eigensolvers for Large Scale Nanoscience Simulations

We present results for new iterative eigensolvers based on conjugate gradients and Jacobi-Davidson in the context of semi-empirical plane wave electronic structure calculations. These new methods give significant speedup over existing conjugate gradient methods used in electronic structure calculations. The new methods will be demonstrated for CdSe quantum dots as well as quantum wires constructed from layers of InP and InAs. These systems are studied in the context of a semi-empirical potential where we typically solve for a few states around the gap allowing us to study large scale nanaosytems. The parallelization of this approach will also be discussed as well as scaling results to large processor counts.

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CP27

On Eigenvalues/Partial Eigenvectors Assignment in Multi-Input Controllable Linear System

The main objective of the present paper is to utilize the power of the advanced analysis and synthesis method embedded in eigenstructure assignment technique to construct a state feedback controller that improves the closed loop systems performance when goals beyond precise eigenvalues assignment are to be met, namely partial eigenvectors assignment. The proposed procedure fared well towards precisely shaping right eigenvectors and implementing a feedback controller. The null space of the system matrix is exploited to construct parts of the achievable eigenvectors. The resulting state feedback controller is unique. The existence of a solution to the assignment problem is ensured, and an algorithm is presented to design the concerned controller. A numerical illustrative example is presented to reveal ease of computations required for designing the controller

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CP27

Eigenvalue Grid and Cluster Computations, Using Task Farming Computing Paradigm and Data Persistency

Recent progress has made possible to construct high performance distributed computing environments, such as computational grids and cluster of clusters, which provide access to large scale heterogeneous computational resources. Exploration of novel algorithms and evaluation of performance is a strategy research for the future of computational grid and cluster scientific computing for many important applications. We adapted the well-known parallel iterative Lanczos method to compute Hermitian eigenvalues of large sparse matrices for a GRID platform and for a cluster of clusters worldwide deployed between France and Japan. Parts of the proposed GRID algorithm use an efficient task-farming computing paradigm, with data persistency scheduling strategies.

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CP27

Robust and Efficient Solution of Hermitian Eigenproblems Using Primme

PRIMME, or PReconditioned Iterative MultiMethod Eigensolver, is a comprehensive, open source software package for solving large, sparse, hermitian eigenvalue problems. We review some of its enhancements since its first release in October 2005, that include complex hermitian eigenproblems, an interface for solving SVD problems, complete Fortran interface, and full interoperability among the different operation modes. We present experimental results from two electronic structure applications and from data mining showing its robustness and efficiency.

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CP27

The Use of Bulk Information to Improve The Scalability of Parallel Band Gap Computations For Quantum Dots

We consider the parallel computation of interior eigenstates of large Hermitian matrices arising from plane-wave discretization of effective single-particle Schrodinger equations. We apply a folded-spectrum approach based on Preconditioned Conjugate Gradient (PCG) to compute only a small number of eigenstates close to the band gap whose location determines electronic and optical properties of the system. We show how to improve the scalability of the eigensolver from observing that the quantum dot band states can be well approximated by states of bulk systems. We make use of these cheaply computable bulk eigenstates to improve the choice of the starting vector and the preconditioner for the eigensolver.

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CP27

Computing Eigenvector Derivatives for Repeated Eigenvalues

Eigenvalues and eigenvectors often occur in engineering problems. This eigensystem may depend on some parameter. The sensitivity of the eigenvector with respect to a change of this parameter is expressed by its derivative. Currently, eigenvector derivatives can be computed when the eigenvalues themselves, or the first and/or second order derivatives of a repeated eigenvalue, are distinct. We show how this method can be generalized for an arbitrary matrix.

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CP28

Parameter Optimization Algorithm for Differential Equations in Market Return Prediction

We combine an implementation of a state-of-the-art computational optimization algorithm, a dynamic initial parameter pool and a system of nonlinear differential equations to describe price dynamics. Given an n-day period of market price (MP) and net asset value (NAV) from day i to day $i+n-1$, we obtain four optimal parameters in the differential equations derived by Caginalp. We then solve the initial value problem to predict MP and return on day $i+n$ or later. The results of our statistical methods in real data support the model. We provide out-of-sample prediction that is more successful than random walk.

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CP28

The Importance of Rare Events in Kelly's Algorithm

John Kelly's 1956 paper, *A New Interpretation of Information Rate*, describes an algorithm for exploiting inside information to optimize capital deployment across uncertain opportunities. Kelly models the inside information as a noisy channel and shows, under fair odds and no transaction fees, that the maximal capital growth rate is precisely the Shannon information rate of the channel. The algorithm's optimal strategy, however, is valid for more general odds and in the presence of transaction fees. A paradox arises in the general case because the algorithm can place capital at risk on outcomes with a known negative expected return. This paper provides an alternative derivation of Kelly's results that emphasizes the cases where such counterintuitive strategies arise. The explanation lies with the outsized effects of low-probability events in the context of compounding investments. We also extend the information-theoretic interpretation of the maximum capital growth rate to the general case, where transaction fees can be viewed as additional noise in the channel.

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CP28

Robust Numerical Schemes for Pricing and Hedging Exotic Options

We present numerical schemes for pricing options with non-smooth payoffs, multiple strike prices, and discrete barriers. These exotic options induce discontinuities in the solution for which Standard numerical methods may cause large spurious oscillations, thereby giving misleading estimates for options valuations and hedging parameters. The proposed numerical methods do not incur such oscillations while efficient to implement on parallel as well as serial machine. Numerical experiments are presented to demonstrate the robustness of the methods.

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CP28

Finite Element Methods with Three Levels for Pricing American Put and Call Options

To compute numerically the price and its free boundary of American options, we present algorithms of finite element methods with three levels for the time-marching. Our algorithms are based on the Jamshidian equation which is a version of the Black-Scholes equation. We prove the existence and uniqueness of the numerical solutions at a given time level. Also, to compare with other methods, we present some numerical results obtained through extensive numerical experiments.

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CP29

Fct Algorithms for the Euler Equations on Overlapping Grids

High resolution numerical methods are critical for the efficient computation of fluid flow problems. These methods should use high order discretizations on smooth portions of the flows while maintaining physical consistency near

discontinuities. In this talk we discuss the implementation of flux corrected transport (FCT) algorithms on overlapping grids with the motivation to investigate monotonicity preserving methods for fluid flow problems. The algorithm will be applied to the Euler equations for an inviscid compressible gas. Convergence of the method is investigated using both the method of manufactured solutions and for a series of simple flow problems. We then present results for a series of problems involving both moving and stationary obstacles. These results are compared to results obtained using a high-resolution Godunov method. Finally the method is applied to a number of prototype problems of relevance to the Z-pinch experiments at Sandia National Labs including Sedov's blast wave and Noh's problem.

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CP29

Numerical Symmetry Capture

For reliable fluid dynamic simulations the numerical errors must be small. Symmetries are fundamental in physics that leave a Partial Differential Equation invariant after a transformation. In this paper Lie Groups will be used to extend this philosophy to discretised equations. It will be shown that errors occur due to the breaking of symmetry. We will introduce a new class of SYNC based numerical methods that eliminate these errors; SYmmetries Numerically Captured.

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CP29

Adaptive and Implicit Immersed Boundary Method with Advection-Electrodiffusion

Immersed boundary method is a mathematical and computational framework involving the interaction of fluid and structure. Advection-electrodiffusion of ions(solutes) dissolved in fluid in a biological system is considered in the context of fluid-solute-structure. For a chemical barrier across a boundary, a chemical potential is placed for each solute(ion) along the boundary. An implicit numerical scheme is proposed. For numerical accuracy and efficiency, adaptive mesh refinement around boundaries is applied. Stokes equations are solved with hybrid approximate projection method with cell-centered grid. Advection-electrodiffusion equations are solved with the combination of geometric and algebraic multigrid methods. With advection of the boundaries, advection of ions is observed. With local change of the amplitude of chemical potentials, diffusion of each ion across the boundaries is regulated. The results show electroneutrality except in space charge layers near membranes, and agree with the Nernst equation for the potential difference across membranes.

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CP29

A Hybrid Method for Unsteady Aerodynamics

We develop a stable and accurate hybrid method that can handle locally highly nonlinear phenomena in complex geometries as well as efficient and accurate signal transportation in domains with smooth flow and geometries. Two separate solvers, one using high order finite difference methods and another using the node-centered unstructured finite volume method is coupled in a truly stable way. The two flow solvers run independently and recieve and send information from each other by using a third coupling code. Exact solutions to the Euler equations are used to verify the accuracy and stability of the new computational procedure. We also demonstrate the usefulness of the new method in a calculation of the flow around a device with complex geometry.

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CP29

Comparison of Different Techniques for the Study of Nonlinear Laminar Flow Between Parallel Permeable Disks

The equations describing similarity solutions for flow between infinite parallel permeable disks with equal rates of suction or injection at the interface are analyzed. The nonlinear ODE is found to admit a solution for all Reynolds number R, using Leray Schauder degree theory. Uniqueness of solution for small Reynolds number is proved analytically. The nonlinear ODE is then solved computationally using regular perturbation technique and numerical finite difference method fail for large value of Reynolds number, where as Padé approximation gives converging solution for all values of R and this solution shows the disapperance of boundary layer as $R \to \infty$, and as a consequence shock is developed. For many practical applications, we

also calculated the skin friction and pressure distribution. The results are found good agreement with the physical theory.

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CP30

A Numerical Method for the Simulation of a Gravitationally Stratified Atmosphere Over a Mountain Range

Although long-wavelength gravity waves may have a negligible influence on the overall dynamics of the atmosphere, they pose a computational challenge by sharply restricting the time step. We present a new algorithm to solve the compressible Euler equations using a splitting to separate the fast acoustic dynamics from the slower anelastic dynamics, as well as a strategy based on normal mode analysis to filter out the fastest modes, thereby allowing for a larger time step. UCRL-ABS-223491.

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CP30

Simulation of the Climate of the Last 600 Years

We will run the Educational Global Climate Model from Columbia University for the past six centuries, and compare the output with global reconstructions of annual surface temperature patterns. The project's goal is to verify if the mean annual surface temperature of the Northern Hemisphere in the model results shows any noticeable warming distinct from natural climate variability.

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CP30

Modified Finite Difference Schemes for Geophysical Flows

We describe a method to improve both the accuracy and computational efficiency of a given finite difference scheme used to simulate a geophysical flow. The resulting modified scheme is at least as accurate as the original, has the same time step, and often uses the same spatial stencil. However, in certain parameter regimes it is higher order. As examples we apply the method to the shallow water equations, the Navier-Stokes equations, and to a sea breeze model.

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CP30

Coupling of Ocean Acoustics and Seismic Waves

The interaction of acoustic and seismic waves with geometric features such as bathymetry is of great practical interest. Using a newly developed finite difference technique for wave propagation we are studying and evaluating a number of problems with interacting acoustic and elastic materials. Results from parallel computations involving very large data sets will be reported.

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CP30

Numerical Adjoints, Ffts and Generalized Linear Stability

A generalized (finite-time) linear hydrodynamic stability theory has recently been developed and shown to provide a theoretical explanation of observed transition events at odds with predictions from traditional asymptotic theory. However, creating a numerical model, *ab initio*, to apply this methodology to different flow regimes requires consideration of important numerical aspects. In this talk, these issues will be considered and illustrated using an example from atmospheric dynamics.

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CP31

Self-Consistent Hartree-Fock Calculations for the Effect of Pressure on the Electronic Structure of Diamond

A self-consistent Hartree-Fock formalism on the basis of semi-empirical INDO (Intermediate Neglect of Differential Overlap) Hamiltonians has been used to study the electronic and pressure dependent properties of diamond. The increase of pressure on diamond is predicted to cause an increase of the valance and conduction band widths with a decrease of the direct band gap, an increase of the electronic occupation probability for p orbital, and a decrease of x-ray scattering factors.

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CP31

Simple Numerical Ab-Initio Program for Molecular Orbital Calculations

A concise simple numerical ab-initio program for molecular calculations is written using trapezoidal rule for carrying molecular Hartree-Fock integrals. the program accepts any kind of basis functions to perform the calculations such as Gaussian or Slater type functions or numerically input functions. In spite of long execution time, the program is very limited in its size. The program can be used as a

whole or to check single values of molecular integrals.

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CP31

Computational Workflow for Petaflops-Scale Bio-Molecular Simulations: Opportunities and Challenges

Petaflops-scale processing capabilities are essential for breakthrough bio-molecular simulations, which are widely-used in many fields including bio-fuel and protein-folding simulations. Supercomputing systems at this scale will however be significantly different from conventional cluster systems, and are likely to have unique combinations of processor, networking and IO characteristics. This talk will overview the key workflow components of a bio-molecular simulation. We will also identify opportunities and challenges for large-scale system simulations (>500,000 atoms) on Petaflops-scale supercomputers.

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CP31

Estimating Accuracy in Molecular Dynamics Simulation

In molecular dynamics, accuracy and efficiency of a numerical method should be measured with respect to statistical averages, rather than deviations from an "exact trajectory". In this talk I will survey some results from backward error analysis and show how (under certain assumptions) these results can be applied to compute estimates of the error in averages from molecular dynamics simulations. Results from several test problems will be explored including examples from constant temperature molecular dynamics.

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CP31

Molecular Property Prediction Using Kernel Molecular Dynamics

Molecular dynamics can be used to simulate the behavior of molecular structures with high accuracy on a small scale. Supervised learning methods can be used to make chemical property predictions less accurately but on a large scale. We propose the marriage of these two methods using a Support Vector Machine kernel function. We introduce a novel kernel function which incorporates molecular dynamics. We apply the approach to existing datasets to test its effectiveness.

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CP31

Using the Method of Weighted Residuals to Compute Potentials of Mean Force

The potential of mean force (PMF) describes the change in free energy along a reaction coordinate and determines the strength and likelihood of association in molecular systems. We propose a general framework for approximating the PMF in conformational space. This framework, based on the method of weighted residuals, can be viewed as a generalization of thermodynamic integration and direct histogram methods. Comparisons between the new weighted residual methods, thermodynamic integration, and WHAM are performed.

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CP32

A Primal-Dual Interior-Point Method for Dynamic Constrained Global Minimization in Thermodynamic Phase Calculations

The global minimization of non-convex energy functions arises in thermodynamic calculations where phase equilibrium is characterized by the convex envelope of the energy function. A primal-dual interior-point algorithm is presented for computing the convex envelope. It is extended then to evolutive problems with time-dependent constraints, by coupling the optimization problem with differential equations. The time discretization of the differential-algebraic system leads to a block-structured KKT system. Applications to the modeling of atmospheric particles are given.

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CP32

Inexact Sqp Methods for Equality Constrained Optimization

The high cost of step computations in sound nonlinear optimization algorithms presents a number of challenges for

their application to large-scale equality constrained problems, e.g., those defined by systems of partial differential equations. We outline a simple set of easily calculable criteria to evaluate any potential primal-dual step as an inexact Sequential Quadratic Programming step, the incorporation of which into any algorithm will lead to a globally convergent method allowing for relatively cheap step computations.

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CP32

Uncertainty Estimation for Large-Scale Ill-Posed Inverse Transport Problems

We consider the problem of estimating the uncertainty in the initial condition field of a convection-diffusion problem describing the transport of atmospheric contaminants. The uncertainty results from measurement of the contaminant concentration at a limited number of sensors. Estimation of the covariance matrix is facilitated by a low rank (truncated Lanczos) approximation of the compact part of the Hessian matrix of the inverse problem, under the assumption of Gaussian statistics. Examples demonstrate the ability to estimate uncertainty at a small multiple of the cost of solving the forward problem.

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CP32

Optimization of the Geometry of Materials

Materials scientists are interested in determining the geometry of a material in its ground-state configuration in order to predict its physical and chemical properties. Our research seeks to determine which optimization methods are the most effective for the geometry optimization problem (also known as the structural relaxation problem) of finding a low-energy configuration of a material. In this talk, we compare the performance of several quasi-Newton and nonlinear conjugate gradient methods on various materials.

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CP32

An Optimization Procedure For Model Updating Via Physical Parameters

The matrices of many finite elements models can be expressed in terms of physical parameters and known substructure matrices. A new optimization-based method is proposed for updating of such models by improving the physical parameters only. Thus, the important structural properties, including the connectivity, structure, are preserved by the updating. An appropriate gradient formula is developed for the solution of the corresponding optimization problem.

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MS0

Pathway Modeling of Shewanella Denitrificans OS217

The bacterium Shewanellas ability to reduce compounds of several metals, some of which may be toxic to humans and to other organisms, make it an ideal candidate for bioremediation of contaminated areas. The metabolic pathway modeling software, Pathway Tools, was used to model specific metabolic pathways of the bacterium Shewanella denitrificans OS217. The results of this study are expected to provide insight into Shewanella metabolism and to assist in the design of bioremediation programs.

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MS0

Adaptive Temporal Integration of ODEs with Interval Computations

The area of Interval Computations is of growing interest for rigorous and error bounded computations. By using interval arithmetic routines in the Matlab toolbox Intlab, error bounds can be propagated throughout an algorithm to yield reliable enclosures of solutions. We examine the use of interval arithmetic applied to adaptive temporal integration of stiff ODEs and solutions to nonlinear systems.

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MS0

Resolving Systematic Errors in using Discrete Data to Fit Continuous Functions

We recorded the motion of oscillating springs, fit continuous functions to data sequences using Excel Solver to fit parameters by minimizing the sum of squared error, and analyzed the patterns of the residuals. The residuals showed systematic errors indicating our theoretical model or data were flawed. Our procedure for examining the error allowed us to verify our theoretical model using discrete data, and investigate the sources of systematic error in the model or data.

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MS1

Scalable High Fidelity Modeling of Semiconductor Devices

Abstract not available at time of publication.

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MS1

High Performance Modeling of Circuits Using the Multitime PDE Algorithm

Abstract not available at time of publication.

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MS1

Novel Algorithms SPICE_Diego for Circuit Simulation

Abstract not available at time of publication.

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MS2

Specialized Computing Architectures for Biological Computations

This talk describes the current state of the art in biomolecular simulation and explores the potential role of high-performance computing technologies in extending current capabilities. Efforts within our own lab to develop novel architectures and algorithms to accelerate molecular dynamics simulations by several orders of magnitude would be described, along with work by other researchers pursuing alternative approaches. If such efforts ultimately prove successful, one might imagine the emergence of an entirely new paradigm in which computational experiments take their place alongside those conducted in "wet" laboratories as central tools in the quest to understand living organisms at a molecular level.

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MS2

Climate Modeling at the Petaflop Scale Using Semicustom Computing

We present the performance requirements of an atmospheric general circulation model at ultra-high resolution and describe alternative technological paths to realize a solution in the relatively near future. It is estimated that a credible kilometer scale atmospheric model would require at least a sustained ten petaflop computer to provide scientifically useful climate simulations. Analysis shows that embedded processor technology could be exploited to tailor a custom machine designed to ultra-high climate model specifications at surprisingly affordable cost and power considerations.

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MS2

Domain-Oriented Processors for Power-Efficient Multi-PetaFLOP HPC

This informal talk discusses the potential and outlines one possible design for a highly efficient petascale system (10-petaFLOPS peak and roughly 1 petaFLOPS sustained) oriented towards important high-performance parallel computing problems such as climate modeling. The proposed system is at least one order of magnitude more energy efficient than extrapolations from existing HPC cluster systems for two reasons: 1) a sharp focus on an application domain for which local mesh topologies permit efficient, low-contention communications, and 2) utilization of configurable processor technology derived from high-efficiency, multiple processor applications in embedded consumer and communication products.

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MS2

MDGRAPE-3 : A Petaflops Special-Purpose Computer for Molecular Dynamics Simulations

We have developed a special-purpose computer system for molecular dynamics simulations named MDGRAPE-3,

which has nominal peak performance of 1 PFLOPS. It consists of 4,778 fully-customized processors of 216 GFLOPS for calculations of forces between atoms. The specialization enables highly-parallel operations inside the processor by the "broadcast memory architecture". By using many parallel pipelines at moderate speed of 300 MHz, our processor consumes a low power of 17 W, or 0.1 W/GFLOPS.

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MS3

Bifurcation Analysis of a Liquid State Theory: Multiple Solutions and Phase Transitions

This talk presents bifurcations of the Ornstein-Zernike(OZ) equation with hypernetted chain and Perkus-Yevick closures using several intermolecular potentials. We show that spinodal solution branches, precursors to a liquid-vapour phase transition, cannot be reproduced numerically, and that the existence of a so-called no-solution region causes fold bifurcations along the vapour isothermal solution branch when density is used as the bifurcation parameter. This provides an explanation for previous inconclusive attempts to compute near-critical solutions with Newton-Picard methods.

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MS3

Advanced Numerical Methods for Density Functional Theories

We discuss numerical methods developed for the solution of Density Functional Theories for inhomogeneous fluids in complex 3D geometries. The nature of the equations makes application of generic parallel iterative solvers less than optimal. We discuss a Schur complement based approach that improves the performance and stability of the methods. Solution complexity and identification of phase transitions with arc-length continuation methods will be discussed in the context of a variety of applications.

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MS3

Why Sampling Efficiency is the Key to Using Molecular Theory as an Implicit Solvent for Monte Carlo Molecular Simulations

Simulations of mixtures with at least one large component in a small solvent are challenging. The larger components are the focus of the simulation, but the solvent has significant effects. Implicit solvent methods trade off accuracy in solvent effects for computational speed. In Monte Carlo (MC) simulations, convergence depends on efficiently sample phase space. We discuss how new MC methods for sampling coupled with a molecular theory based implicit solvent may provide a route for MC based investigation of these systems.

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MS3

Morphometric Approach: Theory and Application in Biophysics

Fluids in confined geometries develop an inhomogeneous structure and their thermodynamic properties depend in a complicated way on the geometry. The morphometric approach discussed here allows one to transfer the insight gained in simple geometries to complicated ones. This is accomplished by the separation of the grand potential into four geometrical measures, describing the shape of the confinement, and corresponding thermodynamic coefficients. We discuss protein folding as an application of the morphometric approach.

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MS4

An Asynchronous Parallel Generating Set Search Algorithm for Handling Nonlinear General Constraints

Many real-life optimization problems present formidable challenges despite having a relatively small number of independent variables. Difficulties can arise from nonsmoothness, discontinuities, and noise. Further, function evaluations typically involves calling unwieldy CPU-intensive simulation software that may periodically crash. In this context, we present a globally convergent derivative-free method for nonlinear programming based on generating set search. Linear constraints are handled using conforming search directions. Several options for handling nonlinear constraints are explored, including an augmented Lagrangian approach. All methods are implemented asynchronously in parallel. We present extensive test results using the CUTEr test set as well as real-life applications.

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MS4

Surface Structure Determination of Nanostructures Using a Mesh Adaptive Optimization Method

Many properties of nanostructures depend on the atomic configuration at the surface. One common technique used

for determining this surface structure is based on the low energy electron diffraction (LEED) method, which uses a sophisticated physics model to compare experimental results with spectra computed via a computer simulation. While this approach is highly effective, the computational cost of the simulations can be prohibitive for large systems. In this work, we propose the use of generalized pattern search methods in combination with a simplified physics surrogate for the full fidelity physics model. The generalized pattern search method handles both discrete and continuous variables, which allows the simultaneous optimization of the atomic coordinates as well as the chemical identity. In addition, the calculation time of the surrogate scales linearly with the number of atoms on the unit cell (N), compared to the N^3 scaling behavior of the full LEED calculation. We will present some numerical results based on this simplified physics surrogate within a mesh adaptive direct search (MADS) algorithm.

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MS4

Function Approximation Algorithms for Local and Global Optimization Including Applications to Expensive Engineering Simulations

Global optimization methods are often necessary for complex simulation models because there is no guarantee the problem is unimodal. We discuss numerical comparisons of variety of existing global optimization methods with local optimization methods implemented with multi-start. We will also present convergence theorem and numerical results for a new method that is a hybrid between a global and a multistart method, which outperforms alternative algorithms on number of multimodal test problems and expensive engineering simulations.

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MS4

Optimization of Simulation-Based Optimization Problems with Constraints on the Computational Budget

We consider simulation-based optimization problems where the function evaluation is expensive and the computation of derivatives is not feasible. Pattern-based algorithms or surrogate-based algorithms, which repeatedly build and optimize over cheap-to-evaluate approximations of the objective function, often make unsatisfactory progress in reducing the function within a fixed computational budget. We propose an algorithm that finds an approximate local minimizer in fewer function evaluations than current derivative-free alternatives.

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MS5

A Regularized Gauss-Newton Method for Ill-Posed Nonlinear Problems Applied to Diffuse Optical Tomography

Many reconstruction problems take the form of a nonlinear least-squares problem for a set of parameters. The traditional methods, damped Gauss-Newton (GN) and Levenberg-Marquardt (LM), are generally effective but they require a considerable number of function and Jacobian evaluations to determine the correct step length and/or damping parameter. To deal with ill-conditioned Jacobians and (usually) noise in the data, we propose a regularized, trust-region-based Gauss-Newton approach for determining search directions. Our method systematically evaluates the potential contribution of each of the spectral components corresponding to the GN-direction and constructs the new direction relative to this contribution within the confines of a trust-region. Examples show the success of our method in minimizing function evaluations with respect to other well-known methods.

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MS5

On the Use of Krylov-Secant Updates to Accelarate the Convergence of Nonlinear Ill-posed Problems

This work proposes an inexact Newton-Krylov framework based on Krylov-secant updates. This entails to recycle or extrapolate the Krylov information generated for the solution of the current Jacobian equation to perform a sequence of secant steps restricted to the Krylov basis. In other words, the Newton step is recursively composed with Broyden updates constrained to the reduced Krylov subspace. This is repeated until no further decrease of the nonlinear residual can be delivered, in which case, a new nonlinear step yielding another Jacobian system is performed.

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MS5

A Hybrid Optimization Approach for the Automated Parameter Estimation Problem

We propose two hybrid optimization approaches based on the coupling of the simultaneous perturbation stochastic approximation (SPSA) (a global and derivative free optimization method) with two local and derivative-dependent optimization methods: (1) the globalized Newton-Krylov interior-point and, (2) the global Levenberg-Marquardt . The former implies the generation of a surrogate model whereas the latter gradually incorporates derivative information as sufficient progress is made towards the solution. Numerical examples show their appealing capabilities for parameter estimation

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MS6

Model Reduction and Mode Computation for Damped Resonant MEMS

In the design of resonant micro-electro-mechanical systems, controlling the amount of damping is critical. Simulations which incorporate realistic damping models typically lead to non-Hermitian problems which depend nonlinearly on a frequency parameter. In this presentation, we discuss our work on developing methods that use the structure of the damped model equations to efficiently compute modes and reduced order models of these problems. We illustrate our methods with models of thermoelastic damping in resonant microstructures.

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MS6

AMLS Method for Sparse Eigenvalue Problems

We describe an efficient implementation and present a performance study of an algebraic multilevel sub-structuring (AMLS) method for sparse eigenvalue problems. We assess the time and memory requirements associated with the key steps of the algorithm, and compare it with the shift-invert Lanczos algorithm in computational cost. Our eigenvalue problems come from two very different areas: the accelerator cavity design and the normal mode vibrational analysis of the polyethylene particles. We show that the AMLS method is very competitive with the traditional method in broad application areas, especially when large numbers of eigenvalues are sought.

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MS6

Modal Dynamic Solutions - Current State and Challenges

This presentation will briefly review the concept of modal dynamic solutions and present some of their structural engineering industry use, a topic not well understood by academia. The state of the current technology and remaining numerical and computational challenges will also be discussed.

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MS6

Solving Structural Eigenproblems with KKT Matrices

Lagrange multiplier techniques are a popular method for modeling constraints in structures stemming from contact, nonlinear rigid elements, inertia relief, and other applications. The resulting KKT matrices are indefinite, posing a significant challenge for the prevailing eigenvalue solution techniques in normal modes and buckling analysis. This talk will describe a Lanczos eigensolver which has been modified to handle KKT matrices.

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MS7

Interoperable Mesh and Geometry Technologies

Interoperable mesh and geometry technologies developed by the ITAPS center allow domain scientists to leverage both software and the expertise of tool developers. Critical to our interoperability goal is the creation of the creation

of common interfaces for a wide variety of mesh and geometry tools that will allow them to work with each other to provide fundamentally increased capabilities and to allow application scientists to switch among them easily. I describe the current status of our interface definition effort, the tradeoffs required to balance performance and flexibility, the tools used to address language interoperability issues, and many of the tools now available through the ITAPS interfaces.

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MS7

On the Interoperability Between FronTier and Other Scientific Application Software

The FronTier code features high quality tracking of a dynamically moving interface and the coupling of between the front and interior solutions. A combined operation between front tracking and other adapted mesh software such as the Overture and KIVA codes enables highly resolution scientific applications such as the study of combustion problems.

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MS7

Adding Adaptive Mesh Control to Fusion and Accelerator Applications

The ability to support adaptive computations starting from existing non-adaptive analysis programs requires determining where and how the mesh needs to be improved and then executing those mesh improvements. This presentation will describe a tool capable of performing the mesh modification needed to alter a given mesh to match a specified anisotropic mesh size field. Its use in the creation of adaptive analysis loops for multiple applications will also be presented.

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MS7

Applications of the TSTT Geometry, Mesh, and Relations Interfaces

The Interoperable Tools for Advanced Petascale Simulations (ITAPS) center has developed API specifications for interfaces to geometry, mesh, and relations data. These interfaces allow the construction of tools which operate on the associated data, without depending on one particular implementation of those interfaces. These interfaces also allow the assembly of advanced components and services based on third party tools interacting though these interfaces. This presentation will describe several such components and services, including partitioning/load balancing and parallel mesh generation. Geometry and mesh support for shape optimization will also be described.

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MS8

A Parallel And Generic Algebraic Multigrid Algorithm Based on Agglomeration

Sparse matrices obtained from finite element discretizations exhibit a lot of structure (e.g., discretization of three-component system with linear finite elements and pointwise ordering) already known at compile time. The parallel algebraic multigrid algorithm based on agglomeration presented is capable of exploiting this structure using generic programming techniques. This leeds to shorter setup times, e.g., for systems of linear equations. And the smoothers, coarse grid solvers and surrounding preconditioned Krylow methods become more efficient due to the knowledge of the structure.

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MS8

Scaling Multigrid Libraries to 100K Processors

In this talk, we will first overview the basic issues associated with developing parallel multigrid methods, outlining some of the techniques used to overcome these problems. The remainder of the talk will focus on additional issues that arise when confronting architectures with more than 100K processors (e.g., BlueGene/L), especially when developing multigrid libraries such as hypre. In particular, we will describe our new assumed partition algorithm and

new interpolation schemes for algebraic multigrid.

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MS8

High Performance Parallel Multigrid for Large-Scale Electromagnetics Simulations

Parallel multigrid for large-scale electromagnetics simulations presents unique challenges, due to the need to simultaneously address parallel and algorithmic performance. System resources are often constrained because of demands from other parts of the application, coarse-level problems can have large communication to computation ratios, and load-balancing of the linear systems may be optimized for something other than the linear solver. We discuss our approaches to these challenges, and present numerical results on thousands of processors.

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MS8

Scalable Parallel Multigrid for Finite Element Computations

The hierarchical hybrid grids framework combines unstructured FE meshes with structured refinement to achieve excellent performance on current supercomputer architectures. Scalability is achieved by using multigrid as a very efficient solver and a very careful implementation that exploits systematically the structuredness of subgrids to achieve excellent node performance. In this talk we will present a scale-up study on a 4000 processor SGI altix system.

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MS9

Mathematical Modeling and Computer Simulation for Foamy Oil

There exist nearly one trillion barrels of heavy oil in Venezuela. China has a project with orimulsion production of 6 million tons per year, and expects to have more projects like this. Two crucial issues must be addressed before or during designing these projects: What is a suitable method to evaluate foamy oil driven mechanism that plays a major role during such oil recovery, and how do we get a reasonable number of ultimate oil recovery? Unfortunately, it is still very difficult to give good explanations for these two issues although several studies were performed. This talk attempts to present better explanations for these two issues using experimental results, mathematical modeling, and numerical simulations. This is a joint work with Ruihe Wang, Jishun Qin, and Ming Zhao.

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MS9

A Higher Order Spectral Finite Volume Method for Atmospheric Flows

Advection plays a fundamental role in atmospheric dynamics. In many atmospheric transport problems, it is essential to correctly calculate the 3-dim advective transport of atmospheric constituents over the globe. High-order numerical methods offer the promise of accurately capturing these advective processes in atmospheric flows and have been shown to efficiently scale to large numbers of processors. The spectral finite volume (SFV) method was developed by Wang for conservation laws and has been used by Choi et al. for ocean modeling. Recently, we developed a transport scheme based on a high-order nodal SFV on cubed-sphere which relies on a flux-corrected transport (FCT) scheme to enforce monotonicity. The reconstruction procedure which we developed avoids the expensive calculation of the inverse of a matrix used by Choi et al. We are currently working to apply this approach to an SFV based nonlinear shallow water model in curvilinear-coordinates on a cubed-sphere. In this talk, we will discuss global transport scheme combined with FCT. We also anticipate presenting our SFV based results for shallow water model.

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MS9

Characteristic Methods for Reservoir Simulation

Fluid transport is a major process that controls many reservoir simulation applications. Fluid transport is modeled very well by flow along characteristics of advection part of the differential operator. Characteristic methods that utilize these flow directions can effectively predict fluid transport without introducing artificial diffusion phenomena. Finite element and wavelet Eulerian-Lagrangian localized adjoint methods (ELLAM) will be presented , with their analysis and computational examples. This is a joint work with Jiangguo Liu and Hong Wang.

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MS9

Numerical Analysis and Adaptive Computation for

Solutions of Elliptic Problems with Randomly Perturbed Coefficients

We develop and analyze an innovative numerical method for computing solutions to the Poisson equation with randomly perturbed multiscale coefficients in an efficient fasion. We derive *a posteriori* error estimates for the method and use this to devise an adaptive algorithm for automatic tuning of the method parameters such as mesh size and sample size. The goal of the adaptive algorithm is to minimize the error in the distribution function generated by taking a desired linear functional of the solutions. The method is successfully applied to a problem that arises in oil reservoir simulation.

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MS10

Adaptive Multilevel Mesh Refinement for the Solution of Large Scale Inverse Problems

In this talk we study an efficient method for the solution of distributed parameter estimation problems. We are particularly interested in problems where the regularization operators allow jumps in the solution such as Total Variation and Huber. Even for relatively simple problems the computational cost of solving the inverse problems can be substantial. This is because the forward problem can be difficult to solve, especially when the coefficients are discontinuous. Solving the inverse problem is therefore challenging and advanced computational techniques are needed. In this talk we explore the use orthogonal but non-conforming finite difference or finite volume methods. We show that they can be very efficient for the solution of inverse problems and dramatically reducing the computation.

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MS10

Multigrid Methods for Optimal Control Problems Governed by Advection Diffusion Equations

Linear-quadratic optimal control problems governed by advection-diffusion equations arise in a variety of applications. The optimality conditions for these problems lead to large-scale, symmetric indefinite linear systems of equations, which have to be solved iteratively. These systems involve two discretized advection-diffusion equations with advection in one equation given by the negative advection in the other. In this talk we discuss multigrid methods for these optimality systems and explore differences in behavior of MG methods applied to a single PDE and MG methods applied to the optimality system.

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MS10

Multilevel Methods for Nonlinear Conjugate Gradient Methods

We analyze the performance of nonlinear conjugate gradient methods for mesh-based optimization problems. We show, in particular, that the use of scaling and limited-memory techniques results in significant improvements in performance. We present results for both single-processor and multi-processor environments.

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MS10

Assessing the Performance of Optimization-Based Multigrid Methods

Many large nonlinear optimization problems are based upon discretizations of underlying continuous functions. Optimization-based multigrid methods are designed to solve such discretized problems efficiently by taking explicit advantage of the family of discretizations. The methods are generalizations of more traditional multigrid methods for solving partial differential equations. We discuss techniques whereby the multigrid method can assess its own performance, with the goal of adaptively deciding appropriate levels of discretization.

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MS11

Reduced Order Approaches for Variational Data Assimilation in a Model of the Tropical Pacific Ocean

A reduced order approach for 4D-Var data assimilation is presented in the context of a tropical Pacific ocean model. The control space is defined as the span of a few vectors representing a significant part of the system variability. It is shown that such an approach can lead to significant improvements, both in terms of the quality of the solution and of the computational efficiency. A first step toward an hybrid variational-sequential algorithm is also discussed.

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MS11

Analysis of a POD Approach to Order Reduction in 4D-Var Data Assimilation

The proper orthogonal decomposition method to order reduction in 4D-Var data assimilation is implemented for a two dimensional global shallow water model. Specification of appropriate weights to the snapshots and the norm used to quantify the projection error are discussed. A reduced second order adjoint model is used to perform a Hessian condition number analysis in the POD space. A dual weighted procedure based on adjoint sensitivity fields is shown to provide improved results.

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MS11

Direct and Inverse POD Model Reduction Applied to Imperial College Ocean Model

A POD-based reduced model is developed for an advanced 3-D adaptive finite element ocean model. The aim of this study is to explore the: (a) feasibility of significant reduction in the computational cost of an adaptive mesh model; (b) number of snapshots that contain enough information to model the behaviour of flow dynamics throughout the data assimilation process; (c) efficiency of the reduced model in accelerating the inversion procedure; (d) estimation of model error in POD.

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MS11

POD-Based Reduced Order Ocean Modeling and Applications to Variational Data Assimilation

The proper orthogonal decomposition (POD) is a model reduction technique for the simulation of physical processes governed by partial differential equations. In this presentation, the method is applied to a simple reduced gravity ocean model in the tropical Pacific. Three issues are discussed here: (1) Numerical comparison of the POD modeling to the original modeling; (2) Error analysis of the POD modeling, both from theoretical and numerical aspects; (3) Application to variational data assimilation.

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MS12

A Posteriori Error Control for Coupled Systems

We extend our a posteriori error analysis for one-way coupled elliptic systems to the general setting of coupled elliptic systems solved via operator decomposition and single-physics solvers. We decomposte the non-iteration error into a error contributions from inherited error, single physics residuals, and projection error, all computable by formulating the appropriate single-physics adjoint problem. We then give several numerical illustrations of the features of this approach.

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MS12

An A Posteriori Analysis of Operator Splitting for Reaction-Diffusion Ode

In this talk, we present the aposteriori error analysis of an operator splitting procedure to solve a system of ordinary differential equation governing a reaction-diffusion problem. A discontinuous Galerkin Finite Element method is used to solve the resulting analytical splitting. An a priori error estimate is presented that uses a decomposition of the error into one that corresponds to the analytical splitting and one that corresponds to the discontinuous Galerkin Finite Element used to numerically solve it. An a posteriori analysis is described to derive an error representation that is computable. The analysis uses the notion of adjoint problems that correspond to the linearization of the original problem. Some numerical examples will also be presented.

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MS12

Accuracy and Stability of Operator Splitting Methods Applied to Diffusion/Reaction and Convection/Diffusion/Reaction Systems with Indefinite Operators

In this talk results are reviewed that demonstrate that common second-order operator-splitting methods can exhibit subtle instabilities for diffusion/reaction (DR) and

convection/diffusion/reaction (CDR) systems. We evaluate the relative accuracy and asymptotic order of accuracy of methods on problems that exhibit an approximate balance between competing component time scales. We consider first- and second-order semi-implicit, fully-implicit, and operator-splitting techniques. The problems include a propagating nonlinear DR and CDR wave, a Brusselator problem and a simplified CDR chemotaxis model.

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MS12

A-Posteriori Analysis of An Operator Decomposition Method for Time-Dependent Transfer of Informationthough An Interface

We consider operator decomposition methods to be a special form of operator splitting in which a real or artificial interface provides a natural partition. We present an a-posteriori adjoint-based analysis of the stability and accuracy of an operator decomposition method for a time-dependent reaction-diffusion problem which involves the exchange of information across a physical boundary. We illustrate our approach with an application to core-edge transport simulations in fusion modeling.

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MS12

Cost of Accuracy for Coupled Diffusion and Reaction Systems

Many applications give rise to coupled and nonlinear mathematical models. Due to advances in solver technologies, implicit methods have become viable solution alternatives to traditionally-applied operator splitting methods in many application areas. We present results exploring the relative costs of the most common operator splitting and implicit methods for coupled diffusion and reaction systems. We discuss the practical application of recently developed stability theory (Ropp & Shadid, 2005) on these systems and point out both advantages and disadvantages of split and implicit strategies. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48

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MS13

Moderator

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MS14

Parallel AMG Setup Phase Algorithms

The performance of AMG depends heavily on the quality of the coarse grids and transfer operators constructed during the setup phase. New theory and setup phase algorithms have been developed in recent years in an effort to make AMG more robust. These algorithms are often inherently sequential, and developing efficient, scalable algorithms in parallel remains a principle challenge. This talk focuses on recent algorithmic work on parallel coarse grid selection and parallel transfer operator construction.

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MS14

Algebraic Multigrid Methods for Systems of PDEs

Modifications to classical AMG are required when solving linear systems derived from systems of PDEs involving multiple unknowns. Two accepted approaches are treating variables corresponding to the same unknown separately (the "unknown" approach) and treating variables corresponding to the same physical node together (the "nodal" approach). We discuss the applicability and parallel performance of each approach as well as our investigation into alternative interpolation and coarsening algorithms.

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MS14

Parallel Auxiliary Space AMG for Maxwell Problems

Recently, Hiptmair and Xu introduced a new auxiliary space preconditioner for constant coefficient definite Maxwell problems. We present numerical experiments with a parallel version of their method, which utilizes two internal AMG V-cycles for scalar and vector Poisson-like matrices. Our tests include problems with variable coefficients and zero conductivity, and clearly demonstrate the scalability of this preconditioner on hundreds of processors. The implementation is part of the *hypre* library and is based on

its algebraic multigrid solver BoomerAMG.

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MS14

Long-Range Interpolation for Parallel Algebraic Multigrid

Algebraic multigrid (AMG) is a very efficient algorithm for solving sparse unstructured linear systems. However, for large three-dimensional problems, traditional coarsening algorithms often generate growing complexities in terms of memory use and computations per AMG V-cycle. The PMIS coarsening algorithm remedies this complexity growth, but leads to non-scalable AMG convergence factors when classical interpolation is used. We study the scalability of AMG methods that use PMIS coarsening combined with long-range interpolation methods for a variety of relevant test problems on parallel computers.

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MS15

Effects of Alcohols and Pore-Forming Peptides on Lipid Bilayers

Lipid bilayers are important inhomogeneous fluid systems that mediate the interaction of cells with their environment. We have applied a classical density functional theory (DFT) to a coarse-grained model of lipid and solvent, designed to self-assemble into a bilayer. We will present two recent results: the effects of alcohols on the mechanical properties of lipid bilayers, and the structure and free energy of pores formed in the bilayer by assemblies of model peptides.

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MS15

Selectivity and Permeation of Ions in Biological Ion Channels

Biological ion channels conduct ions across membranes down chemical potential gradients. Some ion channels can select which ion species they conduct, a property important for physiological function. The region of the pore where this selectivity occurs is usually highly-charged, especially in the case of Ca- and Na-selective channels. Density functional theory of fluids coupled with drift-diffusion equations reproduce and predict experimental channel data and is used to understand the physics of selectivity of channels.

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MS15

Osmotic Pressure and Packaging Structure of Caged DNA

Packaging double-stranded (ds)DNA in a small viral capsid must overcome strong electrostatic repulsion due to backbone charges and the ultimate packing density is limited by the free volume available to the colossal molecule. Multiple length scales make it a formidable task to describe the structure and thermodynamic properties caged DNA from a microscopic perspective. This work presents a theoretical model for aqueous solutions of dsDNA. Predictions of the theory are in good agreement with experiments.

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MS16

Local Calculation of Conservative Edge Fluxes from Finite Element Hydrodynamic Models

A method for calculating conservative edge fluxes for a finite element hydrodynamic model is demonstrated for the 2D shallow water equations. The method is local and relies upon physically relevant parameters such as the nodal flux and circulation. Requirements for using this approach are that the finite element method is in conservative form and the test functions sum to an elemental constant.

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MS16

Development of a Software Toolkit for Consistent-Conservative Flux Computation

Model coupling is a prosperous research field. Independent meshes and different numerical methods commonly exist in each component/model. Theoretically, globally and locally mass conservation has to be preserved when it is checked consistently, or even when the flux is computed inconsistently with the discrete equation being solved. This paper presents a software toolkit to provide coupling model

developers with capabilities for obtaining consistent and conservative flux computation without large investments of effort or time.

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MS16

A Local Conversion From Nodal Flow to Edge Flow

Mass-conservative nodal flow can be received by back substituting the numerical solution into the discretized equations of mass conservation with the finite element method. To compute flow through a desired cross section that is composed of a number of element edges, a local conversion from nodal flow to edge flow is proposed. A two-dimensional subsurface flow example is used to demonstrate this method and discuss its strengths and weaknesses.

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MS16

Locally Conservative Algorithms for Flow

When modeling fluid flow and transport problems, it is desirable to have locally conservative velocities on the transport grid. Lack of local mass conservation can result in spurious sources and sinks to the transport equation. We describe several numerical locally conservative algorithms: discontinuous Galerkin, mixed finite element, and mimetic finite difference methods. We also discuss a priori and a posteriori convergence results and compare advantages and disadvantages of each of these methods with projection approaches.

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MS17

Model Reduction Applied to Large-Scale Structural Dynamics and Control

Structural vibration control continues to be an active topic of investigation. The application to highly complex large-scale systems can involve finite element discretizations with millions of states and similarly large number of unknown parameters. The active control of these complex systems poses many unsolved problems and daunting challenges. A key challenge is designing practical controllers for active control applications of complex structures. Modern control techniques yield controllers of order comparable the physical system model, thus making real-time implementation difficult and often impractical. Therefore generation of lower-dimensional models that closely approximate full order systems are desirable for the analysis and control of large-scale systems. In the literature, model reduction has been studied both in control engineering and structural analysis. A very challenging large-scale control problem that has emerged recently is the protection of civil structures, such as high-rise buildings and long-span bridges, from dynamic loadings such as earthquakes, high wind, and heavy traffic. This presentation provides an overview of model and controller reduction techniques applied to structural dynamics problems in building control. A comparative study is performed using Modal Reduction, Guyan Reduction, Balanced Truncation and Krylov Techniques in a large-scale setting together with extensions to the closed-loop controller reduction problem.

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MS17

An Algebraic Krylov Substructuring for Model Order Reduction

Substructuring techniques are usually based on the superposition of the eigenmodes. In this talk, we present a Krylov mode based substructuring method, which is similar to the popular component mode synthesis technique; however, no eigenmodes of the interior substructures are evaluated. This new scheme replaces the eigenmodes of interior substructures by proper Krylov modes of the substructures, which take the force and the coupling among substructures into account. The accuracy improvements of this new scheme are demonstrated by numerical results from structural dynamics in both frequency and time domains.

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MS17

A Parallel Scheme for Solving Large-Scale Lyapunov Equations

We present a parallel preconditioned iterative scheme for solving the large-scale Lyapunov equations that arise when one attempts to obtain a reduced-order model of large-scale structures subjected to strong ground motion. Numerical experiments are presented to explore the effectiveness of this scheme compared to others, and to demonstrate its performance on parallel computing platforms.

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MS17
Advancing Analysis Capabilities with ANSYS

The CAD/CAE software environment has now become an accepted tool in engineering design. In its most effective use computer simulation is an integrated part of the design and manufacturing process from concept to production. This talk describes some major efforts at ANSYS that continue to advance analysis capabilities. These major efforts include software innovation and initiatives to maximize the capabilities of high performance computing. The ability to solve complex assemblies with detailed models has been advanced to new levels by ANSYS breakthrough achievements in parallel processing and large memory computing. This talk will describe current and future hardware developments as well as algorithmic breakthroughs that have made these achievements possible. Examples will be given that illustrate the current state-of-the art capabilities of ANSYS today and motivate the future goals for further developments in the world of CAD/CAE software.

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MS18
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MS19
ELLAM for Resolving Kinematics of Resistive Magnetohydrodynamic (MHD) Flows

The kinematics of MHD studies the influence of the velocity of an electrically conducting fluid on the magnetic field, which conserves the solenoidal property for all time. For the 2-dim case, a scalar potential can be introduced and the magnetic field induction equation can be converted into a convection-diffusion-reaction equation, which can be efficiently solved by the Eulerian-Lagrangian localized adjoint method (ELLAM). For the 3-dim case, locally divergence-free finite elements are used to satisfy the solenoidal property and the discontinuous Galerkin method comes into play very naturally. Simulations for some interesting MHD eddy flows will be presented, including analysis on distortion and energy evolution of magnetic fields. This is a joint work with Hongsen Chen, Richard Ewing, Shuyu Sun, and Simon Tavener.

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MS19
Data Assimilation into Some Wildfire Models

A wildfire is modeled by a system of nonlinear reaction-convection-diffusion equations. Solutions of such equations exhibit traveling waves, which consist of a reaction zone and a cool-down zone. The width of the reaction zone is less than the modeling scale and thus modeling in the reaction sheet limit is also considered, which leads to fireline evolution and fire spread models. The wildfire model stands alone or it is coupled with an atmospheric model (weather forecasting). Data is assimilated into a running model by a version of the Ensemble Kalman Filter (EnKF). Originally, EnKFs attempt to fit the measurements by a least squares fit using linear combinations of ensemble members, and the ensemble is derived by adding perturbation to a given initial state. This makes fitting thin reaction interfaces difficult. So, in addition to additive perturbation and correction, we use also spatial deformation, level-set techniques, and a new class predictor-corrector ensemble filters. The predictor-corrector filters combine the ideas of EnKF, empirical data assimilation such as nudging, and sequential Monte-Carlo methods. The predictor delivers a proposal ensemble that may not have the correct statistics, but it should be close the to analysis ensemble (i.e., ensemble with new data incorporated). The corrector then uses density estimation to assign weights to members of the proposal ensemble to obtain correct statistics.

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MS19
A-Posteriori Analysis of an Operator Splitting Method for Heat Transfer Through a Fluid-Solid Interface

We consider operator decomposition methods to be a special form of operator splitting in which a real or artificial interface provides a natural partition. For example, non-overlapping domain decomposition methods may be considered as a type of operator decomposition. We present an *a-posteriori* adjoint-based analysis of the stability and accuracy of an operator decomposition method for a multiphysics problem which involves the exchange of information across a physical boundary. We illustrate our approach with a heat transfer problem in which a cool solid is embedded within a hot Newtonian fluid.

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MS19

A Computational Flow Simulation in Multiphysics Environment

The aim of this talk is to introduce a coupled surface and subsurface flow problem arising from flood prediction and control. The mathematical and computational challenges are: (1) model deveoplement and model reduction, (2) numerical approximation for shallow water equation with complex physics, (3) algorithm design, (4) computer simulation/implementation, and (5) validation. The first four challenges shall be discussed in this talk, and particularly emphasis will be given to the model development and algorithm design. The talk should be accessible to general audience in applied/computational mathematics and hydraulogy.

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MS20

New Developments of Fast First Principles Computational Methods for Biochemical Simulations

Methods of directly simulating the behavior of complex strongly interacting atomic systems (molecular dynamics, Monte Carlo) have provided important insight into the behavior of many biochemical systems such as DNA, enzymes, and membranes. The limitation of the even wider application of these methods is the difficulty of developing representations of potential interactions in these systems at the molecular level that capture their complex chemistry that is commonly encountered in these systems (reactions, polarization, etc.). Static quantum chemistry methods have provided a means to calculate reactive mechanisms in cluster approximations to mineral systems. These methods are limited to small atomic sizes and generally cannot be applied to problems in which dynamics play a role. In this talk new developments in the implementations of methods to simultaneously simulate the electronic structure and molecular dynamics of nanoscale materials will be described (ab-initio molecular dynamics, AIMD). These methods have at their core the calculation of interatomic forces from the fast iterative solution of the density functional approximation to the electronic Schrdinger equation and, therefore, avoid problems of force development limiting the application of MD. They are designed to efficiently provide the DFT solutions to problems of very large size and so generalized the application of quantum chemistry to very large system while at the same time removing the limitation of quantum chemistry methods to static systems. This talk will focus on the development in three areas: the implementation a local basis/plane wave method (projector augmented plane-wave method, PAW) that removes the use of pseudopotentials, the development of a plane wave implementation of exact exchange, and the development of an adaptive multilevel finite element first principles solver. The talk will focus on the fundamentals of these methods and the realities in terms of system size, computational requirements and simulation times that are required for their application.

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MS20

Simulation of Diffusion Tensor Imaging (DTI) in Realistic Neural Tissues

MRI measurement of diffusion in realistic neural tissues models has many complexities. By using Monte Carlo simulation environment MCELL with computational models of neural tissues, we developed a computational environment that simulates the signal in diffusion weighted MRI experiments in neural tissues, including the influence of tissue geometry and pulse sequence parameters. Allowing for the assessment of physiological parameters on the MR DWI signal, the efficacy of data analysis techniques, and the optimality of pulse sequence parameters.

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MS20

Chemical Transformations in Complex Biological Systems: Hybrid Quantum Mechanical and Molecular Mechanics Methodologies

Accurate description of chemical transformations in complex biological systems remains one of great challenges in computational biology. This problem is inherently multiscale and requires efficient integration of several levels of theory to bridge fine description of the electronic structure effects with large scale dynamical fluctuations of the surrounding protein environment. One particular methodology that was found successful in describing problems of this type is based on combined quantum mechanical and molecular mechanical (QM/MM) methodologies. The focus of this talk will be to give a general overview of QM/MM methods, as well and discuss latest developments and challenges in this field. As a particular application example DNA photostability problem will be considered.

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MS20

Large Scale First Principles Simulations of Signaling Phosphoryl Transfer Reactions

A major limitation to simulating reactive biochemical processes is the development of accurate representations of the many-body forces that lead to their interesting properties, while retaining large enough particle numbers in the simulation to correctly describe their chemistry. Recently

progress has been made in the development of simulation methods for very large systems based on forces calculated directly from the electronic Schrdinger equation. In order to carry out these calculations is necessary to solve a very large nonlinear eigenvalue problem on the fly. These methods combine the essential features of high level quantum chemistry with those molecular dynamics to produce a 1st principles based parameter free method of simulation. While they are leading to new insights into biochemical problems, there are significant numerical limitations to their application. In this talk these problems will be discussed in the context of our recent calculations on the kinase reaction mechanism. The kinase enzymes catalyze the most important signaling events in eukaryote cells. They catalyze the transfer of the _-phosphoryl group of ATP to serine, threonine, and tyrosine residues in proteins. Even after careful structural characterization and many years of study the mechanism of the phosphoryl transfer reaction in these systems is still poorly understood. In this project we use a combined quantum mechanical and molecular mechanics approach (QM/MM) to analyze the mechanism of the phosphorylation reaction in a well characterized member of the kinase family – cAMP dependent serine protein kinase (cAPK). In order to obtain reliable results we had to include roughly 150 atoms in a full B3LYP calculation coupled with an additional 54,000 molecular mechanics atoms representing the protein environment. Our calculations support a dissociative mechanism for the reaction process with a late proton transfer to a catalytic base residue. This mechanism is consistent with observations.

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MS21

Domain-Decomposition and Operator-Split Smoothers for Inverse Problems with Parabolic PDEs

Parabolic PDEs model physical systems in science and engineering. We are interested in devising efficient numerical schemes for inverse and control problems related to such systems. In this talk we present results for the linear heat equation with a non-constant coefficient reaction-like term. First we discuss space-time smoothers for the forward problem. We propose a new smoother, inspired by operator-splitting methods, which can be combined with domain decomposition. Second we discuss the spectral properties of the inverse operator (reduced Hessian) and discuss smoothers. The basic single level techniques are the King-Kaltenbacher class preconditioners, Borzi pointwise smoothers, and space-time domain decomposition techniques. We conclude with analysis of complexity and convergence rates, their effectiveness when used in a full multigrid scheme, verify the analysis with numerical results, and compare them with the proposed smoothers.

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MS21

Mesh Adaptivity for Inverse Problems

The numerical solution of inverse problems governed by PDEs is often challenging, since it involves the discretization of both a state variable and the unknown parameter (for example material properties). In adaptive schemes, they should be discretized on separate meshes. This, and the saddle point structure of the problem, makes the construction of efficient solvers such as multigrid difficult. We present a scheme for independent discretization and efficient solution, and point out challenges to this approach.

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MS21

Multilevel Methods in Image Registration

Abstract not available at time of publication.

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MS21

Model Problems in PDE-Constrained Optimization

We hope to aid in benchmarking algorithms for PDE-constrained optimization problems by presenting a set of such model problems. We specifically examine a type of PDE-constrained optimization problem, the parameter estimation problem. We present three model parameter estimation problems, each containing a different type of partial differential equation in the constraint. We also describe different discretization and solution techniques for each problem, presenting numerical results to compare such techniques.

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MS22

Images: New Perspectives in Data Assimilation

Assimilation of satellite images is an attempt to conjugate the information contained in atmospheric or oceanographic models and images. We will discuss the main directions of research in this field. The first approach is to estimate from images some pseudo observations such as velocities then to assimilate them in a classical scheme of data assimilation. The other approach is to add to the classical variational analysis a space of images with a metric structure and an operator from the space of the solutions of the numerical model toward the space of images in order to be able to compute the discrepancy between the model

and the images then to plug it in a variational method. In this communication we will present both approaches with applications to actual situations, the comparison between these approaches will be discussed.

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MS22

Localized Ensemble Kalman Data Assimilation for Atmospheric Chemical Transport Models

The task of providing an optimal analysis of the state of the atmosphere requires the development of dynamic data-driven systems that efficiently integrate the observational data and the models. In this paper we discuss practical aspects of nonlinear ensemble data assimilation applied to atmospheric chemical transport models. We highlight the challenges encountered in this approach such as filter divergence and spurious corrections, and propose solutions to overcome them, such as background covariance inflation and filter localization. The predictability is further improved by including model parameters in the assimilation process. Results for a large scale simulation of air pollution in North-East United States illustrate the potential of nonlinear ensemble techniques to assimilate chemical observations.

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MS22

The Inverse Ocean Model: A Toolkit for Creating Geophysical Data-Assimilation Systems

The Inverse Ocean Model system is a modular software package that implements Weak-constraint, Four-Dimensional Variational (W4DVAR) assimilation for any dynamical model and observing array, both of which may be nonlinear but functionally smooth. Program templates, coded in Parametric Fortran, enable custom code generation for user's models, which have included primitive equations and shallow water models on structured and unstructured grids, with numerics ranging from finite-differences to spectral elements.

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MS22

Issues in Ensemble Assimilation/Prediction for Extreme Events

By definition, the extreme values belong to the tails of a probability distribution function (PDF). The consequence of using a typical Gaussian framework is that the extreme event observations will be rejected, or given a negligible weight, thus discarding the important new information. We will discuss challenging issues and present a maximum likelihood ensemble methodology designed to assimilate extreme value observations, based on the use of mixed Gaussian and Extreme Value PDFs.

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MS23

NOMADm: A MATLAB Software Package for Surrogate-Based Black Box Optimization

In this talk, we discuss the implementation of both interpolatory and simplified physics surrogates as an aid in numerically solving nonlinear and mixed variable optimization problems, in which objective and constraint functions are computationally expensive and derivatives are generally not available. The NOMADm software package is a MATLAB code based on the class of mesh adaptive direct search (MADS) algorithms for derivative-free optimization. The flexibility of the search step in MADS allows for the construction and optimization of less expensive surrogate functions. The talk focuses on different types of surrogates, strategies for using surrogates on mixed variable problems (especially when nonnumeric categorical variables are present), simplified physics surrogates, and additive surrogates that make use of both interpolation and simplified physics models. A few applications will be discussed.

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MS23

Formulations for Surrogate-Based Optimization Using Data Fit and Multifidelity Models

Surrogate-based optimization (SBO) methods have become established as effective techniques for engineering design problems through their ability to tame nonsmoothness and reduce computational expense. Possible surrogate modeling techniques include data fits (local, multipoint, or global), multifidelity model hierarchies, and reduced-order models, and each of these types has unique features when employed within SBO. We discuss a number of SBO algorithmic variations and their effect for each of the surrogate modeling cases. First, general facilities for constraint management will be explored through approximate subproblem formulations (e.g., direct surrogate), constraint relaxation techniques (e.g., homotopy), merit function selections (e.g., augmented Lagrangian), and iterate acceptance logic selections (e.g., filter methods). Second, techniques specialized to particular surrogate types will be described. Computational results will be presented for a selected set of test problems using the DAKOTA software.

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MS23

Generation of Optimal Artificial Neural Networks Using a Pattern Search Algorithm: Application to Approximation of Chemical Systems

A pattern search optimization method is applied to the generation of optimal artificial neural networks (ANNs). Optimization is performed using a mixed variable extension to the generalized pattern search method. When used with a surrogate, the resulting algorithm is highly efficient for expensive objective functions. Results of this approach applied to a chemistry approximation problem demonstrate the effectiveness of this method.

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MS23

Derivative-Free Trust-Region Methods Using Radial Basis Functions

We implement a derivative-free trust-region optimization method using different types of radial basis function (RBF) models. We compare the performance of these Trust-Region RBF algorithms to alternative local optimization methods, including Newuoa, Pattern Search, and a Quasi-Newton method, on a variety of test problems. We also compare these algorithms on two environmental applications, namely, groundwater bioremediation and the calibration of a watershed model. The results indicate that the Trust-Region RBF approach is very promising in derivative-free optimization. Finally, we will explore some parallelization strategies for Trust Region RBF algorithms.

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MS24

Computational Science PhD at San Diego State University

San Diego State University (SDSU) offers a doctoral degree in computational science, the first in California, in collaboration with Claremont Graduate University (CGU), Claremont, CA. the program involves graduate level courses and research projects under the supervision of SDSU faculty from the departments of engineering, physics, mathematics, computer science, chemistry, and biology with cooperating faculty from CGU. the ph.d. degree is awarded jointly by the two institutions. We will describe the program curriculum and highlite some of the research projects.

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MS24

The Growing Role of the TeraGrid in the Computational Science Education Pipeline

The NSF-funded TeraGrid is the worlds first large-scale and production grid infrastructure for open scientific research. The San Diego Supercomputer Center (SDSC) serves as the data-intensive site lead for the TeraGrid. SDSC has a vested interest in the computational science education pipeline not only as a user of computational science resources but also as a potential future employer of students currently interested in computational science and engineering. In response to an NSF mandate that users from HPC Expert to K-12 student should benefit from the TeraGrid, TeraGrid partners are developing a series of Gateways. TeraGrid Gateways are web-based portals consisting of front-end grid services that provide teragrid-deployed applications used by a discipline-specific community. Gateways are intended to: streamline the process of doing research that depends on high-performance computing, reach a broader community of users, and help define the specifications for a computational science education pipeline, An important long-term goal of TeraGrid Gateways is to engage communities that are not traditional users of the supercomputing centers by providing community-tailored access to TeraGrid services and capabilities so they may take advantage of existing community investment in software, services, education, and other components of Cyberinfrastructure. Ten Gateways are currently under development in a diverse range of disciplines including nanotechnology, atmospheric science, bioinformatics, and traffic flow. Gateways feature workflow management tools and expert technical support to maximize productivity. The Grid Computing Environments Research Group solicits and analyzes Gateway user feedback to help improve the interface and respond to user needs. Teragrid partners or Resource Providers offer workshops, institutes, seminars and provide on-line learning resources to support and promote the effective use of TeraGrid resources.

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MS24

3d Game Programming as a CS Service-Learning Curriculum for High School Science Courses

3d computer games are undeniably popular today and

many university Computer Science (CS) majors are eager to gain skills at programming their own game. We have been able to capitalize on this interest to develop a course where students learn to code effective games using the Torque 3d Game Engine from garagegames.com. This course requires appropriate CS content to understand the 3d environment and the Object Oriented Scripting language. The course goal is to collaborate with an educator who can pose the 3d topic to be explored. With the accepted high school science standards, this module can be characterized and can be useful to a large wide body of high school science teachers. Since current high school students are of a generation that was born digital, they are comfortable and engaged when exploring topics delivered within the game environment. This scientific visualization application can be further applied to topics in computational science.

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MS24

Undergraduate Computational Science Curricula: Programs and Educational Materials

There is a growing number of undergraduate CSE curricula. This presentation will first highlight the different versions of computational science programs (e.g., B.Sc. programs, minor programs, certificate programs, etc) that depend on the type of institution and local resources. We will also present a model curriculum and provide specific examples of educational materials developed by the Keck Undergraduate Computational Science Education Consortium.

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MS25

The Entrainment and Optimal Control of Circadian Phase Dynamics

Circadian rhythms are observed at all cellular levels affecting cell function, division, and growth. These approximate timekeepers synchronize organisms to the environment and to one another through entrainment factors such as light. An inability to entrain the biological clock leads to a variety of circadian-related disorders. Our objective is to better understand and control circadian entrainment through development and application of a closed-loop model predictive control algorithm, where light serves as the manipulated control input.

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MS25

A Molecular Model for Intercellular Synchronization in the Mammalian Circadian Clock

Abstract not available at time of publication.

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MS25

Period Determination Among Circadian Pacemakers

Abstract not available at time of publication.

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MS25

BioSens: A Sensitivity Analysis Toolkit for Systems Biology

Sensitivity analysis guides the development of ordinary differential equation models of biological systems. The sensitivity of characteristic behaviors to parametric perturbation identifies areas requiring refinement. For many oscillatory systems, such as the circadian clock, phase behavior is the feature that best elucidates clock performance and, therefore, is the key behavior to analyze. We discuss period and phase sensitivity for oscillatory systems and BioSens, a software toolkit for general systems.

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MS26

Direct and Inverse Algorithms for Stochastic Models of Microrheology

The field of microrheology exploits experimental tracking of micron-scale beads suspended in viscoelastic materials to infer properties of the material. Passive microrheology is based on entropic bead fluctuations, the fluctuation-dissipation theorem, and a generalized Stokes-Einstein drag law to deduce frequency-dependent storage and loss moduli of the material. Since the 1995 PRL of T. Mason and D. Weitz, this method or variants of it have been applied as an alternative to bulk methods, or in biology, to soft matter materials for which very small volumes are available. In addition to the standard application as an inverse characterization method, we are interested in direct simulations of pathogens in pulmonary fluids. The lecture will highlight direct and inverse methods and algorithms developed in our group based on generalized Langevin equation models and the statistical tools of maximum likelihood estimators from noisy time series data.

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MS26

Implicit Solvent Models: Level-Set Relaxation and Generalized Born Approximations

Understanding biomolecules and their interaction with solvent such as water is essential to revealing mechanisms and functions of biological systems. While atomistic simulations that treat both solvent and solute molecules explicitly are accurate, the recently developed implicit solvent models for biomolecules greatly reduce the degree of freedom in simulations. In this talk, I will first introduce a class of variational implicit solvent models for biomolecules. I will then present my recent work, jointly with L.-T. Cheng, J. Dzubiella, and J. A. McCammon, on level-set calculations of equilibrium solvent-solute interface and free-energy for nonpolar solvation systems. Finally, I will introduce generalized Born models for the electrostatics calculations in implicit solvent models; and examine the validity of various formulas of generalized Born radii.

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MS26

Continuum-Discrete Computation of Viscoelastic Flows

Abstract not available at time of publication.

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MS26

Applications of An Energetic Variational Phase-Field Method for Numerical Simulation of Multiphase Flows

Abstract not available at time of publication.

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MS27

Error Representation and Estimation in Compressible MHD

Error representation and estimation of numerically approximated functionals arising in time dependent compressible magnetohydrodynamics (MHD) is considered. The discrete MHD stability theory [Barth, "On the Role of Involutions in Discontinuous Galerkin Discretization of Maxwell and MHD Systems", IMA Volume on Compatible Spatial Discretizations, Vol. 195, 2006] motivates several hybrid FEM discretizations strategies for compressible MHD depending on

- strong or weak satisfaction of $\operatorname{div} \mathbf{B} = 0$ in element interiors
- strong or weak satisfaction of $[\mathbf{B} \cdot \mathbf{n}]^+_- = 0$ on element interfaces

where $\mathbf{B}$ denotes the magnetic induction field in MHD. We then consider the representation and estimation of errors in computed MHD functionals for these discretizations using error estimation techniques developed by Becker and Rannacher [Becker and Rannacher, "Weighted A-Posteriori Error Control in FE Methods", Proc. ENUMATH-97, Heidelberg, 1998]. A critical comparison of the various discretization methods and error representation formulas reveals rather significant differences in computational cost and ease of implementation which are verified via numerical experiments.

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MS27

Coupled a Posteriori Error Estimation and Uncertainty Quantification for a Nonlinear Elasticity MEMS Problem

Quantification of both numerical error and probabilistic uncertainties is important for proper design of micro-electro-mechanical systems (MEMS). We present a goal-oriented a posteriori error estimator for the average surface force in a nonlinear elasticity problem that models a MEMS device. Our results demonstrate the performance of the error estimator for both stand-alone deterministic models and for models that are embedded in calculations for uncertainty quantification and reliability-based design optimization.

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MS27

Error Estimation and Adaptivity Tools for Nonlinear Thermal Applications

We discuss tools for error estimation and adaptivity based on least squares recovery, element residual indicators, and adjoint-based estimators for local quantities of interest. We examine the practical implementation of these tools in a production parallel finite element code that approximates solutions of nonlinear elliptic and parabolic equations. We present results for transient heat conduction with contact

and enclosure radiation. The use of these tools is discussed in the wider context of code and solution verification.

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MS27

Adaptive Anisotropic Meshing Control for Cardiovascular Flow Modeling

Many physical problems exhibit strong phenomena that introduce a need for anisotropic meshes. In viscous flow simulations better results for key quantities of interest in regions of boundary layers can be obtained with a semi-structured boundary layer mesh. We will present an adaptive procedure that adapts a boundary layer mesh to an anisotropic mesh size field defined such that the structure of the boundary layer mesh is maintained.

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MS28

Experimental Data Visualization: Some Alternatives to Equal-Width Binning

We report on a set of adaptive-multiresolution binning approaches, specially designed for data visualization in experimental sciences where counting statistics follow poisson distributions. Fields of possible applications of algorithms here described stem from astrophysics to condensed matter sciences. Our main focus of interest concerns neutron spectroscopy data from single crystal samples where signals span a fourdimensional space comprised by three spatial plus time dimensions. This makes a priori equal width binning schemes inadequate since physically relevant information is often concentrated within rather small regions of such a space. Our aim is to generate optimally-binned data sets from 1D to 3D volumes to enhance the experimenters ability to carry out searches within a 4D space. Several binning algorithms are then scrutinized against experimental as well as simulated data.

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MS28

Adaptive Methods for PDEs and Conforming Centroidal Voronoi Delaunay Triangulations

In this talk, we will discuss a new mesh adaptivity algorithm for elliptic PDEs that combines a posteriori error estimation with centroidal Voronoi/Delaunay tessellations of domains in two dimensions. The ability of the first ingredient to detect local regions of large error and the ability of the second ingredient to generate superior unstructured grids result in an mesh adaptivity algorithm that has several very desirable features, including the following. Errors are very well equidistributed over the triangles; at all levels of refinement, the triangles remain very well shaped, even if the grid size at any particular refinement level, when viewed globally, varies by several orders of magnitude; and the convergence rates achieved are the best obtainable using piecewise linear elements.

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MS28

Reduced Order Modeling of Partial Differential Equations Via CVT

A reduced-basis method based on centroidal Voronoi tessellations (CVTs) is introduced. A discussion of reduced-ordering modeling for partial differential equations is given to provide a context for the application of reduced-order bases. Then, detailed descriptions of CVT-based reduced-order bases including their construction from snapshot sets their application to the low-cost simulation of partial differential equations and its control problems are given. An adaptive method using density functions will also be introduced.

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MS28

Radially Projected Finite Elements

We develop and analyze finite element discretizations for domains with spherical geometry. In particular, we describe the method used to approximate solutions (as well as eigenvalues and eigenvectors) of partial differential equations posed on the sphere, ellipsoidal shell,and cylindrical shell. These novel, so-called, "radially projected finite

elements" are particularly attractive for numerical simulations since the resulting finite element discretization is "logically rectangular" and may be easily implemented in existing finite element codes.

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MS29

Use of a Manufactured Solution for Verifying CFD Flux Schemes and BCs

Order-of-accuracy verification is necessary to ensure that software correctly solves a given set of equations. One method for verifying the order of accuracy of a code is the method of manufactured solutions. A manufactured solution is presented and deomonstrated that allows verification of not only the Euler, Navier-Stokes, and Reynolds-Averaged Navier-Stokes equation sets, but also some of their associated boundary conditions: slip, no-slip (adiabatic and isothermal), and outflow (subsonic, supersonic, and mixed).

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MS29

Verification of Overflow 2.0 through the Method of Manufactured Solutions

The overset grid code, OVERFLOW2.0y, is subject to verification via the method of manufactured solutions (MMS). In this investigation, a prescribed, time-and-space-varying solution is inserted into the governing equations using symbolic software. The analytic remainder is then used as a forcing term within the numerical algorithm to be verified. Through successive space and/or time refinement, the solution error, produced via comparison to the prescribed solution, may then verify the theoretical order-of-accuracy of a given discretization.

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MS29

An Extreme Accuracy Benchmark via Convergence Acceleration for the McCormack Model for Binary Gas Mixture Channel Flow

Verification of computational algorithms for internal channel flow of rarefied gases is an essential ingredient of reliable code development. The analytical discrete ordinates (ADO) method has recently emerged as an efficient algorithm to generate highly accurate numerical benchmark solutions for a variety of internal flows of binary mixtures including Poiseuille, thermal-creep and diffusion flows. While the ADO method is computationally fast, its implementation may not be readily accessible to those who are not transport aficionados. For this reason, this presentation will address the question, Can a simpler, more fundamental, transport algorithm provide benchmarks comparable to the ADO method for internal gas flow?

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MS29

Overview of Scientific Code Verification

Computer simulations have been increasingly contributing to the understanding of physical processes, analysis, and design of engineering systems. Terminology such as virtual prototyping and testing is being used in the development of engineering systems. Users of computational simulation tools face a critical question as how to evaluate the confidence in simulations. Verification, Validation, and Uncertainty Quantification are the primary tools to establish and quantify this confidence. An overview of scientific code verification will be presented. This work was performed under the auspices of the U. S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

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MS30

How Scalable is Your Load Balancer?

Load-balancing (also known as partitioning) is a critical component in parallel scientific computing to achieve higher degree of parallelism. The goal is to assign computation to processors evenly while trying to minimize the communication volume. Graph and hypergraph partitioning have served as useful approaches for this purpose over the last decade. In this talk, we will discuss and present scalability performance of the state-of-the-art parallel graph and hypergraph partitioning tools.

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MS30

Parallel Hypergraph Repartitioning and Load Balancing

Hypergraph partitioning is highly effective for many scientific applications. Its accurate communication model enables higher quality than graph partitioning. Hypergraphs also represent greater varieties of data, including non-square, non-symmetric data. Adaptive computations, however, require periodic repartitioning; hypergraph partitioning can incur significant costs for data migration. We present parallel hypergraph repartitioners that account for existing partition assignments in computing new partitions, thus reducing migration costs. We compare our repartitioners with both hypergraph partitioners and graph repartitioners.

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MS30

Performance Improvement in a Mesh Quality Optimization Application

We describe the use of combinatorial algorithms and related techniques to improve the performance of a Newton-based mesh quality improvement application. We emphasize the use of runtime reordering transformations to improve data locality and the use of graph algorithms in automatic differentiation to reduce the cost of gradient and Hessian evaluations.

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MS30

Graph Coloring Problems for Computing Derivatives: Recent Developments and Future Plans

We provide an overview of the research plans for the CSCAPES Institute, funded by the Department of Energy's SciDAC program for five years. Then we discuss new graph models and algorithms for the specialized graph coloring problems that arise in computing Jacobians and Hessians. Among these is the first practical algorithm for acyclic coloring and its use in estimating Hessians by an indirect method. We also evaluate the performance gained through our coloring software in an automatic differentiation code.

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MS31

Uncertainty Analysis for Flows with Temperature Dependent Material Properties

In this talk, we discuss the use of sensitivity analysis (the computation of derivatives of fluid quantities with respect to model parameters) in performing uncertainty analysis for fluids with temperature dependent material properties. Experimental measurements of the free convection of corn syrup and nonlinear, temperature dependent models of viscosity and thermal conductivity are evaluated.

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MS31

Moment Closure for the Macro-Micro FENE Model of Complex Fluids

We present some systematic moment closure models for the FENE models of polymeric fluids, and we illustrate their various extensions and demonstrate the good agreement with the fully coupled macro-micro model for the simple shear flow and extensional flows. The talk is based on the joint works with YunKyong Hyon, Chun Liu and Peng Yu.

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MS31
A Two-Level Smagorinsky Model

A two-level method for discretizing the Smagorinsky model for the numerical simulation of turbulent flows is proposed and analyzed. The two-level algorithm consists of solving a small nonlinear system of equations on the coarse mesh, and then using that solution to solve a larger linear system on the fine mesh. For an appropriate choice of grids, the two-level algorithm is significantly more efficient than the standard one-level algorithm.

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MS31
New Numerical Techniques for Some Non-Newtonian Flow Simulations

In this talk, we report efficient methods to simulate various rate-type non-Newtonian fluid models in a unified framework. The method is developed from a simple observation that various rate-type constitutive equations can be recast into the well-known symmetric matrix Riccati differential equations. We discuss and show how such an observation can be crucially used for the stability with respect to the high Weissenberg number. The multigrid solution strategy for the discrete system will also be presented and analyzed.

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MS32
Moderator

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MS33
IMPETUS for Career Success

We present our Roller Coaster Camp outreach program designed for 7th-12th graders. We use an integrated math-physics curriculum to teach students about roller coaster design. The program helps build students basic skills while introducing them to exciting applications of computational science and engineering. We describe the hands-on learning experiences, including a trip to Six Flags for roller coaster research. We also incorporate professional development for teachers, undergraduate and graduate students to ultimately increase the awareness of STEM college programs and careers.

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MS33
The St. Lawrence Mathematics Partnership

This talk focuses on a partnership developed with NY State funding. The partnership is focused on professional development activities for 300 teachers in a very widely scattered, low income, rural part of northern New York. The primary objective is helping teachers appreciate the interactions among science, mathematics and technology for solving real-world problems CSE at the K-12 level. Teachers work in triads throughout the year and attend week-long institutes in the summer. Content examples and structure will be presented.

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MS33
Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS34
Formulation of a Target-Matrix Paradigm for Mesh Optimization

A new target-matrix paradigm for improving mesh quality by node repositioning via optimization is formulated to place most application goals within a single theoretical framework. The paradigm shifts the focus from quality metrics that measure quality in an absolute sense to metrics that measure quality relative to application requirements. In this talk, properties of mesh-based matrices, of quality metrics and examples of objective functions will be presented.

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MS34
Implementation of the Target-Matrix Paradigm in

Mesquite

The design of the Mesquite quality improvement library has been modified and extended to support a target-based smoothing paradigm. The design has been modified such that definition of the sample points at which a quality metric is evaluated in a patch of mesh has been abstracted. The design has been extended to allow target-based metrics evaluated at user-specified element sample locations.

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MS34

The Effect of Node Ordering on 2D Local Mesh Smoothing

Local mesh smoothing is widely used for quality improvement of unstructured meshes due to its simplicity. One interesting aspect of this approach is the role of node ordering within a single pass over the mesh. We investigate various ordering schemes based on mesh quality, and the trade-offs involved between ordering and overall performance of the optimization algorithm in terms of speed and quality improvement. The study uses the FeasNewt solver within the Mesquite package.

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MS34

Convexity of Mesh Optimization Metrics Using a Target Matrix Paradigm

We discuss sufficient conditions for establishing convexity of mesh metrics within a target-matrix paradigm for mesh optimization that Patrick Knupp introduced at Sandia National Laboratories in 2006 in his SAND document SAND 2006-2730J, titled A Target-Matrix Paradigm for Mesh Optimization. We develop fairly simple criteria for proving convexity of mesh metrics and certain objective functions derived from those mesh metrics.

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MS35

High Order Mimetic Differential Operators

Mimetic Operators satisfy a discrete analog of the divergence theorem and they are used to create or design conservative andreliable numerical representations to continuous models. We will present a methodology to construct mimetic versions of the divergence and gradient operators which exhibit high order of accuracy at the grid interior as well as at the boundaries. As a case of study, we will show the construction of fourth order operators in a one-dimensional staggered grid. Mimetic conditions on discrete operators are stated using matrix analysis and the overall high order of accuracy determines the bandwidth parameter. This contributes to a marked clarity with respect to earlier approaches of construction. As test cases, we will solve 2-D elliptic equations with full tensor coefficients arising from oil reservoir models. Additionally, applications to elastic wave propagation under free surface and shear rupture boundary conditions will be given.

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MS35

Mimetic Discretizations for a Scalar Convection-Diffusion Operator

In this work, we presents two mimetic discretizations for a scalar convection-diffusion operator in 2D using Robin boundary conditions. Also, we have implemented other discretization called support operator method. The numerical results show the performance about of the sparse linear solver and the convergence rate. We can observe that the mimetic methods has a good future

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MS35

Mimetic Discretization of Elliptic Problems with Full Tensor Coefficients

This work concentrates on the Mimetic discretization of elliptic partial differential equations (PDE), derived from the application of Darcys law to flows in Reservoir Simulation. Numerical solutions are obtained and discussed for one-dimensional equations on uniform and irregular grids and two-dimensional equations on uniform grids. The focal point is to develop a scheme incorporated with the full tensor coefficients on uniform grids in 2-D. The results of the numerical examples are then compared to previous well-established methods. Based on its conservative properties and global second order of accuracy, this Mimetic scheme shows higher precision in the tests given, especially on the boundaries.

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MS35

A Compatible Arbitrary Lagrangian-Eulerian Discretization of the Magnetic Dynamo Equation

We are concerned with the simulation of coupled electromagnetic-hydrodynamic-thermal systems, and we have adopted an unstructured finite element Arbitrary Lagrangian-Eulerian formulation for this problem. The focus of this presentation is on the magnetic dynamo equation, which is a vector advection-diffusion equation with an implied divergence-free constraint. We derive a variant of constrained transport with flux correction that is valid for 3D unstructured grids, the algorithm relies heavily upon the compatible (mimetic) curl operator.

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MS36

Benchmarking Adaptive Multivariate Surrogate Modeling Techniques

The increasing computational complexity of computer simulation codes and the need for high fidelity simulation of large scale systems, has caused cheap meta-models to become standard practice in engineering design. Due to their compact representation and efficient implementation, these surrogate models allow fast exploration of the design space and extensive what-if analysis. In this contribution we compare three multivariate surrogate modeling techniques: rational functions, multi-layer perceptrons and support vector machines. Both predefined functions and real world engineering problems are used to check the performance of the meta-models. The results reveal the strengths and weaknesses of the different metamodel types and demonstrate the importance of adaptive metamodeling and sequential design.

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MS36

Structure-Preserving Model Reduction without Using Explicit Projection

In recent years, there has been a lot of progress in Krylov subspace-based structure-preserving model reduction of large-scale linear dynamical systems. However, all existing methods first generate a basis matrix of the underlying Krylov subspace and then employ explicit projection using some suitable partitioning of the basis matrix to obtain a structure-preserving reduced-order model. There are two major problems with the use of such explicit projections. First, it requires the storage of the basis matrix, which becomes prohibitive in the case of truly large-scale linear dynamical systems. Second, the approximation properties of the resulting structure-preserving reduced-order models are far from optimal, and they show that the available degrees of freedom are not fully used. In this talk, we discuss Krylov subspace-based recduction techniques that do not require explicit projection and thus overcome the two major problems of projection methods.

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MS36

All Levels Reduced Order Models of Passive Integrated Components

Abstract not available at time of publication.

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MS36

Linear and Nonlinear Model Order Reduction for Nanoelectronics

Simulation for nanoelectronics requires that circuit equations are coupled to electromagnetics, semiconductor equations, and involves heat transfer. Model Order Reduction (MOR) is a means to speed up simulation. We discuss approaches to generalize existing MOR techniques to be applicable to the resulting system of (Partial) Differential-Algebraic Equations. Also the inclusion of nonlinearity will be taken into account. Experiences with several approaches will be shown.

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MS37

Scalability and Run Time Support Issues

Traditional approaches to implementing scalable applications are based on synchronous parallelism, which divides an application into distinct phases of communication and computation. However, in some cases an asynchronous model is more appropriate. Such a model is better matched to applications modeling asynchronous processes; it can simplify the design of algorithms that tolerate communication delays by overlapping them with computation. This talk will explore asynchronous programming techniques currently under investigation and discuss experiences with applications.

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MS37

On a Future Software Platform for Demanding Multi-Scale and Multi-Physics Problems

Demanding problems in computational biology and medicine span a range of scales and involve many different types of mathematical models (for example, ODEs for cell biology; PDEs for flow, tissue deformation, and eletrical signals). Successful software must flexibly combine a variety of models and numerical techniques in legacy and new codes. In this talk we propose a Python-based platform

for future simulation software, where alternative legacy libraries (such as PETSc, Trilinos, DOLFIN, Diffpack) can be invoked in convenient ways and where new optimized code can be automatically generated. Examples on useful tools to realize such a platform will be given. We will also demonstrate current progress with building complete solvers.

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MS37

Multi-Scale Computational Modeling of the Heart

Computational models of the heart can be integrative in several important ways. In particular, multi-scale computational models aim to achieve structural integration across physical scales of biomedical organization from molecule to organism. We describe and illustrate a strategy for developing multi-scale models of the electromechanical properties of the heart that integrate across the following scales: DAE network models of the biophysical mechanisms of cell excitation and contractile processes and their biochemical regulation. Structurally based constitutive models of multi-cellular tissue electrical and mechanical properties. PDE continuum models of cardiac wall mechanics and electrical impulse propagation in anatomically detailed models of the ventricles Closed loop systems models of pulmonary and systemic circulatory dynamics.

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MS37

Design Principles of Neurotransmitter Release during Synaptic Transmission: Calcium Imaging, Electrophysiology, and Spatially Realistic Monte Carlo Simulations

Intracellular calcium is tightly regulated and is critical to many processes, including nerve-evoked release of neurotransmitter molecules during synaptic transmission. Calcium imaging can be used to visualize spatiotemporal changes that occur with nerve stimulation, and electrophysiological recordings can provide a readout of resulting neurotransmitter release. To understand the biophysical coupling between the two, we have created a 3-D model of the nerve active zone, the region from which neurotransmitter is released. The model is based on anatomical data from electron microscopy, was created with computer-aided design software, and subsequently was imported into the MCell/DReAMM environment for spatially realistic microphysiological simulations (www.mcell.psc.edu). Using a variety of experimental constraints and validations, we simulate stimulus-driven calcium influx and binding within an entire active zone using Monte Carlo diffusion-reaction algorithms. We thus are able to predict important spatial and chemical kinetic relationships between voltage-gated calcium channels, synaptic vesicles, calcium binding sites, and neurotransmitter release. Model predictions then can be tested using experimental (pharmacological) perturbations that change the incoming calcium signal in different ways. This combination of experiment and spatially realistic Monte Carlo modeling yields insights that cannot be obtained in other ways, and that illustrate physiologically important design principles for high sensitivity, fidelity, and adaptability of neurotransmitter release. Supported by NIH R01 GM068630 and P41 RR06009.

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MS38

A Multilevel Optimization Approach to PDE-Constrained Optimization

We examine an approach to the design of complex systems governed by coupled PDE. The term multilevel refers to the optimization problem formulation, the solution algorithm and the use of several layers of models in representing a particular discipline at various stages of design. We investigate analytical and computational properties of the approach and examine a numerical demonstration.

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MS38

Optimal Control of Elliptic Variational Inequalities

The class of control problems considered in this talk falls into the area of mathematical programs with complementarity constraints (MPCCs) in function space. These problems typically violate classical constraint qualifications (such as the Mangasarian-Fromovitz constraint qualification) and, hence, the existence of (Lagrange) multipliers does not follow from standard theory. In this talk, based on a relaxation scheme for the complementarity constraint we derive first order optimality characterizations, which, after passing to the limit, provide first order conditions for the MPCC. Then an algorithmic framework is presented which is based on a Moreau- Yosida-based path-following concept in order to deal with poor multiplier regularity. The talk ends by a report on numerical results.

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MS38

Solution of Optimal Control Problems Arising in the Modeling and Design of Semiconductors

Optimization problems governed by the drift–diffusion equations that arise in the modeling of semiconductor devices present many algorithmic and analytic challenges. The first part of the talk focuses on algorithmic issues in solving a real–world large–scale semiconductor design problem, in particular the use of a novel trust–region SQP algorithm that allows inexact (e.g. iterative) linear system solves. The second part addresses analytic issues related to the fact that the objective functionals of interest involve flux terms, which have fundamentally different discrete representations depending on which FE scheme is used for the discretization of the underlying PDEs.

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MS38

Approximate Reduced SQP Approaches for Aerodynamic Shape Optimization

Aerodynamic shape optimization is still a challenging subject. Recently, novel highly efficient algorithms based on approximate reduced SQP methods have been developed. Numerical results for practical problems provided by DLR Germany within the joint effort MEGADESIGN are presented as well as theoretical insights.

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MS39

3D Multi-Material Interface Reconstruction with General Polyhedral Meshes

We present a 3D volume tracking multi-material interface reconstruction algorithm for general polyhedral meshes. Multiple piecewise linear interfaces are reconstructed within polyhedral cells containing more than two materials. Second order accurate interface reconstruction algorithms, such as LVIRA and MoF, are applied for general polyhedral mesh environment. Multi-material ordering algorithms are presented for proper sequence of interface reconstruction. For maximum flexibility of handling complex geometries as well as arbitrary mesh motion, general polyhedral meshes are utilized.

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MS39

Mimetic Discretization Methods

Compatible discretizations are model reduction techniques to replace PDE's by algebraic equations that mimic their fundamental structural properties. We provide a common framework for such discretizations using algebraic topology to guide our analysis. This results in discrete notions of differentiation and integration that are mutually consistent in the sense that they obey a discrete Stokes theorem. Furthermore, the invariants of DeRham homology groups are preserved in a discrete sense, which allows, among other things, for an elementary calculation of the kernel of the discrete Laplacian. The key components of the framework are a restriction operator defined by the DeRham map and a consistent reconstruction operator. We show that many of the existing compatible discretizations by finite elements, finite volumes and finite differences are obtained from the framework by specific choices of the reconstruction operator. This opens up an attractive possibility to develop a common convergence and stability analysis for a broad range of discrete models.

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MS39

Stabilized Lagrangian Hydrodynamics

A new SUPG-stabilized formulation for Lagrangian Hydrodynamics of materials satisfying the Mie-Grüneisen class of constitutive laws is presented [(Guglielmo Scovazzi, Mark A. Christon, Thomas J. R. Hughes, and John N. Shadid, "Stabilized shock hydrodynamics: I. A Lagrangian method", (accepted, Computer Methods in Applied Mechanics and Engineering, 2006),Guglielmo Scovazzi, "Stabilized shock hydrodynamics: II. Design and physical interpretation of the SUPG operator for Lagrangian computations", (accepted, Computer Methods in Applied Mechanics and Engineering, 2006).]. The proposed method can be used in conjunction with simplex-type (triangular/tetrahedral) meshes, as well as the more commonly used brick-type (quadrilateral/hexahedral) meshes. Simplex-type meshes offer significant advantages in the automatic mesh generation process, and they are usually preferred in multi-physics problems involving radiation effects. The proposed method results in a globally conservative formulation, in which equal-order interpolation (P1 or Q1 isoparametric finite elements) is applied to velocities, displacements, and thermodynamic variables, namely pressure. As a direct consequence, a natural representation of the pressure gradient on element interiors bypasses all problematic issues related to pressure gradient reconstruction, typical of standard, cell-centered, multidimensional hydrocode implementations. SUPG stabilization in the Lagrangian context involves specific design requirements such as Galilean invariance [Guglielmo Scovazzi, "A discourse on Galilean invariance, SUPG stabilization, and the variational multiscale framework", (accepted, Computer Methods in Applied Mechanics and Engineering, 2006).], an overlooked aspect in the literature on the subject. A discontinuity capturing operator in the form of a Noh-type viscosity with artificial heat flux is used to preserve stability and smoothness of the solution in the shock regions. Numerical results for the Euler equations of gas dynamics will be presented.

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MS39

Closure Models for Mixed Cells in Multi-Material Flow Simulations

High-speed multi-material flows with strong shear deformations occur in many problems. Due to the nature of shock wave propagation in complex materials, the Arbitrary Lagrangian-Eulerian (ALE) methods are currently the only proven technology to solve such problems. In ALE methods, the mesh does not move with the fluid, and so it is unavoidable that mixed cells containing two or more materials will appear, and special closure model is needed for such cells.

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MS40

Computational Studies of Nematic Liquid Crystalline Polymers in Planar Shear Flow

Abstract not available at time of publication.

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MS40

Numerical Results on Flow-Driven Responses for Anisotropic Nematic Liquid Crystals and Particle Suspensions

Abstract not available at time of publication.

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MS40

Comprehensive Study of 2D Nematic Polymers Under a Shear

We study the behavior of 2D nematic polymers under s shear of arbitrary magnitude. When the shear is weak, the previous asymptotic analysis showed that there exists a threshold (U0) for the normalized polymer concentration (U) such that for U¡U0 the polymer orientation distribution converges to a steady state; for U¿U0 the polymer orientation distribution tumbles and does not converge to a steady state. Numerical results show that as the magnitude of the shear increases the magnitude of the threshold also increases. We will discuss the change of U0 and the change in behaviors of the polymer orientation distribution as the magnitude of the shear increases.

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MS40

Anchoring-Induced Texture and Shear Banding of Nematic Polymers in Shear Cells

We numericall explore texture and shear banding of nematic polymers in shear cells, allowing for one-dimensional morphology in the gap between parallel plates. We solve the coupled Navier-Stokes and Doi-Marrucci-Greco orientation tensor model, considering both confined orientation in the plane of shear and full orientation tensor degrees of freedom. This formulation makes contact with a large literature on analytical and numerical as well as experimental studies of nematic polymer texture and flow feedback.

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MS41

A One-Dimensional Conservative Method to Track Discontinuities in a Compressible Medium

We present a multi-fluid method where a moving interface cuts out time-varying control volumes. A consistent finite-volume discretization is derived by applying the divergence theorem in space and time, and the resulting method is fully conservative even at the discontinuities. The truncation errors are expected to be first-order at the interface, which is one order higher than conventional methods. Both shock waves and contact discontinuities are presented as possible interfaces in the results. UCRL-ABS-223489.

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MS41

A Second-Order Accurate Level Set Method on Non-Graded Adaptive Cartesian Grids

We will present a level set method on non-graded adaptive Cartesian grids, i.e. grids for which the ratio between adjacent cells is not constrained. We use quadtree and octree data structures to represent the grid and a simple algorithm to generate meshes with the finest resolution at the interface. In particular, we will present (1) a locally third order accurate reinitialization scheme that transforms an arbitrary level set function into a signed distance function, (2) a second order accurate semi-Lagrangian methods to evolve the linear level set advection equation under an externally generated velocity field, (3) a second order accurate upwind method to evolve the nonlinear level set equation under a normal velocity as well as to extrapolate scalar quantities across an interface in the normal direction, and

(4) a semi-implicit scheme to evolve the interface under mean curvature. Combined, we obtain a level set method on adaptive Cartesian grids with a negligible mass loss. We will exemplify the performance of the method in two and three spatial dimensions.

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MS41

A Volume-of-Fluid Method for Compressible Multiphase (Resolved) Flow

A finite volume method will be presented for the modeling of compressible flows consisting of multiple spatially-resolved material phases. The approach uses well-known high-order Godunov methods to advance individual material regions. Interfaces are reconstructed from volume-of-fluid fields advected with velocities obtained from interfacial 2-material Riemann problems. Cut cell conservation and stability is maintained with the mass-redistribution formalism. This approach is stable and globally O(h) for characteristic variables. Example solid-solid-vacuum calculations in 3d will be presented. The convergence properties will motivate higher-order methods being developed by C. Bono and P. Colella.

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MS41

A N-Dimensional Conservative Front-Tracking Method

We present a N-dimensional conservative interface tracking algorithm with a convex hull control volume reconstruction method based on a grid-based space-time interface. The algorithm is derived from an integral formulation of PDEs. Near tracked discontinuities in the solution, the proposed algorithm improves by one order in its errors commonly found near a discontinuity.

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MS42

Verification Analysis of NNSA Tri-Lab Test Suite Problems

Three DOE laboratories identified test problems used to evaluate hydrocode performance. We describe error models used in these assessments and propose how they could be expanded. Automated analysis of two- and three-dimensional problems provide results on how well hydrocodes retain fidelity to the underlying physics when motions and gradients are not grid-aligned. We include an assessment of whether solutions using an adaptive mesh refinement algorithm are as accurate as solutions on corresponding uniform grids.

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MS42

Code Verification for Astrophysical Simulation Codes

Verification of astrophysical simulation codes poses unique challenges. Codes may have to solve equations that describe the dynamics of matter, radiation, magnetic fields, and the gravitational field. It is important that each of these components be verified using standard techniques appropriate for specific sets of equations, e.g. the Euler equations. Verification of the coupled sets of equations is equally important. We will discuss verification of astrophysical simulation codes and areas where more work is needed.

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MS42

Qualitative and Quantitative Accuracy of the Lattice Boltzmann Method

Many methods have been developed to study hydrodynamics. While very accurate, some approaches require laborious set-up and suffer from computational complexities, such as, frequent re-meshing. The lattice Boltzmann method, a discretized form of the Boltzmann Transport Equation, has shown promise for solving complex fluid problems. A brief overview of the method is presented and results are compared with theory and other established computational methods. Examples include porous media and particulate flows, natural convection, and microfluidics.

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MS42

Verification of Multiphysics Codes

We will present results of a formal a verification effort of a multi-physics code through use of observed spatial and temporal order-of-accuracy. Formal verification requires

development of appropriate test cases targeting important codes modules, construction and review of input decks for the code, and grid refinement studies. We will discuss decision points in the formal verification and outline advantages and disadvantages of each choice. This work was performed under the auspices of the U. S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

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MS43

New Approaches to Optical Flow and Digital Inpainting

In this talk, new formulation for the optical flow problem and digital inpainting problem are presented. For determining optical flows, an optimal control approach is presented where the velocity field are interpreted as bilinear control functions of the optimal control problem of tracking a sequence of given frames. This approach was originally proposed in A. Borz, K. Ito, and K. Kunisch, SIAM J. Sci. Comput., 24(3) (2002), 818-847. For digital inpainting, a new approach based on the solution of a Ginzburg–Landau equation is discussed. This approach was first proposed in H. Grossauer and O. Scherzer, Scale Space Methods in Computer Vision, Lecture Notes in Computer Science 2695, Springer, 2003.

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MS43

Super Fast OcTree Representations

Abstract not available at time of publication.

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MS43

Registration and Intensity Correction

In many medical applications, registration and intensity correction problems do intertwine. We propose a new methodological framework for a joint registration and intensity correction (RIC). This framework is based on minimization of a joint energy J with various degrees of freedom. The essential advantages of the RIC approach are: combination of registration and intensity correction into one unified framework and thus joint minimization. The performance of the RIC approach is demonstrated on a variety of applications ranging from MRI to histology.

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MS43

Volume Preserving Image Registration

There exist many instances particularly in medical imaging which demand for registration. Many applications require that the transformation that deforms the template image has to be one-to-one. We force bijectivity by controlling the change of volume of the transformation and present variational techniques to prove the existence of a minimizing element of this constrained optimization problem. Furthermore we propose conditions on registration functionals that guarantee the existence of minimizing elements.

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MS44

Computing Viscoelastic Fluid Flows at High Weissenberg Number

The numerical simulation of viscoelastic fluid flow becomes more difficult as a physical parameter, the Weissenberg number, increases. Specifically, for a given discretization scheme and set of problem parameters, standard nonlinear solution approaches fail to converge beyond a critical value of the Weissenberg number. In this talk we discuss the steady-state Johnson-Segalman model for viscoelastic fluid flow and the high Weissenberg number problem. We examine the behavior of computed solutions near the critical Weissenberg value, and investigate approaches to computing solutions at and above the critical Weissenberg number.

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MS44

Numerical Approximation of a Non-Linear Generalized Newtonian Fluid with Defective Boundary Conditions

We study the numerical approximation of a non-linear generalized Newtonian fluid where only the flow rates are specified for the inflow and outflow boundaries. A variational formulation of the problem is developed based on the Lagrange multipliers rule in order to enforce the stated flow

rates. Existence and uniqueness of the solution to the continuous, and discrete, variational formulation will be shown. An error estimate for the numerical approximation and some numerical results will be discussed.

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MS44

Advances in MHD Flow Simulation

Magnetohydrodynamics (MHD) is the theory of the macroscopic interaction of electrically conducting fluids with a magnetic field. It is of importance in connection with many engineering problems such as plasma confinement, liquid-metal cooling of nuclear reactors, the CZ crystal growth process, and electromagnetic casting. In the viscous incompressible case, MHD flow is governed by the Navier-Stokes equations and the pre-Maxwell equations giving rise to challenging problems of mathematical analysis and numerical approximation. We will discuss recent advances in MHD flow simulation.

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MS44

Index Reduction Approaches for Feedback Control of the Navier-Stokes Equations

Linear feedback control is considered for large systems of differential algebraic equations arising from discretization of saddle point problems. Necessary conditions are derived by applying the Maximum Principle and have the form of constrained Riccati equations. We consider two approaches for solving the feedback control problem as well as practical numerical methods. Numerical studies using examples derived from a constrained heat equation and the Stokes equation demonstrate the effectiveness of the approaches we consider.

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MS45

Moderator

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MS46

Patterns on Growing Square Domains Via Mode Interaction

We consider reaction-diffusion systems on growing square domains with Neumann boundary conditions (NBC). As suggested by numerical simulations, we study the simpler problem of mode interactions in steady-state bifurcation problems with both translational symmetry and square symmetry, combined with the symmetry constraint imposed by NBC. We show that the transition between different types of squares can be generically continuous. Also, we show that transitions between squares and stripes can occur generically via a jump, via steady-states or via steady-states and time-periodic states. We point out some differences between stable patterns in the NBC problem and in the periodic boundary conditions problem. This is joint work with Martin Golubitsky.

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MS46

Modelling the Origin of Pattern in Naevoid Skin Disease: A Survey of Recent Results

A diffusing system of interacting chemical species restricted to the ectodermal surface of the primitive embryo is shown, via a two-species reaction-diffusion mdoel, to be capable of generating spatial inhomogeneity of chemical concentration. Depending on local concentrations, these chemical "pre-patterns" can then act as centres of organisation via genetic switching, chemotaxis or differential rates of growth. It is suggested the process may account for the origin of the patchiness of naevoid skin disease. Many types of morphologies - from simple unilateral asymmetries to lines-of-Blaschko-like - can be generated by this simple and universal scheme. Here some recent results are reported and the implications for the pathogenesis of mosaic skin disease is discussed.

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MS46

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS46

Numerical Solutions of Reaction-Diffusion Systems on Continuously Growing Domains

We examine the implications of mesh structure on numerically computed solutions of a reaction-diffusion model system on two-dimensional growing domains. The incorporation of domain growth creates an additional parameter – the grid-point velocity – which greatly influences the selection of certain symmetric solutions for the ADI finite difference scheme. Domain growth coupled with grid-point

velocity stabilises certain patterns which are unstable to any kind of mesh perturbation.

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MS47

Simulation of Magneto-Hydrodynamic Physics Associated with Evolving Interfaces Via ALEGRA/MESQUITE

Simulation of physics associated with severe deformations and evolving interfaces may be treated with Arbitrary Lagrangian Eulerian (ALE) techniques. The use of a Lagrangian interface and evolving ALE regions introduces a number of challenges for ALE mesh smoothing. We explore the application of the MESQUITE library to address some of these issues. Specifically, we discuss several important ALEGRA-HEDP simulations where MESQUITE was employed to improve the usability of ALEGRA relative to more traditional approaches. *Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

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MS47

Using Mesquite in Distributed Memory Applications

We discuss the development of an infrastructure that supports the use of Mesquite mesh quality improvement algorithms in distributed memory applications. We start with the application's decomposition of the mesh data and use an iterative process to select independent sets of vertices to resposition in each pass. We experiment with a mix of local and global techniques from Mesquite and report on the scalability and performance or our methods.

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MS47

R-Adaptivity Using Finite Element Theoretical Error Bounds

Mesh quality is critical for accuracy in the numerical solution of partial differential equations. In this talk, we will review briefly theoretical bounds for the finite element analysis. We will emphasize the role of mesh quality in these theoretical bounds. Then we will discuss how these theoretical results can influence the design of mesh optimization algorithms by vertex repositioning. Numerical examples will illustrate the performance of this approach.

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MS47

Improvement of Remapped Meshes Using Mesquite in ALE Applications

Adaptive Lagrangian Eulerian (ALE) techniques are commonly used in numerical simulations of multidimensional fluid flow. ALE methods typically use relatively simple geometric approaches to combat deteriorating mesh quality as the number of remaps increase. In these schemes, there are often no barriers to mesh element inversions and solution behaviors are neglected which may lead to inaccuracies. To help address these issues, we apply the optimization-based approaches in the Mesquite mesh quality improvement software library to a particular ALE hydrodynamics code. We show that this approach preserves large-scale features of the remapping, honors fixed internal and boundary nodes, and prevents element inversion.

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MS48

Hierarchical Model Reduction of Structured Matrices

The talk concentrates on the treatment of (large) structured matrices in general, and in particular on matrices that have multiple hierarchical structure of the semi separable type. Such matrices occur e.g. in bulk or surface finite-element like systems, encountered in solving partial differential equations in the direct form or as integrals with a Green's function. In the 1D case the resulting structure is invariably close to semi-separable matrix, and there exists a well developed theory of model reduction for this case (which will be reviewed). In higher dimensions, the situation is much more complicated, but not hopeless. The problem gets its richest expression when one considers efficient methods for matrix inversion, in which the hierarchical structure of the original matrix is exploited to obtain efficiency. We give a survey of techniques that can be used to handle this case, develop some theory on the model reduction properties that can be obtained and illustrate the methods by example.

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MS48

PPV-HB: Harmonic Balance for Oscillator/PLL Phase Macromodels

Oscillators feature unboundedly increasing phase characteristics when perturbed by external signals, making standard harmonic balance (HB) inapplicable to their phase macromodels. In this talk, we rectify this situation by presenting a novel extension of HB that is capable of handling oscillator phase macromodels. Key to the new method, termed PPV-HB, is a formulation that separates unboundedly increasing terms of phase characteristics from

bounded, periodic components. PPV-HB can be used not only on individual oscillators, but crucially, it enables the application of HB-like techniques for simulating system-level equation systems composed of higher-level macromodels of blocks. We validate PPV-HB on individual oscillators and a PLL system, demonstrating perfect matches with transient simulation using phase macromodels. Speedups of 1-2 orders of magnitude are obtained, in addition to speedups of another 2-3 orders of magnitude that stem from using macromodels as opposed to full circuit simulation.

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MS48

Model-Compiler Driven Model Order Reduction and VLSI Circuit Simulation

Abstract not available at time of publication.

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MS48

Direct Methods for Model Order Reduction of RC Circuits

In this presentation we will introduce direct techniques, as opposed to iterative (projection based) techniques, for simplification of very large RC circuits arising during the electrical modeling of integrated circuits. The principal advantage of such techniques is to stay closer to the electrical domain, rather than loosing essential properties related to the physics of the problem as a result of the mathematical process. As a result, the so-called realization problem is avoided or alleviated.

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MS49

Iterative Methods for Nonconvex PDE Constrained Optimization

Interior methods are proposed for the numerical solution of general nonlinear PDE-constrained optimization problems. The talk will focus on methods based on sequential unconstrained optimization and the use of multilevel preconditioned iterative methods for the constituent linear systems. Based on joint work with Randolph Bank, Anders Forsgren and Joshua Griffin.

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MS49

Parallel Solution of Large-Scale Nonlinear Parameter Estimation Problems with IPOPT

We present the next generation version of IPOPT with capabilities for efficient parallel solution of large, structured nonlinear programming problems. This nonlinear interior point framework allows straightforward customization of the linear algebra data structures and calculation routines. A parallel Schur-complement decomposition has been implemented and scaleup results are demonstrated on a real dynamic parameter estimation problem.

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MS49

Inexact Primal-Dual Methods for Constrained Optimization

Very large constrained optimization problems, such as those arising in PDE-constrained optimization, can be solved using inexact methods in which the search direction is computed using iterative linear algebra techniques. To make such an approach robust for nonlinear problems, it is necessary to know when an approximate solution of the primal-dual system makes sufficient progress toward optimality. In this talk we consider conditions that ensure global convergence using models of an exact penalty function.

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MS49

Primal Dual Interior Point Methods for PDE Constrained Optimization

Primal-dual interior-point methods have proven to be very efficient in the context of large scale nonlinear programming. In this talk, we present a convergence analysis of a primal-dual interior-point method for PDE-constrained optimization in an appropriate function space setting. Considered are optimal control problems with control constraints in L^p. It is shown that the developed primal-dual interior-point method converges globally and locally superlinearly. Not only the L^∞-setting is analyzed, but also a more involved L^q-analysis, $q < \infty$, is presented. In L^∞, the set of feasible controls contains interior points and the Fréchet differentiability of the perturbed optimality system can be shown. In the L^q-setting, which is highly relevant for PDE-constrained optimization, these nice properties are no longer available. Nevertheless, using refined techniques, a convergence analysis can be carried out. In particular, two-norm techniques and a smoothing step are required. Numerical results are presented.

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MS50

A Novel In Silico Approach For De Novo Protein Design

The primary objective in de novo protein design is to determine the amino acid sequences which are compatible with specific template backbone structures that may be rigid or flexible. It is of fundamental importance since it addresses the mapping of the space of amino acid sequences to known protein folds or postulated/putative protein folds. It is also of significant practical importance since it can lead to the improved design of inhibitors, design of novel sequences with better stability, design of catalytic sites of enzymes, and drug discovery. The de novo protein design problem involves three key decisions: (a) the definition of the template backbone structure; (b) the sequence selection; and (c) the validation of the fold specificity and fold stability. The template backbone structure can be (i) a single rigid backbone (e.g., the average NMR structure for a protein); (ii) a set of rigid backbone structures (e.g., all NMR structures for a protein or a discrete number of randomly selected rigid structures based on some algorithmic procedure or a discrete set of rigid structures based on a parameterization of the backbone); or (iii) a flexible backbone structure defined by lower and upper bounds on the distances between the alpha carbon atoms and the backbone dihedral angles. It is apparent that true backbone template flexibility is reflected in (iii) since it allows for all possible combinations of distances and backbone dihedral angles within their specified ranges, while (ii) considers only a small subset of flexible structures, and (i) is restricted to a single structure only. In this presentation, we will discuss a novel two stage approach which takes into account explicitly the flexibility of the templates. The first stage addresses the in silico sequence selection problem via a novel mathematical modeling and optimization approach which corresponds to the class of quadratic assignment-like models. It will be shown that these models can be solved to global optimality rigorously. The second stage addresses the fold specificity by performing structure prediction calculations using atomistic level force fields and the first principles approach, Astro-Fold. The probabilities of each sequence to fold specifically to the flexible templates are calculated. The theoretical prediction results for several systems that include variants of Compstatin, human beta defensins, C3a, and gp41 of HIV-1 virus will be presented.

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MS50

Optimization with Categorical or Integer Variables

Many optimal design applications are modeled using categorical variables, that are not integers, and express for example material choices. Such models do not allow standard optimization techniques to be used, leading scientists to use heuristic search procedures. We show, that categorical variables can be modeled using standard 0-1 variables. We illustrate our approach on a thermal insulation system, which has a number of insulators of different materials (the categorical variables) to minimize the heat flow.

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MS50

Optimizing Sensor Placement for Municipal Water Network Security

We wish to optimally place sensors in water networks to minimize expected damage due to intentional or accidental contamination. We track the movement of contamination through a network using a simulator. In its simplest form, placing sensors to detect a suite of events is a p-median problem. We describe integer programming models and heuristics for effectively solving full-scale problems. We discuss modifications to address uncertainties in impact values, contamination event distribution, objective, and sensor performance.

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MS50

Vulnerability Analysis on The Electric Power Grid

We present our work on detecting the vulnerabilities of the electric power system, i.e., a small group of lines that can cause a significant blackout, if they fail concurrently. We model the problem as a mixed integer nonlinear optimization problem, and our analysis on the structure of an optimal solution reveals a reduction to a pure combinatorial problem, which enables us to adopt graph theoretical techniques. In this talk, we will present our formulations, algorithms, and experimental results.

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MS51

Optimization for Wave Propagation Problems: From the Design of Acoustic Components to Microwave Tomography

We consider several different optimization problems that involve waves interacting with geometric details of dimensions comparable with the wavelength. One example concerns the design of devices that efficiently transmit and favorably distribute acoustic energy in the far field, such as acoustic horns designed using shape optimization techniques, or more general acoustic labyrinths designed utilizing topology optimization methods. A second example concerns microwave tomography, that is, the reconstruction of illuminated objects permittivity distribution.

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MS51

Hamilton-Jacobi Equations in Infinite Dimension for Approximation of Optimal Design and Reconstruction Problems

Many inverse problems, e.g. in optimal design and reconstruction, can be formulated as optimal control problems. Optimal control problems for low, d, dimensional differential equations, can be solved computationally by their corresponding Hamilton-Jacobi-Bellman partial differential equation in R^{d+1}. We will show how to use Hamilton-Jacobi equations in infinite dimension to regularize and solve optimal design problems for partial differential equations.

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MS51

Musical Wind Instrument Design: Transmission Line Analogy And Shape Optimization

Musical wind instrument design is an interesting example of a PDE constrained optimization problem. This work presents how gradient based shape optimization schemes are used to improve the function of brasswinds. Their shape is described by a large number of degrees of freedom, and different techniques are presented in order to comply with visual and manufactural geometrical preferences. A transmission line analogy is employed where applicable with respect to the solution of the PDE.

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MS51

Design of Composite Structures with Optimal Focusing Properties

In this talk, we study the problem of designing a flat lens, which focuses a monochromatic wave emanating from a point source on one side, to a well localized spot on the other side. The lens is realized as a periodic composite structure, which emerges as a solution to a well-defined optimization problem. This problem is motivated by the recent intense interest in so-called "superlenses", which attempt to accomplish the same task using left-handed materials.

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MS52

Not Available at Time of Publication

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MS52

The Structure and Dynamics of the Ribosome Studied by Cryo-EM and Computer Image Processing: Molecular Mechanism of Translocation

My research involved using cryo-electron microscopy and computer image processing to study the structure and dynamics of the ribosome during translation. I obtained a 3D reconstruction of the ribosome with the antibiotic fusidic acid. Fusidic acid stops translocation after GTP hydrolysis by preventing the dissociation of EF2. This reconstruction will be compared with other ribosomal complexes with different inhibitors that stop translocation at different steps to see how translation works.

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MS52

A Thermal Model of the Crust of Saturn's Satellite Enceladus

The icy terrain of the Saturnian moon, Enceladus, suggests a violent history of bombardment–a history which is actively overwritten by geological mechanisms. Thermal imaging of the southern polar region suggests heat flows beneath the ice may be responsible. Furthermore, an early 2006 flyby of NASA's Cassini spacecraft imaged water ice jetting from Enceladus' south pole. We investigate the

effects of these suggested heat flows by modeling the thickness of Enceladus surface ice layer.

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MS52

A Nodal Spectral Element Method Using Curl-conforming Vector Basis Functions on Tetrahedra

Nedelec basis functions are commonly used in the finite element method (FEM) solution of electromagnetic field problems. Higher-order finite and spectral elements are classified as either hierarchical (modal) or interpolatory (nodal). Here we use the Vandermonde matrix to express the interpolatory vector basis in terms of a hierarchical basis utilizing the scalar orthonormal polynomials on tetrahedra. In an effort to increase efficiency, integration and differentiation operations are developed using matrix-matrix multiplications.

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MS52

Plume Containment Using Particle Swarm Optimization

We will describe an optimal design problem from water resources management. The goal is to design a well-field that alters the groundwater flow to control the migration of a contaminant plume. The resulting problem is a simulation based optimization problem where gradient information is unavailable. We solve the problem using particle swarm optimization (PSO) and point the way towards future work.

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MS53

What Can the Theory of Radiation Boundary Conditions Contribute to a Theory of Multi-Physics Interfaces?

In the past decade there have been substantial practical advances in the imposition of radiation boundary conditions for the standard models of linear wave propagation. These include fast, low-memory methods for evaluating exact nonlocal conditions, improved implementations of local boundary condition sequences, and absorbing layers with reflectionless interfaces. In this talk we will examine the extension of these techniques to more complex interfaces separating regions where different physical models are solved.

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MS53

Interface Tracking Using Face Offsetting and Anisotropic Mesh Adaptation

Moving interfaces arise in many applications, such as multiphase flows and fluid-solid interactions. A surface triangulation is frequently used to represent the interface, posing significant challenges in interface tracking and mesh adaptation. We present a new method for moving interfaces, called *face offsetting*, and an anisotropic mesh adaptation technique to meet these challenges, based on a unified asymptotic and singularity analysis. We report applications of our methods in multi-physics simulations of solid-rocket combustion.

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MS53

Algorithms for Shock Wave Propagation in Coupled Fluid/Solid Environments

Finite volume methods using Riemann solvers are convenient for solving wave propagation problems in heterogeneous media. If material interfaces align with cell boundaries then each grid cell contains a distinct material and the Riemann solver resolves jumps into appropriate waves in each medium. I will discuss application of this approach to shock wave propagation near fluid/solid boundaries where compressible fluid equations are coupled to nonlinear elasticity, with particular application to the study of shock wave therapy in medical applications. I will also discuss Cartesian grid approaches to problems with geometrically complex interfaces that cut through grid cells so that some cells contain a mixture of materials.

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MS53

Back and Forth Error Compensation and Correction for Advections with Applications to Interface and Fluid Simulations

Level set method uses a level set function, usually an approximate signed distance function, Phi, to represent the interface as the zero set of Phi. When Phi is advanced to the next time level by a transportation equation, its new zero level set will represent the new interface position. We update the level set function Phi forward in time and then backward to get another copy of the level set function, say Phi_1. Phi_1 and Phi should have been equal if there were no numerical error. Therefore Phi-Phi_1 provides us the information of error and this information can be used to compensate Phi before updating Phi forward again in time. One nice property is that it has the convenience of possibly improving the temporal and spatial order of an odd order scheme simultaneously. We found that when applying this idea to semi-Lagrangian schemes, e.g., CIR scheme(which has no CFL restriction, a nice feature for local refinement), the property is still valid. This technique coupled with a simple yet less diffusive redistancing technique produces a very efficient algorithm even for unstructured triangle meshes. Numerical results for interface movements with level set equation computed by the new method will be presented in the talk. Also we would like show some interesting theoretical results for applying this idea to a general linear scheme. Further more, the application of this algorithm to semi-Lagrangian velocity advection in the Navier Stokes' fluid simulation has greatly reduced the advection

diffusion while essentially keeping the compactness and simplicity of a first order semi-Lagrangian scheme. Collaborators: Todd F. Dupont, ByungMoon Kim, Ignacio Llamas and Jarek Rossignac.

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MS54

Mobile Actuator Networks for Distributed Feedback Control of Diffusion Process Using Multiscale Central Voronoi Tessellations

In this paper, we address the problem of path planning for a group of networked mobile robots (sprayers) which can release neutralizing chemicals, known as mobile actuator networks, to neutralize the toxic 2D diffusion process modeled by an unknown parabolic distributed parameter system. We assume that static mesh sensors can inform the networked mobile sprayers the local concentration level. The desired trajectory of the robot is decided by Centroidal Voronoi Tessellations (CVT). Although the collision avoidance among the mobile sprayers is automatically build-in due to CVTs, the potential field method is embedded in the CVT for the mobile robots to avoid dynamic obstacles in its working space. In addition, since each mobile sprayer can only carry limited amount of neutralizing agent, we investigate the advantage of using multiscale CVT that can dynamically group more than one mobile sprayers within one Voronoi cell when the concentration is high. Simulation results are presented to illustrate the proposed solution to the hard smart spraying problem.

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MS54

Optimal and Anisotropic CVTs and Their Applications

In this talk, we discuss some recent works on the optimal and nisotropic centroidal Voronoi tessellations (CVTs). The optimal CVTs are related to the Gersho's conjecture. The anisotropic CVTs are associated with given Riemann metric tensors and they are defined in a novel way via directional distance functions. We present algorithms for the construction of such CVTs and discuss their various applications such as 3d and surface meshing and optimal clustering.

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MS54

Multidimensional Energy-Based Multilevel Quantization Scheme and its Applications

We present a multidimensional generalization of the recently introduced optimization based multilevel algorithm for the numerical computation of the centroidal Voronoi tessellations. Rigorous proof of the uniform convergence of the one-dimensional method has been obtained and it has been conjectured that the scheme would preserve its superior numerical properties when extended to higher dimensional domains. We build a generalized multidimensional algorithm by means of barycentric coordinate based interpolation and maximal independent set coarsening procedure. The uniform convergence is demonstrated for a variety of two-dimensional examples with arbitrary densities, guaranteeing a significant speedup when the number of variables increases. Taking image analysis and quantization applications as particular examples, we show that the method can handle large sets of data for both discrete and continuous densities and gives significant time reduction and attains better quality of limiting solutions comparing to the commonly used methods.

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MS54

An Adaptive Strategy for Convection Dominated Problems with Anisotropic Mesh Refinement

A new numerical approach to solve convection dominated problems is proposed. The goal is to design an adaptive algorithm which utilizes three main ingredients: a stabilization method, a reliable and efficient a posteriori error estimator, and an adapted metric tensor to align the anisotropic mesh with the computed solution. Due to the presence of layers in the solution, the stabilization scheme is necessary to reduce discretization errors and to improve convergence of the iterative solver. The a posteriori error estimator is used for estimating the local errors so that adaptive mesh refinement can be controlled. The mesh refinement turns out to satisfy the alignment and equidistribution conditions which can be guaranteed by the optimal metric tensor and the anisotropic centroidal Voronoi/ Delaunay mesh generator.

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MS54

Using Spherical Centroidal Voronoi Tessellations in Climate System Modeling

Spherical Centroidal Voronoi Tessellations (SCVTs) offer great potential to improve our climate system model simulations. Unfortunately, only a fraction of this potential has been exploited to date. In the initial search for point sets that span the surface of the sphere, emphasis was placed on uniformity in terms of cell area and distance between cell centers. This emphasis on uniformity arose from problems encountered on latitude-longitude grids in the region of the grid poles. The Voronoi point sets have been highly successful in this regard, and applications involving atmospheric modeling, ocean modeling, and sea-ice modeling will be presented. When we seek uniformity in our Vononoi point sets on the sphere, the centroidal Voronoi point sets are not substantially different than other Voronoi point sets, such as those generated on the sphere through recursive bisection of the inscribed icosahedron. The powerful aspect of centroidal Voronoi points sets is their ability to produce variable resolution grids that maintain a high degree of local uniformity. This is precisely the aspect that has yet to be exploited in climate system modeling. It is often the case in climate system modeling that the important length scale of interest varies substantially throughout the domain, often by an order of magnitude or more in terms of spacing between generators. Examples will be provided to demonstrate that SCVTs do an exceptional job in allowing us to place resolution where we need it, while at the same time producing a locally uniform grid. Potential applications of variable-resolution SCVTs to land-ice, sea-ice, and ocean modeling will be presented.

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MS55

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS55

Primal-Dual Techniques in Image Restoration

This talk focuses on TV-regularization in image restoration. Based on the Fenchel-duality claculus we introduce the predual of the TV-problem, which turns out to be a bound constrained minimization problem in a Hilbert space. Then an active-set-type algorithm is introduced and analysed for the numerical solution of the predual. The talk ends by a report on numerical tests.

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MS55

Segmentation Under Occlusions Using Prior Shape Information

Here, we address the problem of segmenting multiple objects, with possible occlusions, in a variational setting. To handle occlusions, we use prior shape information of objects to fill in missing boundary information in overlapping regions. A novelty in our approach is that prior shape is introduced in a selective manner, only to occluded boundaries. Further, a direct application of our framework is that it solves the segmentation with depth problem for certain classes of images.

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MS55

Volumetric MRI Brain Segmentation Using a Multilayer Surface Evolution Approach

This talk will present a novel multilayer level set approach for the segmentation of anatomical structures in 3D MRI data. In particular, a nested structure of evolving surfaces represented by a single implicit function will be used to segment and classify the white matter, gray matter and cerebro-spinal fluid. Experimental results with prior (probabilistic atlas based) and without prior will be presented, together with comparison and validation. This work is supported by the Center for Computational Biology, UCLA.

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MS56

A Krylov-Based Descent Algorithm for Optimal H2 Model Reduction

In this work, we introduce a Krylov-based descent algorithm for optimal H2 approximation of large-scale dynamicals systems where the interpolation points are the variables of the underlying optimization problem. After deriving the gradient and Hessian of the H2 cost function with respect to interpolation points, a numerically effective optimal H2 model reduction method is developed. Convergence properties and effectiveness of the algorithm are presented through numerical examples.

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MS56

Adaptive Concepts in Reduced Order Modelling

Proper orthogonal decomposition (POD) is proposed for deriving low order models of large scale dynamical systems. These low order models serve as surrogates for the dynamical system in the optimization processes. In the context of pde constrained optimal control this approach may suffer from the fact that the POD basis elements are computed from reference trajectories containing features which are different from those of the optimally controlled trajectory. Adaptive POD concepts are discussed which avoid these shortcomings.

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MS56

Reduced Order Models and Optimization Methods

Abstract not available at time of publication.

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MS56

Model-Constrained Methods for Reduction of Large-Scale Systems

For large-scale optimal design, optimal control, and inverse problem applications, a key challenge is deriving reduced models to capture variation over a parametric input space, which, for many optimization applications, is of high dimension. This talk presents recent methodology developments in which the task of determining a suitable reduced basis is formulated as a sequence of optimization problems. The methodology is demonstrated for a steady design problem, an unsteady turbomachinery probabilistic analysis problem, and a large-scale contaminant transport inverse problem.

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MS57

PCA and Consensus Ensemble Clustering to Stratify Breast Cancer into Clinically Useful Subtypes

We describe a technique to integrate principal component analysis and consensus ensemble clustering to identify the optimum cancer subtypes from gene microarray data. Applied to a breast cancer dataset, we find that it stratifies into eight subtypes with distinct molecular signatures, clinical course and prognosis. A novel discovery is the identification of two subtypes of primary Her2+ tumors with different natural survival rates. The low recurrence (low metastasis) tumors are marked by a strong up-regulation of immunoglobulin genes. These predictions were validated on unseen data.

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MS57

Correlations in Complex Disease Association Studies

Association studies for complex disease phenotypes, such as cell apoptosis rates and age of onset of cancer, entail multiple hypotheses testing with many combinations of single nucleotide polymorphisms. However, these tests are usually far from independent because linkage disequilibrium across the genome induces strong correlations between loci. The problem is compounded by correlations between combinations of distant loci. A mathematical formalism is developed that correctly accounts for correlations amongst null association tests by explicitly evaluating the multi-information among polymorphisms. This permits an effective evaluation of synergistic or antagonistic genetic interactions with respect to the phenotype.

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MS57

Correlating Mitochondrial SNPs and Complex Disease Phenotypes.

Using complete mtDNA sequences from 672 unrelated Japanese individuals stratified into seven phenotypes: Diabetics with Angiopathy, Normal Diabetics, Healthy Non-Obese, Obese Normal, Alzheimer patients, Parkinson patients and Centenarians we describe methods to find correlations between phenotype, mtDNA mutations and haplogroups. Using t-tests, clustering methods and exhaustive pattern searches, we identify sets of mutations correlated with the phenotypes. We find that individuals in certain haplogroups are protected against diabetes and others are selected for longevity. We discuss and apply methods to identify the causative mechanisms and the time of occurrence of the mutational events responsible for these effects.

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MS57

Finding Optimum Viral Vaccine Targets for HIV and Avian Flu

HLA polymorphism and high mutation rates make it difficult to create effective viral vaccines. We describe a genomic scanning method across candidate peptides that creates a large number of epitopes per HLA and optimizes the vaccine to prevent viral escape by mutations. We compute peptide cleavage probability and transfer through TAP and MHC binding for many HLA alleles to prune out poorly

conserved and similar-to-self peptides. We then create an optimal vaccine ordered for cleavage using a genetic algorithm. Application of our method to HCV, HIV-I, Influenza H3N2 and the Avian Flu Virus will be presented.

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MS58

Optimizing Tetrahedral Element Quality Using Output from Black-Box Mesh Generators and Mesh Smoothing Techniques

An algorithm for rapid, large-scale mesh generation will be presented in the context of studying near-surface phenomena. This procedure takes advantage of open-source (black-box) mesh generation software, and a post-process, mesh-smoothing technique to ensure quality elements in the final tetrahedral mesh. The result is an optimization problem with possibly 100k or more degrees of freedom. The entire procedure will be presented with a specific focus on the smoothing algorithm and the treatment of buried objects.

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MS58

Parameter Estimation for Large-scale Groundwater Problems

The Engineer Research and Development Center models groundwater flow and transport for monitoring and remediation purposes. Data provided for these sites such as borehole data, head values, and concentration values are spatially sparse. Physics based models for some of these sites are very large and require parallel computer resources. Optimization techniques for these parallel numerical models will be presented that utilize the sparse data to provide the best estimates of the model input parameters.

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MS58

Calibration of Ground Water Models with POD

We present some preliminary results which apply the method of proper orthogonal decomposition (POD) to an elliptic parameter identification problem which arises in the calibration of ground water models. We generate the POD basis from the sensitivities taken from a small number of fine-scale nonlinear iterations. We solve the nonlinear least squares problems at both the fine and reduced scales with a variant of pseudo-transient continuation.

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MS58

Heuristic Optimization and Algorithm Tuning Applied to Sorptive Barrier Design

While heuristic optimization is applied in environmental applications, ad-hoc algorithm configuration is typical. We use a multi-layer sorptive barrier design problem as a benchmark for an algorithm-tuning procedure, as applied to three heuristics (genetic algorithms, simulated annealing, and particle swarm optimization). Design problems were formulated as combinatorial optimizations where the sorptive layers of a landfill liner were selected to minimize contaminant transport. Results indicate that formal pretuning can improve algorithm performance and provide insight into the physical processes that control environmental systems.

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MS59

Numerical Methods for Boundary Value Problems in Stochastic Domains

Efficient methods for the numerical realization of elliptic PDEs in domains depending on random variables are presented. Mappings or Fictitious Domain techniques are used to handle the domain randomness. Generalized Wiener expansions are invoked to convert such stochastic problems into deterministic ones, depending on an extra set of real variables (the stochastic variables). Discretization is accomplished by finite elements in the physical variables and G-NI (Galerkin projection with numerical integration) in the stochastic variables.

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MS59

Finite Element Methods for Stochastic Parabolic PDEs in High Dimensions

Abstract not available at time of publication.

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MS59

Stochastic Galerkin and Stochastic Collocation for SPDEs

We will discuss Stochastic Galerkin and Stochastic Collocation methods combined with sparse approximation techniques as alternatives to the classical Monte Carlo approach for the approximation of SPDEs. The mathematical analysis of these methods and the characterization of their convergence is extremely relevant to decide in which cases they should be used. We will present novel results, discussing the efficient implementation and the mathematical analysis of the different sources of approximation error in the numerical solutions.

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MS59

An Adaptive Multi-Element Generalized Polynomial Chaos Method for Elliptic Problems with Random Coefficients

We develop an adaptive multi-element generalized polynomial chaos (ME-gPC) method for elliptic equations with random coefficients of a moderate number (≤ 10) of random dimensions, where we employ low-order polynomial chaos ($p \leq 3$) and refine the solution adaptively in the random space. We generate local and global a-posterior error estimators. To reduce to the cost of solving the error equations, we construct a reduced space, where a much smaller number of terms in the enhanced polynomial chaos space are used to capture the errors.

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MS60

The Synergy of Computer Science and Scientific Computing

Scientific computing and computer science have a long symbiotic history which is perhaps not easily perceived since most problems of computer science are discrete as opposed to the continuous aspect of numerical analysis. However, the use of topics such as combinatorics, compiler design, datamining, etc, are being increasingly prevalent in scientific computing. This presentation will review how some of these areas are being applied to improve and extend numerical techniques and software.

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MS60

A Self-Adapting System for Linear Solver Selection

A self-adapting system integrates several components: feature extraction, a database for storage of features and runtime results, a modeller that builds recommendation strategies from the information in the database, and a runtime recommender. We will describe the general ideas of the SALSA system, and its implementation, in particular the statistical and machine learning techniques used for the recommender component.

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MS60

Enabling Adaptive Algorithms in Component Applications

Component-based software engineering has been gaining popularity in scientific computing, facilitating the creation and management of large multi-disciplinary, multi-developer application codes, and providing opportunities for improved performance and numerical accuracy by enabling selection among multiple solution approaches. We present a component infrastructure for the support of dynamic algorithm selection and adaptation in applications involving the solution of nonlinear PDEs. We also describe a general architecture for providing quality of service for numerical software in component-based environments.

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MS60

Domain-Specific Program Analysis with OpenAnalysis

Program analysis is necessary in many application domains

including software engineering, high performance computing, scientific computing, data mining, and operating systems. However, reusing analysis implementations is difficult because they are typically coupled to a particular intermediate representation (IR). The OpenAnalysis toolkit separates analysis from the intermediate representation of the program. In this talk I will present some of the research questions involved in automating the generation of domain-specific, data-flow analysis implementations.

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MS61

An Extensible Framework for the Mathematical Manipulation of Music

The goal of this project was the creation of an extensible sound manipulation architecture using Mathematica. The two essential phases were the implementation of a structure to play sounds, and a system for the exploration of granular synthesis. The first phase includes functions for the basic implementation of a song. The more important granular synthesis phase consists of functions for the engineering and of sound clouds, collections of thousands of very short enveloped waveforms (sound grains).

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MS61

Talk Title Not Available at Time of Publication

To Be Announced
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MS61

Using COMSOL to Develop a Hydrodynamic Model of the Chesapeake Bay

This talk displays results from using COMSOL to develop a hydrodynamic model of the Chesapeake Bay. The model itself was initially divided into two separate sets of problems. The first deals with running the non-linear Navier-Stokes equations in simple rectangular geometries. The other half of the project solves linear PDEs in the complete geometry of the Chesapeake. When the two halves of the project are completed, they are combined together, creating a full non-linear model.

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MS61

Hydrocode Simulations of Impacts in the Outer Solar System

Imaging of the icy surfaces of outer solar system bodies by the Voyager, Galileo and Cassini missions reveals an extensive history of bombardment, predominantly by comets. To analyze the physics of such events, a Smoothed Particle Hydrodynamics (SPH) model was used to simulate the impact of a comet on an icy surface. One focus of this study was the extent of pyrolysis of pre-existing organic material in the icy target resulting from the impact shock.

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MS61

Spectral Collocation for Resolving Spike Dynamics

In this work the Gierer-Meinhardt model is analyzed using Chebyshev collocation methods. This reaction-diffusion system is governed by activator and inhibitor concentrations. Initially, the system is considered in one dimension and then in two dimensions; numerical results are presented for both cases. The algorithmic complexity and accuracy are compared to a moving finite element method. Finally, observations are made concerning when to use the proposed spectral method as opposed to the established moving mesh method.

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MS62

Simulating Potential Hydrogen Explosions in Nuclear Reactor Containment Buildings

We describe the use of a high resolution finite method based wave propagation algorithms for simulating potential hydrogen explosions in nuclear reactor containment buildings. In this work, the reactive Euler equations are solved on an adaptively refined, mapped grid representing the containment building. The flame front is modeled using either level set like approach for deflagration, or an Arrhenius law for detonations. Peak over-pressures and impulses on the containment structure are sought, along with peak temperatures inside the structure. A general equation of state modeling the dependence of specific heats on temperature may be used.

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MS62

A Wave Propagation Analysis of the October 2, 2004 Tremor at Mount St. Helens, Washington

On October 2, 2004, three component, broad-frequency band seismometers detected a prominent low-frequency resonance within Mount St. Helens associated with the onset of eruptive volcanic activity. The energy is dominantly in the 0.5 to 10 Hz range. I test the idea that this signal is generated by sudden extension of a long, viscoelastic magma body as it forces its way through a brittle crust using the finite volume method of Leveque (2002).

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MS62

Finite Volume Methods and Adaptive Refinement for Global Tsunami Propagation and Local Inun-

dation

Modeling global tsunami propagation as well as inundation requires resolving diverse flow regimes and spatial scales with a single numerical method. The shallow water equations, a commonly accepted governing system, are a set of hyperbolic conservation laws—demanding specialized numerical methods. I will describe the extension of a class of finite volume methods developed for such systems, as well as unique modifications and attributes necessary for using these methods for tsunami modeling.

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MS62

Numerical Models for the Interaction of Volcanic Flows with Water

Modeling a pyroclastic surge interacting with a body of water requires a coupling of compressible gas dynamics for a hot dusty gas with fluid equations for the liquid, ideally including heat transfer and phase change as well as penetration of the water by the solid phase. An approach to this problem well be presented based on high resolution wave propagation algorithms for a dusty gas developed by Pelanti and LeVeque and previously used to model volcanic jets and plumes.

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MS63

Aspects of Unstructured Finite Volume Method and Optimal Design in the European Project "New Aircraft Concepts Research" (NACRE)

Gradient-based aerodynamic shape optimization based on Computational Fluid Dynamic is used in the context of the European Project "New Aircraft Concepts Research" (NACRE) in the prospect to speed up the design of new aircrafts. The core of the computer program used here is the Unstructured Finite Volume solver Edge, which solves the flow and adjoint flow equations. Aspects of the gradient computation, for example involving the mesh deformation and the pre-processing, will also be presented.

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MS63

Modeling Fluid Structure Interactions in Underwater Cavities

Fluid Structure modeling is used to study the occurrence of Helmholtz resonance due to coupling of the structural deflections with the shear layer oscillations in underwater cavities. The method employs an edge based multi-element finite volume flow solver coupled loosely with a similarly structured finite volume structural solver. Mesh motion to accomodate surface deflection is handled by treating the mesh as an elastic structure. The details of the solver, coupling methods and some results are presented.

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MS63

An Accurate and Conservative Load Transfer Scheme for Fluid/Structure Interaction Simulations with Non-Matching Interface Discretizations

In aeroelastic simulations, the precision of fluid-induced load transfer across non-matching fluid/structure interfaces plays a key role in the accuracy of the coupled scheme. In this work, we compare the performance of a novel load transfer scheme based on a common refinement of the discretized interface to state-of-the-art point-to-element load transfer schemes. Through a set of fluid/structure problems involving flat and curved interfaces, we quantify the substantial improvement in accuracy achieved by the new scheme.

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MS63

Multiphase Flow Simulations of Solid-Propellant Rockets on Unstructured Grids

A multiphase flow simulation framework for solid-propellant rocket motors is presented. Unstructured grids are used to enable representation of geometrically complex domains. Detailed information is provided about the droplet-localization algorithm and its parallel implementation. A distinguishing feature of our droplet-localization algorithm is that it gathers automatically data about droplet impacts on boundaries. Results are provided for the AFRL BATES and RSRM motors.

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MS63

Aspects of Reconstruction Schemes on Unstructured Mesh Flow Solvers

Data reconstruction techniques used in unstructured mesh flow solvers are investigated in the context of gradient limited and flux limited TVD schemes. Of particular concern is reconstruction on meshes containing highly curved large aspect ratio cells (e.g., boundary layer regions). Gradient

based MUSCL reconstruction is compared to a collinear edge reconstruction that only requires a modest modification to existing edge data structures. While somewhat restricted, the collinear edge reconstruction provides improved robustness.

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MS64

A Stochastic Immersed Boundary Method Incorporating Thermal Fluctuations: Toward Modeling Flexible Micromechanics

The mechanics of many physical systems arising in the modeling of biological processes and technological devices involve elastic structures which interact with a fluid. The Immersed Boundary Method is one approach which has been applied with some success to macroscopic systems, including blood flow in the heart, wave propogation in the inner ear, and lift generation in insect flight. However, at sufficiently small length scales thermal fluctuations become significant and must be taken into account. We shall discuss an extension of the Immersed Boundary Method framework which incorporates thermal fluctuations through appropriate stochastic forcing terms in the fluid equations. This gives a system of stiff SPDE's for which standard numerical approaches perform poorly. We discuss a novel stochastic numerical method which exploits stochastic calculus to handle stiff features of the equations. We further show how this numerical method can be applied in practice to model the basic microscopic mechanics of polymers, polymer knots, membrane sheets, and vesicles. We also discuss preliminary work on modeling the micromechanics of cellular structures.

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MS64

Operator Splitting for Fluid Flow in Deformable Domains

Fluid flows with free surface and fluid-structure interaction problems are examples of fluid flows in deformable domains. We formulate the flow problem in a reference domain and we use a time discretization by operator splitting to reduce the solution of the original flow problem to that of simpler sub-problems. We combine the time-splitting scheme with an isoparametric Bercovier-Pironneau finite element approximation of the Navier-Stokes equations. The wave-like equation methodolog is used to handle the pure advection problems resulting from the time-splitting and from the domain transformation. The resulting methodology is modular, relatively easy to implement, and it introduces very little numerical dissipation.

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MS64

A Fictitious Domain Method Based Novel Numerical Scheme for the Viscoelastic Particulate Flow

We present a fictitious domain method based novel numerical scheme for the particulate flows in Oldroyd-B fluid by combining Stokes solvers, a wave-like equation treatment of the advection, and the rigid body motion projection via operator-splitting. The new scheme takes advantage of matrix decomposition and guarantees positive definiteness of the configuration tensor at all times. The 2D numerical simulations of sendimentations of a particle and several particles in the fluid will be presented.

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MS64

Domain Decomposition Method for Wave Propagation in Heterogeneous Media

In this talk we address the numerical solution of a wave equation with discontinuous coefficients by a finite element method using domain decomposition and semimatching grids. A wave equation with absorbing boundary conditions is considered, the coefficients in the equation essentially differ in the subdomains. The problem is approximated by an explicit in time finite difference scheme combined with a piecewise linear finite element method in the space variables on a semimatching grid. The matching condition on the interface is taken into account by means of Lagrange multipliers. The resulting system of linear equations of the saddle-point form is solved by a conjugate gradient method.

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MS64

Two Efficient Projection Methods

The MAC projection method has been a very successful method for solving the Navier-Stokes equations. Its spatial allocation enables achieving the divergence-free condition exactly, and more importantly ensures numerical stability. On the other hand, the different spatial allocation for each velocity component make numerical schemes complicated especially with implicit treatment of the visous terms. We introduce two novel projection methods that sample all the velocity component at one location and achieve numerical stability and second order accuracy.

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MS65
Moderator

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MS66
Application of Averaging-Based Error Estimation to Problems in Adaptive Atmospheric Modeling

Adaptive methods for atmospheric modeling are becoming more and more popular for simulating phenomena with localized features. In general, adaptive computational methods heavily rely on the quality of criteria to control the adaptation process. So far, most adaptive atmospheric simulation approaches utilize gradient based heuristical or physically induced refinement criteria. In this presentation we report on recent results in the construction of averaging-based rigorous error estimators for adaptive atmospheric simulation problems. A short introduction of the derivation of such error estimation is given and a comparison with common gradient-based methods is shown.

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MS66
An Adaptive Method with Error Control for High-Order Discontinuous Galerkin Methods Applied to Hamilton-Jacobi Equations

We propose and study an adaptive version of the discontinuous Galerkin method for Hamilton-Jacobi equations which, given a tolerance and the polynomial degree of the approximate solution, finds a mesh on which the approximate solution has a distance (in the uniform norm) to the viscosity solution no bigger than the prescribed tolerance. Our numerical experiments show that the method achieves its goal with optimal complexity independently of the tolerance and the polynomial degree.

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MS66
A 3D Self-Adaptive, Goal-Oriented hpFEM with a Multigrid Solver. Applications to Electromagnetics

We describe the development of a self-adaptive hp goal-oriented 3D Finite ElementMethod (FEM) applied to the simulation of borehole resistivity measurements for the assessment of rock formation properties. The self-adaptive algorithm delivers (without any user interaction) a sequence of optimal hp-grids that converges exponentially in terms of a user-prescribed quantity of interest with respect to the CPU time. The self-adaptive algorithm iterates along the following steps. Given a (coarse) conforming hp mesh, it is first globally refined in both h and p to yield a fine mesh, i.e. each element is broken into eight new elements, and the discretization order of approximation p is raised uniformly by one. Subsequently, the problem of interest is solved on the fine mesh. The next optimal coarse mesh is then determined as the one that maximizes the decrease of the projection based interpolation error averaged by the added number of unknowns. Since the mesh optimization process is based on the minimization of the interpolation error rather than the residual, the algorithm is problem independent, and it can be applied to different physics (acoustics, elasticity, etc.), nonlinear and eigenvalue problems as well. The fine mesh problem contains typically 20-30 times more unknowns than the corresponding coarse mesh problem. Thus, an efficient multigrid (two grids only) solver of linear equations for hp-finite elements has been developed. It utilizes a block-Jacobi smoother on the fine grid combined with a global solution on the coarse grid (also called coarse grid correction). A fine grid edge-based overlapping block-Jacobi smoother has been employed to avoid degeneration of convergence properties due to the presence of elongated elements. This two-grid cycle is accelerated by using a goal-oriented steepest-descend method. Numerical results indicate that the iterative solver converges typically in less than fifteen iterations, even in presence of elongated elements with an aspect ratio up to 100000:1. Visit www.ices.utexas.edu/Pardo for details and the most updated progress on this research.

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MS66
The Computation of a-Posteriori Bounds for Functional Outputs of PDEs Using Discontinuous Galerkin Methods

We present a formulation to calculate upper and lower bounds for functional outputs of the exact weak solution of coercive partial differential equations. It turns out that when using DG formulations most of the necessary ingredients required for the computation of bounds are readily available and as a consequence, the computation of bounds results in a minimum overhead. We will present convection-diffusion equations at low and high Peclet numbers, the Stokes equation as well as our initial investigation into the extension of the approach to the low Reynolds number steady state incompressible Navier-Stokes equations.

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MS67
Diffuse Interface Methods

We consider diffuse interface methods for modeling and simulation of fluid interfaces and for problems in image inpainting. We show how to design efficient and fast numerical schemes for such problems and how asymptotic analysis combined with bifurcation theory can suggest approaches for efficient topological reconnection in image inpainting. For fluid interfaces we show how such methods can be quantitatively compared to experimental data.

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MS67
Modeling and Computing the Blink Cycle in the Tear Film

A tear film is left on the front of the eye with each blink. Formation and evolution of the film over multiple blink cycles is studied using lubrication theory. Different numerical methods are implemented and compared on a moving domain. Comparison of the results with in vivo interferometry for a half blink is favorable. For many conditions, only 7/8 of full lid closure is required to completely restart the film according to fluid dynamics.

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MS67
Modeling and Simulation of Simple Locomotors in Stokes Flow

Motivated by the locomotion and modeling of heavily flagellated micro-organisms and by recent experiments of chemically driven nanomachines, we study the dynamics of bodies of simple geometric shape that are propelled by tangential surface stresses. For a Stokesian fluid, we have developed a mathematical model of the body dynamics based on a mixed-type boundary integral formulation. We will discuss the effect of body geometry on the dynamics, as well as interactions between multiple bodies.

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MS67
Shape Optimization of Swimming Sheets

Motivated by the propulsion mechanisms adopted by gastropods, we consider shape optimization of a flexible sheet which propels itself over a thin layer of viscous fluid by propagating deformation waves along its body. We use a lubrication approximation to model the dynamics and derive the relevant Euler-Lagrange equations to optimize swimming speed and efficiency. We present a fast, highly accurate method for solving the optimization equations and explore the solution in various singular limits. We also monitor the validity of the model using a new rigorous error estimate for Reynolds' approximation.

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MS68
Internships and Work Experience in Undergraduate CSE Education

An internship or work experience can be the climax of a CSE undergraduate's education. With exposure to many new ideas, techniques, and applications at another institution, such an experience can greatly broaden and deepen the student's understanding of computational science and make the classroom education more meaningful. Moreover, work with a professional computational science team and contacts made during the summer can greatly enhance opportunities and options available to the CSE undergraduate.

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MS68
Introduction to the Working Group Report

This presentation will provide an overview of the report on Undergraduate CSE Education and an introduction to the minisymposium. We will begin with our working definition of CSE, outline the sections and the topics for the presentations to follow. Attention will be paid to the differing forms and needs an undergraduate education in CSE can take and must try to meet.

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MS68
Undergaduate Computational Science and Engi-

neering Programs

The Minisymposium is organized and presented by the working group on the SIAM report of Undergraduate CS&E education. This presentation will highlight the different versions of computational science programs at the undergraduate level. (e.g., B.Sc programs, minor programs, certificate programs, etc). The session will also provide information on educational materials for the teaching and learning of CS&E at the undergraduate level.

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MS69
Moderator

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MS70
Implementation of Flow Solvers in COMSOL Multiphysics: Overview and Demonstration

As computational science progresses, the need for a general multiphysics platform (or at least strategy) has become evident. A multiphysics framework may not, however, be easily compatible with the sophisticated discretization and solution methods required by specialized fields in science and engineering, such as incompressible flow. This presentation will give an overview and demonstration of the COMSOL Multiphysics platform and the challenges associated with integrating flow solvers into a general multiphysics environment.

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MS70
IFISS: A Matlab Toolbox for Modelling Incompressible Flow

IFISS is a MATLAB package for the interactive numerical modelling of incompressible flow problems. It includes algorithms for discretisation by mixed finite element methods and a posteriori error estimation of the computed solutions. It can also be used as a computational laboratory for experimenting with state-of-the-art preconditioned iterative solvers for the discrete linear systems that arise in incompressible flow modelling. Here we will discuss its main features and demonstrate its use on some practical problems.

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MS70
Groundwater Flow Modelling Using the IFISS Toolbox

Mixed finite element approximation of the PDEs modelling steady incompressible flow leads to symmetric indefinite linear systems of equations. We describe a generic block preconditioning technique for such systems based on algebraic multigrid and describe an implementation in MATLAB and COMSOL. Some numerical results are presented showing the effectiveness of our approach in the context of diffusion equations that arise in modelling ground-water flow in porous media that exhibit random spatial variability.

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MS70
Comparing Incompressible Flow Preconditioners with IFISS

In CFD, there is a strong need for fast and robust iterative solvers for the discretized incompressible Navier Stokes equations. Popular methods are preconditioned Krylov solvers. The most important part is to find a good preconditioner. We present a new ILU with reordering preconditioner, which is compared with the pressure convection diffusion (PCD), least squares commutator (LSC), and augmented Lagrangian based (ALB) preconditioners. We compare these preconditioners for a number of problems obtained from the IFISS package.

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MS71
An Overview of the LSMLIB Library: Design and Usage

The Level Set Method Library (LSMLIB) is a C++/C/Fortran/MATLAB software library that provides support for the serial and parallel simulation of implicit surfaces and curves dynamics in two- and three-dimensions. It is designed to deliver high-performance, level set method algorithms to the application's developer while requiring only a high-level understanding of the level set method formalism. We present an overview of the LSMLIB software including a few examples demonstrating it usage in various modes.

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MS71
Surface Area Minimization of Triply-Periodic Surfaces with Volume Fraction Constraint Via the Level Set Method

We present a variational level set approach for theoretically and computationally studying triply-periodic surfaces that minimize the total surface area when there is a constraint on the volume fraction of the regions that the surface sepa-

rates. We demonstrate that optimal surfaces are precisely those possessing constant mean curvature. We then study the optimality of several well-known minimal surfaces and explore the properties of optimal surfaces when the volume fractions of the two phases are not equal. Parallel LSMLIB is used to handle the computational cost of the three-dimensional shape optimization problem.

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MS71

Investigating Spontaneous Capillarity-Controlled Events Via the Level Set Method

An accurate description of the mechanics of pore level displacement of immiscible fluids could significantly improve the macroscopic parameter predictions from pore network models in real porous media. Assuming quasi-static displacement, we describe a simple but robust model based on the level set method for determining critical events for throat drainage and pore imbibition. The method arrives at geometrically correct interfaces while robustly handling topology changes and is independent of the pore space complexity.

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MS71

Solving Two-Phase Incompressible Stokes Equations Using the Immersed Interface Method and LSMLIB

Two-phase incompressible Stokes equations appear in many physical and biological applications. We use the second-order Immersed Interface Method (IIM) coupled with the Level Set Method (LSM) to solve multiphase Stokes flows with singular interface force and piecewise constant viscosity coefficient. The Stokes equations are decoupled into Poisson equations using the projection method. To use the IIM for the decoupled Poisson equations, we first derive the jump conditions for both the pressure and the velocity in the case where the two fluids may have unequal viscosity coefficients. Since the jump conditions for the kinematic variables can be decoupled by introducing augmented variables, we use the Generalized Minimal Residual (GMRES) method to solve for the augmented variables, and then solve the Stokes equations. The interface between two fluid phases is implicitly represented using a level set function. We couple the LSM with IIM for moving interface problems such as mean curvature flows for both 2D and 3D. Numerical simulations show that our algorithm implemented using LSMLIB is both efficient and second-order accurate.

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MS72

Local Quasicontinuum-Like Reduction of Optimization Problems in Materials Science

We present a local quasicontinuum-like approach for model reduction of minimum energy problems in materials science, and we give sufficient conditions for the well-posedness of the reduced problem. The approach includes a recent multiscale model reduction approach for orbital-free density functional theory electronic structure calculations that was proposed by the authors as well as the local quasicontinuum approach for potential-based calculations. Numerical results validate our findings.

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MS72

Algorithms for Inverse Problems Under Uncertainty: Applications to Dynamic Data Driven Assimilation of Nonlinear Dynamical Systems.

Data driven assimilation algorithms are typically applied to problems in geophysics and weather prediction. The key ideas however, extend to many systems that operate under uncertainty. In this talk we present a new algorithm for data assimilation that is inspired on ensemble Kalman filter but is based on algorithms from large-scale PDE-constrained optimization. We apply the new ideas to nonlinear chaotic dynamical systems, first proposed by E.N. Lorenz.

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MS72

Multigrid Schemes for Distributed Parameter Estimation Problems

Distributed parameter estimation problems represent a class of inverse problems with a bilinear structure. In these

cases, an optimization approach is considered where the inherent ill-posedness of these problems is accommodated by appropriate regularization and solution techniques. For this purpose, the experience gathered with the multigrid solution of singular optimal control problems and with the concept of strong coupling of optimization variables will be instrumental for the development of the multilevel algorithms presented in this talk. The inherent optimization and globalization properties of the resulting multigrid processes will be discussed.

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MS72

Inexact Adaptive Multilevel Methods for PDE-Constrained Optimization

We present a class of inexact multilevel SQP-methods for the efficient solution of PDE-constrained optimization problems. The algorithm starts with a coarse discretization of the underlying optimization problem and provides 1) implementable criteria for an adaptive refinement strategy of the current discretization and 2) implementable accuracy requirements for iterative solvers of the PDE and adjoint PDE on the current grid such that global convergence to the solution of the infinite-dimensional problem is ensured. Numerical results are presented.

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MS73

Coupling Molecular and Continuum Modeling for Detailed Reaction Kinetics of TRISO Fuel Coating

Chemical vapor deposition of silicon carbide is applied in TRISO coatings for uranium kernels used as nuclear fuel in high-temperature gas-cooled reactors. The gas-phase reaction mechanisms will be determined using *ab initio* electronic structure theory to provide initial parameters needed to predict rate constants, namely activation energies and structural features, to calculate the appropriate partition functions. The detailed chemical kinetics will be used as input into simulations using a continuum-based code, MFIX.

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MS73

Quadrature-Based Moment Methods for Polydisperse Multiphase Flows

The fundamental description of gas-solid flows begins with a kinetic equation for the particle-velocity distribution function. In the Eulerian representation of gas-solid flow, the moments of the kinetic equation are used to describe the particle density, the mean velocity, and selected second moments of velocity. However, the transport equations for these moments are not closed due to (at least) two terms: (i) spatial transport by the fluctuating velocity, and (ii) particle-particle interactions (e.g. collisions). In addition, systems with a distribution of particle properties (i.e., polydisperse systems) lead to a kinetic equation of higher dimensionality, and moment transport equations with even more unclosed terms. In this talk we will demonstrate how quadrature methods applied to the kinetic equation can be used to derive consistent closures for the moment equations. In particular, we will show that even the simplest case of non-interacting particles with finite Stokes number can be treated correctly using a quadrature approach, whereas "standard" multi-fluid models fail. We also show that the Boltzmann collision kernel can be succesfully treated using quadrature to capture nonequilibrium flows.

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MS73

Wavelet-Based Multiscale Approach for Heterogeneous Chemically Reactive Flows: A Simple Case Study of Diffusion/Reaction Problem

This talk will give an overview of a general wavelet-based multiscale methodology called Compound Wavelet Matrix (CWM) and how it can be used to bridge spatial and temporal scales. In particular, the effectiveness of this method in bridging scales in a simple reaction/diffusion problem will be presented as an illustration of the CWM strategy for multiscale/multiphysics models. In conclusion, the next steps needed to generalize the current methodology for arbitrary heterogeneous chemically reacting flows will be presented.

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MS73

Multiscale/Multiphysics Methods Used in Heterogeneous Chemically Reacting Flows

This talk will provide an overview of modeling multiphase chemical reactors and the various methods currently used which span ¿10 orders of magnitude in both temporal and spatial scales. This includes a wide-variety of models like DFT, Lattice Boltzmann methods, Discrete particle simulations, CFD and process models. This presentation will also address the obstacles that need to be addressed to improve the integration across the scales and predictability of the overall device scale simulations.

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MS74

A Bridging Domain Method for Coupling Continua with Molecular Dynamics

A bridging domain method for coupling continuum models with molecular models is described. In this method, the continuum and molecular domains are overlapped in a bridging subdomain, where the Hamiltonian is taken to be a linear combination of the continuum and molecular Hamiltonians. We enforce the compatibility in the bridging domain by Lagrange multipliers or by the augmented Lagrangian method. An explicit algorithm for dynamic solutions is developed. Results show that this multiscale method can avoid spurious wave reflections at the molecular/continuum interface without any additional filtering procedures, even for problems with significant nonlinearitics. The method is also shown to naturally handle the coupling of the continuum energy equation with the molecular subdomain. A multiple-time-step algorithm is also developed within this framework.

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MS74

Generalized Mathematical Homogenization of Atomistic Media at Finite Temperatures in Three Dimensions

We derive thermo-mechanical continuum equations from Molecular Dynamics (MD) equations using the Generalized Mathematical Homogenization (GMH) theory developed by the authors for 0K applications. GMH constructs an array of atomistic unit cell problems coupled with a thermo-mechanical continuum problem. The unit cell problem derived is a molecular dynamics problem defined for the perturbation from the average atomistic displacements subjected to the deformation gradient and temperature extracted from the continuum problem. The coarse scale problem derived is a constitutive law-free continuum thermo-mechanical equation. Attention is restricted to heat transfer by lattice vibration (phonons). The method is verified on several model problems against the reference molecular dynamics solution.

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MS74

Phonon Heat Bath Approach for the Atomistic and Multiscale

A novel approach to modeling the crystalline solid as a heat bath is proposed. The approach is reducing the physical domain to an MD-solvable size. Interface with the hypothetic exterior region is non-reflective for outward elastic waves, and provides adequate statistical correlation for the atomic thermal vibration by utilizing Gibbs canonical distribution for the phonon gas in thermodynamic equilibrium at constant temperature. All method parameters are derived from the interatomic potential. Benchmark applications are shown.

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MS74

Perfectly Matched Multiscale Simulations

A multiscale method is proposed. It combines the so-called bridging scale method and the perfectly matched layer method to form a robust and versatile multiscale algorithm. The method can efficiently eliminate the spurious reflections/diffractions from the artificial atomistic/continuum interface by matching the impedance at the interface of the molecular dynamic region and the perfectly matched layer. Moreover, it is shown in this paper that the method can capture anharmonic interaction among nonuniformly distributed atoms in a local region.

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MS75

High-Resolution Central Schemes for Kinetic and Fluid Plasmas Models

In this work we present high-reslution central schemes for two-species plasmas described by the microscopic Vlasov model and by the macroscopic Euler-Poisson fluid model. Finite volume schemes for both models have been recently developed so as to asess the validity of the fluid model by comparing the results obtained to those obtained with its kinetic counterpart. We propose the development of finite volume schemes based on central differencing. Central schemes avoid the costly use of Riemann solvers for the fluid model, resulting in simple numerical schemes.

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MS75

A Hybrid Particle/Continuum Simulation Method for Coulomb Collisions in a Plasma

For small Knudsen number, simulation of of particles dynamics by Monte Carlo becomes computationally intensive. In the context of rarefied gas dynamics, we have developed an accelerated, hybrid method that combines DSMC and a continuum solver. The molecular distribution function f is represented as a linear combination of a Maxwellian distribution M and a particle distribution g; i.e., $f = bM + (1-b)g$. The density, velocity and temperature of M are governed by fluid-like equations, while the particle distribution g is simulated by Monte Carlo. In addition there are interaction terms between M and g. The coefficient b is determined automatically, by a thermalization approximation. This talk will describe an extension of the hybrid method to Coulomb collisions in a plasma. For this extension, the underlying Monte Carlo method is Nanbu's method for Coulomb collisions.

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MS75

Numerical Heating and Particle Codes

Plasmas (ionized gases) have rich and complex behavior which often need multiple lines of attack to fully understand their rich dynamics. Depending on the length scales involved, the plasma may be described by either a kinetic or a fluid model, the kinetic model being the more fundamental of the two. In this talk we will give a brief overview of the relation between these two models and then discuss Lagrangian particle methods for kinetic plasma problems. In particular, we will discuss the issue of numerical heating in a verity of grid-based and grid-free particle methods (time stepping errors, mesh based effects, particle shape functions and nonlinear coupling of statistical errors to long range fields.)

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MS75

An Unstaggered Constrained Transport Method for 3D Ideal MHD

The ideal magnetohydrodynamic (MHD) system is a fluid model for a perfectly conducting quasi-neutral plasma. One of the main challenges in numerically solving these equations is the requirement from Maxwell's equations that the magnetic field remain divergence-free for all time (no magnetic monopoles). The continuous equations automatically preserve this relationship, but standard numerical discretizations do not. Furthermore, in many numerical computations, the failure to satisfy a discrete divergence-free constraint leads to (sometimes violent) numerical instabilities. In this talk we will review the constrained transport framework of Evans and Hawley [Astrophysical Journal, 1988] and describe a new version of their approach that is spatially unstaggered and relies on a magnetic potential to maintain discrete divergence-free magnetic fields. A key ingredient in this approach is a new flux limiting strategy that maintains essentially non-oscillatory magnetic fields indirectly through the use of limiters on the magnetic potential equations. Several 2D and 3D simulations will be presented to show the merit of the proposed method.

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MS76

Low-Rank Tensor Product Approximations for Stochastic PDEs

One way to quantify uncertainty is via stochastic models, resulting often in a stochastic PDE (SPDE). Galerkin discretisations of such linear and non-linear SPDEs result in huge and complex systems of linear or non-linear equations. As the information amount in such a stochastic/physical discretisation can be enormous, it is important to have some way of compressing it. Low-rank tensor-product approximations are one possibility for this, and their use is described in this context.

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MS76

Stochastic Collocation and Stochastic Galerkin for Time Dependent SPDEs

We study numerical approximations for the statistical moments of the solution of a time dependent PDE, illustrating on the computation of the expected value and deriving a priori estimates of the resulting numerical errors. We apply a non-intrusive Stochastic Collocation Method which is very versatile. It entails solving a number of standard deterministic PDEs, precisely like in the Monte Carlo method. We will discuss implementation issues and present numerical examples.

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MS76

Sparse Second Moment Analysis of Elliptic Problems in Stochastic Domains

We consider the numerical solution of elliptic problems in domains with a class random boundary perturbations. Assuming perturbations with small amplitude and known mean field and two-point correlation function, we derive, using a second order shape calculus, deterministic equations for the mean field and the two-point correlation function of the random solution in the stochastic domain. Using a variational boundary integral equation formulation on the unperturbed, 'mean' boundary and a wavelet discretization, we present and analyze an algorithm to approximate the random solution's two-point correlation function at essentially optimal order in essentially $\mathcal{O}(\mathcal{N})$ work and memory, where N denotes the number of unknowns required for consistent discretization of the boundary of the domain. Joint work w. Reinhold Schneider (Kiel) and Helmut Harbrecht (Bonn).

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MS76

Spectral Methods for Random Differential Equations

This talk focuses efficient spectral methods for PDEs with random inputs. Spectral expansions based on the generalized polynomial chaos (gPC) are employed in random space to approximate the random quantities. Stochastic Galerkin or stochastic collocation method is then employed to convert the stochastic PDEs into a set of deterministic PDEs, which can be solved via standard methods. Examples for practical applications are presented.

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MS77

OOF: Analyzing Material Microstructure

The OOF program, developed at NIST, analyzes the properties of materials with complicated microstructures. OOF allows a user to assign various material properties to the features in a real or simulated microstructure, and uses finite element analysis to predict the behavior of the microstructure in virtual experiments. I will present the current version of the program, OOF2, and discuss features of its structure designed to make it easy to integrate with computations on different scales.

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MS77

RheoPlast: Open-Source Modular Parallel Finite Difference Phase Field Software

RheoPlast is a multi-physics finite difference simulation code which includes modules for: binary and ternary Cahn-Hilliard and vector-valued Allen-Cahn phase field, transport-limited electrochemistry, velocity-vorticity and velocity-pressure flow, elastic shear strain for fluid-structure interactions, and heat conduction; these can be combined arbitrarily at runtime. Based on the PETSc suite of parallel solvers and data objects, RheoPlast runs in two or three dimensions, features flexible time stepping, and can use periodic, symmetry, and module-specific programmed boundary conditions.

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MS77

Computational Informatics for Materials Design

In this presentation we discuss how statistical learning techniques can be used to augment more classical approaches to computational based design of materials. The role of data mining to identify dominant parameters influencing phase stability calculations is demonstrated. The use of such informatics based techniques to accelerate the computational approaches for first principle calculations is discussed. Examples are provided for a variety of multi-component alloy design platforms.

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MS77

On-Line Microstructure Repository for Predictive Analyses

Many materials properties can be understood by analyzing the temporal and spatial evolution of microstructures under different conditions. Performing such analysis requires compact representation to store and manipulate a large set of microstructures and techniques to determine relationships between properties, structure and processing parameters from such large data sets. We discuss how these challenges can be addressed through computational and software techniques implemented in our web-portal applications for designing Aluminum-rich alloys.

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MS78

Simulation of Supersonic Combustion Phenomena in Evolving Geometries with Cartesian Upwind Methods

Accurate numerical simulation of gaseous high-speed combustion in evolving domains requires the integrated application of several advanced techniques: consideration of stiff chemical kinetics, parallelization, and (in our case) embedding of moving boundaries into a dynamically adaptive Cartesian mesh. The core component though is a reliable high-resolution upwind scheme for gas-mixtures with complex equation of state. The presentation compares wave-propagation-based methods with standard shock-capturing schemes and evaluates suitability and performance for simple and practically relevant configurations.

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MS78

High-Resolution Finite Volume Methods for a Biological Problem

Extracorporeal Shock Wave Therapy is a noninvasive technique for the treatment of a variety of musculoskeletal conditions such as bone fractures and plantar fasciitis. In lithotripsy, a shock wave is generated in a liquid bath, focused by an ellipsoidal reflector, and it then propagates into the body where it strikes the treatment area. We use high-resolution finite volume methods to solve the nonlinear elasticity equations and model the shock wave propagation in bone and tissue.

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MS78

Numerical Simulations of a Multi-Scale Model for Suspensions of Rod-like Molecules

We consider the Doi model for suspensions of rigid rod-like molecules. The model couples a microscopic Fokker-Planck type equation (the Smoluchowski equation) to a macroscopic Stokes equation. The Smoluchowski equation describes the evolution of the distribution of the rod orientation. It is a drift-diffusion equation on the sphere which is solved in every point of the macroscopic flow domain. The coupled flow problem shows interesting behavior, in particular the spurt phenomenon. In the spurt regime, the drift term in the Smoluchowski equation is dominant and thus a discretization based on the wave propagation algorithm is used to approximate the coupled micro-macro flow problem.

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MS78

Finite Volume Modeling of Acoustic and Elastic Waves in Periodic Media

I will briefly present the basic ideas of WENOCLAW, a high order accurate finite volume method built within the CLAWPACK framework. WENOCLAW combines the ideas of wave propagation and high order WENO reconstruction. I will then discuss the application of WENOCLAW to acoustics and elastics in heterogeneous media. The wave propagation algorithm easily handles the numerical difficulties associated with discontinuous material parameters, while the WENO reconstruction yields high order accuracy. I will show results of calculations of bandgaps in sonic crystals, focusing via acoustic lenses, and solitary waves in periodic two-dimensional elastic media.

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MS79

A Posteriori Error Estimation For Discontinuous Galerkin Methods

Discontinuous Galerkin methods (DGM) have gained in popularity during the last 30 years because of their ability to address problems having discontinuities, such as those that arise in hyperbolic conservation laws. The DGM use a discontinuous finite element basis which simplifies *hp* adaptivity and leads to a simple communication pattern across faces that makes them useful for parallel computation. In order for the DGM to be useful in an adaptive setting, techniques for estimating the discretization errors should be available both to guide adaptive enrichment and to provide a stopping criteria for the solution process. We will present new superconvergence results on triangular elements and show how to construct effective estimates of the finite element discretization error using superconvergence of DG solutions. First, we present new $O(h^{p+2})$ pointwise superconvergence results for first-order hyperbolic problems on triangular meshes consisting of one-outflow-edge elements as well as on meshes having both one- and two-outflow-edge elements. We will present efficient techniques to compute asymptotically correct a posteriori error estimates obtained by solving local problems.

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MS79

A Posteriori Error Estimates, Error Control, and Model Sensitivity

Investigating and exploiting the sensitivity of a model with respect to data and parameters is a fundamental problem in CS&E. This involves computing solutions correspond-

ing to different data and parameter values, and therefore having different properties. This raises a critical need for error estimation and control since otherwise numerical error can mask the true responses. In this talk, we develop the computational aspects of dealing with model sensitivity by means of a posteriori error analysis.

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MS79

A Posteriori Error Estimates for Eigenvalue Analysis of Heterogeneous Elastic Structures

For eigenvalue analysis of heterogeneous elastic structures, a posteriori error estimators are less studied than the estimators for traditional static elliptic or time-dependent problems. In this talk, we will present an explicit estimator that treats the cases of high order finite elements and discontinuous material coefficients. This estimator is equivalent with the error in the eigenvector, independently of the variation of the materials properties. We will assess the efficiency of this estimator with numerical experiments.

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MS79

Adaptive Simulation of Multiphysics Problems

In this talk we outline a basic framework for adaptive simulation of multiphysics problems. The adaptive algorithms are based on a posteriori error estimates that account for the overall effect on output goal quantities of the errors caused in the individual single physics solvers and in the transfer of data between these solvers. The framework is illustrated on several applications including multiphysics simulation of oil reservoirs, mems devices, and electronics cooling.

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MS80

Overlapping Grids for Interface and Moving Boundary Problems

The overlapping grid approach can be used to accurately treat problems with interfaces and moving boundaries. In a typical grid construction, narrow boundary fitted grids are used to represent the moving boundary or interface, and these grids overlap with stationary background Cartesian grids. In this talk I will discuss several examples of using overlapping grids to handle problems with interfaces and moving boundaries including results for the reactive-Euler equations, incompressible fluid flow and Maxwell's equations.

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MS80

Front Tracking Simulation of Shock Bubble Interaction

In this presentation, we study shock-bubble multiple interactions through reflecting boundaries using the front tracking method. We make a systematic exploration of the single shock passage problem in a range of dimensionless parameters. We then extend our computational study to multiple re-shocks produced by reflecting boundaries. We use fast Fourier transform (FFT) to analyze the spectra of kinetic energy and vorticity and compare with the non-tracking simulations.

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MS80

The Moving Contact Line Problem

The moving contact line problem is a classical problem in fluid mechanics. The difficulty stems from the fact that the classical continuum theory with no-slip boundary condition predicts a non-physical singularity at the contact line with infinite rate of energy dissipation. Many modified continuum models are then proposed to overcome this difficulty. They all succeed in removing the singularity, but they leave behind the question: which one of these models is a good description of the microscopic physics near the contact line region? We will review the results obtained using continuum theory, molecular dynamics and the more recent multiscale techniques. We will also discuss how these techniques can be combined to give us a better understanding of the fundamental physics of the moving contact line and formulate simple and effective models

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MS80

A High-Resolution Godunov Method for Reactive and Nonreactive Multi-Material Flow on Overlapping Grids

A numerical method is described for reactive and nonreactive multi-material flow. The flow is governed by the multi-material reactive Euler equations with a general mixture equation of state. Composite overlapping grids are used to handle complex flow geometry and block-structured adaptive mesh refinement (AMR) is used to locally increase grid resolution near shocks, material interfaces and reaction zones. The discretization is based on a high-resolution Godunov method, but includes an energy correction designed to suppress numerical errors that develop near a material interface for standard, conservative shock-capturing schemes. Nonreactive flow involving shock interactions with planar and curved inhomogeneities and reactive flow involving detonation diffraction are discussed to illustrate the numerical approach.

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MS81

Theory and Discretization of Operator Riccati Equations

In this paper we focus on the problem of developing numerical schemes that yield convergent and mesh independent approximations of the infinite dimensional Riccati equation

$$\mathcal{F}(\mathcal{X}) = \mathcal{A}^*\mathcal{X} + \mathcal{X}\mathcal{A} - \mathcal{X}\mathcal{B}\mathcal{B}^*\mathcal{X} + \mathcal{C}^*\mathcal{C} = \imath,$$

where $BB^*, CC^* \in \mathcal{L}(\mathcal{H})$ and A generates a strongly continuous semigroup on a Hilbert space H. We consider a sequence of approximating problems defined by (H^N, A^N, B^N, C^N), where $H^N \subset H$ is a sequence of finite dimensional subspaces of H, $A^N \in \mathcal{L}(\mathcal{H}^\mathcal{N}, \mathcal{H}^\mathcal{N})$, $B^N \in \mathcal{L}(\mathcal{U}, \mathcal{H}^\mathcal{N})$ and $C^N \in \mathcal{L}(\mathcal{H}^\mathcal{N}, \mathcal{Y})$ are bounded linear operators. Let $P^N : H \to H^N$ denote the orthogonal projection of H onto H^N satisfying $\left\|P^N\right\| \leq 1$ and assume that $\|P^N x - Px\| \to 0$ as $N \to \infty$ for all $x \in H$. Define the finite dimensional approximating Riccati equations by

$$\mathcal{F}^\mathcal{N}(\mathcal{X}^\mathcal{N}) = (\mathcal{A}^\mathcal{N})^*\mathcal{X} + \mathcal{X}\mathcal{A}^\mathcal{N} - \mathcal{X}^\mathcal{N}\mathcal{B}^\mathcal{N}(\mathcal{B}^\mathcal{N})^*\mathcal{X}^\mathcal{N} + (\mathcal{C}^\mathcal{N})^*\mathcal{C}^\mathcal{N} = \imath.$$

Let $X_k \in \mathcal{L}(\mathcal{H})$ denote the iterates of the Newton method for the infinite dimensional Riccati equation $\mathcal{F}(\mathcal{X}) = \imath$. Likewise, $X_k^N \in \mathcal{L}(\mathcal{H}^\mathcal{N})$ denotes the iterates of the Newton method for the discretized Riccati equation $\mathcal{F}^\mathcal{N}(\mathcal{X}^\mathcal{N}) = \imath$. Roughly speaking, the MIP may be broken down into convergence under mesh refinement and Newton interation counts on a given mesh. We first review the conditions on the approximating scheme (H^N, A^N, B^N, C^N) which are sufficient to imply that the approximating Riccati equation admits a unique nonnegative solution X_∞^N, and $X_\infty^N P^N$ converges to the unique nonnegative solution X_∞ of the infinite dimensional operator Riccati equation. We then focus on the issue of mesh independence for the Kleinman-Newton algorithm. In particular, we present results that relate mesh independence to dual convergence and the preservation of control system properties under approximation. Finally, we provide applications and numerical examples to illustrate the ideas.

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MS81

A Comparsion of Multigrid and H-ADI for Large Scale Riccati Equations

We compare two related multilevel methods for the solution of large scale algebraic matrix Riccati equations $AX + XA^T - XFX + C = 0$: A (nonlinear) multigrid method and an ADI iteration based on hierarchical matrices. Both approaches can be adapted in order to preserve the low rank structure of the $n \times n$ solution X induced by low rank right-hand sides C, so the equation can be solved in almost linear complexity $\mathcal{O}(n \log^c n)$.

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MS81

Iterative Solution of ARE's Arising in Control of Vibrations

Algebraic Riccati equations (ARE) of large dimension arise when using approximations to design controllers for systems modelled by partial differential equations. A number of approaches to solving such algebraic Riccati equations exist. Most rely on finding a low rank approximation to the exact solution. For some problems, such as heating problems, this low rank approximation exists. Numerical results indicate that for weakly damped problems a low rank solution to the ARE may not exist. Further analysis supports this point.

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MS81

Low Rank Approximate Solution of Algebraic Riccati Equations

A method is developed for the approximate low rank solution of several important problems in control, including the solution of large scale algebraic Riccati equations as they arise in optimal control, H-infinity control and in model reduction. The solutions are obtained through the approximate computation of a basis for a selected invariant subspace of a block structured matrix pencil. The subspace basis is used to construct low rank approximate solutions to Riccati equations, in particular to the maximal and minimal symmetric solutions. This approach yields approximation results that guarantee stability and passivity in model reduction of passive systems.

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MS82

Adaptive Refinement for the Solution of Maxwell's Equations

Abstract not available at time of publication.

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MS82

Talk Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS82

Discontinuous Galerkin Methods for the Time-Harmonic Maxwell Equations

We propose and analyze interior penalty discontinuous Galerkin methods for the numerical discretization of the time-harmonic Maxwell equations. The main advantages of these methods in comparison with conforming finite element approaches lie in their high flexibility in the mesh-design and their accommodation of high-order elements. We derive the methods for the time-harmonic Maxwell equations, and discuss the underlying stability mechanisms. Based on suitable duality arguments, we then derive optimal a-priori error bounds in the energy norm and the L^2-norm. Finally, we present a-posteriori error estimators for the low-frequency approximation of the time-harmonic Maxwell equations where the resulting bilinear forms are coercive. We show the reliability and efficiency of the estimators and demonstrate numerically that they can efficiently resolve the strongest Maxwell singularites in non-smooth domains. We derive the methods for the incompressible Navier-Stokes equations, and discuss the underlying stability mechanisms. We then develop the a-priori and a-posteriori error estimation of hp-adaptive discretizations and present adaptive refinement procedures. All our theoretical results are illustrated and verified in numerical experiments.

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MS82

Algebraic Multigrid and Algebraic Reformulations of the Eddy Current Equations

With the rising popularity of compatible discretizations (edge elements) for the eddy current Maxwell's equations, there is a corresponding need for fast solvers. We propose an algebraic reformulation of the discrete system along with a new AMG technique for this reformulated problem. This technique requires a specialized solver on the fine mesh, but traditional methods can be used on the coarser meshes. We illustrate the new technique for smoothed aggregation AMG and present computational results.

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MS83

BGCE - The Bavarian Graduate School of Computational Engineering

The Bavarian Graduate School of Computational Engineering (BGCE) was established as kind of an umbrella programme, gathering three CSE-related graduate programmes at TU Munich and University of Erlangen-Nuremberg. For the best students there, BGCE offers an elite track which, after successful participation, leads to a master's degree with honours. The talk will present the BGCE as the funding institution of this student prize.

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MS83

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MS84

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MS84

Treed Gaussian Processes for Surrogate Modeling Under Uncertainty

One important contribution of statistics is in the development of surrogate models which can give a computationally fast approximate response surface for a function, such as the output of complex computer code. The traditional approach to surrogate modeling uses Gaussian process models, but they have a number of potential problems. We present a more flexible model, based on a treed partition of the space, with Gaussian processes fit within each parti-

tion. By doing so in a fully Bayesian manner, we can also give complete uncertainty estimates, which can then be used for guiding searches of the input space for either optimization or learning about the unknown function itself. We demonstrate this approach on our motivating example of the adaptive design of a simulation experiment for learning the response surface of flight characteristics of a proposed rocket booster.

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MS84

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MS84

Pattern Search Optimization with a Treed Gaussian Process Oracle

The derivative-free optimization method Asynchronous Parallel Pattern Search (APPS) allows use of an external 'oracle' to help guide the optimization search. Here we incorporate statistical modeling via Treed Gaussian Processes as the oracle. Using a statistical model allows us to explicitly quantify our uncertainty about the function output, leading to a more robust global optimization. We also investigate the use of statistical inference in convergence criteria, so as to include globally informed stopping rules.

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MS85

The Cactus Framework: Design, Applications and Future Directions

The Cactus Code is an opensource, modular framework for collaborative high-performance computing. In addition to including different computational and community toolkits, Cactus provides a range of abstract interfaces to application developers through which a variety of third party libraries and tools can be easily leveraged. In this talk, we review the design of Cactus, describe how it is used by different application communities, and discuss ongoing development plans for supporting new application needs.

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MS85

AMROC - A Cartesian SAMR Framework for Compressible Gas Dynamics

AMROC is an object-oriented C++ framework that provides structured adaptive mesh refinement (SAMR) on distributed memory machines. Being the fluid solver system of Caltech's simulation infrastructure "Virtual Test Facility", the current main applications range from Eulerian-Lagrangian fluid-structure interaction simulation to supersonic combustion and turbulence modeling in complex (evolving) geometries. The presentation details the design and generic components that enable the construction of large-scale parallel simulation codes involving Eulerian compressible gas dynamics in minimal time.

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MS85

Integrating Modeling and Simulation Components within the SIERRA Framework

The SIERRA Framework provides modeling and simulation application codes with a collection of capabilities for parallel execution, distributed adaptive unstructured meshes, and multiphysics coupling. Application codes integrate their physics-specific components into the framework such that these components may be completely insulated from details of parallel communication and distributed data synchronization. The SIERRA Frameworks parallel execution model, distributed mesh model, application components and taxonomy, and framework interactions with application components will be presented.

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MS85

Components for Adaptive Multiscale Simulations

This presentation will discuss a set of functional components being developed to support the execution of adaptive multiscale simulations. The components are designed to accept a general specification of multiscale problems and to coordination the interactions of the simulation domains and fields accounting for the transformations associated with going across the multiple scales in which various discretization processes are used within each scale. Example adaptive applications including continuum to atomistic coupling will be presented.

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MS86

The L^2 Norm Error Estimates for the Div Least-Squares Method

This talk presents L^2 norm error estimates for the *div* least-squares method for which the associated homogeneous least-squares functional is equivalent to the $H(div) \times H^1$ norm for the respective dual and primal variables. Optimal L^2 norm error estimates for the primal variable under the minimum regularity requirement for the second-order elliptic equations, elasticity, and the Stokes equations are established.

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MS86

Least-Squares Methods for Interface and Mesh Tying Problems

In the finite element method, a standard approach to mesh tying is to apply Lagrange multipliers. However, if the adjoining surfaces do not coincide spatially, straightforward Lagrange multiplier methods lead to discrete formulations failing a first-order patch test. A least-squares method is presented here for mesh tying in the presence of gaps and overlaps. The least-squares formulation for transmission problems is extended to settings where subdomain boundaries are not spatially coincident. The new method is consistent in the sense that it recovers exactly global polynomial solutions that are in the finite element space. As a result, the least-squares mesh tying method passes a patch test of the order of the finite element space by construction. This attractive computational property is illustrated by numerical experiments.

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MS86

First-Order System Least Squares FEM Approach for Solving Maxwells Equations in Deforming Media

Deformation of solid media brings the matter flow field and the Cauchy-Green and Piola strain tensors into the electromagnetic constitutive laws, which renders Maxwell's equations hyperbolic with variable coefficients. A numerical solution of the time-diecretized Maxwells equations is deforming solid media based on a first-order system least-squares (FOSLS) variational formalism will be presented.

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MS86

First-Order System Ll* (fosll*) for Maxwell's Equations in 3D with Edge Singularities.

The L^2–norm version of first–order system least squares (FOSLS) attempts to reformulate a given system of partial differential equations so that applying a least–squares principle yields a functional whose bilinear part is H^1–elliptic. This means that the minimization process amounts to solving a loosely coupled system of elliptic scalar equations. An unfortunate limitation of the L^2–norm FOSLS approach is that this product H^1 equivalence generally requires sufficient smoothness of the original problem. Inverse–norm FOSLS overcomes this limitation, but at a substantial loss of real efficiency. The FOSLL* approach described here is a promising alternative that is based on recasting the original problem as a minimization principle involving the adjoint equations. This talk provides a theoretical foundation for the FOSLL* methodology and application to the eddy current form of Maxwell's equations. It is shown that singularities due to discontinuous coefficients are easily treated. However, singularities due to reentrant edges require a further modification. A partially weighted norm is used only on the slack equations. The solution retains optimal order accuracy and the resulting linear systems are easily solved by multigrid methods. Comparison is made to the curlcurl formulation and the weighted regularization approach. The FOSLL* is shown to have equal or better accuracy, obtained at a smaller cost. Numerical examples are presented that support the theory.

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MS87

Mathematical Modeling of Pollution Distribution from Motor Transport in City in Bottom Layer of Atmosphere

In report there are 3D air-dynamics model in bottom layer of atmosphere and advection-diffusion model of transport pollution. Program realization of models based on GIS technology and database for the pollution distribution in case of typical weather conditions. The first regime of program based on direct simulation gas dynamics, humidity and heat transport and finally air pollution distribution modeling. The other variant based on fast searching of most similar variant for given situation from database.

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MS87

LBM Approaches for the Heat-Mass Transfer in Shallow Water Basins

In recent years the lattice Boltzmann method (LBM) has attracted much attention in the physics and engineering communities as a possible alternative approach for solving complex fluid dynamics problems. In particular, the inherent parallelism, the simplicity of programming, and the capability of incorporating complex microscopic interactions have made LBM a very attractive simulation method for fluid flow in complex physical systems, specifically in modeling of heat and mass transfer in shallow water basins.

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MS87

High Resolution Shallow Water Models and Its Ap-

plication to Some Basins in the South of Russia

In report 2D and 3D high precision models for shallow water basins have been presented. These models take into account following factors: complicated form of beach and bottom, wind and bottom friction, Coriolis factor, input and output, evaporation in mass conservation as well as in momentum equations and so on. Also coefficients of turbulent diffusion have been computed. These models have been applied to the Azov Sea modeling and theoretical and experimental results compared.

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MS87

Modeling of Pollution Distribution in the Azov Sea Using Irregular Grids

For numerical realization of high precision hydrodynamic model for shallow water basins the method of finite elements on irregular triangular meshes is used. Unlike regular meshes, irregular meshes are easier to build, they easily adapt for complex geometry of area. It is developed original algorithms of irregular triangular meshes construction based on the mesh refining by moving nodes preserving Delaunay conditions fulfillment. Nodes also moved along borders of the area in iterative process.

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MS88

Challenges and Algorithms for Simulating Alfvenic Turbulence in Collisionless Plasma

Turbulence plays a critical role in plasma systems ranging from laboratory fusion experiments to astrophysics. In nearly collisionless systems, modeling this turbulence is challenging because of the kinetic nature of the dominant dissipation processes and because of the strong nonlinear interactions that control the dynamics. On the other hand, the range of spatio-temporal scales that must be simultaneously resolved is not as large as in neutral fluid turbulence. A new class of "gyrokinetic" codes developed for fusion are facilitating the exploration of plasma turbulence across a broad range of problems. In astrophysics an important issue is how large-scale turbulent energy is absorbed as it cascades to small spatial scales. Whether the energy is dumped into electrons or ions in accretion flows and in other systems impacts both the dynamics of the system and our ability to interpret observations through measurement of radiation from distant sites throughout the universe. Results from the first self-consistent calculations of the collisionless absorption of turbulent energy cascades for astrophysical applications will be presented. A new mechanism for ion heating in Alfvenic plasma turbulence will be discussed, and a short discussion of the accuracy of the algorithms used for this calculation will be presented.

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MS88

Discontinuous Galerkin Methods for Fluid Plasma Modeling with Applications to Plasmoid Accelerators

Plasmoid accelerators are an interesting high energy density propulsion concept currently under investigation at Advatech Pacific in partnership with the Air Force Research Laboratory at Edwards Air Force Base. Approaches to fluid plasma modeling using the discontinuous Galerkin method are being developed to help better understand plasma physics issues important to this thruster concept. One promising approach involves the use of vector potentials to maintain the divergence constraint when time dependent magnetic field boundary conditions are applied. In this talk, discontinuous Galerkin algorithms for fluid plasma models will be presented along with numerical benchmarks and results relevant to plasmoid propulsion.

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MS88

Advances in Mixed Materials Modeling for Resistive MHD on ALE Meshes

There is continued interest in the MHD modeling of mixed materials for a variety of high current plasma applications. The challenge is the constituents may be very small, requiring high spatial resolution. We show the protocol for using "microscopic" simulations, where the individual materials are resolved, to build a "macroscopic" EOS and resistivity tables of a thermodynamically correct mixed, homogenized material at reduced resolution. Simulations will be compared against both microscopic calculations and experimental results.

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MS88

A Boltzmann-PIC-MCC Hybrid Model for Collisional Transport in the Tokamak Diverter Sheath

The plasma sheath and hydrocarbon transport near a carbon diverter plate of a ITER-like tokamak is modeled using a one-dimensional particle-fluid hybrid model, with a hybrid Monte Carlo collision model. Electrons are modeled as an inertia-less (Boltzmann) fluid with conservation of charge enforced by a time-dependent flux balance at the walls for a Maxwellian distribution at a specified temperature. Flux flows in from the edge plasma, and out at the diverter and also in the upstream direction. Ions are modeled using the PIC methodology. The modeling methodology for the iterative nonlinear solver is presented. The hybrid collision model allows particle-particle collisions as well as particle-fuild and fluid-fluid collisions. The hybrid model is shown to run about one hundred times faster than a full PIC model.

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MS89

Model Reduction and Adaptation in Stochastic Galerkin Projections

This paper focuses on addressing issues of computational efficiency of spectral stochastic Galerkin projections for the solution of complex stochastic systems. In particular, an algorithm is developed for the efficient characterization of a lower dimensional manifold occupied by the solution to a stochastic partial differential equation (SPDE) in the Fock space associated with the Wiener chaos. A description of the stochastic aspect of the problem on two well-separated scales is developed to enable the stochastic characterization on the fine scale using algebraic operations on the coarse scale. Moreover, a solid foundation is provided for the adaptive error control in stochastic Galerkin procedures.

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MS89

Uncertainty Quantification in Electromagnetic Scattering

We shall discuss the use of polynomial chaos expansions for quantifing the impact of uncertainty in electromagnetic scattering. Modeling of uncertainty in sources, materials, and geometries will be discussed and we will also compare Galerkin and Collocation forms of the polynomial chaos approach. The EM problem is solved using a high-order DG-FEM approach. We shall illustrate use of such techniques on problems of realistic complexity, including problems requiring a high-dimensional random space.

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MS89

Stochastic Collocation Methods Nonlinear Elliptic PDEs with Random Input Data

This work proposes and analyzes sparse grid stochastic collocation techniques for solving nonlinear elliptic partial differential equations with random coefficients and forcing terms (input data of the model). This method can be viewed as an extension of the Stochastic Collocation method proposed in [Babuska-Nobile-Tempone, Technical report, MOX, Dipartimento di Matematica, 2005] which consists of a Galerkin approximation in space and a collocation at the zeros of suitable tensor product orthogonal polynomials in probability space and naturally leads to the solution of uncoupled deterministic problems as in the Monte Carlo method. The full tensor product spaces suffer from the curse of dimensionality since the dimension of the approximating space grows exponentially fast in the number of random variables. If the number of random variables is moderately large, this work proposes the use of sparse tensor product spaces utilizing either Clenshaw-Curtis or Gaussian interpolants. For both situations this work provides rigorous convergence analysis of the fully discrete problem and demonstrates: (sub)-exponential convergence of the "probability error" in the asymptotic regime and algebraic convergence of the "probability error" in the pre-asymptotic regime, with respect to the total number of collocation points. Numerical examples exemplify the theoretical results and show the effectiveness of the method.

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MS89

Modeling Diffusion in Random Heterogeneous Media: Data-Driven Microstructure Reconstruction Models, Stochastic Collocation and the Variational Multiscale Method

We are interested in modeling diffusion in 3D random heterogeneous microstructures that are defined through limited statistical information extracted from 2D microstructure snapshots. An accurate simulation of diffusion in random heterogeneous media has to satisfactorily account for the twin issues of randomness as well as the multi-length scale variations in the material properties. We propose a general methodology to construct a data-driven, reduced-order microstructure representation model to describe property variations in realistic heterogeneous media. This reduced-order model then serves as the input to the SPDE describing thermal diffusion through random heterogeneous media. A decoupled scheme is used to tackle

the problems of stochasticity and multi-length scale variations in properties. A sparse-grid collocation strategy is utilized to reduce the solution of the SPDE to a set of deterministic problems. A variational multiscale method with explicit subgrid modeling is used to solve these deterministic problems. An illustrative example using experimental data is provided to showcase the effectiveness of the proposed methodology.

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MS90

Arbitrary Order Accurate and Unconditionally Stable Discretization of the 4D Navier-Stokes Equation on Unstructured Meshes

Stablized numerical methods utilizing continuous and discontinuous basis approximations are presented for discretizing the time-dependent compressible Navier-Stokes flow equations about curved geometries using arbitrary mesh complexes containing simplex, brick, prism, and pyramidal elements. Salient features of this formulation and implementation include: (1) arbitrary order accuracy in both space and time (for sufficiently smooth solutions) using machine generated basis representations, (2) provable global nonlinear stability whenever entropy convexity is strictly retained, and (3) parallel implementation using domain decomposition techniques. Numerical results for compressible Navier-Stokes flow are presented to illustrate performance characteristics of the method(s).

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MS90

Accuracy of Mixed-Element Finite-Volume Discretizations

The recent drag prediction workshops have identified lack of reliable accuracy analysis for unstructured discretizations as a critical problem. This paper proposes a unified approach to evaluating accuracy of finite-volume discretizations on mixed-element unstructured grids. The analysis is applied to the inviscid-flow equations discretized with a typical node-based discretization; the first-order convergence on mixed grids is shown and explained. Alternative discretizations, demonstrating convergence with the second and third designed accuracy order, are analyzed and tested.

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MS90

Simulation of Heating on Unstructured Grids in Hypersonic Flows

The quality of surface heat transfer simulation under conditions of hypersonic flow as a function of flux reconstruction algorithm within FUN3D is reviewed. Focus is on all tetrahedral elements in order to preserve flexibility for grid adaptation and remove constraints of semi-structured (prismatic) grids across all shear layers. Context for discussion is provided by a simple test case (flow over a cylinder) and a more complex case (flow over a spacecraft towing a toroidal ballute).

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MS90

Paths Toward Accurate Unstructured Grid Heating

An account of trials and tribulations endured during the quest for predicting aeroheating with unstructured grids.

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MS90

Newton-Krylov Methods on Unstructured Meshes for Aerodynamic Flows

In this presentation two Newton-Krylov algorithms are described for solution of the compressible Navier-Stokes equations on unstructured meshes. In the first, the mean-flow equations are fully coupled with the turbulence model equation; in the second algorithm, the two systems are loosely coupled. Both algorithms use the generalized minimal residual Krylov solver with incomplete lower-upper preconditioning. Results are presented for several two- and three-dimensional flows, including a wing-body-nacelle geometry.

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MS91

Phase Field Modeling and Simulation of Some Interface Problems

We present our on-going works on the phase field modeling and simulations of some interface problems, ranging from microstructure evolution in multicomponent alloy to lipid vesicle deformation and interaction in fluid. We discuss recent development of highly adaptive computational algorithms for large scale phase field simulations. We also address how to effectively retrieve useful statistical information within the phase field framework.

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MS91
Rayleigh-Taylor Turbulent Mixing

Improvements to the Front Tracking method have increased its power and ease of use. The robust treatment of bifurcations was achieved through combination of the robust but less accurate grid based tracking with the accurate but less robust grid free tracking. This, with improved physical modeling (correct modeling of physical transport phenomena, etc.), allows validation of simulations for the 3D Rayleigh-Taylor chaotic mixing problem. We thank the many collaborators who contributed to this work.

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MS91
Regularization for Accurate Numerical Wave Propagation in Discontinuous Media

Structured computational grids are the basis for highly efficient numerical approximations of wave propagation. When there are discontinuous material coefficients the accuracy is typically reduced and there may also be stability problems. In this talk, we consider a technique for modifying the material coefficients close to the material interface, to improve on the order of accuracy of the Yee scheme as well as other (also higher order) methods based on a similar staggered structure.

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MS91
An Eulerian Formulation for Interfacial Flows with Surfactant

An interfacial flow with surfactant involves more complicated physics along the interface as well as more complicated coupling of interface dynamics and bulk dynamics. An Eulerian framework is developed to capture both the surfactant distribution on the interface, the moving interface, and the ambient fluid flow. Extensive computation results will be shown to validate our algorithm. This is a joint work with Z. Li, J. Lowengrub and J. Xu.

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MS92
Speaker Names

To Be Announced
tba
tba

MS93
Shape Determination for Real and Complex Maxwell Eigenvalue Problems

Experimentally observed cavity response differ from that of ideal cavity. This is due to shape deviations resulting from both loose machine tolerance in the fabrication, and tuning process for the accelerating mode. In this talk, we present a shape determination algorithm to solve for the unknown cavity deviations using the real cavity's frequency response. The inverse problem is posed as a least-squares minimization problem. Nonlinear optimization problem is solved using a line search based reduced space Gauss-Newton method, and shape sensitivities are computed with a discrete adjoint approach. We present both real-life and synthetic examples.

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MS93
Shape Optimization in Support of Implantable Blood Pump Design

Several challenges and methods in biomedical flow device design are described. The objective often involves the unique behavior of blood as the flowing medium, necessitating, e.g., accurate modeling of cell damage. The complex constitutive behavior, in particular shear-thinning, may affect the outcome of shape optimization more than it affects direct flow analysis. Finally, target applications often involve intricate time-varying geometry, and thus, realistic solutions can be only obtained on high-performance parallel computers.

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MS93
Optimization of Self-Stability for Periodic Motion of Walking and Running Robots

Abstract not available at time of publication.

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MS93
Determination of Initial Orbits of Satellites After Faulty Launches

Abstract not available at time of publication.

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MS94

Preconditioned Iterative Solvers for Linear Stability Analysis of Incompressible Flows

We explore iterative methods for eigenvalue problems $\mathcal{A}\sqsubseteq = \lambda\mathcal{B}\sqsubseteq$ arising from linear stability analysis of the Navier-Stokes equations. $\mathcal{A}$ is a nonsymmetric indefinite matrix with structure like that of saddle point systems and $\mathcal{B}$ is singular. The matrix-vector products required by methods such as inverse iteration or the implicitly restarted Arnoldi algorithm entail solution of linear systems with coefficient matrix $\mathcal{A}$ or $\mathcal{A} - \theta\mathcal{B}$. For this, we use preconditioned Krylov subspace methods and examine effects of Reynolds number and shifts on performance. Moreover, we study "inexact" solvers and the effects of stopping criteria on the performance and costs of eigenvalue computations.

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MS94

The Effect of Inner Solver Accuracy and Boundary Conditions on Pressure Convection-Diffusion Preconditioners for the Incompressible Navier-Stokes Equations

While numerous studies have demonstrated mesh-independent convergence for *Pressure Convection–Diffusion* preconditioners and their overall efficacy, several potential weaknesses remain in their practical use. The relationship between accuracy of inner sub-problem solves and overall convergence rate of the outer iteration is not well understood for the Navier-Stokes equations or when the inner sub-block solver has less than ideal behavior. We discuss this issue as well as the influence of boundary conditions on overall algorithm convergence.

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MS94

Two-Phase Incompressible Flow Problems: Discretization and Preconditioners

In this talk we consider a standard model for a two-phase flow problem, namely the incompressible Navier-Stokes equations with a localized force term at the interface between the two phases. The levelset approach is used for the implict representation of the interface. Special finite elememt spaces are used for discretization. We present preconditioning methods that have robustness properties with respect to mesh size, time step and jumps in problem parameters (density and viscosity).

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MS94

Least Squares Commutator Preconditioning for Stabilized Mixed Approximation

The focus of this talk is the Least Squares Commutator (LSC) preconditioner developed by Elman, Howle, Shadid, Shuttleworth and Tuminaro. The original version of the preconditioner required that the underlying spatial discretization be uniformly inf-sup stable. Here the definition of the original preconditioner is generalized to cover the case of discrete systems that arise when using stabilized low-order mixed finite element approximation or collocated finite difference methods.

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MS95

Continuation of Sparse Eigendecompositions

The eigenvalues of large parameter-dependent matrices provide insight to engineers designing resonators and to those studying the stability of dynamical equilibria. We describe continuation methods for approximating a few eigenvalues of such parameter-dependent matrices. In particular, we explore how the continuous structure of these problems informs the choice of solver parameters at each step, and how information from the eigensolver can be used to make choices about step size control in the continuation process.

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MS95

Continuation for the Ornstein-Zernike Equation Using LOCA

The Ornstein-Zernike equation together with a closure equation can be solved to find probability distributions of atoms in fluid states. Varying parameters of the state such as density and temperature allows us to understand phase transitions, say, from liquid to vapor. It has been shown, however, that such a continuation study produces incorrect results when using a common closure equation. We seek to perform this study using an alternative closure equation using the software LOCA.

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MS95

Computing Hopf Bifurcations in Large-Scale Prob-

lems

Hopf bifurcations, signified by the birth of an oscillatory periodic solution, are a common means by which dynamical systems become unstable. Examples include flutter, vortex shedding, and chemical oscillators. We describe block elimination and bordered matrix methods for computing Hopf bifurcations that are scalable to problems with millions of unknowns. These methods have been implemented in LOCA, part of the Trilinos solvers collection, and are designed to be easily integrated into existing engineering codes.

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MS95

Periodic Orbit Tracking for Large-Scale Applications

A general-purpose periodic orbit tracking capability is being developed in Sandia's Trilinos framework. We use finite difference discretizations of the time domain and use a Newton's method to solve the entire space-time problem. Parallelism over the space and time domains is implemented, and different preconditioning strategies are investigated. For 3D PDE applications, this formulation is for a "steady" problem in four dimensions, so existing continuation and stability analysis capabilities can be used.

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MS96

Deformable Boundaries on Moving Overset Grids

We consider viscous flow coupled to deformable boundaries. We introduce "essentially Cartesian grid methods" where thin unstructured grids track the deformable boundaries while most of the domain is covered by structured Cartesian grids. This is the natural extension of classical overset (Chimera) schemes which simplifies the treatment of complex surface geometry. Computational examples are presented to illustrate the new features of these algorithms.

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MS96

Turbulent Mixing in Imploding Richtmyer-Meshkov Instability

We study imploding Richtmyer-Meshkov instability to understand the effect of the numerical flow model on late time mixing dynamics, in particular sharp interfaces vs. mixed cell pressure-temperature equilibrium. For early times the models behave similarly, but show completely different late time mixing structures. Mixed cell treatments are dominated by a few fully mixed well defined vortices, while sharp interface treatments show fragmented materials with large temperature spikes and a many fine scale vortices.

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MS96

Numerical Algorithms for MHD of Free Surface Flows of Ablated Materials

New mathematical models, algorithms, and computational software have been developed for the study of magnetohydrodynamics of multiphase flows in the presence of phase transitions. The code is applicable to the simulation of free surface flows of electrically conducting liquids or weakly ionized plasmas ablated by particle or laser beams in magnetic fields. Applications of the developed methods for the simulation of tokamak fueling through the injection of small frozen deuterium - tritium pellets will be discussed. We have performed first systematic studies of the pellet ablation in magnetic fields, and our results disproved some prevailing expectation about the role of the geometry and magnetic field on the pellet ablation rate.

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MS96

Application of the PPB Moment-Conserving Advection Scheme to Multifluid Interface Instability Problems

A moment-conserving finite difference scheme for nonlinear advection, the PPB scheme, has been derived from an extension to 3D of van Leers Scheme VI and with the addition of appropriate constraint conditions. This scheme will be briefly described along with its implementation inside the PPM gas dynamics scheme. A variety of multifluid interface instability problems have been attacked using this PPM/PPB combination, including problems with several distinct fluids. These results will be presented and the advantages of this approach discussed.

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MS97

Convergence of Pseudospectral Methods for Nonlinear Optimal Control Problems

A main problem in control engineering is solving a constrained nonlinear optimal control problem. In recent years, many practical, nonlinear optimal control problems have been solved by pseudospectral (PS) methods. In an effort to better understand the PS approach to solving control problems, we present some convergence results for problems with mixed state and control constraints. It is proved that the PS-discretized optimal control problem is a consistent approximation to the continuous-time optimal control problem. Convergence can be guaranteed under numerically verifiable conditions.

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MS97

Convergence of a Curse-of-Dimensionality-Free Method for HJB PDEs

A nonlinear HJB PDE corresponding to an infinite time-horizon control problem is used as a basis for development of a curse-of-dimensionality-free numerical method. In particular, the method handles PDEs which are written as (or well-approximated by) a point-wise maximum of quadratic Hamiltonian forms. The approach works by exploiting the structure of the semiconvex dual of the associated semigroup as an approximate max-plus summation of max-plus integral operators with quadratic kernels. The solution is obtained over the entire space, with errors in the gradient growing linearly with distance from the origin. Previous results have demonstrated that the computational growth as a function of space dimension is cubic (rather than exponential). The downside is a curse-of-complexity which is best dealt with via various pruning schemes including a convex-programming approach. Convergence rates as a function of the number of iterations will be discussed.

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MS97

Trajectory Optimization using Higher Order Implicit Integration Methods

Trajectory optimization is key to the design and analysis of aerospace vehicles. The use of implicit integration combined with modern nonlinear programming packages has proven to be an effective technique for trajectory optimization. The development of higher order implicit integration schemes will be covered. Computation experiences applying these methods to aircraft and interplanetary spacecraft problems will be shared.

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MS97

Addressing Dimensionality and Complexity Curses in Computational Optimal Control

The Hamilton-Jacobi framework for solving optimal control problems suffers from Bellmans famous curse of dimensionality. It can be easily argued that the Pontryagin framework suffers from a curse of complexity arising from the symplectic structure of the Hamiltonian system. It is possible to delay the onset of dimensionality and complexity by modern computational techniques whose roots can be traced back to the original ideas of Bernoulli and Euler. This talk will explore these issues thru the prism of new insights brought on by the availability of extraordinary computational power on ordinary computers.

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MS98

Linear Systems Arising in Computational Geomechanics

Finite element analysis is widely used in engineering geomechanics. Most problems require solutions of linear systems which are often both very large and include the effects of nonlinear material behaviour. This talk will provide an overview of the types of systems generated and will highlight some of the outstanding research issues in this area.

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MS98

An Element-by-Element Krylov Solver for Dynamic Soil-Structure Interaction

The survivability against aircraft impact of a nuclear containment vessel sited on soft soils poses a challenging dynamic soil-structure interaction problem. The foundation stiffness plays a key role in controlling the stresses experienced by the superstructure. Here the efficient use of the Scaled Boundary Element method (to simulate the dynamic far-field) in conjunction with a Krylov element-by-element NLFE solver is examined. Particular attention is given to reducing compute time when calculating the convolution integral.

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MS98

Block Preconditioners for FE Coupled Consolidation Equations

The repeated solution in time of the large size indefinite linear system resulting from the FE integration of coupled consolidation equations is a major computational effort. Because of ill-conditioning, a suitable preconditioner is necessary to guarantee the convergence of projection methods based on Krylov's subspaces. Novel block preconditioners are theoretically investigated with their practical applica-

tion discussed. Several numerical tests show their efficiency and robustness as compared to standard ILU/ILUT preconditioners.

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MS98

Element-Based Preconditioners for Problems in Geomechanics

The solution of algebraic equilibrium equations lies at the heart of a nonlinear finite element analysis in geotechnical engineering. This problem is usually reduced to a sequence of large sparse linear system solves, so iterative solvers and preconditioners play important roles. Here we review the use of a range of established element-based preconditioners for linear elastic and elasto-plastic problems and compare their performance with a new element-based method which offers a significant improvement in performance.

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MS99

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Abstract not available at time of publication.

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MS99

Gaussian Processes in Trust-Region Optimization Methods

Gaussian process models are often used to emulate expensive computer simulations. Recently, they have also been used to model the "error field" between two levels of fidelity in a computer simulation. This work examines the efficacy of using Gaussian processes in trust-region surrogate-based optimization. Since Gaussian processes account for uncertainties, they offer a potentially powerful way to reduce the number of high-fidelity function evaluations necessary in multi-fidelity optimization, especially in optimization problems which include uncertainty.

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MS99

Title Not Available at Time of Publication

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MS100

Why Advanced PDE Frameworks Should Use a Domain-Specific Language

Application codes need reusable components for meshes, solvers, and different physical components. However, many important processes are governed by PDE. By introducing a domain-specific language for PDE, it is possible to generate many such physical components while still interfacing to a common set of meshes and solvers. Moreover, layering physical components on top of such a unified approach to PDE allows a single entry point for fast algorithms or advanced approximating functions to be shared across physical modules. I will present examples of this concept from the FEniCS project and Sundance.

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MS100

Building High-performance, Optimization-Enabled PDE Simulations with Sundance

The Sundance high-level components allow building high-performance parallel PDE simulations with a convenient symbolic problem description language, also enabling advanced algorithms for PDE-constrained optimization and uncertainty quantification. The symbolic problem description also facilitates automated performance optimizations through which Sundance-built simulators can get runtime performance that is often superior to hand-coded domain-specific PDE codes. We will describe the symbolic engine's design, the architecture enabling its use with other frameworks, and show applications case studies.

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MS100

Automatic Parallelization with Hybrid Analysis

Hybrid Analysis (HA) compiler technology can seamlessly integrate static and run-time analysis of memory references into a single framework that can perform data dependence analysis and generate necessary information for most memory related optimizations. HA is used for automatic parallelization of programs. It extracts run-time assertions from loops and generates minimum overhead run-time tests. The technology has been implemented in the Polaris compiler and has parallelized 22 benchmark codes

with 99% coverage and scalable speedups.

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MS100

Plug-n-Play Linear Solvers: Abstraction of Linear System Assembly

Sparse linear systems arise in many engineering applications, and their solution often dominates runtime. Optimal linear system solution can be highly problem specific, which motivates the need to switch among various solver libraries. Widely varying solver interfaces makes switching difficult, so we have developed abstraction layers that encapsulate solver-library-specific interfaces and data types. The process of assembling and manipulating linear systems will be described, as well as access to solution methods and other operations.

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MS101

Enabling and Comparing Weak to Strong Multiphysics Coupling

This talk addresses development of stronger coupling algorithms approaching monolithic coupling using as little problem information beyond weak coupling as possible. Candidate algorithms involve matrix-free and Broyden-based approaches. Practical realization of these algorithms via solver libraries is discussed. The relative performance and cost associated with the various algorithms is comapred leading to an understanding of (dis)advantages and appropriate use. Examples ranging from coupled prototype systems to coupled production scale analysis codes will be presented.

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MS101

Algorithmic and Numerical Aspects of Coupled Problems

Coupled problems arise naturally in many areas, such as fluid-structure interaction. Often, there are good methods for each single problem. This leads to a partitioned approach. Here one wants to obtain the same results as fully monolithic. Assuming solvers for each subproblem, we look at numerical methods to solve the coupled problem, explaining some effects. Aditionally, we consider the separate pieces of subproblem software as components in a software engineering sense.

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MS101

Globalization-Preserving Coupling Techniques for Circuit-Device Coupling

This talk presents an algorithm to solve coupled circuit simulation between a low-fidelity lumped parameter circuit simulator and a high-fidelity PDE simulatior for drift diffusion. Each code is highly nonlinear and requires specific Globalized Newton-based techniques. Each application's globalization is incompatible with the other. Strong and robust coupling is achieved using a nonlinear elimination technique that preserves each application's globalization technique. Results will be shown for large-scale parallel circuits using production codes at Sandia.

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MS101

Modular Coupling Strategies for Melt Crystal Growth Models

We desire to construct a model for melt crystal growth processes that is both computationally expedient and mathematically self-consistent by employing codes that solve nonlinear, boundary value problems coupled along a common domain boundary. We present several strategies to implement a loose coupling of such codes. A block Gauss–Seidel iteration procedure is simple to implement but not robust. Much more promising is an approximate, Block-Newton approach implemented using a Jacobian-free Newton-Krylov algorithm.

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MS102

MKL Intel's Numerical Library on Multicore

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MS102

Solving Dense Symmetric Positive Definite Systems of Linear Equations Using Cholesky Factorization on the CELL Processor

We present a mixed-precision algorithm for solving symmetric positive definite systems of linear equations on the CELL processor. The algorithm is based on Cholesky factorization in single precision and iterative refinement of the single precision result to achieve double precision accuracy. Parallel Cholesky factorization is based on pipelining of consecutive steps of the algorithm in order to achieve

excellent load balance and almost complete hiding of communication latency.

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MS102

Extra-Precise Iterative Refinement for Least Squares Problems

We present the algorithm, error bounds, and numerical results of the extra-precise iterative refinement for overdetermined linear least squares (LLS) problems. We apply our linear system refinement algorithm to Bjorck's augmented linear system formulation of the LLS problem. Our algorithm reduces the forward normwise and componentwise errors to $\sqrt{n}\varepsilon$ unless the system is too ill-conditioned. In contrast to linear systems, we provide two separate error bounds for the solution x and the residual r.

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MS102

LAPACK For Clusters: Productivity Meets High Performance

LAPACK For Clusters (LFC) allows seamless parallelization of numerically intensive computations through the familiar environments such as Mathematica, MATLAB, and Python. These client environments naturally hide the inherent complexity of the parallel code in their sequential user interface. The computational resources reside on the server side in a form of a parallel cluster that allows remote manipulation of distributed objects and execution of parallel code. The integration between the server and client environments happens through the standard function overloading features of the clients and thus allows effortless scaling of existing sequential codes as well as writing new algorithms with the functionality of the server that extends built-in capabilities of the clients.

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MS103

Inverse Seismic Wave Propagation

Inverse problems in seismic wave propagation are difficult to solve due to their highly nonlinear nature. A successful strategy here is to use multiscale hierarchies both in the space discretization and the signal frequencies. Alternatively, experience from computational seismology suggests to amend the misfit term by traveltime measurements or more general integral transform operators. We combine these ideas for the solution of inversion problems on real geological data and provide a variety of numerical results.

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MS103

Dimensionality Reduction and Polynomial Chaos Acceleration of Bayesian Inference in Inverse Problems

In the Bayesian setting for inverse problems, the cost of likelihood evaluations with computationally intensive forward models may be prohibitive. This problem is compounded by high dimensionality, as when the unknown is a spatiotemporal field. We address these difficulties by combining a Karhunen-Loeve representation of Gaussian process priors with a Galerkin/polynomial chaos construction to propagate prior uncertainty through the forward model. The result is a lower-dimensional surrogate posterior which may be explored at negligible cost.

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MS103

Comparison of Advanced Large-Scale Minimization Algorithms for the Solution of Inverse Ill-Posed Problems

We compare performance of several robust large-scale minimization algorithms applied for unconstrained minimization of cost functional in the solution of ill-posed inverse problems applied to parabolized Navier-Stokes equations. The methods compared consist of the nonlinear conjugate gradient method, BFGS, the limited memory Quasi-Newton (L-BFGS) , Truncated Newton method and a new hybrid algorithm . For all methods employed the gradient of the cost function is obtained via an adjoint method. The hybrid method emerged as the best performer for an adequate choice of parameters controlling the number of L-BFGS and Truncated Newton iterations to be interlaced.

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MS103

Real-Time Reliable Parameter Estimation for Systems Described by Partial Differential Equations

We present a reduced-basis technique for the reliable real-time parameter estimation in parametrized partial differential equations. We first formulate a parameter estimation problem of identifying a compact set of all possible parameter values consistent with the interval measurements. We then replace the truth approximation outputs with the reduced-basis output bounds to obtain a new problem formulation of several orders of magnitude lower computational cost than the original problem. Finally, we propose efficient algorithms to construct approximate bounding regions for the solution of the new problem. Numerical results of a nondestructive evaluation problem is presented to demonstrate several features of our approach.

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MS104

Augmentation Preconditioners for Saddle Point Systems

In this talk we provide an overview of augmentation preconditioners for saddle point systems of the form $[A\ B^T; B\ 0]$. Those preconditioners come in a few flavors. Defining W as a weight matrix, the basic form is block diagonal, with $A+B^TW^{-1}B$ in the (1,1) block and W in the (2,2) block. The preconditioned matrix has the interesting property that the higher the nullity of the (1,1) block is, the faster a minimal residual Krylov solver (such as MINRES) converges. When the nullity of A is equal to the number of constraints, convergence (in the absence of roundoff errors) is expected to occur within two iterations. When applied to discretized PDEs, it is desirable to exploit the properties of the differential operators in a way that will allow for fast inversion of the augmented (1,1) block. This issue and other computational properties of the preconditioner will be discussed.

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MS104

Augmented Lagrangian and Schur Complement Preconditioners for the Oseen Equations

We discuss several block preconditioners for the discrete Oseen system. In one group preconditioners make use of special approximations to the pressure Schur complement of the problem. We will consider and compare several options of building such approximations. To avoid constructing sophisticated pressure Schur complement approximations we further consider a block preconditioner for an augmented Lagrangian formulation of the corresponding saddle point system. In this approach the crucial ingredient is an appropriate solver for the (1,1) block of the system. We discuss available theoretical and numerical results for different preconditioning techniques with respect to the mesh and viscosity dependence. This presentation is based on a joint research with M.Benzi.

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MS104

Block Preconditioning for Stabilized Finite Elements and Microfluidic Applications

Over the past several years, considerable effort has been placed on developing efficient solution algorithms for the incompressible Navier-Stokes equations. The effectiveness of these methods requires that the solution techniques for the linear subproblems generated by these algorithms exhibit robust and rapid convergence. These methods should be insensitive to problem parameters such as mesh size and Reynolds number. This study concerns a class of preconditioners derived from a block factorization of the coefficient matrix generated in a Newton nonlinear iteration for the primitive variable formulation of the system. These preconditioners are based on the approximation of the Schur complement operator using a technique proposed by Elman, Howle, Shadid, Shuttleworth, and Tuminaro [H. Elman, V. Howle, J. Shadid, R. Shuttleworth, R. Tuminaro, Block Preconditioners Based on Approximate Commutators, SIAM J. on Sci. Comp. 27 (2006) 1651 - 1668], Kay, Loghin, and Wathen [D. Kay, D. Loghin, and A. J. Wathen, A preconditioner for the steady-state Navier-Stokes equations, SIAM J. on Sci. Comp. 24 (2002) 237-256.], and Silvester, Elman, Kay, and Wathen [D. Silvester, H. Elman, D. Kay, A. Wathen, Efficient preconditioning of the linearized Navier-Stokes equations for incompressible flow, J. Comp. Appl. Math. 128 (2001) 261-279.]. It is derived using subsidiary computations (solutions of pressure Poisson and convection-diffusion-like subproblems) that are significantly easier to solve than the entire coupled system, and a solver can be built using tools, such as smooth aggregation multigrid for the subproblems. We discuss two computational studies we performed using MPSalsa, a stabilized finite element code, and Sundance, a high-level symbolic differentiation finite element code. Using MPSalsa, we compare parallel versions of the pressure convection-diffusion preconditioners with an overlapping Schwarz domain decomposition preconditioner. Using Sundance, we apply these techniques to realistic microfluidic problems where the flow is driven by an electric potential field. Our results show nearly ideal convergence rates for a wide range of Reynolds numbers with both enclosed and in/out flow boundary conditions on both structured and unstructured meshes.

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MS104

High-Order-in-Time Factorizations for Solving and

Preconditioning the Incompressible Navier-Stokes Equations

Algebraic Yosida-like fractional-step methods for solving the unsteady Navier-Stokes equations are presented. These methods (Quarteroni, Saleri, Veneziani, J Math Pur Appl, 1999, Saleri, Veneziani, SIAM J Num An, 2004, Gervasio, Saleri, Veneziani, J Comp Phys 2005) rely on approximate LU block factorizations of the matrix of the discrete Navier-Stokes system. We address time accuracy of these schemes and performances as preconditioners of the coupled Navier-Stokes system, using both finite elements and spectral space discretizations.

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MS105

Improved Boundary Conditions for Electromagnetic Particle-in-Cell Algorithm

Particle-in-cell (PIC) calculations based on the electromagnetic finite-difference time-domain method (FDTD) are simple, robust, and successful. However, the structured, Cartesian grids employed by the FDTD method result in staircase approximations that cannot accurately model curved surfaces. We will compare the accuracy of Cartesian grids, cylindrical grids, and a cut-cell embedded boundary. The particle currents must be weighted to these grids in a charge conserving manner. The charge conserving current weights are derived from finite element method (FEM) vector (edge) basis functions for the Cartesian (well known Villasenor-Buneman current weights), cylindrical, and cut-cell embedded boundary.

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MS105

Lagrangian and SemiLagrangian Models of Breakdown

Simulation of breakdown presents computational challenges because of the wide variation in spatial and temporal scales, and the need to keep numerical diffusion to an absolute minimum. We discuss attempts to develop a very accurate fully Lagrangian (mesh-free) approach. Semi-Lagrangian approaches which are faster and attempt to achieve the accuracy of the particle simulation are also discussed.

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MS105

Grid-Free Particle Simulations for Electrostatic Plasmas

A grid-free particle method for electrostatic plasma simulations is presented. The method employs techniques from vortex methods in computational fluid dynamics including: (1) treecode algorithm for evaluating the electric field induced by a set of point charges, (2) kernel smoothing to handle the Coulomb singularity, and (3) adaptive particle insertion to maintain resolution of the charge distribution. Simulations are presented for the instability of collisionless electron beams. This work is supported by AFOSR and NSF.

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MS105

Recent Applications of 3D Finite-Element Analysis for Electrostatic and Magnetostatic PIC

MICHELLE is a new two-dimensional and three-dimensional steady-state and time-domain particle-in-cell (PIC) code that employs electrostatic and now magnetostatic finite-element field solvers. Over the past several years the code has been employed successfully by industry to design and analyze a wide variety of devices that include multistage depressed collectors, electron guns, and ion thrusters. This paper will present applications of the MICHELLE code, including parametric optimization for design applications.

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MS106

Additive Schwarz Methods for Stochastic Elliptic

Equations

We present a parallel multilevel domain decomposition preconditioned recycling Krylov subspace method for the numerical solution of elliptic equations with stochastic uncertainties in the operator. Karhunen-Loeve expansion and Galerkin method with double orthogonal polynomial basis are used to transform the stochastic problem into a sequence of deterministic equations. We report results obtained from a PETSc based parallel implementation of a recycling Krylov subspace method preconditioned with the additive Schwarz method.

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MS106

Solving the Stochastic Steady-State Diffusion Problem Using Multigrid

We study multigrid for the stochastic steady-state diffusion problem where the diffusion coefficient has a finite Karhunen-Loève expansion. The problem is discretized in space using linear finite elements and in the "stochastic component" with a polynomial chaos method. The resulting discrete system is solved using multigrid where the spatial discretization varies from grid to grid while the stochastic discretization is held constant. We establish a "textbook" multigrid convergence rate independent of spatial mesh size, and we demonstrate performance with experiments. In addition, we explore extension of these ideas to the case where the diffusion equation is posed as a first order system discretized by mixed methods.

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MS106

Adaptive Multi-Element Collocation Method for Flow Problems

Abstract not available at time of publication.

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MS106

Stochastic Galerkin Method for Elliptic Spdes: A White Noise Approach

We present and explain several advantages of using the *White Noise* probability space as a natural framework for this problem. Applying properly the Wiener-Itô Chaos decomposition and a modification of the Karnunen-Loeve expansion, we obtain statistically stationary log normal permeability field and symmetric positive definite linear system of equations whose solutions are the coefficients of a Galerkin-type approximation to the solution of the original equation.

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MS107

Parallel Adaptive Methods and Domain Decomposition

We discuss a parallel adaptive meshing strategy due to Bank and Holst. The main features are low communication costs, a simple load balancing procedure, and the ability to develop parallel solvers from sequential adaptive solvers with little additional coding. In this talk we will discuss some recent developments, including variants of the basic adaptive paradigm, improvements in the adaptive refinement algorithm itself, and a domain decomposition linear equations solver based on the same principles.

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MS107

Adaptive Methods for Time-Dependent Problems Using Classical and Adjoint Approaches

Global error control for initial value problems relies on predicting the impact of accumulated error as it evolves in time. Methods based on Adjoint methods offer an attractive but potentially expensive solution. The alternative is to consider simple classical global error estimation for the forward PDE problem. Both these approaches are described and compared and an attempt made to undertsand when one method should be used rather than the other.

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MS107

Convergence of Adaptive Methods with Applications in Physics and Geometric Analysis

We consider two-scale models of electrostatics in biological materials, and similar nonlinear problems arising in geometric analysis. We establish well-posedness and derive max-norm estimates. We then prove similar results for Galerkin approximations, and use these results to derive a priori and a posteriori error estimates. We describe an adaptive algorithm and prove convergenece for the first model, and indicate the obstacles for a similar result for the second. We finish with examples using FETK.

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MS107

A fully Implicit Adaptive Multigrid Scheme for the Solution of Nonlinear Time-Dependent PDEs Arising in Phase-Field Models of Rapid Solidification

One of the most powerful techniques for modelling dendritic micro structures is the Phase Field method. The resulting governing equations are highly nonlinear time-dependent PDEs which we solve using adaptivity in both space and time. The temporal error control requires a fully implicit integration scheme to overcome stability restrictions: the resulting nonlinear algebraic equations at each time step are solved using a composite multigrid scheme. The method will be demonstrated for both pure metal and binary alloy solidification.

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MS108

Accelerating Scientific Exploration with Workflow Automation Systems

The increasing complexity of modern scientific investigations - a series of structured activities and computations that arise in scientific problem-solving, requires an integrated network-based support framework that allows scientists to reduce information technology overhead and focus on scientific research and discovery. This presentation discusses long-term practical experiences of the U.S. Department of Energy Scientific Data Management Center with automation of large scientific workflows. We will describe the current status and usage of a scientific workflow system, called Kepler, to automate the scientific exploration process.

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MS108

High-Performance Parallel Data and Storage Management

Parallel data access support for computational science has evolved into a sophisticated set of layered components designed to attain high performance and to provide convenient abstractions for data access. In this talk we will discuss the architecture of these "I/O software stacks". We'll start by describing the challenges in providing effective data access to computation science applications, and then we will discuss how the components in the I/O software stack work together to meet these challenges, citing examples from real applications. We'll conclude by discussing areas that researchers are exploring in order to enable applications to make even better use of data storage systems on high-end machines.

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MS108

Mining Science Data

The data from scientific simulations, observations, and experiments is now being measured in terabytes and will soon reach the petabyte regime. The size of the data and its complexity make it difficult to find useful information in the data. This is disconcerting to scientists who wonder about the science still undiscovered in the data. The Sapphire project (http://www.llnl.gov/casc/sapphire) is addressing this concern by applying data mining techniques to problems ranging in size from a few megabytes to a hundred terabytes. Using examples from fluid mixing, astronomy, remote sensing, and experimental physics, I will discuss our experiences in mining science data.

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MS108

High Performance Statistical Computing with Parallel R and Star-P

Tera- and peta-scale scientific data sets generated by contemporary simulations or high-throughput experiments bring new challenges to existing environments for statistical computing. New paradigms for ultrascale data analytics are emerging to address these challenges. Parallel R aims to provide efficient parallel statistical computing environment that: (a) automatically detects and executes task-parallel analyses in sequential R codes; (b) allows to easily plug-in data-parallel analyses codes in MPI-based C/C++/Fortran. Star-P exploits a similar paradigm for multiple languages: MatLab, Mathematica, Python, etc. We will present under-the-hood implementation intricacies of both systems, and demonstrate their usage by scientific applications in biology, climate, and nanoscience.

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PP0

Computer Simulation and Rheological Study of Xanthan Gum

Xanthan gum is a natural polysaccharide used as a food additive and rheological modifier. It is produced by the bacterium Xanthomonas campestris. Viscosity and elasticity properties of xanthan gum were studied for various pH using AR2000 rheometer with cone and plate geometry. The temperature and frequency dependence of loss and storage modules were also studied and data were fitted with well known model. Same experimental data were used to do computer simulation. In computer simulation, we designed the same geometry and used the experimental data to compare with the simulation data.

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PP0

A Hybrid Optimization Approach for the Optimal Design of Traveling Wave Tubes

We will present a hybrid optimization approach for the optimal design of electron device based on two independent physics-based design and simulation codes. In particular, we use the CHRISTINE suite of large signal codes to model the slow wave circuit, in conjunction with Beam Optics Analysis to model a multi-stage depressed collector. These two simulation codes will be combined in a hybrid framework to automate the process of optimizing several physical parameters while realizing several design constraints. The equations describing the device properties as well as the objective functions will be discussed, and examples of optimized TWTs will be presented.

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PP0

Computational Theory Using Gene Regulatory Network

Complex networks found in biological beings are in fact mysterious. Mimicking the networks has been practiced in many types of mathematical models. Boolean networks, Petri nets, Bayesian networks, graphical Gaussian models, Stochastic Process Calculi are examples of this imitation. Within this presentation, we introduce another approach to biology imitation. Using the gene regulatory network we develop a generic model, which we suspect useful for engineering computation.

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PP0

Implementing Machine Learning for Solver Selection

Machine learning techniques have proven to be effective in selecting efficient solvers for linear systems. Linear systems are represented by a set of matrix properties and application parameters combined into "feature-vectors". This poster highlights some factors that affect the accuracy of solver selection. We present a comparison of two classification methods, Boosting and Support Vector Machines. We also discuss the process of generating feature-vectors and the optimal composition of their element set.

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PP0

Accurate Model Selection Computations

I will discuss a model selection methodology which includes models for deterministic individual dynamics and random population effects in the context of HIV infection dynamics. Preliminary results concerning the numerics of the inverse problem and the realistic distinguishability of a class of models will be presented. In particular, I will focus on the relationship between random sources of error and those arising from the numerical discretization.

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PP0

Application of URVD Updating Techniques to the

Template Tracking Problem

Template tracking is a well studied problem in computer vision which refers to tracking an object through a video sequence by extracting an image of the ob ject (template) from the first frame and using it to find the regions in the remaining frames that correspond, as closely as possible, to the template. This framework has been extended by allowing parametric deformations of the template and linear appearance variations. One of the challenges in template tracking is how to update the template so that it remains a good model of the ob ject being tracked. A solution proposed recently by Matthews et al. (2003) is to update the template and the appearance variation parameters at every iteration. Since this matrix changes every time a new frame arrives, these updates involve calculation of the principal components of the augmented image matrix at every iteration. Traditionally, the principal components are computed at every iteration; we suggest algorithms to update the principal components obviating the need to recompute them from scratch at every iteration.

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PP0
Relating Mesh Quality Metrics to Sparse Linear Solver Performance

Large scale computational modeling and simulation involves unstructured finite difference or finite element meshes and solution of related sparse linear systems. We now attempt to relate well known mesh quality metrics to convergence characteristics of sparse krylov space linear solvers. We analyze the behavior of these quality metrics for a suite of different meshes and their perturbations and relate them to the performance of the underlying sparse krylov space solver.

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PP0
Hyperspectral Imaging

A hyperspectral image typically has more than 200 spectral bands that can include not only the visible spectrum, but also the infrared and ultraviolet spectra as well. The extra information in the spectral bands can be used to classify objects in an image with greater accuracy. Due to the high information content of a hyperspectral image and redundancy in the data, dimension reduction is an integral part of analyzing a hyperspectral image.

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PP0
Stability and Scalability of 2D Swarming Patterns

A swarming system is used to describe the aggregation of animals in biology and autonomous vehicles in engineering. We observe various distinct states with a dynamic model by changing its parameters. While these patterns exhibit different scalability properties, we apply H-stability from statistical mechanics to investigate such a difference. To further analyze the system, a continuum description is derived from the discrete model. Its validity is tested and a linear stability analysis is given.

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PP0
Strong Stability Preserving Multirate Schemes for Hyperbolic Conservation Laws

This work will consider the problem of designing 3-D electron guns using computer optimization techniques. Several different design parameters related to gun geometry and physical properties will be manipulated while considering multiple design criteria related to beam properties. The equations modeling the electron beam dynamics and the optimization routines will be described. Finally, examples of guns designed using these techniques will also be presented.

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PP0
A Parallel Lagrangian-Eulerian Coupling Algorithm for the Simulation of Floating Bodies in In-

compressible 2-Phase Flows

This poster concerns the parallel and accurate simulation of floating rigid bodies in incompressible two-phase flows. The coupling between the fluid and the solid response will be achieved with an Eulerian-Lagrangian coupling algorithm based on the Level-Set method. The underlying conservation laws at the interface are enforced by applying proper interface boundary conditions to the fluid which additionally have to prevent geometrically inadmissible penetrations.

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PP0
The Variational Brain

The Center for Computational Biology at UCLA has been developing computational methods to help understanding quantitatively the brain. For example, we investigate methods to detect morphological variations of brain structures as empirical evidences have suggested that shape and size play an important role in the assessment of the brain in health and disease. We will present a collection of variational energy minimization approaches and their results supporting the Center's mission. These include cortical surface segmentation with multiple level sets, brain image registration using large deformation log-unbiased fluid models, direct mapping of cortical and hippocampal surfaces with landmark constraints, and total variation based filtering and feature detection, modeling, and registration of brain images.

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PP0
Electron Gun Design Using Computer Optimization

This work will consider the problem of designing 3-D electron guns using computer optimization techniques. Several different design parameters related to gun geometry and physical properties will be manipulated while considering multiple design criteria related to beam properties. The equations modeling the electron beam dynamics and the optimization routines will be described. Finally, examples of guns designed using these techniques will also be presented.

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PP0
Adaptive Global Surrogate Modeling

Due to the scale and computational complexity of current simulation codes, metamodels (or surrogate models) have become indispensable tools for exploring and understanding the design space. Consequently, there is great interest in techniques that aid the construction and evaluation of such models while minimizing the computational cost and maximizing metamodel accuracy. We present a novel, adaptive, integrated approach to global metamodeling based on the Multivariate Metamodeling Toolbox (M3-Toolbox).

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PP0
Fully Implicit Solutions for Reduced Magnetohydrodynamics Models

We describe fully implicit solutions for one- and two-fluid, reduced, time dependent, magnetohydrodynamics models. Our approach uses Newton-Krylov-Schwarz techniques and is second order accurate in space and up to fourth order accurate in time. The advantage of implicit solutions over their explicit counterparts follows from the larger implicit time step sizes, constrained only by accuracy requirements and not by stability requirements as in the explicit case. We illustrate this by comparisons with explicit solutions, reporting computational results obtained on a parallel platform using thousands of processors.

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PP0

A Numerical Algorithm for MHD of Free Surface Flows at Low Magnetic Reynolds Numbers

We present a numerical algorithm which uses front tracking and embedded boundary method for the study of the magnetohydrodynamics (MHD) of free surface flows at low magnetic Reynolds numbers. The code has been validated through the numerical simulations of a liquid metal jet entering a non-uniform magnetic field and is currently being used for the simulation of liquid targets for future accelerators and pellet fueling of thermonuclear reactors (tokamaks).

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PP0

Multigrid Preconditioning for One-Shot Newton-Krylov Methods in PDE-Constrained Optimization

We present a multigrid one shot method for the solution of PDE-constrained optimization problems. Linearization of the coupled nonlinear optimality system is done with an inexact Newton method, the resulting linear systems are solved with a Krylov method. Since the arising KKT-type systems are indefinite and ill-conditioned, effective preconditioning is mandatory for their efficient solution. As preconditioner we use parallel multigrid with smoother and coarse grid solver adapted to optimal control problems.

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PP0

Meshless Formulations of PDEs Governing Electromagnetic Transients

In this paper an advanced meshless particle method for electromagnetic transient analysis is presented. The aim is to obtain numerical solutions for electromagnetic problems by avoiding the mesh generation and by employing a set of particles arbitrarily placed in the problem domain. The meshless Smoothed Particle Hydrodynamics method has been reformulated for solving the time domain Maxwells curl equations. Test problems, dealing with even and uneven particles distribution, are simulated to validate the proposed methodology.

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PP0

A New Theory Extending Continuum Mechanics to the Nanoscale and Applications

We present a new theory extending continuum mechanics to the nanoscale. While several successful applications have been developed, we will focus on one one which illustrates the theory by studying a nonlinear boundary value problem resulting from a novel approach to modeling fracture of a brittle material.

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PP0

A Comparative Study of Preconditioned Iterative Sparse Linear Solver Packages

This study evaluates a suite of preconditioners based on incomplete factorization, approximate inverse and algebraic multilevel schemes available in packages such as PETSC, Trilinos, HYPRE, PARMS and WSMP. We compare the performance of these preconditioners on a set of benchmark problems using the recommended set of parameters. Our observations provide insight into the strengths and weaknesses of the preconditioners in each package. These results can be used to guide the selection of the best package.

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PP0
TSP on Multi-Digraphs

The problem is to find a lightest tour in a given weighted multi-digraph. The tours can be presented with circular permutation matrices. The matrices are vectors in the vector space of square matrices. Decomposition of tours over the spaces basis reduces the problem to a non-symmetrical LP problem.

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PP0
Combined Parareal/reduced Order Modeling Method for Time-dependent PDEs

Due to the computational intensity of solving nonlinear partial differential equations, there has been much interest in developing algorithms which improve the ability to perform real-time calculations. One approach to reducing computational costs is the development of low-dimensional models; a second approach is to distribute the work over multiple processes by the development of parallel algorithms. In this work we combine both approaches by using POD based reduced order modeling in space and a parallel-in-time algorithm for the temporal integration known as the parareal algorithm.

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PP0
PDE-Based Parameter Reconstruction Through a Parallel Newton-Krylov Method

We consider distributed parameter identification problems for the FitzHugh-Nagumo system that models the propagation of transmembrane electrical potentials in excitable media such as neurons or heart tissues. We have developed a parallel algorithm of Newton-Krylov type for such an inverse problem. The method combines Newtons method for numerical optimization with Krylov subspace solvers for the reduced KKT system. We show by numerical simulations that the excitation parameter can be recovered from boundary measurements.

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PP0
Combinatorial Algorithms Enabling Computational Science

Combinatorial Scientific Computing is concerned with the development, analysis and utilization of discrete algorithms in scientific and engineering applications. Graph and geometric algorithms are the fundamental tools of combinatorial scientific computing. They play a crucial enabling role in numerous areas, including sparse matrix computation, partitioning for parallelization, mesh generation, and automatic differentiation. In this poster we report on some recent developments in this highly interdisciplinary and rapidly evolving field.

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PP0
Using Supervised Machine Learning Techniques to Predict Preconditioner Behavior

Choosing the right preconditioner is a critical component of using iterative methods to solve $Ax = b$ for large, sparse A. However, given a specific matrix A, few guidelines exist for choosing a preconditioner and setting its parameters effectively. With the goal of providing useful guidelines, we explore the use of supervised machine learning techniques, such as neural networks, for predicting the behavior of preconditioned iterative methods.

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PP0

A Model for Timely Decision as a Competitive Edge

Making timely decisions is considered to be a major factor as a competitive edge in the business world. To quantify this factor, we consider a model with two competitive businesses that differ in the delay time of making and implementing decisions. A time-delayed dynamic system is used to simulate the effect of delays in decisions. Results show that business with shorter decision delays experiences less fluctuation and is more adaptive to the changing business environment.

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PP0

Long Time Behavior of Numerical Solutions for Problems with Coarsening

We use the Cahn-Hilliard equation as a model of coarsening systems to study its long time behavior under the influence of discretization errors. In particular, we investigate the scaling properties of discretization errors to guide the design of a gradient stable time stepping method, the ultimate goal being to compute the slow dynamics both efficiently and accurately. The solution procedure and results from various time stepping approaches will be presented.

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PP0

Nonlinear Dynamical Analysis of Multi-Channel Neonate EEG Time Series During Sleep

Nonlinear dynamical analysis of the EEG time series during sleep is used to investigate the dynamics of neurodevelopment. As an alternative to reconstructing the state vector using time-delay embedding a single-channel of the recorded EEG time series, a 14 individual channels measuring electrical activity from different regions of the brain is used for the computation of correlation dimension. Brain activity as quantified by correlation dimension provides a good indicator of neurodevelopment.

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PP0

Cooperative Boundary Tracking with Embedded Nonlinear Filter

In this work, we consider the problem that using multiple autonomous underwater vehicles (AUVs) to track environmental boundaries. Assuming each AUV has a simple density detector, we demonstrate that, with our boundary estimation and motion control algorithms, AUVs track the boundary efficiently. Also, embedded nonlinear filters greatly improve the reliability against sensor noise. Moreover, a cooperative scheme is proposed so that multiple AUVs can track and estimate the boundary optimally using limited communication bandwidth.

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PP0

Modeling of Contaminant Transport in Groundwater Via Exact Simulation of Diffusions

It is well known that a advection-dispersion equation (ADE) can be interpreted as forward-Kolmogorov equation, also called Fokker-Planck equation, of a diffusion process given by a stochastic differential equation. Such solute transport can be simulated by generating paths of this process. 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) to obtain a 'particle solution' of the ADE. We compare the results with those obtained by the forward reverse method of *Milstein et al.* (Bernoulli 2004, vol. 10(2), 281- 312) for transition density estimation. Furthermore we adress sensivity analysis of exceedance probabilities with respect to variations of the transmissivity field, porosity and dispersivity.

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PP0

An Efficient Direct Parallel Elliptic Solver by the Spectral Element Method

An efficient direct elliptic solver based on the spectral element discretization is developed. The direct solver is based on a matrix decomposition approach which reduces multi-dimensional problems to a sequence of one-dimensional problems that can be efficiently handled by a static condensation process. Thanks to the spectral accuracy and the localized nature of a spectral element discretization, this elliptic solver is of spectrally accurate and can be efficiently parallelized.

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PP0
Benchmarking OpenMPI

OpenMPI, the successor to LA-MPI, FT-MPI, LAM/MPI, and PACX-MPI, offers significant improvements over the current implementations. These include fault tolerant networking and check-point/restart capabilities. The need for these features will increase as demand for petascale computing grows. While development continues on OpenMPI, it is important to maintain and improve work from previous MPI implementations on optimization of bandwidth and latency for network transfers. We compare OpenMPI to other implementations at the network and application level.

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PP0
Microfluidics of an Electrowetting Drop

We propose a diffuse interface model for drop motion, due to electrowetting, in a Hele-Shaw geometry. In the limit of small interface thickness, asymptotic analysis shows the model is equivalent to Hele-Shaw flow with a voltage-modified Young-Laplace boundary condition. The details of the contact angle significantly affect the timescale of motion in the model. The shape dynamics in the model agree well with the experiment, down to the length scale of the diffuse interface thickness.

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PP0
Phase-Aware Hardware Adaptivity for Energy-Aware High Performance Computing

For large multiprocessor installations improving the thermal and energy efficiency of scientific workloads is becoming increasingly critical. We conjecture that scientific codes consist of distinct phases. We therefore propose runtime phase detection schemes for adaptive hardware selection to improve energy efficiency. Our preliminary results indicate that by adaptively selecting power aware caches, CPU gears, data prefetchers and a load miss predictor, we can achieve power reduction of 14%, energy reduction of 43% while reducing the execution time by 32%.

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PP0
General Approach for the Numerical Solution of Inverse Problems

We need to use some sort of regularization techniques for the numerical solution of inverse problems. Especially for the cases where some features of the solution exhibit different patterns, along its different subspaces , the usual fixed regularization techniques can not compute a satisfactory solution. In this work, we develop an algorithm for adaptive regularization techniques based on the concept of Tikhonov regularization method. The basic idea is to use multiple regularization parameters.

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PP0
Verification Tests for Computational, Multigroup, Radiation Hydrodynamics in Two Spatial Dimensions

We have developed a computational radiation-hydrodynamics algorithm, in two spatial dimensions, designed to model astrophysical problems in stellar-core collapse, shock propagation, and proto-neutron-star evolution. Accurate modeling of such phenomena requires a rigorous verification process. We present here a test suite designed to stress diverse aspects of our code by comparing its output to known analytic solutions. It includes tests of pure hydrodynamics, pure radiation, and problems that couple these components together.

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PP0
Large-Scale Coupled Simulations for Seismic Response of Multiple Oil-Storage Tanks

This work is a part of gIntegrated Predictive Simulation System for Earthquake and Tsunami Disasterh, a 5-year project from FY.2005, supported by Japanese Government. In this poster, frameworks, such as data structure, and application interface, for large-scale parallel coupling simulations for seismic response of multiple tanks for oil-storage with fluid-structure interaction using finite-element methods are described. Preliminary results of coupled simulations on PC cluster with 64 corefs will be also demonstrated.

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PP0

BCCD/LittleFe - Computational Science Education on the Move

One of the principle challenges to computational science, high performance computing, and Grid education is that many institutions do not have access to appropriate platforms for demonstrations and laboratories. LittleFe is an inexpensive design for a 4-8 node portable computational cluster. LittleFe uses the Bootable Cluster CD (BCCD), a standard Linux environment with a complete set of parallel and distributed computing tools. LittleFe is an inexpensive, easy to use solution for computational science education.

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DNA Micro-Array Optimization with Synthesis and Sequence Composition Constraints

DNA micro-array hybridization is a high-throughput technology extensively used in genomic analysis. Recent advances in high density microarray technology - increased probe density and specificity allow efficient probing of large eukaryote genomes. Whole genome probing however requires efficient algorithms for oligonucleotide selection and synthesis. We propose here local search algorithms for optimizing oligonucleotide selection with synthesis and sequence similarity constraints. The optimization method was used for designing high density isoTM tiling arrays. We discuss here the performance of proposed optimization algorithms.

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PP0

Implementation of Meshless Finite Difference Method for Schrodinger Equation

Meshless methods have recently become popular for solving varieties of differential equations, with many applications in science and engineering fields. One of these methods, the meshless finite difference method, approximates a differential operator by using directional difference quotients and their combinations. Here we present numerical results of implementing the meshless finite difference method for solving Schrodinger equation.

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PP0

Nonlinear Spectral Viscosity for the Navier-Stokes Equations

Fluid turbulence in three dimension is a challenge both in analysis and computation due to the need to resolve the effects of small scales. In order to resolve this difficulty, various modeling strategies are employed. Ladyzhenskaya proposed the use of the nonlinear diffusion operator to model the small scale fluctuations. On the other hand, we must also preserve the large-scale dynamics described by the Navier-Stokes equations. Thus we use nonlinear diffusion in combination with spectral viscosity filter which attempts to limit the nonlinear viscosity effects to high modes. We analyze one such hybrid model, and prove existence and regularity, as well as derive certain restriction on the nonlinearity to preserve consistency with respect to the Navier-Stokes equations. Thus we use nonlinear diffusion in combination with spectral viscosity filter which attempts to limit the nonlinear viscosity effects to high modes. We analyze one such hybrid model, and prove existence and regularity, as well as derive certain restriction on the nonlinearity to preserve consistency with respect to the Navier-Stokes equations.

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The Double Globe Method: A Novel Adaptive Neighborhood Controller for Meta-Heuristic Algorithms

In a meta-heuristic optimization algorithm, at each iteration, a neighborhood is defined in which new solutions would be generated. We propose a novel adaptive scheme for controlling the stochastic search neighbourhood. The proposed "double globe" method features two hyper-spheres around the current optimum whose radii are dynamically enlarged or shrunk in order to adapt the degree of "exploration" and "exploitation." Numerical experiments and further analysis demonstrate the effectiveness of the proposed scheme in conjunction with several meta-heuristic algorithms for combinatorial optimization problems.

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PP0

Mode Pursuing Sampling Method for Discrete Variable Optimization in Mechanical Design

Based on the previously developed Mode Pursuing Sampling (MPS) method for continuous variables, a variation for discrete variable global optimization problems is devised. The proposed discrete-MPS method controls the convergence behavior by dynamically resizing two hyper-spheres centered at the current optimum. The radii of the spheres adapt the extent of exploration and exploitation. Application of the proposed method to two challenging mechanical design problems, namely pressure vessel and gear train, shows promising results compared to other commonly used algorithms

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PP0

Parallel Hydrodynamic Simulations Using New Generation of the Multicore Processors

Multi-core revolution in the processor designs allows shifting the parallel hydrodynamic simulations from the distributed CPU farms to a server or even a laptop while maintaining similar performance characteristics. The combination of the compact size, low cost, and energy consumption of a typical server with the power of a distributed parallel cluster gives the new generation of the multi-core platforms a potential to redefine the way hydrodynamic simulations for oil and gas reservoirs are run. Since calculations used in modeling require intensive CPU and memory usage, one needs to verify that the multi-core hardware architecture is efficient for this kind of calculations, on one hand, and that the software performance scales well with the number of the available cores, on the other hand. With four cores of two Intels Woodcrest processors used in Bensley server, the simulation acceleration achieved on a number of real full-field models exceeded factor of 3. Results for Tulsa server platform are also discussed.

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Using Adaptive Proper Orthogonal Decomposition to Model Reacting Flow

We develop an adaptive proper orthogonal decomposition (aPOD) method to simulate reacting flow with detailed chemical kinetics. The scheme is based on the method of snapshots and uses different POD basis vectors in different regions of the computational domain. We demonstrate the use of aPOD on an unsteady one-dimensional reaction-diffusion model equation corresponding to a laminar premixed methane-air flame. The observed speed-up factor is approximately 3.5.

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A Gradient-Based EM Algorithm for Maximizing the Likelihood Function of an ARMA Process

The maximum likelihood estimate of an ARMA process can be computed using a gradient-based EM algorithm coupled with a reparameterization. Using the EM algorithm, an exact gradient can be computed while holding the predicted values at the current state fixed. The predicted values are then updated in the expectation step. This approach avoids the use of a numerical approximation to the gradient. Software demonstrating the approach will be presented.

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PP0

Wavelet Lgorithm for High-Resolution Image Reconstruction

Low-resolution samples of a scene, shifted by sub-pixel length, are used in an iterative process to obtain a high-resolution image. Obtaining a better approximation to the true image is modeled as a linear system $Lf = g$, where L is a blurring matrix, f is the true image and g is constructed from the low-resolution frames. This system is solved for f using reconstruction and decomposition algorithms derived from wavelet theory.

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PP0

Efficient and Load Balanced Force Decomposition Algorithm for Parallel Molecular Dynamics Simulations

An algorithm, based on equal partitioning of the force matrix onto processors is presented. Asynchronous communications efficiently hide communication between processors. Communication is reduced by i) exchanging only non-redundant information between processors and ii) sorting particles according to a space-filling Hilbert curve. Load-balancing is implemented by i) distributing equal number of interactions on each processor or ii) balancing the time spent in the force routine. Results show good scaling behavior especially for non-homogenous systems.

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A Parallel 2-Dimensional Wavelet Transformation

The 2-dimensional Wavelet transform T, formulated as a product of three matrices $T = W^t AW$, is parallelized. The sparsity of W is used explicitly to implement the algorithm as a double loop over an upper triangular matrix. Parallelization is performed by a scaled version of equal sub-areas of the triangular matrix, where processors work independently on each sub-area. Scalability is shown, but not limited, up to 128 processors.

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Novel Computational and Statistical Approaches to Whole Genome Association Analysis

In human genetics, recent technological developments have created an explosion of whole genome single nucleotide polymorphism (SNP) data and, consequently, substantial analytical challenges. We describe an analysis toolset, PLINK, offering efficient implementations of existing methods (basic association statistics, sample matching based on inferred ancestry) as well as novel approaches including a shared segment analysis using hidden Markov models. We describe the algorithms and their implementation in PLINK and also a user-friendly GUI, gPLINK.

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Strongly Anisotropic Cahn-Hilliard Models

We compare different approaches for modeling strongly anisotropic crystal and epitaxial growth using regularized, anisotropic Cahn-Hilliard-type equations. When the surface anisotropy is sufficiently strong, sharp corners form and unregularized anisotropic Cahn-Hilliard equations become ill-posed. Our models contain high order Willmore and linear regularizations to remove the ill-posedness. Then we provide matched asymptotic analysis to show the convergence of the diffusive interface model to the usual sharp interface model. We also present 2D and 3D numerical results by adaptive finite-difference methods.

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PP0

Polarizability of Zeolitic Broensted Acidic Sites

The interacting induced-dipoles polarization model, implemented in POLAR, is used for calculation of effective polarizability of zeolitic bridged OH group, which results much higher than that of the free silanol group. A high polarizability is also calculated for the bridged OH group with a Si^{4+}, in absence of Lewis-acid promotion of silanol by Al^{3+}. Only when cations are located in the zeolite micropore, next to tetrahedra that contain trivalent cations, are large electrostatic fields generated.

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PP0

An Efficient Computational Tool Approaching Multiscale Environments

In designing multiscale models process information are reported at multiple levels of resolution commonly involving

operations such as discrete convolution and upsampling. In this paper a non recursive computational tool which allows to follow the evolution of a process across the scales by using suitable vectors weight and involving only initial data sampling is provided. B-spline functions are well-known in designing representation at different scales; experiments involving centered cardinal B-spline functions are provided.

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PP0

Performance Scalings of the Extended MHD NIMROD Code

The NIMROD code is a production-level code for solving the extended magnetohydrodynamic equations for fusion applications and is part of the Center for Extended Magnetohydrodynamic Modeling (CEMM) SciDAC. In this work, we will show results of studies aimed at understanding the various factors influencing the parallel performance of the time consuming matrix solves for production-level problems. We will especially focus on the performance of the SuperLU preconditioner, and the effectiveness of using METIS graph partitioning for the matrix reordering.

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PP0

Atomistic Psuedopotential Simulation of Nanometer Sized CMOS Devices

When the size of a CMOS is shrunk to 10-20 nm, quantum mechanical device simulation becomes necessary. We have developed a method to calculate the electronic structures and I-V curves of million atom CMOS devices using atomistic pseudopotentials. The electronic structure is described by an empirical pseudopotential, and the Hamiltonian is diagonalized using a linear combination of bulk band algorithm. This approach is more accurate than the traditional effective mass method.

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Model-Based Xampling for Bayesian Inverse Problems

For large scale problems, the computational cost of evaluating the forward model is one of the limiting factors of using the Bayesian approach for inverse problems. The standard methods used to sample the posterior distribution generally only use evaluations of the forward problem as input information. We investigate using model-based information, (e.g., the Hessian of a misfit function), to reduce the computation cost of sampling the posterior distribution.

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PP0

Components of a Hybrid Algorithm for Stochastic Compressible Navier-Stokes

The Landau-Lifshitz Navier-Stokes (LLNS) equations use stochastic fluxes to describe fluctuating hydrodynamics. This poster examines explicit Eulerian discretizations of LLNS; we find that the third-order Runge-Kutta integrator accurately produces density fluctuations while advancing with large time steps. A variety of numerical tests are considered, comparing candidate stochastic LLNS PDE solvers with theory and with molecular simulations. The PDE solver and molecular simulation will be coupled to form a multiscale hybrid method.

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Flux Surface-Following Discretization of Magnetic Reconnection

A dynamic flux surface-following solution-adaptive grid algorithm is proposed for the numerical simulation of the magnetic reconnection problem expressed by 2D resistive Hall magnetohydrodynamic equations. The transformation is designed to capture solution features, especially the x-point and o-point structures of the reconnection with precision, while reducing resolution requirements tangent to the surfaces. The parallel, fully coupled, nonlinearly implicit Newton-Krylov-Schwarz algorithm is used to allow a time step based on accuracy and independent of stability considerations.

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Generalized Analytic Functions in 3D Axially Symmetric Stokes Flows

A class of generalized analytic functions, defined by a special case of the Carleman system that arises in 3D asymmetric problems of hydrodynamics of Stokes flows, stationary electromagnetic fields in conductive materials, etc., has been considered. Hilbert formulas, establishing relationships between the real and imaginary parts of a generalized analytic function from this class, have been derived for the domains exterior to the contour of spindle, lens, bi-spheres and torus in the meridional cross-section plane. This special case of the Carleman system has been reduced to a second-order difference equation with respect to either the coefficients in series or densities in integral representations of the real and imaginary parts. For spindle and lens, the equation has been solved in the framework of Riemann boundary-value problems in the class of meromorphic functions. For torus, the equation has been solved by means of the Fourier transform, while for bi-spheres, it has been solved by an algebraic method. As examples, analytical expressions for the pressure in the problems of the 3D axially symmetric Stokes flows about rigid spindle-shaped body, lens-shaped body, bi-spheres and torus have been derived based on the corresponding Hilbert formulas.

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PP0

Linear Scaling 3D Fragment Method for Petascale Nanoscience Simulations

$O(N)$ methods are needed to solve large-scale nanoscience problems (with 1000-1000000 atoms) effectively, where N is the number of atoms in the system. Unfortunately, most of $O(N)$ methods studied in the last decade have various numerical convergence problems and computer parallelization issues. We present a new $O(N)$ method which has an ab initio accuracy and scales linearly upto thousands of processors. This approach provides a practical way for future petascale computation in materials/nanomaterials science.

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Runge-Kutta-Chebyshev Projection Method

We present a fully explicit, stabilized projection method called the Runge-Kutta-Chebyshev (RKC) Projection method for the solution of incompressible Navier-Stokes systems. This method preserves the extended stability property of the RKC method for solving ODEs, and it requires only one projection per step. An additional projection on the time derivative of the velocity is performed whenever a second order approximation for the pressure is desired.

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Crystal Dissolution and Precipitation in Porous Media

We consider a one-phase Stefan problem modelling a dissolution and precipitation process in a porous medium. The model involves nonlinear and multi-valued exchange rates at the free boundary. Analytic results are presented for a one dimensional setting and computational results for one and two dimensional settings. For the one dimensional simulations, a coordinate transform and a finite difference method is used. The two dimensional simulations use an Arbitrary Lagrangian Eulerian method.

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