Ninth Copper Mountain Conference
on
Iterative Methods
April 2 – April 7, 2006

1. Workshops

• Monday 3 April, **Simulation Based Optimization**, George Biros and Eldad Haber

Simulation is a powerful tool in science and engineering for predicting the behavior of physical systems, particularly those that are governed by partial differential equations. Moreover, progress in algorithms and computational hardware has been responsible for improvements in simulation.

Using today's simulation tools it has now become practical to consider complex design problems, where we wish to determine parameters of large systems that maximizes a certain objective, and inverse problems where we wish to determine parameters whose behavior matches measured data. Examples of design problems include structural optimization, antenna design and process optimization. Geophysical imaging, biomedical imaging, weather data assimilations are just a few examples of inverse problems where the physics is governed by partial differential equations.

While these types of problems are naturally posed as optimization problems, they offer new challenges because of their large size, inexact derivatives (when available), and ill-posedness. Current software cannot be used because matrices of constraint gradients cannot be factored, and computing with null space bases can be exceedingly expensive. The goal of this workshop is to review methods for PDE-optimization problems and to expose researches to some open problems in the field.

• Wednesday 5 April, **Dynamic Data Driven Liquid Flows**, Craig Douglas

This workshop will be strictly hands on. It will introduce DDDAS techniques (see http://www.dddas.org) including dynamic modeling, errors, sensor operation, and the symbiotic relations between the sensors and the application.

We will simulate the level of a liquid in media that is porous in one boundary edge only and design from scratch an algorithm to maintain it at a fixed level on average even though the liquid is disappearing through the open boundary using a random step function.

We will develop convergence results initially using a semi-direct method, but some of the participants may end up with a random walk by the end of the workshop. We will iterate on the liquid problem until we develop a fast iterative (and convergent) algorithm that we have thoroughly tested. We will use the data from experiments to drive the entire methodology and the algorithms will drive how and when data is collected.

This workshop will be held in one of the local watering holes, not in the conference center. Sensor oversight and correction will be provided at the tables.

2. Presentations

Abstracts are presented in alphabetical order by speaker's surname.

Uncertainty and reliability analysis-based design optimization capabilities in the DAKOTA toolkit

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When using computational models to design devices or systems, appropriate modeling of uncertainties is crucial to ensure robust and reliable designs. This talk offers a survey of uncertainty quantification and reliability analysis techniques and demonstrates how they can be tightly integrated with optimization algorithms to determine designs that meet reliability and robustness constraints in addition to optimality criteria. Such optimization under uncertainty (OUU) capabilities, developed and implemented in Sandia National Laboratories' DAKOTA toolkit, will be surveyed. Novel problem formulations for reliability-based design optimization in realistic physical applications will be presented and examples of how advanced reliability methods can provide more accurate estimates of output uncertainty given.

Parallel coarse grid selection strategies

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Traditional coarse grid selection algorithms for algebraic multigrid use a strength of connection measure to select coarse degrees of freedom. The strength of connection is a heuristic used to determine the influences between degrees of freedom in M-matrices. Coarsening algorithms using a strength of connection are known to select ineffective coarse grids for some cases where the operator is not an M-matrix. Additionally, these methods do not consider other information such as the smoother to be used in the solve phase. Alternatively, compatible relaxation selects coarse grids without explicitly using a strength of connection measure. Instead, a smoother is applied to identify degrees of freedom where the smooth error is large. This information is then used to select the coarse grid. Recent work on compatible relaxation has produced viable serial implementations and useful theoretical results. The goal of this work is to produce effective and efficient parallel compatible relaxation methods. In this talk, parallel compatible relaxation implementations will be introduced and discussed, along with results from experiments on both structured and unstructured problems.

An additive Schwarz parallel approach to space-time finite elements for hyperbolic equations

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We study a time parallel space-time finite element approach for the nonhomogeneous wave equation using a continuous time Galerkin method and a time decomposition strategy for preconditioning. Space-time finite elements provide some natural advantages for numerical relativity in black hole simulations. With space-time elements, time-varying computational domains are straightforward, higher-order approaches are easily formulated, and both time and spatial domains can be discretized using a more general mesh. We present fully implicit examples in $1+1$, $2+1$, and $3+1$ dimensions using linear quadrilateral, hexahedral, and tesseractic elements. Krylov solvers with additive Schwarz preconditioning are used for solving the linear system. We introduce a time decomposition strategy in preconditioning which significantly improves performance when compared with unpreconditioned cases. Parallel performance results are also given.

A priori error bounds for eigenvalues approximated by the Ritz values

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The Rayleigh-Ritz method finds the stationary values of the Rayleigh quotient, called Ritz values, on a given trial subspace as optimal, in some sense, approximations to eigenvalues of a Hermitian operator A. When a trial subspace is invariant with respect to A, the Ritz values are some of the eigenvalues of A. Given two finite dimensional subspaces X and Y of the same dimension, such that X is an invariant subspace of A, the absolute changes in the Ritz values of A with respect to X compared to the Ritz values with respect to Y represent the absolute eigenvalue approximation error.

We estimate the error in terms of the principal angles between X and Y. There are several known results of this kind, e.g., for the largest (or the smallest) eigenvalues of A, the maximal error is bounded by a constant times the sine squared of the largest principal angle between X and Y. The constant is the difference between the largest and the smallest eigenvalues of A, called the spread of the spectrum of A.

We prove that the absolute eigenvalue error is majorized by a constant times the squares of the sines of the principal angles between the subspaces X and Y, where the constant is proportional to the spread of the spectrum of A, e.g., for Ritz values that are the largest or smallest contiguous set of eigenvalues of A, we show that the proportionality factor is simply one. Our majorization results imply a very general set of inequalities, and some of the known error bounds follow as special cases. Majorization results of this kind are not apparently known in the literature and can be used, e.g., to derive novel convergence rate estimates of the block Lanczos method.

Multilevel homogenization techniques for the cardiac bidomain equations

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The cardiac bidomain equations are a set of nonlinear partial differential equations that are used to model the flow of current within cardiac tissue by treating intracellular and extracellular space as two interpenetrating domains. In the past 10 years research groups around the world have been using the bidomain equations in a variety of sophisticated ways, from modeling fibrillation in the human heart to understanding how plunge electrodes affect potential fields during in vitro experiments on cardiac tissue. The Bioengineering Institute at the University of Auckland has been a world leader in imaging cardiac tissue at a microscale resolution, and discovering specialized features that can be incorporated into the bidomain model.

In this talk, I will briefly introduce the Bioengineering Institute's imaging work, and then focus on how we are using these imaging results in our modeling framework. This discussion will focus on how we are using Black Box Multigrid to generate homogenized models that take into account the discontinuities found at the mezoscale. Such models allow the effect of the discontinuous cardiac structures to be seen in the potential fields at a reduced cost. This work is founded upon the multilevel upscaling approach of MacLachlan and Moulton (Water Resources Research, 2005), and begins exploring their ideas in three-dimensions and in a time-dependent framework.

The representer method for data assimilation of two phase flow in porous media

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Advances in instrumenting and imaging the subsurface are yielding large data sets, making data assimilation vital to modeling flow through porous media. We derive and implement the representer method applied to the oil/water model for reservoirs, a nonlinear model. The representer method, like the Kalman filter, solves the Euler-Lagrange (E-L) system for the minimizer of a least-squares functional of the misfit between the model and measurements. Because the representer method uses the superposition principle, a nonlinear model requires linearization of the E-L system. A key concern is finding a linearization that converges appropriately. We show that convergence is strongly affected by the choice of weights in the least-squares functional. We also compare the effects of linearization and the computational costs of the representer method with the ensemble Kalman filter.

A numerical bifurcation analysis of the Ornstein-Zernike equation

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The isotropic Ornstein-Zernike (OZ) equation

$$h(r) = c(r) + \rho \int_{\mathbb{R}^3} h(\|\mathbf{x} - \mathbf{y}\|)c(\|\mathbf{y}\|)d\mathbf{y}, \qquad (1)$$

that is the subject of this paper was presented almost a century ago to model the molecular structure of a fluid at varying densities. In order to form a well-posed mathematical system of equations from (1) that can be solved, at least in principle, we assume the existence of a closure relationship. This is an algebraic equation that augments (1) with a pointwise constraint that is deemed to hold throughout the fluid and it forces a relationship between the total and direct correlation functions (h and c respectively).

Some closures have a mathematically appealing structure in the sense that the total correlation function is posed as a perturbation of the *Mayer f-function* given by

$$f(r) = -1 + e^{-\beta u(r)}.$$

This perturbation depends on the potential u, temperature (essentially $1/\beta$) and the indirect correlation function through a nonlinear function that we denote G:

$$h = f(r) + e^{-\beta u(r)}G(h - c), \qquad (G(0) = 0), \qquad (2)$$

so that (1-2) are solved together with β and ρ as bifurcation parameters. There are many closures in use and if we write $\exp_1(z) = -1 + e^z$ then the hyper-netted chain (HNC) closure

$$G(\gamma) = \exp_1(\gamma) \qquad (3)$$

has the form of (2) and is popular in the physics and chemistry literature.

The purpose of the talk is show that *any reasonable* discretisation method applied to (1-2) suffers from an inherent defect if the HNC closure is used that can be summarised as follows: phase transitions lead to fold bifurcations. The existence of a phase transition is characterised by the existence of a bifurcation at infinity with respect to h in an L^1 norm at a certain density, such that boundedness of h is maintained in a certain L^p norm. This behaviour is difficult to mimic computationally by projecting onto a space of fixed and finite dimension and, as a result, projections of (1-2) can be shown to undergo at least one fold bifurcation if such a bifurcation at infinity is present. However, other popular closure relations do not necessarily suffer from the same defect.

Model reduction of large scale second-order systems with modal damping

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An approach is described for model reduction of second-order systems with types of normal mode damping that include the most common varieties: proportional damping and square-root damping. We show that unlike the general case that requires usage of a second-order Krylov subspace structure, one can build up instead approximating subspaces satisfying all required conditions much more cheaply as direct sums of standard rational Krylov subspaces within much smaller component subspaces.

We give a detailed analysis of the distribution of system poles, and then, through descriptive bounds that carry the flavor of classical approximation theory, we are able to exploit the structure of these poles to obtain asymptotically optimal shift selection strategies. Numerical examples are provided to illustrate and support the analysis.

An augmented Lagrangian approach for the Oseen problem

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We describe an effective solver for the discrete Oseen problem based on an augmented Lagrangian formulation of the corresponding saddle point system. The proposed method is a block triangular preconditioner used with a Krylov subspace iteration (BiCGStab). The crucial ingredient is a novel multigrid approach for the (1,1) block, which extends a technique introduced by Schöberl for elasticity problems to nonsymmetric problems. Our analysis indicates that this approach results in fast convergence, independent of the mesh size and largely insensitive to the viscosity. We present experimental evidence for both isoP2-P0 and isoP2-P1 finite elements in support of our conclusions. We also show results of a comparison with a state-of-the-art coupled multigrid solver, showing the competitiveness of our approach.

Discrete network approximation for singular behavior of the effective viscosity of concentrated suspensions

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We present a new approach for calculation of effective properties of high contrast random composites and illustrate it by considering highly packed suspensions of rigid particles in a Newtonian fluid.

The main idea of this approach is a reduction of the original continuum problem, which is described by PDE with rough coefficients, to a discrete random network. This reduction is done in two steps which constitute the "fictitious fluid" approach. In Step 1 we introduce a "fictitious fluid" continuum problem when fluid flows only in narrow channels between closely spaced particles, which reflects physical fact that the dominant contribution to the dissipation rate comes from these channels. In Step 2 we derive a discrete network approximation for the latter continuum problem.

Next we use this approach to calculate the effective viscous dissipation rate in a 2D model of a suspension. We show that under certain boundary conditions the model exhibits an anomalously strong rate of blow up when the concentration of particles tends to maximal. We explore physical ramification of this phenomenon.

We will also discuss how an iterative procedure of the network construction which may be used in the study of dynamics of highly packed suspensions.

Algebraic multigrid and convection diffusion problems

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The talk discusses the use of algebraic multigrid (AMG) when solving discrete convection diffusion problems. For practical applications, e.g. modeling incompressible fluid flow, the interest is in using AMG as a preconditioning component within a Krylov subspace solver like GMRES. To be effective in this role, the AMG method should be 'black box', i.e. require no user tuning, and be effective in the sense that if applied as a solver for a convection-diffusion subproblem then iteration counts are independent of mesh size and other problem parameters.

When designing AMG for convection diffusion, it is necessary to consider the interplay between wind direction and AMG smoothing scheme. Numerical test data is presented showing performance for AMG applied to streamline diffusion stabilized finite element discretizations of model problems. The results demonstrate the crucial importance of choosing an appropriate smoothing scheme. The performance of a "well-chosen" AMG method in the context of pressure-convection diffusion preconditioning of the Navier-Stokes equations will also be discussed.

This is ongoing work. It is funded by EPSRC grant EP/C000528/1.

Compatible relaxation and coarsening in algebraic multigrid

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Algebraic multigrid (AMG) has been shown to be an efficient iterative solver for many of the large and sparse linear systems arising from the discretization of partial differential equations. There remain, however, many classes of problems for which conventional AMG setup algorithms, based on the properties of M-matrices, are inappropriate.

In this talk, we consider the use of compatible relaxation (CR) as a tool for extending the applicability of AMG. A CR-based coarsening algorithm is presented along with numerical results demonstrating that the variational multigrid solver resulting from the proposed approach maintains multigrid-like optimality, without the need for parameter tuning, for some problems where current algorithms exhibit degraded performance.

Quasi-Newton preconditioners for the iterative solution of nonlinear equation in porous media

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In this work preconditioners for solving the linear systems of the Newton method in each nonlinear iteration are studied. The preconditioners are defined by means of a Broyden-type rank-one update at each nonlinear iteration, as described in [1]. We report numerical results of the application of this approach for the solution of the nonlinear system of algebraic equations arising from the finite element discretization of two-phase flow model in porous media. Sequential and parallel results show that the efficiency of the proposed method. The parallel version of the algorithm uses the FSAI approximate inverse as initial preconditioner [2]. The obtained performances show that the high cost of the FSAI evaluation is amortized by the efficiency of the subsequent Broyden updates.

[1] L. Bergamaschi, R. Bru, A. Martinez and M. Putti, *Quasi-Newton Preconditioners for the Inexact Newton Method*, to appear in Electr. Trans. on Num. Analysis, 2006.

[2] L. Yu. Kolotilina and A. Yu. Yeremin, *Factorized sparse approximate inverse preconditionings. I. Theory*, SIAM J. Matrix Anal. Appl., **14** (1993) 45–58.

Improving coarsening and interpolation for algebraic multigrid

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Algebraic multigrid (AMG) is one of the most efficient algorithms for solving large sparse linear systems on unstructured grids. Classical coarsening schemes such as the standard Ruge-Steuben method [1] can lead to adverse effects on computation time and memory usage that affect scalability. Memory and execution time complexity growth is remedied for various large three-dimensional (3D) problems using the parallel modified independent set (PMIS) coarsening strategy developed by De Sterck, Yang, and Heys [2]. However, this coarsening strategy often leads to erratic grids without a regular structure that diminish convergence. This talk looks at a modification of the PMIS algorithm that consistently produces more uniform coarsenings, and significantly improves convergence properties over the original PMIS algorithm. Improvements of existing interpolation schemes and application of the resulting methods to several problems are also examined.

[1] J. Ruge, K. Stueben, *Algebraic multigrid (AMG)*, Multigrid Methods v.3, Frontiers in Applied Mathematics, S. McCormick, ed., SIAM (1987) 73–130.

[2] H. De Sterck, U. M. Yang, and J. J. Heys, *Reducing Complexity in Parallel Algebraic Multigrid Preconditioners*, to appear in SIAM J. Matr. An. and Applications, 2006.

New iterative eigensolvers and preconditioners for electronic structure calculations in nano and materials science

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Density functional based electronic structure calculations have become the most heavily used approach in materials science to calculate materials properties with the accuracy of a full quantum mechanical treatment of the electrons. This approach results in a single particle form of the Schrödinger equation which is a non-linear eigenfunction problem. The standard self-consistent solution of this problem involves solving for the lowest eigenpairs corresponding to the electrons in the system. In non-self-consistent formulations the problem becomes one of determining the interior eigenpairs corresponding to the electrons of interest which are typically around the gap in the eigenvalue spectrum for non-metallic systems.

In this talk I will present results for new iterative eigensolvers based on conjugate gradients (the LOBPCG method) in the context of plane wave electronic structure calculations. This new method gives significant speedup over existing conjugate gradient methods used in electronic structure calculations. I will also present results for a new preconditioner based on first solving the bulk structure corresponding to a given nanosystem and then using that as a preconditioner to solve the nanosystem.

This new preconditioner gives significant speedup compared to previously used preconditioners based on the diagonal of the matrix. These new methods will be demonstrated for CdSe quantum dots as well as quantum wires constructed from layers of InP and InAs. This work was supported by the Director, Office of Advanced Scientific Computing Research, Division of Mathematical, Information and Computational Sciences of the U.S. Dept. of Energy and the Laboratory Directed Research and Development Program of Lawrence Berkeley National Laboratory under contract number DE-AC03-76SF00098.

A fully implicit extended 3D MHD solver

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We present results from our research on Jacobian-free Newton-Krylov (JFNK) methods applied to the time-dependent, primitive-variable, 3D extended magnetohydrodynamics (MHD) equations. MHD is a fluid description of the plasma state. While plasma is made up of independent (but coupled) ion and electron species, the standard MHD description of a plasma only includes ion time and length scales (one-fluid model). Extended MHD (XMHD) includes nonideal effects such as nonlinear, anisotropic transport and two-fluid (Hall and diamagnetic) effects. XMHD supports so-called dispersive waves (whistler, ion acoustic), which feature a quadratic dispersion relation $\omega \sim k^2$. In explicit time integration methods, this results in a stringent CFL limit $\Delta t_{CFL} \propto \Delta x^2$, which severely limits their applicability to the study of long-frequency phenomena in XMHD.

A fully implicit implementation promises efficiency (by removing the CFL constraint) without sacrificing numerical accuracy [1]. However, the nonlinear nature of the XMHD system and the numerical stiffness of its fast waves make this endeavor very difficult. Newton-Krylov methods can meet the challenge provided suitable preconditioning is available.

We propose a successful preconditioning strategy for the 3D primitive-variable XMHD formalism. It is based on "physics-based" ideas [2,3], in which a hyperbolic system of equations (which is diagonally submissive for $\Delta t > \Delta t_{CFL}$) is "parabolized" to arrive to a diagonally dominant approximation of the original system, which is multigrid-friendly. The use of approximate multigrid (MG) techniques to invert the "parabolized" operator is a crucial step in the effectiveness of the preconditioner and the scalability of the overall algorithm. The parabolization procedure can be properly generalized using the well-known Schur decomposition of a 2×2 block matrix. In the context of XMHD, the resulting Schur complement is a system of PDEs that couples the three plasma velocity components, and needs to be inverted in a coupled manner. Nevertheless, a system MG treatment is still possible since, when properly discretized, the XMHD Schur complement is block diagonally dominant by construction, and block smoothing is effective.

In this presentation, we will discuss the derivation and validity of the physics-based preconditioner for resistive MHD and its generalization to XMHD, the connection with Schur complement analysis, and the system-MG treatment of the associated systems. A novel second-order, cell-centered, conservative finite-volume discretization has been recently developed [4] for the XMHD system above, and will be used in this work. It is suitable for general curvilinear geometries, solenoidal in **B** and **J**, numerically non-dissipative, and linearly and nonlinearly stable. We will demonstrate the algorithm using the GEM challenge configuration [5]. Grid convergence studies will demonstrate that CPU time scales scale optimally as $\mathcal{O}(N)$, where N is the number of unknowns, and that the number of Krylov iterations scales as $\mathcal{O}(N^0)$. Time convergence studies will demonstrate a favorable scaling with time step $\mathcal{O}(\Delta t^\alpha)$, with $\alpha < 1.0$.

[1] D. A. Knoll, L. Chacón, L. G. Margolin, and V. A. Mousseau, J. Comput. Phys. **185** (2003) 583.

[2] L. Chacón, D. A. Knoll, and J. M. Finn, J. Comput. Phys., **178** (2002) 15.

[3] L. Chacón and D. A. Knoll, J. Comput. Phys., **188** (2003) 573.

[4] L. Chacón, Comp. Phys. Comm., **163** (2004) 143.

[5] J. Birn et al., J. Geophys. Res., **106** (2001) 3715.

Preconditioning analysis for weighted Toeplitz regularized least squares problems

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We consider preconditioners for weighted Toeplitz regularized least squares (WTRLS) problems

$$\min_z \|Az - b\|_2^2$$

where the rectangular coefficient matrix A and the right-hand side vector b are of the form:

$$A = \begin{bmatrix} W_1 H \\ \mu W_2 L \end{bmatrix} \in \mathbb{R}^{(m_1+m_2)\times m_1} \quad \text{and} \quad b = \begin{bmatrix} W_1 f \\ 0 \end{bmatrix} \in \mathbb{R}^{m_1+m_2}.$$

Here $H \in \mathbb{R}^{m_1\times m_1}$ is a Toeplitz matrix, $L \in \mathbb{R}^{m_2\times m_1}$ is the first-order or second-order difference matrix, $W_1 \in \mathbb{R}^{m_1\times m_1}$ and $W_2 \in \mathbb{R}^{m_2\times m_2}$ are non-scalar diagonal matrices with real positive entries, $f \in \mathbb{R}^{m_1}$ is a given right-hand side vector and $\mu > 0$ is a regularization parameter.

Iterative methods using circulant preconditioners has been proposed since 1980s. The efficiency of solving systems are greatly enhanced by these indirect methods. Since then, preconditioners based on circulant matrices were suggested for solving the WTRLS problems. However, most of them do not perform satisfactorily and the results of convergence rates can be disappointing.

Benzi and Ng considered the above system where $W_2 L$ is replaced by I, and proposed a new approach to solve it which is based on an augmented system formulation. We now adopt a similar approach that transforms the problem into a 3×3 block linear system.

The WTRLS problems turn out to be a quadratic minimization problem, which is equivalent to solving the linear system

$$(H^T W_1^{-2} H + \mu^2 L^T W_2^{-2} L) z = H^T W_1^{-2} f \ .$$

The above linear system can overall be rewritten as the following 3×3 block system:

$$\begin{bmatrix} W_1^{-2} & 0 & H \\ 0 & W_2^{-2} & \mu L \\ H^T & \mu L^T & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -H^T W_1^2 f \end{bmatrix} \ .$$

There are not any particular results discussing how to solve a general 3×3 system effectively. The four upper left blocks are considered as one single block and the corresponding two upper right blocks $[H^T \ \mu L^T]^T$ together still attain full rank, so we treat this system as a 2×2 block case and consider methods developed for solving indefinite systems. Here we shall adopt constraint preconditioner and Hermitian skew-Hermitian splitting (HSS) preconditioner and investigate them in details.

The formulation and actual preconditioning settings for WTRLS problems will be discussed. A test problem is performed to demonstrate the convergence behaviour using these iterative methods. We shall see that the number of iterations mainly depend on the condition numbers of W_1 and W_2 as well as some factors related to each preconditioners. In particular, this effect is more significant in the case of using HSS preconditioner. The iteration results and the weaknesses for both preconditioners can be explained with some analyses on the spectra for them.

Some new results in derivative free optimization

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Some new results on derivative free methods will be presented. These have broader implications for, for example, second-order trust-region methods.

Uniformly well-conditioned pseudo-arclength continuation

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Numerical continuation is the process of solving nonlinear equations of the form

$$G(x, \lambda) = 0$$

for various real number parameter values, λ. The obvious approach, called natural parameterization, is to perturb λ with each continuation step and find the corresponding solution x via a nonlinear solver (Newton's method). While this approach is reasonable for paths containing only regular points (points (x, λ) where the Jacobian matrix of G is nonsingular), the approach breaks down at simple fold points where the Jacobian matrix of G becomes singular and Newton's method fails.

In order to remedy this, one may implement pseudoarclength continuation (PAC) which introduces a new parameter based on the arclength s of the solution path. In order to implement PAC, one converts the old problem $G(x, \lambda) = 0$ to a new problem

$$F(x(s), \lambda(s)) = 0.$$

Using PAC on the new problem requires the Jacobian matrix of F, F', which ought to be nonsingular at both regular points and simple folds if we have indeed bypassed the problem that natural parameterization presents.

While the nonsingularity of F' at regular points and simple folds is a known fact, we present a theorem that gives conditions under which F' is uniformly nonsingular for a path containing simple folds. We do this by bounding the smallest singular value of F' from below. The theorem justifies the use of PAC in a practical way for solution curves containing nothing "worse" than a simple fold.

Interpolation operators for algebraic multigrid by local optimization

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An approach is presented to construct the interpolation operators of algebraic multigrid (AMG) based on solving a series of local optimization problems. Given a set of coarse nodes, the approach first attempts to maximize the support of these nodes without introducing additional nonzeros in the stiffness matrix of the next coarser level. By doing so, it is possible to reduce the energy of coarse interpolations without increasing operator complexity.

The local optimization problems are formulated in such a way that the problem null space can be represented exactly at each multigrid level. In addition, a condition ensuring nonsingularity of a local matrix highlights the need for special considerations when the null space dimension exceeds the number of unknowns for each node. Numerical examples for the Poisson equation and linear elasticity demonstrate the effectiveness of the approach and the optimal performance of an ensuing AMG preconditioner. Connections with element-free AMGe are also described.

Constraint-style preconditioners for regularized saddle point problems

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The problem of finding good preconditioners for the numerical solution of a certain important class of indefinite linear systems is considered. These systems are of a saddle point structure

$$\begin{pmatrix} A & B^T \\ B & -C \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} c \\ d \end{pmatrix},$$

where $A \in \mathbb{R}^{n\times n}$, $C \in \mathbb{R}^{m\times m}$ are symmetric, and $B \in \mathbb{R}^{m\times n}$ has full rank.

In *Constraint preconditioning for indefinite linear systems*, SIAM J. Matrix Anal. Appl. **21** (2000), Keller, Gould and Wathen analyzed the idea of using constraint preconditioners that have a specific 2 by 2 block structure for the case of C being zero. We shall extend this idea by allowing the (2,2) block to be non-zero. Results concerning the spectrum and form of the eigenvectors are presented, as are numerical results to validate our conclusions. We will also introduce the idea of implicit-factorization constraint preconditioners which allow us to efficiently carry out the required preconditioning steps.

Filter factor analysis of an iterative multilevel regularizing method

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Recent results have shown that iterative methods of multigrid type are very effective for regularizing purposes. In short, the reconstruction quality is of the same level or slightly better than that related to well-known regularizing procedures such as Landweber or conjugate gradient (CG) for normal equations, but the associated computational cost is highly reduced.

Here we analyze the filter features of one of these multigrid techniques in order to provide a theoretical motivation for the excellent regularizing characteristics experimentally observed in the discussed methods.

Scaling models and data for solving large sparse linear systems: a comparison of methods

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As industrial problems may involve different kinds of physical parameters and different types of coupled equations, ill-conditioned sparse linear systems may arise from the discretization method. Let $Au = f$ be a nonsingular sparse linear system where $A \in \mathbb{C}^{n\times n}$, and $u, f \in \mathbb{C}^n$. If the spectral condition number $\kappa(A)$ is too far from one, direct solvers can lack of accuracy and iterative methods can fail to converge. An economical way of avoiding these difficulties is to find two diagonal matrices D_r and D_c such that $\kappa(D_r A D_c) \approx \min_{D_1,D_2} \kappa(D_1 A, D_2)$. Then, the solving process becomes

1. compute $\hat{u}$ such that $\hat{A}\hat{u} = \hat{f}$
2. compute $u = D_c\hat{u}$

where $\hat{A} = D_r A D_c$ and $\hat{f} = D_r f$. Numerical properties of $\hat{A}$ differ according to the scaling method; it can have normalized rows/columns [2] or it can be approximately doubly stochastic [3]. Other methods make the matrix have arbitrary row/column sums [1]. In this paper, we propose to make clear the interests of scaling corrections for supernodal and multifrontal direct solvers and for preconditioned iterative methods on industrial applications based on Maxwell equations (coupled problems, nonlinear materials, moving structures, transient problems) and discretized by means of nodal or edge finite elements.

[1] N. Linial, A. Samorodnitsky, A. Wigderson, *A deterministic strongly polynomial algorithm for matrix scaling and approximate permanents*, Combinatorica **20** (200) 531–544.

[2] O. E. Livine, G. H. Golub, *Scaling by Binormalization.*

[3] D. Ruiz, *A Scaling Algorithm to Equilibrate Both Rows and Columns Norms in Matrices*, RAL-TR-2001-034.

Actually doing dynamic data-driven application simulations (in 4 parts)

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This is a four part talk to introduce DDDAS concepts before the Wednesday night workshop.

Part I: Introduction to DDDAS and Its Impact on High Performance Computing Environments
Craig Douglas

DDDAS is a paradigm whereby an application (or simulation) and measurements become a symbiotic feedback control system. DDDAS entails the ability to dynamically incorporate additional data into an executing application, and in reverse, the ability of an application to dynamically steer the measurement process. Such capabilities promise more accurate analysis and prediction, more precise controls, an d more reliable outcomes. The ability of an application to control and guide the measurement process and determine when, where, and how it is best to gather additional data has itself the potential of enabling more effective measurement methodologies. Furthermore, the incorporation of dynamic inputs into an executing application invokes new system modalities and helps create application software systems that can more accurately describe real world, complex systems. This enables the development of applications that intelligently adapt to evolving conditions and that infer new knowledge in ways that are not predetermined by the initialization parameters and initial static data.

DDDAS creates a rich set of new challenges for applications, algorithms, systems software, and measurement methods. DDDAS research typically requires strong, systematic collaborations between applications domain researchers and mathematics, statistics, and computer sciences researchers, as well as researchers involved in the design and implementation of measurement methods and instruments. Consequently, most DDDAS projects involve multidisciplinary teams of researchers.

In addition, DDDAS enabled applications run in a different manner than many traditional applications. They place different strains on high performance systems and centers. In this talk, we will also categorize some of these differences.

Part 2: Problem Solving Environments for DDDAS
Chris R. Johnson and Steven G. Parker

One of the significant challenges for DDDAS is to create software infrastructure and tools that help DDDAS researchers tackle the multidisciplinary, often large-scale, dynamically coupled problems described in the previous presentation.

DDDAS problems often require using multiple software frameworks and packages, which leads to the significant software architecture challenge of integrating and providing interoperability of different software frameworks, packages, and libraries. Our approach to this challenge is to create software "bridges" using a meta-component model that allows the user to easily connect one software framework or package to another.

The new system (currently called SCIRun2, but that will change very soon) support the entire life cycle of scientific applications by allowing scientific programmers to quickly and easily develop new techniques, debug new implementations, and apply known algorithms to solve novel problems. SCIRun2 also contain many powerful visualization algorithms for scalar, vector, and tensor field visualization, as well as image processing tools.

In this presentation, we will provide examples of DDDAS software integration.

Part 3: The Impact of DDDAS on Wildland Fire Modeling and Fire Front Tracking
Janice Coen and Jan Mandel

In this talk, we will describe an application to which DDDAS concepts are being applied. Wildland fire modeling involves a numerical weather prediction model that is two-way coupled to a fire behavior model, so that the fire can create its own weather. This is an extremely challenging computational problem with limited predictability because of the uncertainty in fire behavior in addition to uncertainties in weather modeling. It is also difficult to obtain observations near a wildfire. Thus, DDDAS concepts have great potential in advancing this area. In this work, we will describe techniques we have been applying to introduce DDDAS concepts into what was a traditional modeling approach. We define a novel partial differential equation based model for wildland fires instead of the usual stochastic based model. We will show where a DDDAS approach can provide a breakthrough in fire front tracking that can be transmitted to the people on the mountainsides through both computational science and high tech advances.

Part 4: Out of Time Order Kalman Filtering for DDDAS Data Assimilation
Jan Mandel and Jonathan Beezley

We present the basic principles of data assimilation by ensemble filtering. These methods run a collection of randomly perturbed simulations, called an ensemble. From time to time, the ensemble is modified by creating linear combinations found by solving a least squares problem to match the data. We describe new developments needed to accommodate strongly nonlinear wildfire models and sparse data. The new methods include Tikhonov-like regularization in a Bayesian probabilistic framework and new hybrid deterministic/stochastic ensemble methods for non-Gaussian distributions, based on the theory of probability measures on Sobolev spaces. We also discuss a space-time ensemble approach to assimilate data arriving out of order.

Wednesday night, April 5, Workshop on Dynamic Data Driven Liquid Flows
Douglas, Johnson, Coen, Mandel

This workshop will be strictly hands on. It will introduce DDDAS techniques (see http://www.dddas.org) including dynamic modeling, errors, sensor operation, and the symbiotic relations between the sensors and the application.

We will simulate the level of a liquid in media that is porous in one boundary edge only and design from scratch an algorithm to maintain it at a fixed level on average even though the liquid is disappearing through the open boundary using a random step function.

We will develop convergence results initially using a semi-direct method, but some of the participants may end up with a random walk by the end of the workshop. We will iterate on the liquid problem until we develop a fast

iterative (and convergent) algorithm that we have thoroughly tested. We will use the data from experiments to drive the entire methodology and the algorithms will drive how and when data is collected.

This workshop will be held in one of the local watering holes, not in the conference center. Sensor oversight and correction will be provided at the tables.

An abstract method for extending two-level preconditioners to multilevel preconditioners of comparable quality

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We present an abstract method for designing a multilevel preconditioner given a two-level preconditioner for an operator with positive definite symmetric part.

If we denote by A_{fine} and A_{coarse} two discrete versions of a continuous operator, then a two-level preconditioner T_{fine} for A_{fine} can be described in general by a function $T_{\text{fine}} = \mathcal{F}(A_{\text{coarse}}^{-1}, A_{\text{fine}})$, where it is assumed that the evaluation of $\mathcal{F}$ requires a level-independent number of applications of A_{fine} and k applications of A_{coarse}^{-1} ($k = 1$ or 2). The natural extension to a multilevel preconditioner, consisting in replacing in T_{fine} the call to A_{coarse}^{-1} with a recursive call to $\mathcal{F}$, is known to sometimes produce multilevel preconditioners of lower quality (e.g., for certain types of inverse problems). Based on the idea that inverting A_{fine} essentially means to solve the nonlinear equation $X^{-1} - A_{\text{fine}} = 0$, we define our multigrid preconditioner to be the first Newton iterate of the map $X \mapsto X^{-1} - A_{\text{fine}}$ starting at the "natural" multilevel preconditioner. For $k = 1$, the resulting algorithm has a W-cycle structure, and differs only slightly from the textbook version of the W-cycle. Moreover, the method guarantees that the resulting preconditioner maintains the approximation quality of the initial two-level preconditioner. The quality of approximation is measured using a certain distance function, which determines the degree to which two operators with positive definite symmetric parts are spectrally equivalent. We apply this method to designing and analyzing a multigrid preconditioner for a linear advection-diffusion-reaction equation.

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On the convergence of additive Schwarz preconditioned GMRES

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Additive Schwarz preconditioners, when a coarse grid correction is added, are said to be optimal for certain discretized PDE problems, in the sense that bounds on the convergence of iterative methods are independent on the mesh size. Cai and Zou [1] showed with an example that in the absence of a coarse grid correction the usual GMRES bound has a factor of the order of $1/\sqrt{h}$. In this paper we consider the same one-dimensional example (as well as a two-dimensional counterpart) and show that the behavior of the method is not well represented by

the above mentioned bound. We use a different bound for GMRES from Simoncini and Szyld [2] and show that the relevant factor is bounded by $c - O(h)$, so that as $h \to 0$, it approximates a constant. Furthermore, for a sequence of meshes the convergence curves are almost identical and the number of GMRES iterations needed for convergence has a very slow growth.

[1] Numer. Linear Algebra Appl. **9** (2002) 379–397.

[2] SIAM Rev. **47** (2005) 247–272.

A note on GMRES preconditioned by a perturbed LDL^T decomposition with static pivoting

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This paper is concerned with solving the set of linear equations $Ax = b$ (1) where the coefficient matrix A is a symmetric indefinite sparse matrix. Our hope is to solve this system using a direct method that uses an accurate factorization of A but sometimes the cost of doing this is too high in terms of time or memory. We have therefore looked at the possibility of using static pivoting to avoid these problems which are particularly acute if the matrix is highly indefinite as for example can happen for saddle-point problems.

As our direct method we will use a multifrontal approach. In this approach we first determine an order for choosing pivots based on the sparsity structure of A (called the analysis step), and we then accommodate further pivoting for numerical stability during the subsequent numerical factorization phase. The problem when the matrix is highly indefinite is that the resulting pivot sequence used in the numerical factorization can differ substantially from that predicted by the analysis step. In the multifrontal context, the factorization can be represented by a tree at each node of which elimination operations are performed on a partially summed frontal matrix $\begin{pmatrix} F_{11} & F_{12} \\ F_{12}^T & F_{22} \end{pmatrix}$ (2) and pivots at that stage can only be chosen from within the fully summed block F_{11}. The problem occurs when it is impossible or numerically suicidal to eliminate all of F_{11} resulting in more work and storage (sometimes dramatically more) than forecast. A simple way to avoid this problem is to force the elimination of all of F_{11} through static pivoting.

We thus assume that the matrix A has been factorized using the HSL package `MA57` with the option of using static pivoting [1]. The static pivoting strategy will set the diagonal entry to $\pm\tau$ when it is impossible to find a suitable pivot in the fully summed blocks. It is common to choose $\tau \approx \sqrt{\varepsilon}\,||A||$ (ε machine precision).

Therefore, the computed factors $\hat{L}$ and $\hat{D}$ are, in exact arithmetic, the exact factorization of the perturbed problem $A+E = \hat{L}\hat{D}\hat{L}^T$ (3), where the matrix $|E| \leq \tau I$ is a diagonal matrix of rank equal to the number of static pivots used during the factorization. The nonzero diagonal entries in E correspond to the positions at which static pivoting was performed and they are all equal to τ in modulus. Note that if τ is chosen too small then the factorization could be very unstable whereas if it is chosen too large, the factorization will be stable but will not be an accurate factorization of the original matrix (that is, $|E|$ will be large).

Equation (3) gives a splitting of A in terms of $M = \hat{L}\hat{D}\hat{L}^T$ and E, $A = M - E$, and the solution of (1) can be expressed as the solution of the equivalent system $(I - M^{-1}E)x = M^{-1}b$ (4). If the spectral radius of the matrix $I - M^{-1}E$ is less than one, the system (4) can be solved using iterative refinement. This has been used by many authors, including [1] and is successful over a wide range of matrices although is somewhat sensitive to the value of τ. If, however, the spectral radius is greater or equal to one (or ≈ 1), it is necessary to switch to a more powerful

method like GMRES. Although the matrix is symmetric, we choose GMRES since it gives us much more freedom to work with a wide range of preprocessors and preconditionings.

We have found experimentally that using the factorization (3) as a preconditioning for GMRES works in most cases and is, as expected much more robust than iterative refinement. Indeed GMRES gives normwise backward stability in most cases, which is not the case for iterative refinement. However, there are cases where we do not get convergence to a scaled residual at machine precision.

We have, however, found that restarted GMRES performs better and that using FGMRES, even though our preconditioner remains constant, does even better.

We illustrate this through numerical experiment and then show theoretically that, under reasonable assumptions, FGMRES preconditioned by our static pivoting factorization is backward stable so that a small scaled residual can be achieved. Our analysis also holds for the case of restarted FGMRES that we advocate as a measure to control the memory requirement while still achieving the desired accuracy. Indeed we give theoretical arguments why the restarting often greatly improves the convergence.

[1] I. S. Duff and S. Pralet, *Towards a stable static pivoting strategy for the sequential and parallel solution of sparse symmetric indefinite systems*, Technical Report TR/PA/05/26, CERFACS, Toulouse, France, 2005. (Also available as RAL Report RAL-TR-2005-007 and IRIT Report RT/TLSE/05/04.)

Global optimization: for some problems, there's HOPE

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We present a new method for solving unconstrained minimization problems—Homotopy Optimization with Perturbations and Ensembles (HOPE). HOPE is a homotopy optimization method that finds a sequence of minimizers of a homotopy function mapping a template function to the target function, the objective function of our minimization problem. To increase the likelihood of finding a global minimizer, points in the sequence are perturbed and used as starting points to find other minimizers. Points in the resulting ensemble of minimizers are used as starting points to find minimizers of the homotopy function as it deforms the template function into the target function.

We show that certain choices of the parameters used in HOPE lead to instances of existing methods: probability-one homotopy methods, stochastic search methods, and simulated annealing. We use these relations and further analysis to demonstrate the convergence properties of HOPE.

The development of HOPE was motivated by the protein folding problem, the problem of predicting the structure of a protein as it exists in nature, given its amino acid sequence. However, we demonstrate that HOPE is also successful as a general purpose minimization method for nonconvex functions.

Numerical experiments performed to test HOPE include solving several standard test problems and the protein folding problem using two different protein models. In most of these experiments, standard homotopy functions are used in HOPE. Additionally, several new homotopy functions are introduced for solving the protein folding problems to demonstrate how HOPE can be used to exploit the properties or structure of particular problems.

Results of experiments demonstrate that HOPE outperforms several methods often used for solving unconstrained minimization problems—a quasi-Newton method with BFGS Hessian update, a globally convergent variant of Newton's method, and ensemble-based simulated annealing.

Iterative methods for use with the fast multipole method

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For many dense linear systems of size $N \times N$ the availability of an algorithm based on the fast multipole method (FMM) provides a matrix vector product with $O(N \log N)$ time and memory complexity. This reduces the cost of the matrix-vector product step in the iterative solution of linear systems, and for an iteration requiring N_{iter} steps, a complexity of of $O(N_{iter} N log N)$ can be expected. To bound N_{iter} appropriate pre-conditioning strategies must be used. However, many conventional pre-conditioning strategies rely on sparsity in the matrix, and applying them to these dense matrices requires computations that have a formal time or memory complexity of $O(N^2)$, which negates the advantage of the FMM.

We explore the application of two preconditioning strategies to the FMM. In the first, which was applied to the FMM solution of a multiple scattering problem for the Helmholtz equation in three dimensions, the system was solved using the flexible GMRES algorithm. The choice of the (right) preconditioning matrix was based on GMRES solution of a linear system with an approximation to the matrix that is based on a partitioning that is performed in the FMM itself. We describe details of this iterative technique and its performance on some large multiple scattering problems.

In the second iterative solution, we consider an iterative algorithm of Faul et al. [1] for the solution of the radial basis function (RBF) interpolation problem. In this problem the goal is to construct an interpolating function for a set of scattered data points, with the interpolating function expressed as a sum of RBFs centered at the data points. The iterative algorithm of Faul et al. can be accelerated by the use of the FMM for the matrix vector product required at each step. There however is a precomputation stage that requires the construction of approximate cardinal function interpolants centered at each data point and q of its neighbors ($q \ll N$), that are carefully selected. These interpolants are used to provide a Krylov basis for the iteration. The complexity of these preliminary calculations in Faul et al. is $O(N^2)$. We provide a modification to this set-up stage and reduce its complexity to linear order. Results will be presented for the interpolation of large data sets in two and three dimensions using multiquadric and polyharmonic radial basis functions.

[1] A. C. Faul, G. Goodsell, M. J. D. Powell, *A Krylov subspace algorithm for multiquadric interpolation in many dimensions*, IMA Journal of Numerical Analysis **25** (2005) 1–24.

Moment-of-fluid interface reconstruction

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Volume-of-fluid (VoF) methods [2] are widely used in Eulerian simulations of multi-phase flows with mutable interface topology. The popularity of VoF methods is explained by their unique ability to preserves the mass of each fluid component on the discrete level. The strategy of VoF methods consists in calculating the interface

location at each discrete moment of time from the volumes of the cell fractions occupied by different materials. Most VoF methods use a single linear interface to divide two materials in a mixed cell (Piecewise-Linear Interface Calculation (PLIC)) [3,4,5]. Once the direction of the interface normal is know, the location of the interface is uniquely identified by the volumes of the cells fraction. Unfortunately the interface normal can not be evaluated without the volume fraction data from the surrounding cells, which prohibits the resulting approximation to resolve any interface details smaller than a characteristic size of the cell cluster involved in evaluation of the normal.

To overcome this limitation, we designed a new *mass-conservative* interface reconstruction method [1], which calculates the interface based on both *volumes and centroids* of the cell fractions. This choice of the input data allows to evaluate the interface normal in a mixed cell *even without the information from the adjacent elements*. The location of the linear interface in each mixed cell is determined by *fitting the centroid of the cell fraction behind the interface to the reference one*, which leads to $(d-1)$-variate optimization problem in $\mathbb{R}^d$. The technique proposed, called Moment-of-Fluid (MoF) interface reconstruction, results in a *second order accurate* interface approximation (linear interfaces are reconstructed exactly), has higher resolution, and is shown to be *more accurate than VoF-PLIC methods*.

We present a detailed description of MoF interface reconstruction algorithm in 2D, which includes iterative procedure for centroid fitting and a new algorithm for cutting appropriate volume fractions from polygonal cells.

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On the manifold-mapping optimization technique

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Optimization problems in practice often need cost-function evaluations that are very expensive to compute. Examples are, e.g., optimal design problems based on complex finite element simulations. As a consequence, many optimizations may require very long computing times. The space-mapping (SM) technique [1,2] was developed as an alternative in these situations.

In SM terminology, the accurate but expensive-to-evaluate models are called *fine* models, $\mathbf{f} : X \subset \mathbb{R}^n \to \mathbb{R}^m$. The SM method also needs a second, simpler and cheaper and computationally faster model, the *coarse* model, $\mathbf{c} : Z \subset \mathbb{R}^n \to \mathbb{R}^m$, in order to speed-up the optimization process. The key element in this technique is a right-preconditioning for the coarse model, known as the *SM function* $\mathbf{p} : X \to Z$, that aligns the two model responses. The function $\mathbf{c}(\mathbf{p}(\mathbf{x}))$ corrects the coarse model and can be used as a surrogate for the fine model in the accurate

optimization. In most cases the SM function is much simpler than the fine model, in the sense that it is easier to approximate. This fact endows the SM technique with its well-reported efficiency. However, it does not always converge to the right solution.

Defect-correct theory [3] helps to see that, in order to achieve the accurate optimum, the SM function is generally insufficient and also left-preconditioning is needed. In [4] we introduce the mapping $\mathbf{s} : \mathbf{c}(Z) \to \mathbf{f}(X)$ and the associated manifold-mapping (MM) algorithm. MM employs $\mathbf{s}(\mathbf{c}(\bar{\mathbf{p}}(\mathbf{x})))$ as the fine model surrogate. Here, the function $\bar{\mathbf{p}} : X \to Z$ is not the above SM function but an arbitrary simple bijection, often the identity. The MM algorithm is as efficient as SM but converges to the accurate optimal solution [4,5].

In the first part of the presentation the MM algorithm will be briefly introduced and a proof of convergence will be given. The use of more than two models (multi-level approach) and the possibility of having a coarse model with a different dimension than the fine one ($X \subset \mathbb{R}^{n_\mathbf{f}}$ and $Z \subset \mathbb{R}^{n_\mathbf{c}}$ with $n_\mathbf{f} \neq n_\mathbf{c}$) will be the issues dealt with in the second part of the talk.

[1] J. W. Bandler, R. M. Biernacki, C. H. Chen, P. A. Grobelny and R. H. Hemmers, *Space Mapping Technique for Electromagnetic Optimization*, IEEE Trans. on Microwave Theory and Techniques, **42**(12) (1994) 2536–2544.

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IFSS: a MATLAB toolbox for modeling incompressible flow

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We give an overview of the IFISS (*Incompressible Flow Iterative Solution Software*) Package, a graphical MATLAB package for the interactive numerical study of incompressible flow problems. It includes algorithms for discretization by mixed finite element methods and a posteriori error estimation of the computed solutions. The package can also be used as a computational laboratory for experimenting with state-of-the-art preconditioned iterative solvers for the discrete linear equation systems that arise in the modeling of incompressible flow. A unique feature of the package is its comprehensive nature; for each problem addressed, it enables the study of both discretization and iterative solution algorithms as well as the interaction between the two and the resulting effect on overall efficiency.

Development of a 2-D model to simulate convection and phase transition efficiently

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We present a two-dimensional convection phase change model using the incompressible Navier-Stokes equation set and enthalpy as the energy conservation variable. Significant algorithmic challenges are posed for problems of phase change interfaces within convective flow regimes. The equation set is solved with the Jacobian-Free Newton-Krylov (JFNK) nonlinear inexact Newton's method. SIMPLE, a pressure-correction algorithm, is used as a physics-based preconditioner. This algorithm is compared to solutions using SIMPLE as the main solver.

Algorithm performance is assessed for a benchmark problem, phase change convection within a square cavity of a solid pure material cooled below the melting temperature. A time step convergence analysis demonstrates that the JFNK model with second order discretization is second order accurate in time. A Gallium melting simulation is also performed and evaluated; in this configuration multiple roll cells develop in the melted region at early times when the aspect ratio is high. The JFNK-SIMPLE method is shown to be more efficient per time step and more robust at larger time steps when compared to SIMPLE as the main solution algorithm. Overall CPU savings of more than an order of magnitude are realized.

As a further analysis of JFNK-SIMPLE, multigrid is wrapped around SIMPLE, so SIMPLE acts as the smoother within a multigrid preconditioner to JFNK. For phase change conduction, additional gains in efficiency can be accomplished. When SIMPLE is incorporated as a preconditioner and smoother within JFNK, the ability to model more complex and realistic phase change convection problems with increased robustness and efficiency is achieved.

Iterative solver for density functional theory calculations on composite meshes by quadratic finite elements

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Density Functional Theory (DFT) is a simplified quantum model that has proved very successful in real applications. It introduces an independent particles description of the electronic structure of molecules or materials which is much simpler to treat that the original Schrödinger equations. Simulating realistic physical systems by DFT however is still computationally very demanding. More efficient numerical algorithms to reduce computer time and enable larger simulations are always in demand by chemists and physicists who are studying phenomenon at the molecular level.

The finite element (FE) method, a very popular approach to solve partial differential equations, has only recently started being used for solving the Kohn-Sham equations of Density Functional Theory for realistic 3D applications. Traditionally, the pseudo-spectral approach has been the most popular in the field under the denomination Plane Waves method. The regular usage of periodic boundary conditions with simple geometries explains this preference. However with the increase in computer power and the growing interest in studying larger and more diverse systems, more flexible real-space discretizations by finite difference or finite elements have recently attracted more interest.

In this work we focus on FE discretizations with local mesh refinement for the Kohn-Sham equations, and propose an efficient iterative solver and preconditioner for this problem. We present a hierarchical quadratic Finite Elements approach to discretize the equations on structured non-uniform meshes. A multigrid FAC preconditioner is proposed to iteratively minimize the energy functional associated to the Kohn-Sham equations. It is based on an accelerated steepest descent-based scheme. The method has been implemented using SAMRAI, a parallel software infrastructure for general AMR applications. Numerical results of electronic structure calculations on small atomic clusters show in particular a mesh-independent convergence rate for the iterative solver.

Structured matrices, multigrid methods, and the Helmholtz equation

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We wish to present a different approach to the multigrid solution of the Helmholtz equation with constant coefficients. It is primarily based on certain classes of structured matrices and their strong correspondence to generating functions. Discretization of the Helmholtz equation with certain boundary conditions results in structured linear systems which are associated with generating functions. Depending on the kind of boundary conditions, the discretized Helmholtz equation is a linear system of Toeplitz, tau, circulant, or DCT-III type. By solving these systems with normal equations, we have the advantage that the corresponding generating functions are nonnegative, although they have a whole curve of zeros.

The multigrid methods we develop are especially designed for structured matrix classes, making heavy use of the associated generating functions. Over the last ten years, a specific theory of multigrid methods has been developed for structured matrices whose generating functions have isolated zeros. It is based on the AMG approach and the convergence theory of Ruge and Stüben. In this work, we extend some of these theoretical results to the case of

generating functions with whole zero curves, and apply these modified multigrid methods to the solution of the Helmholtz equation. We propose two different strategies how this can be done.

- The first strategy is based on the idea of representing the whole zero curve on all grids. For a multigrid method based on the Galerkin approach, we can prove optimal two-grid convergence, but such a method is computationally too expensive. Therefore we propose a rediscretization technique where the zero curve is approximated on each grid. This results in fast convergence and in coarse grid matrices with the same banded structure as the given matrix. The only disadvantage of this approach is that zero curves become larger on coarser levels, and therefore the number of grids is limited.
- The second strategy consists of splitting the original problem into a fixed number of coarse grid problems. Corresponding to a generating function with isolated zeros, each of these problems locally represents one part of the zero curve. Each coarse grid problem is solved with a standard multigrid method. We combine this splitting technique with the first strategy to construct a faster and more robust multigrid solver.

We wish to discuss the use of our multigrid strategies not only as a solver, but also as a preconditioner for Krylov subspace methods. Moreover, the methods can also be applied to anisotropic linear systems whose generating functions have a whole zero curve.

A flexible conjugate gradient method and its application in power grid analysis of VLSI circuits

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The design and verification of today's very large-scale integrated (VLSI) circuits involve some extremely challenging numerical problems. One of the truly large-scale problems in this area is power grid analysis. Power grids are modeled as networks with up to 10 millions nodes. Steady-state analysis of power grids requires the solution of correspondingly large sparse symmetric positive definite linear systems. The coefficient matrices of these systems have the structure of weighted Laplacians on three-dimensional grids, but with 'boundary' conditions given on a subset of the interior grid points. Strongly-varying weights and the interior boundary conditions have the effect that solutions of these linear systems are often very localized, with components of the solution being near zero in large parts of the grid.

In this talk, we present a flexible conjugate gradient method that is tailored to the solution of the truly large-scale linear systems arising in VLSI power grid analysis. The algorithm allows changing preconditioners and sparsification of the search directions at each iteration. These are the key features to exploit the local nature of the solutions. We also discuss the problem of constructing efficient preconditioners for the linear systems in VLSI power grid analysis, and we present results of numerical experiments.

Extensions of certain graph-based algorithms for preconditioning

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The original TPABLO algorithms are a collection of algorithms which compute a symmetric permutation of a linear system such that the permuted system has a relatively full block diagonal with relatively large nonzero entries. This block diagonal can then be used as a preconditioner. We propose and analyze three extensions of this approach: we incorporate a nonsymmetric permutation to obtain a large diagonal, we use a more general parametrization for TPABLO, and we use a block Gauss-Seidel preconditioner which can be implemented to have the same execution time as the corresponding block Jacobi preconditioner. Since our approach allows for efficient use of level 3 BLAS operations, it outperforms direct solvers and rivals standard ILU preconditioners on many test problems on a single processor system, while having good potential for efficient parallelization.

Solving the stochastic steady-state diffusion problem using multigrid

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We study multigrid for solving the stochastic steady-state diffusion problem. We operate under the mild assumption that the diffusion coefficient takes the form of a finite Karhunen-Loéve expansion. The problem is discretized using a finite element methodology using the polynomial chaos method to discretize the stochastic part of the problem. We apply a multigrid algorithm to the stochastic problem in which the spatial discretization is varied from grid to grid while the stochastic discretization is held constant. We then show, theoretically and experimentally, that the convergence rate is independent of the spatial discretization, as in the deterministic case.

Can information retrieval aid iterative methods?

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Recently, Computational Linear Algebra techniques have started playing an important role in Information Retrieval (IR) research. Indeed, the Vector Space Model and its derivatives, such as Latent Semantic Indexing, are heavily used and investigated. In this presentation we consider the problem in "reverse mode", namely using IR techniques to help in linear algebra and iterative methods in particular. The candidate problem is the solution of large linear systems with multiple right hand sides. The efficiency of solvers is known to depend on the amount of information shared amongst the right hand sides. We specifically investigate the combination of clustering algorithms and schemes from the existing literature to solve such problems.

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The role of optimization in the validation & verification, calibration & validation processes

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A comprehensive study of many of the complex systems in science and engineering may demand physical experimentation. However, in many cases, physical experiments can be prohibitively expensive or even impossible to perform. Fortunately, the behavior of many of these systems can be imitated by computer models, and thus, computer simulation may be a viable alternative or augmentation.

The inclusion of computer simulations does introduce many new challenges. For example, code verification should be used to confirm that the underlying equations are being solved correctly. Calibration or parameter estimation must be incorporated to update the computational model in response to experimental data. In addition, validation is an important process that can answer questions of correctness of the equations and models for the physics being modeled and the application being studied. Moreover, validation metrics must be carefully chosen in order to explicitly compare experimental and computational results and quantify the uncertainties in these comparisons. Overall, the validation and verification verification, calibration, and validation processes for computational experimentation can provide the best estimates of what can happen and the likelihood of it happening when uncertainties are taken into account.

In this talk, we will focus on the validation calibration under uncertainty process. In particular, we will focus on the problem of electrical simulations and elucidate the role of optimization in the parameter extraction problem. We will describe the process, an example problem and our results, and how the inclusion of sensitivity analysis can improve the optimization procedure.

Preconditioners for the discretized time-harmonic Maxwell equations in mixed form

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We introduce a new preconditioning technique for iteratively solving linear systems arising from finite element discretizations of the mixed formulation of the time-harmonic Maxwell equations. The preconditioners are block diagonal with positive definite blocks and are based on discrete augmentation using the scalar Laplacian. They are motivated by spectral equivalence properties of the discrete operators. Specifically, we show that augmenting the curl-curl operator by a discrete grad-div operator, weighed by the scalar Laplacian, yields almost immediate convergence when preconditioned MINRES is used. We also show that if the augmented term is replaced by the vector mass matrix we still obtain fast convergence. Similar (operator-independent) algebraic principles can be applied in general settings and give rise to preconditioners that work effectively for saddle-point linear systems whose (1,1) block is highly singular. Analytical observations and numerical results demonstrate the scalability and the convergence properties of the proposed approach.

An asynchronous parallel derivative-free algorithm for handling general constraints

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We will discuss an asynchronous parallel implementation of a derivative-free augmented Lagrangian algorithm for handling general nonlinear constraints recently proposed by Kolda, Lewis, and Torczon. The method solves a series of linearly constrained subproblems, seeking to approximately minimize the augmented Lagrangian which involves the nonlinear constraints. Each subproblem is solved using a generating set search algorithm capable of handling degenerate linear constraints. We use APPSPACK to solve the linearly-constrained subproblems, enabling the objective and nonlinear constraint functions to be computed asynchronously in parallel. A description and theoretical analysis of the algorithm will be given followed by numerical results.

Cascadic multigrid algorithms for the solution of Helmholtz equations

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In most scenarios, traditional multigrid methods fail to converge in the case of the Helmholtz equation with relatively large wave numbers. One approach for tackling this problem is to use a Krylov type algorithm both as a smoother and as an outer iteration method in the multigrid cycles. In this presentation, we extend this methodology to the iteration methods based on the cascadic principle. Such algorithms are usually referred to as one-way multigrid methods. We consider an adaptive control strategy for the number of iterations on successive refinement levels and present numerical results that illustrate the efficiency of the proposed approach.

Inexact solves in Krylov-based model reduction of large-scale systems

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Dynamical systems are the basic framework for modeling and control of an enormous variety of complex systems. Direct numerical simulation of the associated models has been one of the few available means when goals include accurate prediction or control of complex physical phenomena. However, the ever increasing need for improved accuracy requires the inclusion of ever more detail in the modeling stage, leading inevitably to ever larger-scale, ever more complex dynamical systems.

Simulations in such large-scale settings can be overwhelming and make unmanageably large demands on computational resources, which is the main motivation for model reduction. The goal of model reduction is to produce

a much lower dimensional system having the same input/output characteristics as the original. Recently, Krylov-based methods have emerged as promising candidates for reduction of large-scale dynamical systems.

The main cost in Krylov-based model reduction is due to solving a set of linear systems of the form $(s_o\mathbf{I}_n - \mathbf{A})\mathbf{v} = \mathbf{b}$ where $\mathbf{A}$ is an $n \times n$ matrix, $\mathbf{b}$ is an n-dimensional vector, s_0 is a complex number called the *interpolation point* and $\mathbf{I}_n$ is the identity matrix of size n. Since the need for more detail and accuracy in the modeling stage causes the system dimension, n, to reach levels on the order of millions, direct solvers for the linear system $(s_o\mathbf{I}_n - \mathbf{A})\mathbf{v} = \mathbf{b}$ are no longer feasible; hence inexact solves need to be employed in Krylov-based model reduction.

In this talk, we investigate the use of inexact solves in a Krylov-based model reduction setting and present the resulting perturbation effects on the underlying model reduction problem. We show that for a *good* selection of interpolation points, Krylov-based model reduction is robust with respect to the perturbations due to inexact solves. On the other hand, when the interpolation points are *poorly* selected, these perturbations are magnified through the model reduction process. We also examine stopping criteria, effective preconditioning, and restarting techniques in the particular context of model reduction. Finally, we incorporate inexact solves for the Krylov-based optimal $\mathcal{H}_2$ approximation. The result is an effective optimal model reduction algorithm applicable in realistic large-scale settings.

The block grade of a block Krylov space

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The so-called grade of a vector b with respect to a nonsingular matrix $\mathbf{A}$ is the dimension of the (largest) Krylov (sub)space generated by $\mathbf{A}$ from b. It determines in particular, how many iterations a Krylov space method with linearly independent residuals requires for finding in exact arithmetic the solution of $\mathbf{A}x = b$ (if the initial approximation x_0 is the zero vector). In this talk we generalize the grade notion to block Krylov spaces and show that this and other fundamental properties carry over to block Krylov space methods for solving linear systems with multiple right-hand sides.

We consider s linear systems with the same nonsingular coefficient matrix $\mathbf{A}$, but different right-hand sides $b^{(i)}$, which we gather in a *block vector* $\mathbf{b} := (b^{(1)}, \ldots, b^{(s)})$. The s systems are then written as

$$\mathbf{A}\mathbf{x} = \mathbf{b} \qquad \text{with} \quad \mathbf{A} \in \mathbb{C}^{N\times N}\,, \quad \mathbf{b} \in \mathbb{C}^{N\times s}\,, \quad \mathbf{x} \in \mathbb{C}^{N\times s}\,.$$

Standard block Krylov space methods construct in the nth iteration approximate solutions gathered in a block vector $\mathbf{x}_n$ chosen such that

$$\mathbf{x}_n - \mathbf{x}_0 \in \mathcal{B}_n^{\square}(\mathbf{A}, \mathbf{r}_0)\,,$$

where $\mathbf{x}_0$ contains the s initial approximations and $\mathbf{r}_0$ the corresponding initial residuals, while $\mathcal{B}_n^{\square}$ is the Cartesian product

$$\mathcal{B}_n^{\square} = \underbrace{\mathcal{B}_n \times \cdots \times \mathcal{B}_n}_{s \text{ times}}$$

with

$$\mathcal{B}_n = \mathcal{K}_n(\mathbf{A}, r_0^{(1)}) + \cdots + \mathcal{K}_n(\mathbf{A}, r_0^{(s)})\,.$$

Here, $\mathcal{K}_n(\mathbf{A}, r_0^{(i)})$ is the usual nth Krylov (sub)space of the ith system. It is important, that, in general, the sum in the last formula is not a direct sum, that is, the Krylov spaces may have nontrivial intersections.

The *block grade of* $\mathbf{r}_0$ *with respect to* $\mathbf{A}$ or, the *block grade of* $\mathbf{A}$ *with respect to* $\mathbf{r}_0$ is the positive integer $\bar{\nu} := \bar{\nu}(\mathbf{r}_0, \mathbf{A})$ defined by

$$\bar{\nu}(\mathbf{r}_0, \mathbf{A}) = \min \left\{ n \middle| \dim\ \mathcal{B}_n(\mathbf{A}, \mathbf{r}_0) = \dim\ \mathcal{B}_{n+1}(\mathbf{A}, \mathbf{r}_0) \right\} .$$

Among the results we have established for the block grade are the following ones.

LEMMA 1 For $n \geq \bar{\nu}(\mathbf{r}_0, \mathbf{A})$,

$$\mathcal{B}_n(\mathbf{A}, \mathbf{r}_0) = \mathcal{B}_{n+1}(\mathbf{A}, \mathbf{r}_0) , \qquad \mathcal{B}_n^{\square}(\mathbf{A}, \mathbf{r}_0) = \mathcal{B}_{n+1}^{\square}(\mathbf{A}, \mathbf{r}_0) .$$

LEMMA 2 The block grade of the block Krylov space and the grades of the individual Krylov spaces contained in it are related by

$$\mathcal{B}_{\bar{\nu}(\mathbf{r}_0, \mathbf{A})}(\mathbf{A}, \mathbf{r}_0) = \mathcal{K}_{\bar{\nu}(r_0^{(1)}, \mathbf{A})}(\mathbf{A}, r_0^{(1)}) + \cdots + \mathcal{K}_{\bar{\nu}(r_0^{(s)}, \mathbf{A})}(\mathbf{A}, r_0^{(s)}) .$$

LEMMA 3 The block grade $\bar{\nu}(\mathbf{r}_0, \mathbf{A})$ is characterized by

$$\bar{\nu}(\mathbf{r}_0, \mathbf{A}) = \min \left\{ n \middle| \mathbf{A}^{-1}\mathbf{r}_0 \in \mathcal{B}_n^{\square}(\mathbf{A}, \mathbf{r}_0) \right\} .$$

THEOREM Let $\mathbf{x}_\star$ be the block solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$ and let $\mathbf{x}_0$ be any initial block approximation of it and $\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$ the corresponding block residual. Then

$$\mathbf{x}_\star \in \mathbf{x}_0 + \mathcal{B}_{\bar{\nu}(\mathbf{r}_0, \mathbf{A})}^{\square}(\mathbf{A}, \mathbf{r}_0) .$$

We also discuss the effects of the size of the block grade on the efficiency of a block Krylov space method.

An octree multigrid method for quasi-static Maxwell's equations with highly discontinuous coefficients

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In this work we develop an octree discretization for Maxwells equations in the quasi-static regime. We then use this discretization in order to develop a multigrid method for Maxwells equations with highly discontinuous coefficients. We show that our approach can be interpreted as a semi-algebraic multigrid method with physical base for coarse grid selection. We test our algorithms and compare it to other multilevel algorithms.

Multilevel algorithms for large scale interior point methods in bound constrained optimization

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We develop and compare multilevel algorithms for solving bound constrained nonlinear variational problems via interior point methods. Several equivalent formulations of the linear systems arising at each iteration of the interior point method are compared from the point of view of conditioning and iterative solution. Furthermore, we show how a multilevel continuation strategy can be used to obtain good initial guesses ("hot starts") for each nonlinear iteration. A minimal surface problem is used to illustrate the various approaches.

Multi-level optimization for image registration using local refinement on octrees

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We present a new multi-level approach for non-linear image registration using local refinement techniques.

Standard multi-level approaches for this problem discretize the domain starting with a regular coarse grid and refine every cell from level to level. In our approach, we also start with a regular coarse grid but its refinement for higher levels is done locally. Using local refinement is motivated by the observation that changes in the solution at higher levels appear mainly locally and large areas stay unchanged such that there is no need for a finer resolution. The local refinement in our approach is done by subdividing cells into four (2D) or eight (3D) resulting quad (2D) and octree-grids (3D), respectively.

Compared with the standard multi-level approach, our method requires substantially less memory and arithmetic operations. Therefore, it is in particular well-suited for large-scale problems.

A multiscale perspective on density functional theory for inhomogeneous fluids

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Some modeling and simulations efforts have historically encompassed multiscale phenomena without explicitly handling multiscale features. One such area is density functional theories for inhomogeneous fluids (Fluid-DFTs). In this presentation we look at Fluid-DFTs from a fresh perspective, calling out the fact that Fluid-DFTs incorporate multiple length scales that are introduced in a way such that each longer scale increases the fidelity of the model. By viewing Fluid-DFTs from this perspective, we develop a mathematical framework and a collection of solution algorithms that have a dramatic impact on the robustness, performance and scalability of the implicit equations generated by Fluid-DFTs.

The basic framework for all of our solver algorithms reflects the importance of inter-physics coupling in the extended variable formulation of the Fluid-DFTs. This physics coupling led us to a physics-based block matrix formulation in order to partition critical and nonlocal ancillary variables. The idea is to partition the data into blocks that can be optimally managed or solved. The general 2×2 block matrix is

$$\left(\begin{array}{ccc|ccc} A_{11}^{11} & \cdots & A_{11}^{1j} & A_{12}^{1,j+1} & \cdots & A_{12}^{1k} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ A_{11}^{j1} & \cdots & A_{11}^{jj} & A_{11}^{j1} & \cdots & A_{11}^{jj} \\ \hline A_{21}^{j+1,1} & \cdots & A_{21}^{j+1,j} & A_{22}^{j+1,j+1} & \cdots & A_{22}^{j+1,k} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ A_{21}^{k1} & \cdots & A_{21}^{kj} & A_{22}^{k,j+1} & \cdots & A_{22}^{kk} \end{array}\right)\left(\begin{array}{c} x_1^1 \\ \vdots \\ x_1^j \\ \hline x_2^{j+1} \\ \vdots \\ x_2^k \end{array}\right) = \left(\begin{array}{c} b_1^1 \\ \vdots \\ b_1^j \\ \hline b_2^{j+1} \\ \vdots \\ b_2^k \end{array}\right)$$

where k is the number of DOFs tracked per node. The superscript (p, q) denotes the block of coefficients generated by DOF p interactions with DOF q. The subscripts and partition lines impose a coarser partitioning of the matrix into a 2×2 block system that will be used with a Schur complement approach. We denote by A_{11}, A_{12}, A_{21} and A_{22} the upper left, upper right, lower left and lower right submatrix of the coarse 2×2 block matrix, respectively. Similarly x_1 and x_2, and b_1 and b_2 are the upper and lower parts of x and b, respectively.

Given this two-level structure, the basic strategy for solving each global linear system generated by Newton's method is as follows:

1. Identify and reorder DOFs 1 through j such that A_{11}^{-1} (the inverse of A_{11}) is easy to apply (in parallel).
2. Determine a preconditioner P for $S = A_{22} - A_{21}A_{11}^{-1}A_{12}$, the Schur complement of A with respect to A_{22}.
3. Solve $Sx_2 = (b_2 - A_{21}b_1)$ using a preconditioned Krylov method such as GMRES, with preconditioner P. Note that S may or may not be explicitly formed, depending on other problem details.
4. Finally, solve for $x_1 = A_{11}^{-1}(b_1 - A_{12}x_2)$.

Given this basic framework, we will describe specific solvers for special categories of Fluid-DFT problems, including 2 and 3 dimensional hard-sphere problems and polymer chains. We give results for several problem areas including nanopore and lipid bi-layer models where this Schur complement approach provides one to two orders of magnitude improvement in performance and an order of magnitude reduction in memory requirements.

Improving mass-conservation of least-squares finite element methods

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Interest in least-squares finite element methods continues to grow due to at least two of its major strengths. First, the linear systems obtained after discretization are SPD and often H^1 elliptic so that they can be efficiently solved (often with optimal scalability) using a number of iterative methods, including conjugate gradients and multigrid. Second, the least-squares functional provides a sharp measure of the local error with negligible computational costs. Despite these two major advantages, the methods have not gained widespread use, largely because they are perceived as not providing accurate approximations to the true solution, especially with regards to conservation of mass. The least-squares finite element method is not discretely conservative, but the approximate solutions given by the method are the *most accurate approximate solutions possible in the functional norm for a given finite-dimensional space*. The method converges to the approximation that minimizes the functional, so it gives a relatively accurate solution in the functional norm.

However, anyone would agree that an approximate solution to the Navier-Stokes equations that has an inflow rate that is 100 times the outflow rate is not an acceptable approximation, even if it is 'accurate' in some norm. Unfortunately, some combinations of common least-square functionals and finite element spaces for the Navier-Stokes equations generate solutions that lose 99% of the mass between the inflow and outflow boundaries for some particular boundary conditions. Herein lies the challenge for least-squares methods: how do we formulate a functional and boundary conditions that better represents the type of accuracy we desire?

In this talk, two new first-order system reformulations of the Navier-Stokes equations are presented that admit a wider range of mass conserving boundary conditions. It is common with least-squares methods to rewrite the Navier-Stokes equations as a system of first-order equations using the velocity-vorticity form. The two new first-order systems are based on the velocity-vorticity form, but they include a new variable, $\mathbf{r}$, representing the pressure gradient plus all or part of the convective term. As we will demonstrate, the resulting operator problem can be solved very efficiently using a multigrid or an algebraic multigrid solver, and excellent mass conservation is observed for multiple test problems. A difficulty with the new formulations is obtaining boundary conditions for the new variable, $\mathbf{r}$, but we will demonstrate at least three different methods for overcoming this difficulty.

Implementation and performance of a two-grid method for nonlinear reaction-diffusion equations

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Two-grid methods have been developed by Xu (SIAM J. Num. Anal., 1996) for application to linear and nonlinear PDEs. Of particular interest are methods that can be applied to large nonlinear problems that arise in the simulation of physical processes, such as a method due to Dawson, Wheeler, and Woodward (SIAM J. Num. Anal., 1998). This scheme solves the original nonlinear problem on a mesh coarser than originally specified to capture the nonlinear behavior of the solution, then utilizes a linearized version of the problem to correct the coarse approximation on the original problem mesh.

The two-grid method potentially reduces the overall computational cost by requiring the solution of a smaller nonlinear system and a large linear system in place of the original large nonlinear problem. In this talk we investigate the application of this method to nonlinear reaction-diffusion equations. In particular, we discuss issues that arise in the implementation of the algorithm, and perform numerical experiments on problems designed to gauge the performance of the two-grid method relative to a standard Newton iterative nonlinear solver.

The effect of boundary conditions and inner solver accuracy within pressure convection-diffusion preconditioners for the incompressible Navier-Stokes equations

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Pressure convection-diffusion preconditioners for solving the incompressible Navier-Stokes equations were first proposed by Kay, Loghin, and Wathen and Silvester, Elman, Kay, and Wathen. While numerous theoretical and numerical studies have demonstrated mesh independent convergence for these block methods on several problems and their overall efficacy, there are several potential weaknesses remaining in the practical use of these methods.

Perhaps one of the most poorly understood topics within this block preconditioner family is the influence of boundary conditions on overall algorithm convergence. The notion of differential commuting is the basis for all *pressure convection-diffusion* preconditioners. The main mathematical difficulty is that differential commuting does not hold at the boundaries. Thus, it is unclear what boundary conditions should be enforced in subblocks of the preconditioner. Heuristics have been developed that roughly account for boundary conditions associated with inflow, outflow, and no-slip. However, these rough heuristics often do not properly capture the boundary interactions, and can in fact lead to a degradation in convergence rates as the mesh is refined. We first explore the effect of having "ideal" boundary conditions within the preconditioner. While not computationally feasible, the ideal boundary condition results highlight the importance of choosing suitable boundary conditions. We then explore somewhat more practical approximations to the ideal conditions based on ILU factorizations and probing [Siefert and de Sturler, 2005].

Another important issue is the relationship between the accuracy of inner sub-problem solves to the overall convergence rate of the outer iteration. It has been known for quite some time that when mesh-independent sub-problem solvers are used inexactly within this block preconditioner, the overall convergence of the outer iteration remains mesh independent for the Stokes equations [Silvester and Wathen, 1994]. The situation is not well understood for the Navier-Stokes equations, and it is also not well understood when the inner subblock solver has less than ideal behavior. We have observed a noticeable degradation in the outer iteration convergence rate when a sub-solver is terminated too quickly. We discuss possible solutions to this issue including reusing information from repeated linear solves.

Alternatives to smoothed aggregation multigrid prolongators for anisotrophic problems

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We consider alternatives to the traditional methods in smoothed aggregation for generating prolongator operators. The goal is to produce prolongators that are appropriate for anisotropic operators.

Consider the linear problem $Ax = b$. In the first approach, smoothed aggregation with basis function shifting, we begin with the standard smoothed prolongator, $P^{(sm)} = (I - \omega D^{-1} A)P^{(t)}$, where $P^{(t)}$ is the tentative prolongator. Given a prescribed prolongator sparsity pattern, this method moves basis function support (columns of $P^{(sm)}$) from one aggregate to another to produce a new prolongator, $P^{(shift)}$. The shifting is done in such a way that null space interpolation is maintained.

In the second approach, we consider extensions to building prolongator operators via energy optimization (Vanek, Mandel, Brezina). In this method, the sum of the energies of the prolongator basis functions is minimized, subject to a fixed prolongator nonzero pattern and interpolation of low-energy modes. We consider modifications such as filtering A to account for anisotropies and applying a modified CG method to solve the optimization problem.

We present numerical experiments that compare the two methods to traditional smoothed aggregation on a variety of model problems.

Splittings for iterative solution of linear systems

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Consider iteratively solving a linear system $Ax = b$, with invertible $A \in \mathbb{C}^{n\times n}$ and $b \in \mathbb{C}^n$, by splitting the matrix A as $A = L+R$, where L and R are both readily invertible. In such a case the recently introduced residual minimizing Krylov subspace method [1] can be executed, allowing, in a certain sense, preconditioning simultaneously with L and R.

Splittings satisfying $A = L + R$ result either form the structure of the problem, or are algebraic. Splittings of Gauss-Seidel type belong to the latter category. In this talk we discuss such splittings of A.

[1] M. Huhtanen and O. Nevanlinna, *A minimum residual algorithm for solving linear systems*, submitted manuscript available at www.math.hut.fi/~mhuhtane/index.html.

A preconditioned L-BFGS algorithm with application to protein structure prediction

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The limited-memory BFGS method has been widely used in large scale unconstrained optimization problems, including protein structure prediction. A major weakness of the L-BFGS method is that it may converge very slowly for ill-conditioned problems. We propose a preconditioned L-BFGS method, where we form the preconditioner from parts of the partially separable objective function.

We report results of experiments in the context of the protein structure prediction problem for four different proteins, using a protein energy model as the objective function and multiple initial configurations for each protein. The results show speed-ups with factors between 3 and 10 in terms of function evaluations and with factors between 2 and 7 in terms of CPU time. The difference between CPU time and function evaluation speed-up is due to the extra overhead of calculating and applying the preconditioner. We also compare our results to a method from the other competitive class of large-scale methods, preconditioned truncated Newton method (TNPACK). The limited results indicate that the preconditioned L-BFGS method may be more efficient.

We also tried this approach in a more general context, using limited memory with an incomplete Cholesky factorization of the Hessian as a preconditioner. We compared the performance with the truncated Newton algorithm TRON, which uses a similar preconditioner. Tested on a subset of the CUTER test problems, our results show that, using this preconditioner, the preconditioned LBFGS method is competitive with TRON and much better than the LBFGS algorithm without preconditioner.

Parallel domain decomposition methods for some stochastic partial differential equations

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In this talk, we discuss some parallel multilevel Schwarz type domain decomposition preconditioned recycling Krylov subspace method for the numerical solution of some partial differential equations with stochastic uncertainties in the operator. Using a Karhunen-Loeve expansion and a finite element method with double orthogonal polynomial basis, we transform the stochastic problem into a large number of deterministic equations. We will report results obtained from a PETSc based parallel implementation of a recycling Krylov subspace method with a domain decomposition preconditioning

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Blue Gene/L impacting computational science and engineering

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One year has passed and Blue Gene has been placed at several sites, many of which have a computational science component that involves iterative methods. In this talk, I will review some of the results obtained at some of these sites. I will elaborate on work underway with collaborators and colleagues in the area of computational science. For those unfamiliar with the Blue Gene System, I will very briefly describe the hardware and software environment.

I will describe how Blue Gene might be used to tackle multi-scale problems, many of which will need good parallel iterative solvers. While progress is being made, there remain many challenges for the computational science community to apply the Blue Gene resource to Big science problems with impact on society that until now or in current implementations have fallen short of the mark. Finally, I will elaborate on opportunities that exist for the community to get access to Blue Gene.

Balancing iteration accuracy in control problems governed by PDEs

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We consider the solution of large scale optimization problems governed by parabolic partial differential equations (PDEs). A quadratic functional containing a data misfit term, is minimized to approximately recover the parameter function. The resulting constrained optimization problem is solved by using the reduced Hessian approach. The conjugate gradient method (CG) is employed for the solution of the system involving matrix vector multiplications which are nontrivial. These matrix vector products do not need to be computed exactly. We investigate two approaches for determining the inner iteration tolerance at each CG step and provide numerical experiments comparing these approaches.

A scalable preconditioner for the Wigner-Poisson equations

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In this paper we propose and analyze a scalable preconditioner for the Wigner-Poisson equations for a resonant tunneling diode (RTD), and apply that preconditioner to a matrix-free continuation study of the dependence of the current through the device on the applied voltage.

The equations are a integro-partial differential equation for the distribution of the electrons in the device couples with Poisson's equation for the electrostatic potential. Our preconditioner is the inverse of the kinetic energy operator. We prove that, after elimination of the Poisson equation, the equation after left preconditioning is a compact fixed point problem for the Wigner distribution. We then apply that compactness to show mathematical scalability of the inner Krylov iteration, and use that to show scalability of the continuation. We present numerical results that support the theory.

A regularized Gauss-Newton method for nonlinear imaging problems in diffuse optical tomography

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The goal in diffuse optical tomography for medical imaging is the joint reconstruction of parameterized images of absorption and scattering of light in the body. The reconstruction requires the approximate solution of a nonlinear least squares problem for the image parameters. While traditional approaches such as damped Gauss-Newton (GN) and Levenberg-Marquardt (LM) have been shown to be effective at solving the imaging problem in its various forms, a considerable number of additional function and Jacobian evaluations are involved in determining the correct step length and/or damping parameter. In 3D imaging problems, depending on the particular image model, the cost of one function evaluation is, at a minimum, the cost of a dense matrix-vector product and in the worst, but more realistic, case requires the solution of several large-scale PDEs. A Jacobian evaluation is even slightly more expensive. Therefore, it is crucial to keep the number of function and Jacobian evaluations to a minimum.

The ill-conditioning of the Jacobian, together with the presence of noise in the data, motivates us to devise a regularized, trust-region-based Gauss-Newton approach for determining search directions. Although LM can be thought of as a regularized analogue to determining the GN direction, LM has the property of damping possibly important contributions to the search direction in spectral components corresponding to small singular values. On the other hand, the Gauss-Newton direction is too influenced by components due to small singular values early on, causing the line search to work hard to refine the step length. We propose a method that 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.

A Krylov-Karhunen-Loeve moment equation (KKME) approach for solving stochastic porous media flow equations

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In contrast to the widespread use of Monte Carlo simulations (MCS), stochastic equations have shown remarkable potential to develop efficient, accurate and physical insightful models. The main challenge of solving stochastic equations is to develop tractable descriptions of the system response in terms of stochastic differential operators and random fields. In particular, the solution of stochastic PDEs in porous media flow raises unexplored challenges to the solution of the discretized system of equations due to the significant size of standard reservoir problems combined with the uncertainty induced by error measurements, discontinuities, nonlinearities in the reservoir parameters at different spatial and temporal scales.

This work introduces a Krylov-Karhunen-Loeve moment equation (KKLME) approach for the solution of stochastic PDEs arising in large-scale porous media flow applications. The approach combines recent developments in Karhunen-Loeve moment equation methods with a block deflated Krylov iterative solution of a sequence of deterministic linear algebraic equations sharing the same matrix operator but different right-hand sides (RHSs).

In this approach, the log of the random field (i.e., log of permeability) describing the transmissibility coefficients is decomposed as the sum of a deterministic average log field plus a mean-zero random fluctuation. The covariance function associated with the fluctuation component is further decomposed by means of the Karhunen-Loeve (KL) expansion scheme. This expansion consists of modes (i.e. stochastic orders) of increasing frequency but decreasing magnitude. It has been shown that the KL expansion is of mean square convergence and summation thus implying significant computational savings. Subsequently, a mixed finite element procedure (equivalent to a cell-centered finite difference scheme under a suitable quadrature rule) is employed to derive a system of linear random algebraic equations.

In order to compute higher-order approximations for the different pressure moments, a perturbation approach followed by an expansion of orthogonal random variables is performed to express the variability of pressures with respect to the random field. The algebraic manipulation of modes and moments results in a sequence of deterministic linear systems with multiple RHSs sharing the same matrix operator. This matrix operator corresponds to the discretization of the average random field that, in general, has better algebraic properties than the operator associated with the original random field. A set of independent RHSs becomes available when a lower moment is computed, and each moment involves the solution of several modes or combinations of them with previous moment solutions. Since the associated average system is generally large and sparse, a Krylov subspace iterative solver is suitable in this case. The availability of RHSs describes a particular computational pattern that is amenable for highly scalable implementations and, at the same time, imposes particular challenges for an efficient Krylov subspace implementation.

With regard to the solution of systems with multiple RHSs, significant advances have been made in recycling the information generated by Krylov iterative methods. Deflation methods have been shown to be very effective in these circumstances as they "remove" components of the solution associated with extreme eigenvalues that prevent or slow down convergence. To perform deflation the Krylov subspace is selectively augmented with approximate eigenvectors that are either computed during the iteration or somehow known *a priori* from some geometrical/physical mean.

On the other hand, in order to reduce the negative effects of sequential inner products on memory performance, it is advisable to rely on block implementations or, in other words, process a subset of right-hand-sides in a simultaneous

fashion. A novel block deflation Krylov iterative method is proposed. The main feature of this implementation is to enable changes both in the size of the block and in the augmented subspace as the iteration proceeds. This ensures both numerical stability and flexibility in replacing deflated RHSs (i.e., associated with converging solutions) with new RHSs.

Numerical experiments show that the KKLME approach requires significant less computing time than MCS to converge to the different statistical moments for the pressure response. Results are shown for single phase flow and for pressure system arising in two-phase fully implicit formulations using a block deflation CG iterative method. In light of these preliminary results, extensions to relate random fields with spectrum information are required in order to exploit further efficiencies.

A mathematical framework for equivalent real formulations

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Equivalent real formulations (ERFs) are useful for solving complex linear systems using real solvers. Using the four ERFs discussed by Day and Heroux [1], each can be expressed by multiplying the *canonical* K form of the complex matrix by certain diagonal and permutation matrices on either side. This will allow, for instance, one ERF to be used as a preconditioner and another ERF to be used to iteratively solve the linear system by simply switching back and forth between the forms through scaling and permuting.

Many real world problems result in a complex-valued linear system of the form $Cw = d$, where C is a known $m \times n$ complex matrix, d is a known $m \times 1$ complex vector, and w is an unknown $n \times 1$ complex vector. We can re-write C as a real matrix of size $2m \times 2n$ called the *canonical* K form. If we let matrix A contain the real parts of the complex matrix C and let matrix B consist of the corresponding imaginary parts, we can write $A + iB = C$. The *canonical* K form is created by forming the matrix $K = \begin{pmatrix} A & -B \\ B & A \end{pmatrix}$.

To preserve the sparsity pattern of C, each complex value $c_{pq} = a_{pq} + ib_{pq}$ is converted into a 2×2 sub-block with the structure $\begin{pmatrix} a_{pq} & -b_{pq} \\ b_{pq} & a_{pq} \end{pmatrix}$. For instance, if

$$C = \begin{pmatrix} a_{11} + ib_{11} & a_{12} + ib_{12} \\ 0 & a_{22} + ib_{22} \end{pmatrix}$$

then the *permuted canonical* K form is

$$K = \begin{pmatrix} a_{11} & -b_{11} & a_{12} & -b_{12} \\ b_{11} & a_{11} & b_{12} & a_{12} \\ 0 & 0 & a_{22} & -b_{22} \\ 0 & 0 & b_{22} & a_{22} \end{pmatrix}.$$

The four ERFs that we will concern ourselves with are: $K_1 = \begin{pmatrix} A & -B \\ B & A \end{pmatrix}$, $K_2 = \begin{pmatrix} A & B \\ B & -A \end{pmatrix}$, $K_3 = \begin{pmatrix} B & A \\ A & -B \end{pmatrix}$, and $K_4 = \begin{pmatrix} B & -A \\ A & B \end{pmatrix}$. Each of the ERFs can be obtained from the *permuted canonical* K form by multiplying by diagonal and permutation matrices on both sides. In other words, $K_i = D_l P_l K P_r D_r$,

where D_l, P_l, P_r, and D_r are certain matrices depending on the size of the complex matrix and which ERF we desire. Three diagonal matrices and two permutation matrices (together with their transposes) exist for the ERFs we are considering.

The talk will describe the specific diagonal and permutation matrices needed as well as how to transform from one ERF to another.

[1] David Day and Michael A. Heroux, *Solving Complex-Valued Linear Systems via Equivalent Real Formulations*, SIAM J. Sci. Comput. **23**(2) (2001) 480–498.

Block locally optimal preconditioned eigenvalue xolvers (BLOPEX)

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Block Locally Optimal Preconditioned Eigenvalue Xolvers (BLOPEX) is a package, written in C, that at present includes only one eigenxolver, Locally Optimal Block Preconditioned Conjugate Gradient Method (LOBPCG). BLOPEX supports parallel computations through an abstract layer. BLOPEX is incorporated in the HYPRE package from LLNL and is available as an external block to the PETSc package from ANL as well as a stand-alone serial library. HYPRE and PETSc packages provide high quality multigrid and domain decomposition preconditioning on parallel clusters with distributed or shared memory.

The LOBPCG method, suggested and developed by Andrew Knyazev [1] in the past decade, recently attracts an increasing attention as a potential alternative to the shift-and-invert Lanczos and preconditioned Davidson methods due to its simplicity, robustness and fast convergence. Several MATLAB, C, C++ and FORTRAN implementations of the LOBPCG are developed by different groups, e. g., for such applications areas as structured mechanics and electronic structure calculations. Main LOBPCG features: a matrix-free iterative method for computing several extreme eigenpairs of symmetric positive generalized eigenproblems; a user-defined preconditioner; robustness with respect to random initial approximations, variable preconditioners, and ill-conditioning of the stiffness matrix; apparently optimal convergence speed. Numerical comparisons suggest that LOBPCG may be a genuine block analog for eigenproblems of the standard preconditioned conjugate gradient method for symmetric linear systems.

We present initial scalability results using BLOPEX with HYPRE and PETSc on one BlueGene/L box solving eigenvalue problems of record sizes.

[1] A. V. Knyazev, *Toward the Optimal Preconditioned Eigensolver: Locally Optimal Block Preconditioned Conjugate Gradient Method*, SIAM J. Sci. Comp. **23**(2) (2001) 517–541.

H(curl) auxiliary mesh preconditioning

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In this talk we present a two-level preconditioning scheme for H(curl) bilinear forms. The scheme utilizes an auxiliary problem on a related mesh that is more amenable for constructing optimal order multigrid methods. Combined with a domain embedding (or "fictitious" domain) technique our method can precondition a problem defined on a very complicated mesh by a standard geometric multigrid on a box.

How a step toward wider class of matrices could help improve convergence area of relaxation methods

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Investigations are related to several different relaxation methods for solving systems of linear equations, but the main idea is always the same: knowing that system matrix is strictly diagonally dominant (SDD), we can consider it as an S-SDD (see Lj. Cvetkovic, V. Kostic and R. S. Varga, *A new Gerschgorin-type eigenvalue inclusion area*, ETNA 18, 2004) matrix for every nonempty proper subset S of the set of indices, and from this fact we can derive, in some sense, an optimal convergence area for relaxation parameter(s). This convergence area is usually significantly wider than the corresponding one, obtained from the knowledge of SDD property, only. Instead of S-SDD class, some more subclasses of H-matrices can be used for the same purposes.

Coupled Gauss-Seidel algorithm in multigrid mode for the thin film equation

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In this talk we consider the iterative solution of a nonlinear system arising from a finite element discretisation of the fourth order equation

$$\frac{\partial u}{\partial t} + \nabla \cdot (|u|^\gamma \nabla \Delta u) = 0,$$

where $\gamma > 0$. This equation models a thin liquid film spreading on a solid surface, with u the height of the film. It is well known that for nonnegative initial data, the solution u remains nonnegative for all time. However, this nonnegativity of u is not guaranteed if the equation is discretised in a naive way. Imposing the nonnegativity of u as a constraint leads to a discrete variational inequality to be solved at each time step. Specifically defining S^h to be the space of piecewise linear functions on a uniform mesh and $K^h \subset S^h$ to be the space of nonnegative functions in S^h, given $U^{n-1} \in K^h$ we seek $U^n \in K^h$ and $W^n \in S^h$ such that

$$\begin{aligned} (U^n, \chi)^h + \tau\,(|U^{n-1}|^\gamma \nabla W^n, \nabla \chi) &= (U^{n-1}, \chi)^h \qquad \forall\ \chi \in S^h, \\ (\nabla U^n, \nabla(\chi - U^n)) &\geq (W^n, \chi - U^n)^h \qquad \forall\ \chi \in K^h, \end{aligned}$$

where τ represents the time step, and $(\cdot,\cdot)$ and $(\cdot,\cdot)^h$ represent the L^2 inner product and its trapezoidal rule discretisation respectively.

Well-posedness, stability, unique solvability, and convergence of U^n to u and W^n to $w = -\Delta u$ were established by Barrett, Blowey and Garcke in 1998. To solve the nonlinear system they used an Uzawa algorithm, for which they were able to demonstrate convergence of $U^{n,p} \to U^n$ and of $\int_\Omega |U^{n-1}|^\gamma |\nabla(W^n - W^{n,p})|^2 dx \to 0$, as the number of iterations $p \to \infty$. However, the convergence of this algorithm was found to be extremely slow. Here, we propose instead a coupled Gauss-Seidel algorithm in multigrid mode for the iterative solution of the nonlinear system. Proving convergence for the multigrid algorithm remains an open question, but numerical results indicate mesh independent convergence to the same solution as that achieved with the Uzawa algorithm in most cases tested, with a greatly reduced computational cost compared to iterating on a single grid.

A fast a-posteriori reorthogonalization scheme for the classical Gram-Schmidt orthogonalization in the context of iterative methods

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The year 2005 have been marked by two new papers on the Classical Gram-Schmidt algorithm (see [1,2]). These results offer a better understanding of the Classical Gram-Schmidt algorithm. It is finally proved that the Classical Gram-Schmidt algorithm generates a loss of orthogonality bounded by the square of the condition number of the initial matrix. In the first part of the talk, I will quickly review the proof, explain its key points and its implication in the context of iterative methods. In the second part, I will focus on the new results that we have found related to the Classical Gram-Schmidt algorithm. In particular an a-posteriori reorthogonalization scheme extremely efficient is given in the context of iterative methods. (We borrow ideas developed in [3] in the context of GMRES-MGS.)

[1] A. Smoktunowicz and J. Barlow, *A note on the error analysis of Classical Gram Schmidt*, submitted to Numerische Mathematik (2005).

[2] Luc Giraud, Julien Langou, Miroslav Rozložník, Jasper van den Eshof, *Rounding error analysis of the classical Gram-Schmidt orthogonalization process*, Numerische Mathematik **101**(1) (July 2005) 87–100.

[3] Luc Giraud, Serge Gratton, Julien Langou, *A rank-k update procedure for reorthogonalizing the orthogonal factor from modified Gram-Schmidt*, SIAM J. Matrix An. Appl. **25**(4) (August 2004) 1163–1177.

A preconditioned Newton-Krylov strategy for moving mesh adaptation

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We propose a new approach to adaptive mesh motion based on solving a coupled self-consistent system for the physics equations and for the grid generation equations. The key aspect of the new method is the solution of the non-linear coupled system with a preconditioned Newton-Krylov method. The present work described the approach and focuses on the preconditioning techniques.

Adaptive grids are becoming an ever more common tool for high performance scientific computing. We focus here on the type of adaptation achieved by moving a constant number of points according to appropriate rules, an

approach termed moving mesh adaptation (MMA). The approach we consider here is based specifically on retaining a finite volume approach but allowing the grid to evolve in time according to a grid evolution equation obtained from minimization principles. The approach originates from the seminal papers by Brackbill and Saltzmann [1] and by Winslow [2].

In the present paper we consider the fundamental question in the application of MMA. Is it worth the effort? The literature is very rich and considerable results have been obtained in designing MMA approaches that provide grids that can indeed present the desired properties. But the question of whether once the adaptive grids are used the simulations are actually more cost effective remains largely unanswered.

We have revisited the question and have reached the conclusion that in order to obtain an effective MMA strategy, three ingredients need to be considered.

First is the effective formulation of the moving grid equations. In 1D the problem is benign, as error minimization leads to error equidistribution and to a rigorous and simple minimization procedure. In 2D and 3D the problem is more challenging but we have derived an effective approach based on the classic approach by Brackbill-Saltzmann-Winslow [1,2]. The crucial ingredients of our approach are the formulation of the physics equations in a conservative form and of the formulation of the grid generation equations using harmonic mapping [3,4]. The independent variables of the physics equations are changed from the physical to the logical space and the equations are rewritten in the logical space in a fully conservative form [4].

Second is the solution algorithm for the MMA method. Here we bring a new development. The moving mesh equations and the physics equations, derived by discretizing the problem under investigation on a moving grid, form a tightly coupled system of algebraic non-linear equations. Traditionally, the coupling is broken, the physics and grid equations being solved separately in a lagged time-splitting approach. Each time step is composed of two alternating steps: the physics equations are solved on the current grid, the grid equations are then solved using new information from the solution of the physics equations. However, in presence of sharp fronts or other moving features, breaking such coupling can lead to grid lagging with respect of the physics equations, with adaptation resulting behind rather than on the moving feature.

We avoid breaking the coupling and solve the full non-linear set of physics and grid equation using the preconditioned Newton-Krylov (NK) approach [5].

Third ingredient in a cost-effective grid adaptation is an efficient preconditioning technique. In 1D a simple block tridiagonal approach works effectively [6]. Each set of equations, for physics and for grid generation, is preconditioned with a tridiagonal matrix obtained by numerically approximating the corresponding diagonals in the Jacobian. In 2D, we rely on a multigrid preconditioning strategy where a crucial innovation is how to coarsen the information relative to the adaptivity in the harmonic grid generation equations [4].

In the present paper we describe the approach followed and we report a number of examples to illustrate the performance of the new approach.

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[4] L. Chacón, G. Lapenta, *A fully implicit, nonlinear adaptive grid strategy*, J. Comput. Phys. **212** (2006) 703–717.

[5] C. T. Kelley, *Iterative methods for linear and nonlinear equations*, SIAM, Philadelphia, 1995.

[6] G. Lapenta, L. Chacón, *Cost-effectiveness of fully implicit moving mesh adaptation: a practical investigation in 1D*, J. Comput. Phys., submitted.

Steepest descent and conjugate gradient methods with variable preconditioning

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We show that the conjugate gradient method with variable preconditioning in certain situations cannot give any improvement compared to the steepest descent method for solving a linear system with a symmetric positive definite (SPD) matrix of coefficients. We assume that the preconditioner is SPD on each step, and that the condition number of the preconditioned system matrix is bounded from above by a constant independent of the step number. Our proof is geometric and is based on the simple fact that a nonzero vector multiplied by all SPD matrices with a condition number bounded by a constant generates a circular cone.

Incomplete LU preconditioning enhancement strategies for sparse matrices

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Several preconditioning enhancement strategies for improving inaccurate preconditioners produced by the incomplete LU factorizations of sparse matrices are presented. The strategies employ the elements that are dropped during the incomplete LU factorization and utilize them in different ways by separate algorithms.

The first strategy (error compensation) applies the dropped elements to the lower and upper parts of the LU factorization to computer a new error compensated LU factorization. Another strategy (inner-outer iteration), which is a variant of the incomplete LU factorization, embeds the dropped elements in its iteration process.

Experimental results show that the presented enhancement strategies improve the accuracy of the incomplete LU factorization when the initial factorizations found to be inaccurate. Furthermore, the convergence cost of the preconditioned Krylov subspace methods is reduced on solving the original sparse matrices with the proposed strategies.

A novel algebraic multigrid-based approach for solving Maxwell's equations

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This talk presents a new algebraic multigrid-based method for solving the curl-curl formulation of Maxwell's equations discretized with edge elements. The ultimate goal of this approach is two-fold. The first is to produce a multiple-coarsening multigrid method with two approximately decoupled hierarchies branching off at the initial coarse level, one resolving the divergence-free error and the other resolving the curl-free error, i.e., a multigrid method that couples only on the finest level and mimics a Helmholtz decomposition on the coarse levels. The second consideration is to produce the hierarchies using a non-agglomerate coarsening scheme.

To roughly attain this two-fold goal, this new approach constructs the first coarse level using topological properties of the mesh. In particular, a discrete orthogonal decomposition of the finest edges is constructed by dividing them into two sets, those forming a minimum spanning tree and the complement set forming the cotree. Since the cotree edges do not form closed cycles, these edges cannot support "complete" near-nullspace gradient functions of the curl-curl Maxwell operator. Thus, partitioning the finest level matrix using this tree/cotree decomposition, the cotree-cotree submatrix does not have a large near-nullspace. Hence, a non-agglomerate algebraic multigrid method (AMG) that can handle strong positive and negative off-diagonal elements can be applied to this submatrix. This cotree operator is related to the initial coarse-grid operator for the divergence-free hierarchy.

The curl-free hierarchy is generated by a nodal Poisson operator obtained by restricting the Maxwell operator to the space of gradients. Unfortunately, because the cotree operator itself is not the initial coarse-grid operator for the divergence-free hierarchy, the multiple-coarsening scheme composed of the cotree matrix and its coarsening, and the nodal Poisson operator and its coarsening does not give an overall efficient method. Algebraically, the tree/cotree coupling on the finest level, which is accentuated through smooth divergence-free error, is too strong to be handled sufficiently only on the finest level. In this new approach, these couplings are handled using oblique/orthogonal projections onto the space of discretely divergence-free vectors. In the multigrid viewpoint, the initial coarsening from the target fine level to the divergence-free subspace is obtained using these oblique/orthogonal restriction/interpolation operators in the Galerkin coarsening procedure. The resulting coarse grid operator can be preconditioned with a product operator involving a cotree-cotree submatrix and a topological matrix related to a discrete Poisson operator.

The overall iteration is then a multigrid cycle for a nodal Poisson operator (the curl-free branch) coupled on the finest grid to a preconditioned Krylov iteration for the fine grid Maxwell operator restricted to the subspace of discretely divergence-free vectors. Numerical results are presented to verify the effectiveness and difficulties of this new approach for solving the curl-curl formulation of Maxwell's equations.

The return of the filter method

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Filters have been introduced as an alternative to penalty functions to promote global convergence for nonlinear optimization algorithms. A filter borrows ideas from multi- objective optimization and accepts a trial point when-

ever the objective or the constraint violation is improved compared to previous iterates. We present new filter active set approaches to nonlinear optimization based on a two- phase methodology. The first finds an estimate of the optimal active set, and the second phase performs a Newton step on the corresponding equality constrained problem. The approach allows inexact subsystem solves, making it suitable for PDE constrained optimization. Time permitting we present numerical experience on large structured optimization problems.

Towards an automatic and application-based eigensolver selection

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The computation of eigenvalues and eigenvectors is an important and often time-consuming phase in computer simulations. Recent efforts in the development of eigensolver libraries have given users good algorithm implementations without the need for users to spend much time in programming. Yet, given the variety of algorithms that are available to domain scientists, choosing the "optimal" algorithm for a particular application is a daunting task. In addition, as simulations become increasingly sophisticated and larger, it becomes infeasible for a user to try out every reasonable algorithm configuration in a timely fashion. Therefore, there is a need for an automated tool that is able to guide the user through the maze of various solvers with different configurations.

In this talk, we will describe a high-end, intelligent sparse eigensolver toolbox, EigAdept, which comprises the following components:

- A uniform and extensible interface for a collection of parallel sparse eigensolvers. The collection focuses on a class of solvers based on projection methods which are amenable to scalable implementations, which include ARPACK (implicitly restarted Arnoldi method), BLZPACK (block Lanczos method), TRLan (thick-restart Lanczos method), the Jacobi-Davidson method and the multi-level sub-structuring (AMLS) method. The Arnoldi/Lanczos-based solvers are enhanced with shift-and-invert capabilities using the scalable sparse direct linear solvers such as SuperLU and MUMPS.
- An intelligent engine to guide the user through the maze of various solvers and to automate the process of algorithm selection. To achieve that, a "history" knowledge base (algorithm selection criteria, or decision tree) incorporates initial information from our prior experience as well as from the literature (e.g., from "Templates for the Solution of Algebraic Eigenvalue Problems: a Practical Guide", edited by Bai et al.) The contents of the knowledge base are gradually improved as more problems are solved, and can be "adapted" at runtime through the repeated solutions of similar eigensystems from a specific application domain. An efficient data analyzer takes a user's problem specification at runtime, queries the knowledge base, and finds the best match of an algorithm configuration with the target problem.
- Highly-tuned performance-critical kernels for high-end architectures. We identify and isolate the performance-critical kernels (e.g., parallel sparse matrix-vector multiplication), and provide highly-tuned versions for them. The methodology of automatic performance tuning consists of both off-line optimization guided by detailed performance model, and on-line optimization by running the kernels in the pruned space of possible implementations. Furthermore, these tuned kernels will be made as standard-alone components, so that they can be used directly in any new eigensolver technology, or even in other areas of matrix computations.

EigAdept is implemented in C++ with Fortran interface. We have implemented distinct class structures for eigensolvers, linear equation solvers, and matrix types, so that for each eigensolver algorithm, we can easily support

different sparse matrix formats, or use different linear solvers internally (e.g., for performing shift-and-invert). We use MySQL relational database to facilitate the implementation of the intelligent engine. MySQL is a free open source database software with a reliable C API. We will illustrate, with some case studies, that EigAdept can be a valuable tool for users from application domains, as well as for experts doing algorithm research.

An iterative projection method for solving large-scale nonlinear eigenproblems with application to next-generation accelerator design

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The emerging needs to solve large-scale nonlinear eigenvalue problems arising in many engineering applications have come into notice. More researches have been conducted on efficient algorithm development and computational theory. However, the nonlinearity varying greatly from problem to problem results in a challenging computational task. Instead of considering arbitrary nonlinear eigenvalue problems, we consider a certain type of problems for robust and efficient algorithm developments. This particular type nonlinear eigenvalue problems consist of a dominated linear and positive definite pencil and a "small" nonlinear component. A number of applications give rise of nonlinear eigenvalue problems of such type. Examples include vibration study of fluid solid structures and eigencomputation problem from fiber optic design.

In this talk, a nonlinear eigenvalue problem we particular interested in is from the finite element analysis of the resonant frequencies and external Q of a waveguide loaded cavity, as currently be studied by researchers for next-generation accelerator design. We study iterative subspace projection methods, such as nonlinear Arnoldi method. We focus on the critical stages of algorithms, such as the choice of initial projection subspace, and the expansion and the refinement of projection subspace. We present a notable improvement over the early iterative projection methods in our case study.

Adaptive mesh refinement: in the presence of discontinuities

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Classical multiresolution wavelet techniques have been used successfully to simplify the computation of PDEs by concentrating resources in places where the solution varies quickly. However, classical techniques tend to fail near solution discontinuities, as Gibb's effects contaminate the wavelet coefficients used to refine the solution. Nonlinear adaptive stencil methods, such as the ENO scheme, can reconstruct the solution accurately across jumps, but possess neither the compression capabilities nor the well-understood stability properties of wavelets. Expanding on Harten's ideas, we construct an alternative to wavelets, a multiresolution method that does not suffer from Gibb's effects and has good compression properties. We will present this alternative multiresolution method and compare its performance to other methods by means of several examples.

Preconditioning techniques for the Navier-Stokes equations in rotation form

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We consider preconditioned iterative methods applied to discretizations of the Navier-Stokes equations in 2D and 3D bounded domains. Both unsteady and steady flows are considered. The equations are linearized by Picard iteration. We make use of the rotation form of the momentum equations, which has several advantages from the linear algebra point of view.

We focus on two classes of preconditioners for the resulting nonsymmetric saddle point problems, namely, block triangular preconditioners and some variants of the Hermitian/Skew-Hermitian splitting (HSS) preconditioner. Both types of preconditioners have comparable cost per iteration, and make use of (standard) fast solvers for elliptic scalar PDEs (convection-diffusion and Poisson-type).

We compare the performance of both types of preconditioners with regard to the mesh size, the Reynolds number, the time step, and other problem parameters. Our experiments indicate that fast convergence independent of problem parameters is achieved in many cases. We include comparing experiments for both the rotation form and convection diffusion form of the Navier-Stokes equations the nonlinear iteration.

AMG eigenbasis solver for the Schrödinger eigenvalue problem

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In this talk the AMG algorithm for solving the Scrödinger eigenvalue problem is discussed. Its goal is to approximate the eigenbasis, i.e., all eigenfunctions, of the Schrödinger operator as it appears in the Kohn-Sham equation.

The algorithm employs multilevel eigenvalues/eigenfunction representations that allows approximation of most of the eigenfunctions on the inexpensive coarse grids and leads to a reduction of both computational and storage costs. In addition this structure is beneficial for performance of a variety of applications essential to the Kohn-Sham equations. Also addressed is the issue of quality of the obtained sets of eigenfunctions, such as their accuracy and independence. Numerical results and discussion of the further extension of the approach will conclude the talk.

A domain decomposition method that converges in two steps for three subdomains

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In Schwarz-like domain decomposition methods, a domain Ω is broken into two or more subdomains and Dirichlet, Neumann, Robin or pseudo-differential problems are iteratively solved on each subdomain. For certain problems, it is well-known that the Dirichlet-Neumann iteration for two subdomains will converge in two steps. Let Ω be an open domain and $\Omega_1, \Omega_2, \Omega_3$ a domain decomposition of Ω such that each pair of subdomains shares an interface (for instance, $\Omega = \{z \in \mathbb{C} \mid |z| < 1\}$ and $\Omega_j = \{re^{i\theta} \mid 0 < r < 1 \text{ and } \theta \in (2j\pi/3, 2(j+1)\pi/3)\}$, $j = 1, 2, 3$). We will show a new Schwarz-like domain decomposition method that converges in two iterations in this situation.

A greedy strategy for coarse-grid selection

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In recent years, substantial effort has been focused on developing methods capable of solving the large linear systems that arise from the discretization of partial differential equations. This research has been driven by application scientists' demands of higher accuracy, in both mathematical modeling and computational solution. Efficient solution of many of these linear systems is possible only through the use of multilevel solution techniques. While highly optimized algorithms may be developed using knowledge about the origins of the matrix problem to be considered, much current interest is in the development of purely algebraic approaches that may be applied in many situations, without extensive problem-specific tuning.

In this talk, we present a new algebraic approach to finding the fine/coarse partitions needed in multilevel approaches. The algorithm is motivated by theoretical analysis of the performance of algebraic multigrid (AMG) and algebraic recursive multilevel solvers (ARMS). From the AMG point of view, the coarsening is consistent with the ideas of compatible relaxation, while it may also be motivated by the algebraic criteria central to ARMS. While no guarantee on the rate of coarsening is given, the splitting is shown to always yield an effective preconditioner in the two-level sense. Numerical performance of two-level and multilevel variants of this approach is demonstrated.

Adaptive selection of face coarse degrees of freedom in the BDDC and the FETI-DP iterative substructuring methods

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We propose adaptive selection of the coarse space of the BDDC and FETI-DP iterative substructuring methods by adding coarse degrees of freedom with support on selected intersections of adjacent substructures. The coarse degrees of freedom are constructed using eigenvectors associated with the intersections. The minimal number of coarse degrees of freedom on the selected intersections is added to decrease a heuristic indicator of the the condition number under a target value specified a priori. It is assumed that the starting coarse degrees of freedom are already sufficient to prevent relative rigid body motions of any selected pair of adjacent substructures. It is

shown numerically on 2D elasticity problems that the indicator based on pairs of substructures with common edges predicts reasonably well the actual condition number, and that the method can select adaptively the hard part of the problem and concentrate computational work there to achieve good convergence of the iterations at a modest cost.

A comparison of eigensolvers for large electronic structure calculations

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The solution of the single particle Schrödinger equation that arises in electronic structure calculations often requires solving for interior eigenstates of a large Hamiltonian. The states at the top of the valence band and at the bottom of the conduction band determine the band gap that relates to important physical characteristics such as optical or transport properties.

In order to avoid the explicit computation of all eigenstates, a folded spectrum method has been usually employed to compute only the eigenstates near the band gap. In this talk, we compare the conjugate gradient minimization and the optimal block preconditioned conjugate gradient (LOBPCG) applied to the folded spectrum matrix with the Jacobi-Davidson algorithm.

Solution of high-order discontinuous Galerkin methods using a combined H-P multigrid approach

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The development of optimal, or near optimal solution strategies for higher-order discretizations, including steady-state solutions methodologies, and implicit time integration strategies, remains one of the key determining factors in devising higher-order methods which are not just competitive but superior to lower-order methods in overall accuracy and efficiency. The goal of this work is to investigate and develop a fast and robust algorithm for the solution of high-order accurate discontinuous Galerkin discretizations of non-linear systems of conservation laws on unstructured grids.

We develop a spectral multigrid method, whereby the coarse "grid" levels are constructed by reducing the order (p) of approximation of the discretization using hierarchical basis functions(p-multigrid), keeping the grid elements fixed. This approach is coupled with a traditional agglomeration multigrid (h-multigrid) approach for unstructured grids, by constructing additional coarse levels at the lowest ($p = 0$) spectral level through element agglomeration. The overall goal is the development of a solution algorithm which delivers convergence rates which are independent of "p" (the order of accuracy of the discretization) and independent of "h" (the degree of mesh resolution), while minimizing the cost of each iteration. The investigation of efficient smoothers to be used at each level of the multigrid algorithm is also pursued, and comparisons between different integration strategies are made as well.

AMGLAB: an interactive MATLAB testbench for learning and experimentation with algebraic multigrid methods

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We describe a first step towards a general algebraic multigrid expert system that we expect to become a community project in the multigrid field.

A scalable projection method for the unsteady incompressible Navier-Stokes equations

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We discuss a high order projection scheme for time integration of the incompressible Navier-Stokes equations. The method is based on a projection onto a divergence-free subspace interleaved with a Krylov based exponential time integration. This semi-explicit approach provides stability and high order accuracy without the need for a nonlinear iteration. We present numerical examples to support our claims and provide comparison against a Crank Nicolson scheme.

HP local refinement using FOSLS

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Local refinement enables us to concentrate computational resources in areas that need special attention, for example, near steep gradients and singularities. In order to use local refinement efficiently, it is important to be able to quickly estimate local error. FOSLS is an ideal method to use for this because the FOSLS functional yields a sharp a posteriori error measure for each element. This talk will discuss a strategy for determining which elements to refine in order to optimize the accuracy/computational cost. Set in the context of a full multigrid algorithm, our strategy leads to a refinement pattern with nearly equal error on each element. Further refinement is essentially uniform, which allows for an efficient parallel implementation. Numerical experiments will be presented.

Developments in algebraic multigrid preconditioning for high-order spectral elements

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In this talk we highlight recent attempts to solve systems of equations arising from high-order spectral element discretizations. In particular, we extend the success of Algebraic Multigrid (AMG) preconditioning on structured grids to the unstructured case (using triangles).

We consider high-order nodal spectral elements based on the electrostatic distribution. A low-order finite element preconditioner is utilized and accelerated with Conjugate Gradient. The elements cause a particular challenge as the local grids are also unstructured and suffer from poor aspect ratios. We present numerical evidence in support of this method and discuss the implications of using this approach.

Nonsmooth, nonconvex optimization: theory, algorithms, and applications

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Theory: there are two standard approaches to generalizing derivatives to nonsmooth, nonconvex optimization: the Clarke subdifferential (or generalized gradient), and the MIRW subdifferential (or subgradient sets), as expounded in Rockafellar and Wets (Springer, 1998). We briefly discuss these and mention their advantages and disadvantages. They coincide for an important class of functions: those that are locally Lipschitz and regular, which includes continuously differentiable functions and convex functions.

Algorithms: the usual approach is bundle methods, which are complicated. We describe some alternatives: BFGS (a new look at an old method), and Gradient Sampling (a simply stated method that, although computationally intensive, has solved some previously unsolved problems and has a nice convergence theory).

Applications: these abound in control, but surely in other areas too. Of particular interest to me are applications involving eigenvalues and singular values of nonsymmetric matrices. Sometimes even easily stated problems in a few variables are hard. Our new code HIFOO (H-Infinity Fixed-Order Optimization) is intended for use by practicing control engineers and has solved some open problems in control.

This is all joint work with James Burke and Adrian Lewis. HIFOO is also joint with Didier Henrion.

Additive Schwarz methods for elliptic problems with periodic boundary conditions

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In this presentation we discuss additive Schwarz methods for numerical solutions of elliptic problems with periodic boundary conditions. Unlike Dirichlet or Neumann type conditions that are purely local, periodic conditions are more global, therefore Schwarz type domain decomposition preconditioning techniques do not perform in the same manner as in Dirichlet or Neumann problems. In this work we study the parallel performance of one- and two-level algorithms and report experimental results obtained on the IBM BG/L. We also discuss some applications of additive Schwarz preconditioners for the numerical simulation of magnetohydrodynamics.

Novel preconditioning techniques in matrix computations

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Multiplicative preconditioners are popular for solving linear systems of equations. We introduce additive preconditioners, which are more robust and more readily available. By combining them with aggregation processes, we obtain preconditioners that are nearly as effective as SVD-based multiplicative preconditioners. Besides simplifying and stabilizing the generation of such preconditioners, this technique also preserves the structure of the input matrices, and we also employ it for numerical computation of the sign of the matrix determinant. Our alternative techniques employ additive preconditioners for computing null vectors and null space bases for a singular matrix, and we extend this approach to yield alternative linear solvers and to compute the tails of the SVDs of ill conditioned matrices and matrix eigenvectors. We support our approach with extensive analysis and numerical experiments.

Performance of the predictor-corrector preconditioners for Newton-Krylov solvers

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We investigate an alternative implementation of preconditioning techniques for the solution of non-linear problems. Within the framework of Newton-Krylov methods, preconditioning techniques are needed to improve the performance of the solvers. We use a different implementation approach to re-utilize existing semi-implicit methods to precondition fully implicit non-linear schemes. We use a predictor- corrector approach where the fully non-linear scheme is the corrector and the pre- existing semi-implicit scheme is the predictor [1,2]. The advantage of the proposed approach is that it allows to retrofit existing codes, with only minor modifications, in particular avoiding the need to reformulate existing methods in terms of variations, as required instead by other approaches now currently used.

A classic problem of computational science and engineering is the search for an efficient numerical scheme for solving non-linear time-dependent partial differential equations. Explicit and semi-implicit methods can provide simple solution techniques but are seriously limited by time step limitations for stability (explicit methods) and accuracy (semi-implicit methods).

Recently, significant progress has been made in the development of fully implicit approaches for solving nonlinear problems: the Newton-Krylov (NK) method. The method is developed from the Newton iterative method, by applying a linear iterative solver to the Jacobian equation for the Newton step and terminating that iteration when a suitable convergence criterion holds.

For the solution of the linear Jacobian equation, Krylov methods are often the choice, leading to the Newton-Krylov (NK) approach. However, for most cases, Krylov solvers can be extremely inefficient. The need for good preconditioners techniques becomes a constraining factor in the development of NK solvers.

In a number of fields, recent work based on multi-grid and physics-based preconditioners[3] have demonstrated extremely competitive performances.

In the present study, we discuss a different implementation of preconditioning: the predictor-corrector (PC) preconditioner [1,2]. The approach has two novelties. First, it preconditions directly the non-linear equations rather than the linear Jacobian equation for the Newton step. The idea is not new, but it is implemented here in a new way that leads to great simplifications of the implementation. We note that this simplification is designed also to minimize the effort in refitting existing semi-implicit codes into full fledged implicit codes, representing perhaps a greater advance in software engineering than in computational science. Second, we test new ways of preconditioning the equations by using a combination of predictor-corrector semi-implicit preconditioning.

The fundamental idea is to use a predictor to advance a semi-implicit discretization of the governing equations and use a corrector Newton step to correct for the initial state of the predictor step. The typical NK solver is used to compute the unknown value of the state vector at the end of the time step $\mathbf{x}^1$ from its known value at the previous time step $\mathbf{x}^0$. Instead, we use the Newton method to iterate for a modification of the actual known state $\mathbf{x}^*$ from the previous time step to find a modified *"previous"* state that makes the semi-implicit predictor step give the solution of the fully implicit method.

Two advantages are obvious. First, the actual previous state $\mathbf{x}^0$ is likely to be a better first guess for the modified initial state $\mathbf{x}^*$ of the predictor than it is for the final state of the corrector step. Second, by modifying the non-linear function and consequently modifying the Jacobian equation, the PC preconditioner modifies the spectral properties of the Jacobian matrix in the same way as preconditioners applied directly to the Jacobian equation. Indeed, as shown below the PC preconditioner gives the same type of speed-up of the Krylov convergence without

requiring to formulate an actual preconditioning of the Krylov solver.

We use a suite of problems, including non-linear diffusion [2] and the standard driven cavity flow problem [1], as benchmarks to demonstrate the performance and the reliability of the PC preconditioning method.

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[3] D. A. Knoll, D. Keyes, *Jacobian-free Newton-Krylov methods: a survey of approaches and applications*, J. Comp. Phys. **193** (2004) 357–397.

Theory of molecular fluids

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A quantitative theory of the structure of molecular fluids described by atoms or sites has remained elusive in soft condensed matter theory. Many-body and field theoretic approaches to the correlations liquids have advanced slowly since the 1930s. The qualitative and quantitative inconsistencies of the many-body integral equation theory for predicting the structure and thermodynamic properties of model molecular fluids have been understood for some time.

Several means have been proposed to correct these inconsistencies, many concentrating on the Goldstone theorem. A formally distinct method for constructing a diagrammatically proper theory eliminates terms in the expansion which correspond to unphysical intramolecular interactions, or so-called bad graphs. Unfortunately, while certain qualitative advances using the proper theory have been successful the quantitative results appear to be uniformly disappointing in comparison to simulation.

We present a new derivation from a topological expansion of a model for the single atom activity followed by a topological reduction and low order truncation. This leads to an approximate numerical value for the new density coefficient. The resulting equations give a substantial improvement over the standard construction as shown with a series of simple diatomic model simulations.

Resistive magnetohydrodynamics with implicit adaptive mesh refinement

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Implicit adaptive mesh refinement (AMR) is used to simulate a model resistive magnetohydrodynamics problem. This challenging multi-scale, multi-physics problem involves a wide range of length and time scales. AMR is employed to resolve extremely thin current sheets, essential for an accurate macroscopic description. 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. The preconditioner is implemented using optimal multilevel solvers such as the Fast Adaptive Composite grid (FAC) method. We will describe our initial results highlighting various aspects of problem formulation, optimal preconditioning on AMR grids, and efforts towards achieving parallelism.

Solving bordered systems of linear equations for large-scale continuation and bifurcation analysis

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Solving bordered systems of linear equations where the matrix is augmented by a small number of additional rows and columns is ubiquitous in continuation and bifurcation analysis. Examples include pseudo-arclength continuation, constraint following, and turning point location. However solving these systems in a large-scale setting where the original matrix is large and sparse is difficult. Directly augmenting the matrix destroys the sparsity structure of the original matrix since the additional rows and columns are usually dense, while block elimination methods have difficulty when the original matrix is nearly singular and result in additional linear solves.

In this talk we discuss a simple method for solving systems of this form using Krylov iterative linear solvers based on computing the QR factorization of the augmented rows, and is an extension of the Householder pseudo-arclength continuation method developed by H. Walker. It allows solutions of the bordered system to be computed with a cost roughly equivalent to solving the original matrix and is well-conditioned even when the original matrix is singular.

We then apply this technique to the problem of computing turning point bifurcations in large-scale nonlinear systems. The QR approach allows turning point algorithms that are faster, more robust and scale better to millions of unknowns compared to traditional block elimination schemes. Examples of applying these techniques to large-scale structural and fluid mechanics problems will be presented. These techniques have been implemented in a continuation and bifurcation software package called LOCA, short for The Library of Continuation Algorithms, developed by the authors and publicly available as a part of Trilinos, a set of scalable linear and nonlinear solvers.

Stochastic preconditioning for iterative linear equation solvers

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Stochastic techniques, namely random walks, have been used to form linear equation solvers since the 1940s, but have not been used effectively for preconditioning, to the best of our knowledge. In this talk, we present a new stochastic preconditioning approach: we prove that for symmetric diagonally-dominant M-matrices, an incomplete

LDL factorization can be obtained from random walks, and used as a preconditioner for an iterative solver, e.g., conjugate gradient. The theory can be extended to general matrices with nonzero diagonal entries.

The stochastic preconditioning is performed by a random walk "game" defined as follows. Given a finite undirected connected graph representing a street map, a walker starts from one of the nodes, and goes to one of the adjacent nodes every day with a certain probability. The walker pays an amount of money, m_i at node i, to a motel for lodging everyday, until he/she reaches one of the homes, which are a subset of the nodes. Then the journey is complete and he/she will be rewarded a certain amount of money, m_0. The problem is to determine the gain function:

$$f(i) = E[\text{money earned } | \text{walk starts at node } i]$$

These gain values satisfy the following linear equations:

$$\begin{aligned} f(i) &= \sum_{j \in \text{neighbors of } i} p_{i,j} f(j) - m_i \quad , \quad \forall i \\ f(\text{a home node}) &= m_0 \end{aligned}$$

where $p_{i,j}$ is the transition probability of going from node i to node j, and note that j can be a home node. Thus a random walk game is mapped onto a system of linear equations. Conversely, it can be verified that given $A\mathbf{x} = \mathbf{b}$, where A is a symmetric diagonally-dominant M-matrix, we can always construct a random walk game that is mathematically equivalent, in which the set of f values is equal to the solution vector $\mathbf{x}$. To find the i^{th} entry of $\mathbf{x}$, one may run a number of walks from node i and take the average of the results; to get the complete solution, one may repeat the process for every entry of $\mathbf{x}$. We alter this normal procedure by adding the following rule: every calculated node becomes a new home in the game with an award amount equal to its calculated f value. Without loss of generality, suppose the nodes are in the natural ordering $1, 2, \cdots, N$, then for walks starting from node i, the node set $\{1, 2, \cdots, i-1\}$ are homes where walks terminate (in addition to homes generated from the strictly-diagonally-dominant rows of A), while the node set $\{i, i+1, \cdots, N\}$ are motels where walks pass by.

Define the operator $\text{rev}(\cdot)$ on square matrices such that it reverses the ordering of the rows and reverses the ordering of the columns: $\text{rev}(A)_{i,j} = A_{N+1-i,N+1-j}, \quad \forall i, j \in \{1, 2, \cdots, N\}$. Let the exact LDL factorization of $\text{rev}(A)$ be $\text{rev}(A) = L_{\text{rev}(A)} D_{\text{rev}(A)} \left(L_{\text{rev}(A)}\right)^{\text{T}}$. Again, in the random walk game, assume that the nodes are in the natural ordering $1, 2, \cdots, N$, and that node i corresponds to the i^{th} row of A. We prove the following relations:

$$\begin{aligned} \left(L_{\text{rev}(A)}\right)_{i,j} &\approx -\frac{M_{N+1-j,N+1-i}}{W_{N+1-j}}, \quad \forall i > j \\ \left(D_{\text{rev}(A)}\right)_{i,i} &\approx \frac{W_{N+1-i} A_{N+1-i,N+1-i}}{J_{N+1-i}} \end{aligned}$$

where W_k is the total number of walks that are carried out from node k, M_{k_1,k_2} is the number of walks that start from node k_1 and end at k_2, and J_k is the number of times that the W_k walks from node k pass node k itself. These equations show that we can approximate an LDL factorization by collecting information from random walks. We further prove that if $\left(L_{\text{rev}(A)}\right)_{i,j} = 0$ then $M_{N+1-j,N+1-i} = 0$; in other words, the nonzero pattern of the L factor produced by random walks is a subset of nonzero pattern of the exact $L_{\text{rev}(A)}$. Therefore, we conclude that an incomplete LDL factorization can be obtained from random walks.

We argue that the obtained incomplete LDL factors have better quality, i.e., better accuracy-size tradeoffs, than the incomplete Cholesky factor obtained by a traditional method based on Gaussian elimination. Our argument is based on the fact that each row in the L factor is independently calculated and has no correlation with the computation of other rows. Therefore we avoid the error accumulation in traditional incomplete factorization procedure.

We also discuss, by defining a new set of game rules, how this theory can be extended to general matrices, given that the diagonal entries are nonzero.

To evaluate the proposed approach, a set of benchmark matrices are generated by Y. Saad's SPARSKIT by finite-difference discretization of the 3D Laplace's equation $\nabla^2 u = 0$ with Dirichlet boundary condition. The matrices

correspond to 3D grids with sizes $50 \times 50 \times 50$, $60 \times 60 \times 60$, up to $100 \times 100 \times 100$, and a right-hand-side vector with all entries being 1 is used with each of them. We compare the proposed solver, i.e., random walk preconditioned conjugate gradient, against ICCG with ILU(0) and ICCG with ILUT. The complexity metric is the number of double-precision multiplications needed at the iterative solving stage, in order to converge with an error tolerance of 10^{-6}. The results show up to 2.1 times speedup over ICCG, and a trend that the larger and denser a matrix is, the more the proposed solver outperforms ICCG.

This talk is partially based on [1], and the implementation is available to the public [2].

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[2] H. Qian, S. S. Sapatnekar, *The Hybrid Linear Equation Solver Binary Release*, available at http://www.ece.umn.edu/users/qi

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Preconditioning primal-dual interior point methods for linear programming

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We investigate the application of a class of preconditioners to the problem of solving the linear systems arising from primal-dual interior point methods in linear and quadratic programming. The preconditioners have the attractive property of improved eigenvalue clustering with increased singularity of the (1,1) block of the saddle-point matrix. We analyze spectral properties of the preconditioned matrix utilizing projections onto the null space of the constraint matrix. We then present a practical application of the preconditioners and study their performance on LP and QP problems from the NETLIB and QPS test suites.

Simulating non-Darcy flow through porous media using Sundance

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A non-Darcy partial differential equation (PDE) model for flow through porous media is presented. The focus is on the numerical implementation of the model using Sandia National Laboratories PDE simulation framework, Sundance. In particular, the discussion will include the finite element discretization and how parallelism is accomplished.

Parameter decomposition for iteratively regularized Gauss-Newton solutions in optical tomography

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We extend evaluation of the iteratively regularized Gauss Newton method for the solution of the parameter estimation problem in Optical Tomography. The general problem of optical tomography requires the estimation of the underlying model parameters $\mathbf{q}$, for example the coefficient of diffusion D and the coefficient of absorption μ_a, (i.e. $\mathbf{q} = (D, \mu_a)^T$) that belong to a parameter set Q. The conditioning of the problem with respect to each parameter set is different. We investigate the use of an alternating parameter decomposition approach for solution of the nonlinear inverse problem with regularization. Contrary to statements on the general nonlinear least squares problem in standard references eg Bjorck 1996 , we find that decomposition with respect to the parameter set allows solution of the regularized problem with the use of appropriately chosen weighting schemes.

Krylov-Secant methods for estimating subsidence parameters in hydrocarbon reservoirs

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It is a well known fact that under primary fluid production conditions, pore pressures of hydrocarbon reservoirs and aquifers tend to decline. This decline may lead to severe deformations inside and around the reservoir. The deformation observed at the surface is known as subsidence and can produce negative environmental effects as well as damage to surface facilities and infrastructures. Positively speaking, subsidence observations can be combined with inverse algorithms in order to assess reservoir behavior and detect non-depleted regions that may be subject to further exploitation. The estimation of subsidence usually requires the performance of flow simulations coupled to mechanical deformation. These simulations are computationally intensive and, for this reason, they are seldom performed.

In this work we introduce a Krylov-secant inversion framework for estimating the deformation produced as a consequence of pore pressure reduction in the reservoir. The formulation is based on a solution of the equilibrium equation where perturbations due to pore pressure reduction and elastic modulus contrasts are introduced. The resulting equation for the strain is given in the form of the Lippmann-Schwinger integral, i.e.,

$$\mathbf{e}(\mathbf{x}) = -\int_{\Omega} \Gamma(\mathbf{x} - \mathbf{x}') \{\Delta\mathbf{C}\mathbf{e}(\mathbf{x}') - \alpha\Delta p\} \, d\mathbf{x}', \tag{1}$$

where $\Gamma(\mathbf{x} - \mathbf{x}')$ is the modified half space Green's function; $\Delta\mathbf{C}$ is the elastic module contrast; Δp is the magnitude of the pore pressure drop; and α is the Biot's poroelastic constant, assumed here to be a tensor. Both $\Delta\mathbf{C}$ and Δp are zero outside the reservoir but can be functions of $\mathbf{x}'$. The integration in (1) is performed over the reservoir domain.

A Born-type approximation is implemented, where the total field is assumed to be the incident field by analogy to electromagnetic theory.

Based on the discretization of (1) the resulting inverse problem can be stated as the minimization of the following mismatch functional:

$$\phi = \frac{1}{2}\|\hat{d} - d\|_W^2, \qquad (2)$$

where d and $\hat{d} \in C^n$ are the predicted and observed data vectors respectively, and W is a diagonal weighting matrix, based on the inverse of the covariance of the measurements that compensates for the noise present in the data. In the problem addressed here, the observed data are the subsidence observations at some points, while the predicted data vector d is determined through solution of the forward model (1). The minimization problem (2) is large and ill-posed, especially in the event of high heterogeneities and few measurements. To perform the inversion, a Newton-Krylov procedure based on Krylov-secant updates is proposed.

The Krylov-secant framework entails a recycling or extrapolation of 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.

The proposed framework includes dynamic control of linear tolerances (i.e., forcing terms), preconditioning, and regularization to achieve both efficiency and robustness. Furthermore, this approach may optionally accommodate the latest deflation or augmented Krylov basis strategies for further efficiency. The framework has been previously applied for the solution of several nonlinear PDEs under Newton-Krylov implementations, but the present work explores further issues with respect to inexact Gauss-Newton methods based on Krylov iterative solutions such as LSQR.

Numerical experiments indicate that the current approach is a viable option for performing fast inversion implementations. Comparisons are made against traditional quasi-Newton and gradient-based implementations. It is concluded that the proposed approach has the potential for application to electromagnetic, radar, seismic and medical technologies.

Computing dominant poles of transfer functions

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Recent work on power system stability, controller design and electromagnetic transients has used several advanced model reduction techniques. Although these techniques, such as balanced truncation, produce good results, they impose high computational costs and hence are only applicable to moderately sized systems. Modal model reduction is a cost-effective alternative for large-scale systems, when only a fraction of the system pole spectrum is controllable-observable for the transfer function of interest. Modal reduction produces transfer function modal equivalents from the knowledge of the dominant poles and their corresponding residues. In this talk a specialized eigenvalue method will be presented that computes the most dominant poles and corresponding residues of a SISO transfer function.

The transfer function of a single input single output (SISO) system is defined as

$$H(s) = \mathbf{c}^T(sI - A)^{-1}\mathbf{b} + d, \qquad (1)$$

where $A \in \mathbb{R}^{n\times n}$, $\mathbf{b}, \mathbf{c} \in \mathbb{R}^n$, $d \in \mathbb{R}$ and $I \in \mathbb{R}^{n\times n}$ is the identity matrix and $s \in \mathbb{C}$. Without loss of generality, $d = 0$ in the following.

Let the eigenvalues (poles) of A and the corresponding right and left eigenvectors be given by the triplets $(\lambda_j, \mathbf{x}_j, \mathbf{v}_j)$, and let the right and left eigenvectors be scaled so that $\mathbf{v}_j^* \mathbf{x}_j = 1$. It is assumed that $\mathbf{v}_j^* \mathbf{x}_k = 0$ for $j \neq k$. The transfer function $H(s)$ in equation (1) can be expressed as a sum of residues R_j over first order poles:

$$H(s) = \sum_{j=1}^{n} \frac{R_j}{s - \lambda_j},$$

where the residues R_j are

$$R_j = (\mathbf{x}_j^T \mathbf{c})(\mathbf{v}_j^* \mathbf{b}).$$

A *dominant* pole is a pole λ_j that corresponds to a residue R_j with large magnitude $|R_j|/|\mathrm{Re}(\lambda_j)|$, i.e., a pole that is well observable and controllable in the transfer function. This can also be observed from the corresponding Bode magnitude plot of $H(s)$, where peaks occur at frequencies close to the imaginary parts of the dominant poles of $H(s)$. An approximation of $H(s)$ that consists of $k < n$ terms with $|R_j|/|\mathrm{Re}(\lambda_j)|$ above some value, determines the effective transfer function behavior and is called the transfer function modal equivalent:

$$H_k(s) = \sum_{j=1}^{k} \frac{R_j}{s - \lambda_j}.$$

The problem of concern can now be formulated as:

> Given a SISO linear, time invariant, dynamical system $(A, \mathbf{b}, \mathbf{c}, d)$, compute $k \ll n$ dominant poles λ_j and the corresponding right and left eigenvectors $\mathbf{x}_j$ and $\mathbf{v}_j$.

The algorithm to be presented, called Subspace Accelerated Dominant Pole Algorithm (SADPA) [1], combines a Newton algorithm [2] with subspace acceleration, a clever selection strategy and deflation to efficiently compute the dominant poles and corresponding residues. It can easily be extended to handle MIMO systems as well [3]. The performance of the algorithm will be illustrated by numerical examples of large scale power systems.

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[2] N. Martins, L.T.G. Lima, H.J.C.P. Pinto, *Computing dominant poles of power system transfer functions*, IEEE Trans. Power Syst. **11**(1) (1996) 162–170.

[3] J. Rommes, N. Martins, *Efficient computation of multivariable transfer function dominant poles using subspace acceleration*, UU Preprint (2006) 1344.

Space-time solution of large-scale PDE applications

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Software and algorithms are being developed to efficiently formulate and solve transient PDE problems as "steady" problems in a space-time domain. In this way, sophisticated design and analysis tools for steady problems, such as continuation methods, can be brought to bear on transient (and eventually periodic) problems. This new capability

is being developed in the Trilinos solver framework, and is designed to present a simple interface to application codes. The software allows for parallelism over both the space and time domains.

The main hurdle to make this approach viable is to be able to efficiently solve the very large Jacobian matrix for very large the space-time system, with its characteristic structure. We will present results for a number of preconditioners and solution methods that we have developed for this linear system. Numerical results for a PDE reacting flow application will be presented. These results will shed some light on the underlying question of whether it can pay to parallelize the time domain.

Adaptive smoothed aggregation multigrid for non-symmetric problems

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The performance of the adaptive smooth aggregation multigrid (αSA) algorithm suffers for non-symmetric problems. I will present a non-symmetric version of the algorithm that uses Kaczmarz iteration as a relaxation step and smoothed aggregation of local right and left singular vectors to form a hierarchy of coarse grid operators. Testing has been done on one and two dimensional convection dominated convection-diffusion. I will present the current results and struggles of these tests. Expect some whining.

On large scale diagonalization techniques for the Anderson model of localization

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One of the hardest challenges in modern eigenvalue computation is the numerical solution of large-scale eigenvalue problems, in particular those arising from quantum physics such as the Anderson model of localization [4]. Typically, these problems require the computation of some interior eigenvalues and eigenvectors for systems which have up to several million unknowns due to their high spatial dimensions. Furthermore, their underlying structure involves random perturbations of matrix elements which invalidates simple preconditioning approaches.

We propose an efficient preconditioning algorithm for this Anderson model of localization [6]. The model requires the computation of a few interior eigenvalues and their associated eigenvectors for large scale, sparse, real and symmetric indefinite matrices. Our preconditioning approach for the associated shift-and-invert systems is based on maximum weighted matchings [3,5] and algebraic multilevel, inverse-based incomplete LDL^T factorizations [1,2]. Our numerical examples indicate that recent algebraic multilevel preconditioning solvers can accelerative the computation of the underlying large-scale eigenvalue problem by several orders of magnitude compared with previous approaches [4,6].

[1] M. Bollhöfer and Y. Saad, *Multilevel preconditioners constructed from inverse-based ILUs*, SIAM J. Sci. Comp., to appear (2006).

[2] M. Bollhöfer and O. Schenk, *ILUPACK volume 2.0 — preconditioning software package for symmetrically structured problems* (May 2005).

[3] I. S. Duff and S. Pralet, *Strategies for scaling and pivoting for sparse symmetric indefinite problems*, Technical Report TR/PA/04/59, CERFACS (2004).

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[5] M. Hagemann, O. Schenk, *Weighted matchings for the preconditioning of symmetric indefinite linear systems*, SIAM J. Sci. Comp., to appear (2006).

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Phenomenological comparison of different AMG approaches for the finite element analysis in surgery simulations

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We are dealing with the simulation of maxillo-facial surgeries, especially with distraction osteogenesis. During this treatment the surgeon cuts free the upper jaw (maxilla), which is subsequently relocated into a new position with a distraction device in the course of several weeks. Our simulation tool is set up to predict the displacements of the facial tissues during and after the pulling process and is based on individual CT images of the patient's head before treatment. Its purpose is to support the surgeon in optimizing the treatment plan and avoiding additional post operative plastic surgeries.

The input data for the simulation task is generated by adding the suggested cuts, the geometry of the distraction device and the suggested forces to the CT data of the patient's head. From these data we generate a Finite Element mesh of the head and perform a Finite Element analysis of the distraction process. In order to achieve sufficient accuracy we have to resolve most of the geometrical features of the human head, which leads to a large number of unknowns, typically several millions. In addition to that the computational costs are significantly increased by the finite displacements which can only be properly approximated by non-linear modeling. The resulting systems of equations must be solved on high performance computing resources, such as parallel or vector machines.

Focusing on the efficiency of the Finit Element simulation, the linear solver used to solve the arising systems of equations plays the most crucial role. In our case standard solvers like Krylov methods or ILU methods fail, as we will show in our presentation. Therefore we will focus on the use of Multigrid solvers.

But the complex geometry of the human head in combination with large jumps of the material parameters – Young's modulus jumps about 5 orders of magnitude between bone and soft tissues – prevents standard multigrid approaches to converge at a sufficient rate. In theory they can be dramatically improved by computing the "near null space" of the systems, consisting of the all quasi-rigid body modes, and treat it separately. But we will show, that for our problems a basis of this space needs approximately 10 times the memory of the linear system itself, which rules out this approach.

In our presentation we will demonstrate the performance of the only two solvers we have found to work on our problems so far, which are BoomerAMG from LLNL's HYPRE package and ML from Sandia's Trilinos package. We will show the results of our intensive parameter studies and discuss the extensibility of our performance results for elasto-mechanical Finite Element simulations in general.

Spatial multigrid for transport

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A spatial multigrid algorithm for isotropic neutron transport is presented in x-y geometry. The problem is discretized with discrete ordinates in angle and corner balance finite differencing in space. Spatial smoothing is accomplished by a four color block Jacobi relaxation, where the diagonal blocks correspond to four cell blocks on the spatial grid. A bilinear interpolation operator and its transpose are used for the grid transfer operators. Encouraging preliminary results are presented for homogeneous domains. Heterogeneous domains are also discussed, especially the case of a vacuum region surrounded by a diffusive region.

A new stabilized formulation for the Stokes problem

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I shall introduce a new formulation for the Stokes problem, stemming from the consistent splitting scheme for the time-dependent Navier-Stokes equations introduced by Guermond & Shen (JCP, 2003). I shall present ample numerical results, using spectral and finite element methods, to show that the new formulation leads to positive definite systems and does not require the usual inf-sup condition between the discrete spaces for the velocity and pressure.

A large scale nonlinear finite element solver algorithm with optimal speed and robustness

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The speaker will present a new theory, the related algorithmic and programming architecture for solving nonlinear boundary value problems with *optimal speed and robustness* by using large numbers of finite elements.

The new methodology will achieve the desired optimality over a singularly large spectrum of nonlinear finite element models on bounded domains of R^n with $n = 2$ and $n = 3$. For example, the algorithm will cover the Galerkin formulation of well-posed nonlinear elliptic systems whose principle part is Lipschitz continuous and strongly monotone in a Sobolev space and certain problems that lack unique solutions such as stationary Navier-Stokes equations. Large variations of stiffness will also be permitted in both magnitude and frequency.

The merit of the new algorithm is not only its speed and scope, but also its mathematically rigorous theory, the elegance in algorithmic design, and simplicity in implementation. The approach will be based on the proven success of the speaker's long time effort starting from early 1990s, recently reported in [1], which successfully establishes the corresponding result for second order *quasi-linear* elliptic systems with non-negative lower order terms.

Central to the algorithm, the speaker will reformulate a finite element model by generalized Wiener-Hopf equations. This will make element-wise conditioning an inexpensive process, whereby reducing the solution procedure to the straightforward Banach contraction mapping principle: given f, y_0 and m, compute

$$y_{k+1} = (I - R^*TR)y_k + R^*f, \qquad k = 0, 1, 2 \ldots m.$$

Here the operator $I - R^*TR$ is strictly contractive with the contraction constant independent of the number of unknowns in the system; T is a scaled direct sum of the local stiffness operators; R and R^* are linear operators conjugate to each other, and I is the identity mapping. Computing Ry and R^*y^* for arbitrary y and y^* is equivalent to solving a linear system defined by a fixed class of sparse M-matrices and their close variants, which can be accomplished by algebraic multi-grid method (AMG) in linear computational count.

For a large class of practical problems, they can also be accomplished by a variety of other linear solver techniques, showing the robustness of the algorithm. From the numerical point of view, R and R^* are optimal conditioners of T in terms of cost, efficiency and robustness. They depend only on a discrete function space modulo the kernel of an appropriate linear analog of T. Throughout the algorithmic design and analysis, non-traditional tools such as topological spaces and discrete measures will be systematically deployed for representing and handling the data structure. This is another novelty of the speaker's approach from the standard methodology.

The speaker's new approach is related neither to Newton-Krylov method and its variants, nor to FAS. At the philosophical level, it is a natural extension of AMG to its fully nonlinear analog without using FAS. It can also be viewed as an extreme exercise of the *finite element tearing and inter-connection* (FETI) philosophy coupled with a novel treatment of degrees of freedom.

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A comparison of parallel block multi-level preconditioners for the incompressible Navier-Stokes equations

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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 preconditioner derived from a block factorization of the coefficient matrix generated in a Newton nonlinear iteration for the primitive variable formulation of the system. This preconditioner is based on the approximation of the Schur complement operator using a technique proposed by Kay, Loghin, and Wathen [1] and Silvester, Elman, Kay, and Wathen [2]. 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 a computational study performed using MPSalsa, a stabilized finite element code, in which parallel versions of these preconditioners from the pressure convection-diffusion preconditioners are compared with an

overlapping Schwarz domain decomposition preconditioner. Our results show nearly ideal convergence rates for a wide range of Reynolds numbers on two-dimensional problems with both enclosed and in/out flow boundary conditions on both structured and unstructured meshes.

[1] 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.

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Least squares preconditioners for stabilized mixed approximation of the Navier-Stokes equations

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We consider the Navier–Stokes equations

$$\begin{aligned} -\nu\nabla^2\mathbf{u} + (\mathbf{u}\cdot\operatorname{grad})\,\mathbf{u} + \operatorname{grad} p &= \mathbf{f} \\ -\operatorname{div}\mathbf{u} &= 0 \end{aligned} \qquad (1)$$

on $\Omega \subset \mathbb{R}^d$, $d = 2$ or 3. Here, $\mathbf{u}$ is the d-dimensional velocity field, which is assumed to satisfy suitable boundary conditions on $\partial\Omega$, p is the pressure, and ν is the kinematic viscosity, which is inversely proportional to the Reynolds number.

Linearization and discretization of (1) by finite elements, finite differences or finite volumes leads to a sequence of linear systems of equations of the form

$$\begin{bmatrix} F & B^T \\ B & -\frac{1}{\nu}C \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ g \end{bmatrix}. \qquad (2)$$

These systems, which are the focus of this talk, must be solved at each step of a nonlinear (Picard or Newton) iteration. Here, B and B^T are matrices corresponding to discrete divergence and gradient operators, respectively and F operates on the discrete velocity space. For *div-stable* discretizations, $C = 0$. For mixed approximation methods that do not uniformly satisfy a discrete inf-sup condition, the matrix C is a nonzero *stabilization operator*. Examples of finite element methods that require stabilization are the mixed approximations using linear or bilinear velocities (trilinear in three dimensions) coupled with constant pressures, as well as any discretization in which equal order discrete velocities and pressures are specified using a common set of nodes.

The focus of this talk is the Least Squares Commutator (LSC) preconditioner developed by Elman, Howle, Shadid, Shuttleworth and Tuminaro, and unveiled at the Copper Mountain Conference in 2004. This preconditioning methodology is one of several choices that are effective for Navier-Stokes equations, and it has the advantage of being defined from strictly algebraic considerations. The resulting preconditioning methodology is competitive with the pressure convection-diffusion preconditioner of Kay, Loghin and Wathen, and in some cases its performance is superior. However, the LSC approach has so far only been shown to be applicable to the case where $C = 0$ in (2). In this talk we show that the least squares commutator preconditioner can be extended to cover the case of mixed approximation that require stabilization. This closes a gap in the derivation of these ideas, and a version of the method can be also formulated from algebraic considerations, which enables the fully automated algebraic construction of effective preconditioners for the Navier-Stokes equations by essentially using only properties of the matrices in (2).

Our focus in this work is on steady flow problems although the ideas discussed generalize in a straightforward manner to unsteady flow.

Inexact Newton methods for underdetermined systems

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Extending Newton's method to solving $F(x) = 0$, where $F : \mathbb{R}^m \to \mathbb{R}^n$ is continuously differentiable and $m > n$, requires solving an underdetermined linear system for the Newton step at each iteration. When the step is the pseudo-inverse solution, the resulting method is sometimes called the normal flow method. Like Newton's method, it usually is easy to implement, has a simple and useful local convergence theory and, in its pure form, is not well suited for solving large-scale problems. In this talk I will present variations of the normal flow method analogous to inexact Newton methods and globalized inexact Newton methods. These methods have been developed to improve the robustness and efficiency of the normal flow method on large-scale problems. Preliminary computational results on some simple problems will be presented. This work was done in collaboration with my advisor Homer Walker at Worcester Polytechnic Institute.

Iterative solution techniques for flexible approximation schemes in multiparticle simulations

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The paper examines various parallel iterative solvers for the new Flexible Local Approximation MEthod (FLAME) [5,6] applied to colloidal systems. The electrostatic potential in such systems can be described, at least for monovalent salts in the solvent, by the Poisson-Boltzmann equation (see, e.g., [2]). Classical Finite-Difference (FD) schemes would require unreasonably fine meshes to represent the boundaries of multiple spherical particles at arbitrary locations with sufficient accuracy. In the Finite Element Method, mesh generation for a large number of particles becomes impractical. The Fast Multipole Method works well only if the particle sizes are neglected and the Poisson-Boltzmann equation is linearized [1]. Classical FD schemes rely on Taylor expansions that break down near material interfaces (such as particle boundaries) due to the lack of smoothness of the field. In FLAME, Taylor expansions in the vicinity of the particles are replaced with much more accurate approximations. Namely, the local FLAME bases are constructed by matching (via the boundary conditions) the spherical harmonics for the electrostatic potential inside and outside the particle; see [5,6] for details.

The system matrices of FLAME and classical FD have the same sparsity structure for the same grid stencil on a regular Cartesian grid; for example, the standard seven-point stencil leads to a seven-diagonal matrix. However, the FLAME matrix is generally nonsymmetric. Several parallel iterative solution techniques have been tested with an emphasis on suitable parallel preconditioning for the nonsymmetric system matrix. In particular, flexible GMRES [3] preconditioned with the distributed Schur Complement [4] has been considered and compared with Additive Schwarz and global incomplete ILU(0) preconditionings. It has been observed that Schur Complement preconditioning with a small amount of fill and a few inner iterations scales well and exhibits good solution times

while attaining almost linear speedup. The number of iterations and the computational time depends only mildly on the Debye parameter of the electrolyte.

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PRIMME: PReconditioned Iterative MultiMethod Eigensolver; a robust, efficient and flexible Hermitian eigenvalue software

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The numerical solution of large, sparse, hermitian eigenvalue problems continues to be one of the most computationally intensive tasks. Iterative eigensolvers are routinely called to solve for a large number of eigenvalues of matrices with dimension of excess of a million. As with linear systems of equations, large dimensions almost always necessitate the use of preconditioning. In addition, eigensolvers must also deal with the issue of storing and orthogonalizing an increasingly large set of eigenvectors.

In recent years, many preconditioned eigensolvers have emerged that perform well in many, but not all applications. Notable examples are the many variants of the Jacobi-Davidson method (JDQR, JDCG, JDQMR), the Generalized-Davidson+1 method, and the LOBPCG method, while variations of the traditional RQI and Inverse Iteration methods are still in use. Until recently, however, general purpose software that implements these methods both efficiently and robustly has been very scarce. As a result, application developers could not compare the various algorithms to find the most suitable for their application and computing environment. Often, they would develop in-house implementations of algorithms specifically tuned for their application. Such in-house approaches, however, cannot benefit from current advances in eigenvalue research. Such flexibility in choosing from a variety of methods is missing in todays software.

In some cases of existing software, robustness has taken a secondary role behind efficiency. Ideally, an eigensolver should find all the required eigenvalues, in the shortest possible time, and produce an orthonormal basis for their invariant space. It is well known, that iterative eigensolvers cannot guarantee that eigenvalues are not missed. However, certain algorithmic techniques can increase the confidence in the computed results, albeit at a higher computational cost. This increased confidence is sometimes needed in applications.

Although some of the above eigenvalue methods have been shown to provide nearly optimal convergence for one eigenvalue in terms of matrix-vector operations, the question of efficiency is a much more complex issue.

Actual execution times depend on the computing platform (hardware, compiler, libraries), on the number of eigenvalues required, on the quality of the preconditioner, and often on the problem solved. Block methods have become a prerequisite for good cache performance, yet maintaining good convergence with a large block size is not straightforward. In addition, there is a multitude of techniques for restarting, locking, stopping inner-outer iterations, that when properly implemented can significantly improve the efficiency of the eigensolvers.

In view of the above, our group has developed a robust, efficient multi-method software called PRIMME. PRIMME is based on a Davidson-type main iteration, but it implements various techniques such block, locking, various projections for preconditioning (e.g., Olsen's, Jacobi-Davidson, etc), CG-type restarting (giving rise to JD+1, and LOBPCG-type methods), and adaptive inner-outer iterations (allowing for JDQMR/JDCG or inexact Inverse Iteration type methods). The implementation of all these techniques on top of a common platform, allows PRIMME to transform to any of the above state-of-the-art eigenvalue methods, as well as to hybrids representing arbitrary combinations of techniques.

More than thirty features are controllable and tunable by the user. However, this flexibility is not at the expense of usability. A complete set of defaults is provided, and the user can simply select from a list of twelve predefined methods. Alternatively, a method selection can be further tuned by resetting particular features. Such a multi-layer transparency addresses the different levels of expertise of potential users, from end-users to eigenvalue experts.

Robustness decisions are prevalent in various implementation details of PRIMME, such as multiple levels of convergence checking, validation processes, out of order convergence of required eigenvalues, especially interior eigenvalues, and consideration of numerical error. In cases where a choice between robustness and efficiency has to be made, PRIMME favors robustness by default, but it still implements the efficient approach as a user-defined alternative.

Finally, the software runs both on parallel and sequential machines and can use the optimized BLAS and LAPACK libraries of the target machines. Additionally, the structure of PRIMME allows for a runtime capability of sensing both the computing environment and the problem solved, and adapting the choice of parameters accordingly. The potential of such a fully dynamic multi-method is a particular focus of our current research.

In this talk, we present an overview of PRIMME and its interface, and show some sample numerical results that demonstrate its robustness and efficiency. In particular, we show that JDQMR and GD+1, two of the supported methods, provide minimal execution time and number of iterations respectively to a number of applications. The hope is that the choice between the two can be fully automated within PRIMME. Finally, we show a surprising result that for cases where a preconditioner is not available, block JDQMR can be substantially better than ARPACK, even for large numbers of eigenvalues.

The software is freely available under the lesser GPL license at `http://www.cs.wm.edu/~andreas/software/`.

The convergence of Krylov subspaces methods with recycling

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Many problems in science and engineering require the solution of a long sequence of linear systems, with small changes from one matrix to the next but substantial changes over multiple systems. We are particularly interested in cases where both the matrix and the right hand side change and systems are not available simultaneously. Such sequences arise in time-dependent iterations, nonlinear systems of equations and optimization, (distributed) parameter identification and inverse problems, and many other problems.

In recent papers [1,2,3] we have proposed methods to recycle selected subspaces from the Krylov spaces generated for previous linear systems to improve the convergence of subsequent linear systems. In this presentation, we discuss several important convergence issues:

- the convergence of Krylov methods that recycle approximate solution spaces, approximate invariant subspaces, and other relevant spaces,
- the relevant perturbation theory for the spaces mentioned above for sequences of matrices arising in a range of applications,
- how fast our proposed methods learn to adapt to a changing problem.

We provide experimental results for a range of problems from tomography, nonlinear mechanics, large-scale design optimization, and statistical mechanics.

[1] Michael L. Parks, Eric de Sturler, Greg Mackey, Duane D. Johnson, and Spandan Maiti, *Recycling Krylov Subspaces for Sequences of Linear Systems*, SIAM Journal on Scientific Computing (accepted with minor revisions), 2006, available as Tech. Report UIUCDCS-R-2004-2421, March 2004, from http://www-faculty.cs.uiuc.edu/~sturler.

[2] Misha Kilmer and Eric de Sturler, *Recycling Subspace Information for Diffuse Optical Tomography*, SIAM Journal on Scientific Computing (accepted for publication), 2006, available from http://www-faculty.cs.uiuc.edu/~sturler.

[3] Shun Wang, Eric de Sturler, and Glaucio H. Paulino, *Large-Scale Topology Optimization using Preconditioned Krylov Subspace Methods with Recycling*, International Journal for Numerical Methods in Engineering (submitted), 2006, available as Technical Report UIUCDCS-R-2006-2678 from http://www-faculty.cs.uiuc.edu/~sturler.

Optimal additive Schwarz preconditioning for minimal residual methods with Euclidean and energy norms

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For the solution of non-symmetric or indefinite linear systems arising from discretizations of elliptic problems, two-level additive Schwarz preconditioners are known to be optimal in the sense that convergence bounds for the

preconditioned problem are independent of the mesh and the number of subdomains. These bounds are based on some kind of *energy norm*. However, in practice, iterative methods which minimize the Euclidean norm of the residual are used, despite the fact that the usual bounds are non-optimal, i.e., the quantities appearing in the bounds may depend on the mesh size; see [1]. In this paper, iterative methods are presented which minimize the same energy norm in which the optimal Schwarz bounds are derived, thus maintaining the Schwarz optimality. As a consequence, bounds for the Euclidean norm minimization are also derived, thus providing a theoretical justification for the practical use of Euclidean norm minimization methods preconditioned with additive Schwarz. Both left and right preconditioners are considered, and relations between them are derived. Numerical experiments illustrate the theoretical developments.

[1] X.-C. Cai, J. Zou, Numer. Linear Algebra Appl. **9** (2002) 379–397.

A novel deflation method to solve the 3-D discontinuous and singular Poisson equation

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Recently, simulating bubbly flows is a very popular topic in CFD. These bubbly flows are governed by the Navier-Stokes equations. In many popular operator splitting formulations for these equations, solving the linear system coming from the discontinuous Poisson equation takes the most computational time, despite of its elliptic origins. ICCG is widely used for this purpose, but for complex bubbly flows this method shows slow convergence.

Moreover, new insights are given into the properties of invertible and singular deflated and preconditioned linear systems, where the coefficient matrices are symmetric and positive (semi-) definite. These linear systems can be derived from a discretization of the Poisson equation with Neumann boundary conditions. Sometimes these linear systems are forced to be invertible leading to a worse (effective) condition number. If ICCG is used to solve this problem, the convergence is significantly slower than for the case of the original singular problem.

We show that applying the deflation technique, which leads to the DICCG method, remedies the worse condition number and the worse convergence of ICCG. Moreover, some useful equalities are derived from the deflated variants of the singular and invertible matrices, which are also generalized to preconditioned methods. It appears that solving the invertible and singular linear systems with DICCG leads to exactly the same convergence results.

This new method DICCG incorporates the eigenmodes corresponding to the components which caused the slow convergence of ICCG. Coarse linear systems have to be solved within DICCG. We discuss some methods to do this efficiently which results in two approaches DICCG1 and DICCG2.

Thereafter we show with numerical experiments that both DICCG approaches are very efficient and they emphasize also the theoretical results. Compared to ICCG, DICCG decreases significantly the number of iterations and the computational time as well which are required for solving Poisson equation in applications of 2-D and 3-D bubbly flows.

Fixed-polynomial approximate spectral transformations for preconditioning the eigenvalue problem

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Arnoldi's method is often used to compute a few eigenvalues and eigenvectors of large, sparse matrices. When the eigenvalues of interest are not dominant or well-separated, this method may suffer from slow convergence. Spectral transformations are a common acceleration technique that address this issue by introducing a modified eigenvalue problem that is easier to solve than the original. This modified problem accentuates the eigenvalues of interest, but requires solving a linear system, which is computationally expensive for large-scale eigenvalue problems.

In this talk we will show how this expense can be reduced through a preconditioning scheme that uses a fixed-polynomial operator to approximate the spectral transformation. Three different constructions for a fixed-polynomial operator are derived from some common iterative methods for non-Hermitian linear systems. The implementation details and numerical behavior of these three operators are compared. Numerical experiments will be presented demonstrating that this preconditioning scheme is a competitive approach for solving large-scale eigenvalue problems. The results illustrate the effectiveness of this technique using several practical eigenvalue problems from science and engineering ranging from hundreds to more than a million unknowns.

A fast iterative solver for acoustic scattering by objects in layered media

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We consider the computation of time-harmonic acoustic scattering by objects in layered media. An example of such problem is the scattering by a mine buried in sediment. The computational domain can be tens or hundreds of meters long while the target requires modeling of details smaller than one centimeter. A discretized problem can have several billion degrees of freedom.

We decompose the computational domain into far-field and near-field domains and then we perform a finite element discretization. For the vastly larger far-field domain we use an orthogonal mesh and a preconditioner based on a fast direct solver. For the near-field domain a more standard preconditioner can be used. The combination of these two defines a preconditioner for the GMRES method. An essential implementation detail is the reduction of iterations into a small sparse subspace. Due to this the memory usage is essentially reduced and the GMRES method can be used without restarts.

We present numerical results with two-dimensional and three-dimensional problems demonstrating the efficiency of the proposed approach. For example, we show that it is possible to solve problems with more than a billion degrees of freedom on a modern PC.

Partitioning sparse matrices for parallel preconditioned iterative methods

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We will discuss parallelization techniques for the preconditioned iterative methods that use explicit preconditioners such as approximate inverses or factored approximate inverses. Applications of these preconditioners require sparse matrix-vector multiplication (SpMxV) operations. Roughly speaking, the problem reduces to partitioning two or more matrices together in order to efficiently parallelize the computations of the form $y \leftarrow ABCx$. Note that the computations $y \leftarrow ABCx$ are performed as successive SpMxV operations, and hence there are dependencies among the input and output vectors of these SpMxV operations. Additional dependencies are imposed by the linear vector operations that take part in a full step of the chosen iterative method. We will first discuss how to analyze the preconditioned iterative methods to determine the dependencies between the inputs and outputs of the SpMxV operations. We will give a short account of such dependencies for a number of widely used methods including BiCGStab, preconditioned conjugate gradients, and GMRES. Next, we will develop hypergraph models which capture the dependencies among the input and output vectors of the SpMxV operations with different matrices. We will show that partitioning a single hypergraph amounts to simultaneous partitioning of the matrices in $y \leftarrow ABCx$ computations in such a way that the total volume of communication is minimized and an appropriate balance criterion among the processor loads is maintained. We will present experimental results obtained using a parallel implementation of the right preconditioned BiCGStab method on a PC cluster.

This is a joint work with Prof C. Aykanat of Bilkent University, Ankara, Turkey.

Multigrid for large scale time-dependent Sylvester equations

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We will discuss a multigrid solver for the numerical solution of the time-dependent Sylvester equation

$$\frac{dX}{dt} = AX + XB + F, \qquad \text{with } X \in \mathbf{R}^{N\times N},$$

where A and B are discretisations of an elliptic PDE operator. This type of equation occurs in optimal control problems and in uncertainty propagation algorithms for partial differential equations with random parameters. Common to these applications is the large number of unknowns even for problems with a reasonable mesh width.

Our multigrid solver is built on a recently developed algorithm for the stationary Sylvester equation [1] $AX+XB+F = 0$. We exploit the fact that the iterates can be well compressed when the right hand side F has a low-rank structure. If this compression is used throughout the multigrid cycle, a significant reduction in time and memory can be achieved for large scale problems. This is accomplished by approximating the unknown X by a low-rank matrix

$$X \simeq UV^T, \qquad \text{with} \qquad U, V \in \mathbb{R}^{N\times k}.$$

For a certain precision, this low-rank multigrid typically requires $\mathcal{O}(Nk^2) = \mathcal{O}(N\log^2(N))$ work whereas standard multigrid would require $\mathcal{O}(N^2)$. An adaptive strategy that gradually enlarges the rank to get better precision is explored.

[1] L. Grasedyck, W. Hackbusch, *A Multigrid Method to Solve Large Scale Sylvester Equations*, Technical Report 48 (2004), Max Planck Institute for Mathematics in the Sciences.

Error analysis of BDF Compound-Fast multirate method for differential-algebraic equations

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Analogue electrical circuits are usually modeled by differential-algebraic equations (DAE) of type:

$$\frac{d}{dt}\left[\mathbf{q}(t,\mathbf{x})\right]+\mathbf{j}(t,\mathbf{x})=\mathbf{0}, \qquad (1)$$

where $\mathbf{x}\in\mathbb{R}^d$ represents the state of the circuit. A common analysis is the transient analysis, which computes the solution $\mathbf{x}(t)$ of this non-linear DAE along the time interval $[0,T]$ for a given initial state. Often, parts of electrical circuits have latency or multirate behaviour.

For a multirate method it is necessary to partition the variables and equations into an active (A) and a latent (L) part. The active and latent parts can be expressed by $\mathbf{x}_A=\mathbf{B}_A\mathbf{x},\mathbf{x}_L=\mathbf{B}_L\mathbf{x}$ where $\mathbf{B}_A,\mathbf{B}_L$ are permutation matrices. Then equation (1) is written as the following partitioned system:

$$\begin{array}{l}\frac{d}{dt}\left[\mathbf{q}_A(t,\mathbf{x}_A,\mathbf{x}_L)\right]+\mathbf{j}_A(t,\mathbf{x}_A,\mathbf{x}_L)=\mathbf{0},\\ \frac{d}{dt}\left[\mathbf{q}_L(t,\mathbf{x}_A,\mathbf{x}_L)\right]+\mathbf{j}_L(t,\mathbf{x}_A,\mathbf{x}_L)=\mathbf{0}.\end{array}$$

In contradiction to classical integration methods, multirate methods integrate both parts with different stepsizes. Besides the coarse time-grid $\{T_n, 0\le n\le N\}$ with stepsizes $H_n=T_n-T_{n-1}$, also a refined time-grid $\{t_{n-1,m}, 1\le n\le N, 0\le m\le q_n\}$ is used with stepsizes $h_{n,m}=t_{n,m}-t_{n,m-1}$ and multirate factors q_n. If the two time-grids are synchronized, $T_n=t_{n,0}=t_{n-1,q_n}$ holds for all n. There are a lot of multirate approaches for partitioned systems but we will consider the Compound-Fast version of the BDF methods. This method performs the following four steps:

1. The complete system is integrated at the coarse time-grid.
2. The latent interface variables are interpolated at the refined time-grid.
3. The active part is integrated at the refined time-grid, using the interpolated values at the latent interface.
4. The active solution at the coarse time-grid is updated.

The local discretization error δ^n of the compound phase still has the same behaviour $\delta^n=O(H_n^{K+1})$. Let $\bar{\mathbf{P}}^n,\bar{\mathbf{Q}}^n$ be the Nordsieck vectors which correspond to the predictor and corrector polynomials of $\mathbf{q}$. Then the error δ^n can be estimated by $\hat{\delta}^n$:

$$\hat{\delta}^n=\frac{-H_n}{T_n-T_{n-K-1}}\left[\bar{\mathbf{Q}}_1^n-\bar{\mathbf{P}}_1^n\right].$$

Now $\hat{r}_C^n=\|\mathbf{B}_L\hat{\delta}^n\|+\tau\|\mathbf{B}_A\hat{\delta}^n\|$ is the used weighted error norm, which must satisfy $\hat{r}_C^n<\mathrm{TOL}_C$.
The local discretization error $\delta^{n,m}$ is defined as the residue after inserting the exact solution in the refinement BDF scheme. During the refinement instead of $\delta^{n,m}$ the perturbed local error $\tilde{\delta}^{n,m}$ is estimated. A tedious analysis yields the following asymptotic behaviour:

$$\mathbf{B}_A\delta^{n-1,m}\doteq\mathbf{B}_A\tilde{\delta}^{n-1,m}+\frac{1}{4}h\mathbf{K}_{n-1,m}\mathbf{B}_L\rho^{n-1,m}.$$

Here $\rho^{n-1,m}$ is the interpolation error at the refined grid and $\mathbf{K}_{n-1,m}$ is the coupling matrix. The perturbed local discretization error $\mathbf{B}_A\tilde{\delta}^{n,m}$ behaves as $O(h_{n-1,m}^{k+1})$ and can be estimated in a similar way as δ^n. Thus the active error estimate $\mathbf{B}_A\hat{\delta}^{n-1,m}$ satisfies $\mathbf{B}_A\hat{\delta}^{n-1,m} \doteq \mathbf{B}_A\hat{\tilde{\delta}}^{n-1,m} + \frac{1}{4}h\hat{\mathbf{K}}_{n-1,m}\mathbf{B}_L\hat{\rho}^{n-1,m}$. Let L be the interpolation order, then it can be shown that $\frac{1}{4}\|\hat{\mathbf{K}}_n\mathbf{B}_L\rho^{n-1,m}\|$ is less than

$$\hat{r}_I^n = \frac{1}{4}\frac{H_n}{T_n - T_{n-L-1}}\|\hat{\mathbf{K}}_n\mathbf{B}_L\left[\bar{\mathbf{X}}_1^n - \bar{\mathbf{Y}}_1^n\right]\|.$$

Here $\bar{\mathbf{Y}}^n, \bar{\mathbf{X}}^n$ are the Nordsieck vectors which correspond to the predictor and corrector polynomials of $\mathbf{x}$. This error estimate $\hat{r}_I^n$ has the asymptotic behaviour $\hat{r}_I^n = O(H_n^{L+1})$. It follows that $\|\mathbf{B}_A\hat{\delta}^{n,m}\|$ satisfies:

$$\|\mathbf{B}_A\hat{\delta}^{n-1,m}\| \quad \leq \quad \hat{\tilde{r}}_A^{n-1,m} + h\hat{r}_I^n =: \hat{r}_A^{n-1,m}.$$

If $\hat{r}_I^n \leq \mathrm{TOL}_I = \sigma\mathrm{TOL}_A$ and $\hat{\tilde{r}}_A^{n-1,m} \leq \tilde{\mathrm{TOL}}_A = (1-\sigma h)\mathrm{TOL}_A$ then $\hat{r}_A^{n-1,m} \leq \tilde{\mathrm{TOL}}_A + h\mathrm{TOL}_I = \mathrm{TOL}_A$.

We tested a circuit with 5×10 inverters. The location of the active part is controlled by the connecting elements and the voltage sources. The connecting elements were chosen such that the active part consists of 3 inverters. We did an Euler Backward Compound-Fast multirate simulation on $[0, 10^{-8}]$ with $\sigma = 0.5, \tau = 0$. We get accurate results combined with a speedup factor 13.

An algebraic multigrid preconditioner for a class of singular M-matrices

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We will consider the problem of the computation of stationary distributions of Markov chains which arises in many different application areas. These range from the distribution of drugs in the blood circulation systems to the Page Rank computed by Google. The task is to compute the left eigenvector corresponding to the largest eigenvalue of the transition matrix T or alternatively solve the linear system

$$(I - T^T)x = 0,$$

where the matrix $(I - T^T)$ is a singular M-matrix. In applications, these matrices are large and sparse. Therefore, iterative methods such as GMRES are applied. However, the applicability of GMRES depends on whether it is possible to find a suitable preconditioner. For non-singular, symmetric positive definite M-matrices that are obtained from discretisations of boundary value problems the algebraic multigrid is well known to be a good preconditioner. We show how it is possible to apply the algebraic multigrid method to our special case of singular non-symmetric M-matrices and show numerical examples that illustrate that this leads to significant acceleration of the convergence speed.

Complex shifted-Laplace preconditioners for the Helmholtz equation

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In this paper, the time-harmonic wave equation in heterogeneous media is solved numerically. The underlying equation governs wave propagations and scattering phenomena arising in many area's, e.g., in aeronautics, geophysics, and optical problems. In particular, we look for efficient iterative solution techniques for the Helmholtz equation discretized by finite difference discretizations. Since the number of grid points per wavelength should be sufficiently large for accurate solutions, for very high wavenumbers the discrete problem becomes extremely large, thus prohibiting the use of direct solvers. However, since the coefficient matrix is sparse, iterative solvers are an interesting alternative.

In many geophysical applications that are of our interest, an unbounded domain is used. In our model we approximate such a domain by a bounded domain, where appropriate boundary conditions are used to prevent spurious reflections. As boundary conditions we compare the following possibilities: Dirichlet, Neumann, Sommerfeld, Absorbing Layer and Perfect Matched Layer. Due to the boundary conditions and damping in the heterogeneous medium, the coefficient matrix is complex-valued.

It appears that standard iterative solvers (ILU preconditioned Krylov solver, Multigrid, etc.) fail for the Helmholtz equation, if the wavenumber becomes sufficiently high. In this paper we present a Bi-CGSTAB solution method combined with a novel preconditioner for high wavenumbers. The preconditioner is based on the inverse of an Helmholtz operator, where an artificial damping term is added to the operator. This preconditioner can be approximated by multigrid. This is somewhat surprising as multigrid, without enhancements, has convergence troubles for the original Helmholtz operator at high wavenumbers.

Currently, we are investigating the best choice of the damping term. If the damping term is small Bi-CGSTAB converges fast, but it is difficult to use multigrid for the preconditioner. On the other hand, if the damping term is large the multigrid approximation is very good, but the convergence of Bi-CGSTAB is slow. So a compromise is required to obtain an efficient solver. To find a good value of the damping term we study the spectral properties of the preconditioned matrix. It appears that an eigenvalue analysis of this matrix can be used to predict the convergence of GMRES. In practice it appears that these insights can also be used for the convergence of Bi-CGSTAB. We conclude that Bi-CGSTAB combined with the novel preconditioner converges satisfactorily for all choices of the boundary conditions.

A space-time multigrid approach for acceleration of molecular dynamics simulations

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We present a novel space-time multigrid method for molecular dynamics simulations. It is aimed at bridging discrete scales with either coarse grained discrete or continuum scales. The method consists of the waveform relaxation scheme aimed at capturing the high frequency response of atomistic vibrations and a coarse scale solution in space and time aimed at resolving smooth features of the discrete medium. The formulation of the coarse grained model is based on the variational approach derived from Hamilton's principle. The time integration is performed in windows using the Newmark predictor-corrector method. The method is implicit, possesses superior stability properties and consequently enables larger time steps governed by accuracy considerations of coarse scale quantities of interest.

Performance studies on polymer melts have shown significant speed-up compared to the classical explicit methods, in particular on parallel machines.

Approximate finite-differences in matrix-free Newton-Krylov methods

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Newton-Krylov methods are often implemented in "matrix-free" form, in which the Jacobian-vector products required by the Krylov solver are approximated by finite differences. We consider using approximate function values in these finite differences. We first formulate a finite-difference Arnoldi process that uses approximate function values and give backward-error results for it. We then outline a Newton–Krylov method that uses an implementation of the GMRES or Arnoldi method based on this process and develop a local convergence analysis for it, giving sufficient conditions on the approximate function values for desirable local convergence properties to hold. We conclude with numerical experiments involving particular function-value approximations suitable for nonlinear diffusion problems. For this case, conditions are given for meeting the convergence assumptions for both lagging and linearizing the nonlinearity in the function evaluation.

Constaint preconditioning and Schilders factorization for saddle-point systems

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Saddle-point systems arise widely because they generally result from any problem with constraints. Hence in Fluid Mechanics incompressibility is a constraint on the Navier-Stokes equations, in Optimization algebraic and/or bound constraints are often applied and in PDE constrained optimization the PDEs themselves provide the constraints.

This talk is about preconditioned iterative approaches to the solution of large-scale saddle-point problems based on preconditioners which preserve the constraints: so-called constraint preconditioners. We will briefly review the attractive feature of such preconditioners and then explain how these preconditioners can effectively be realized through a block factorization due to Wil Schilders. This reveals a range of possible approaches where the balance between faster convergence though better preconditioning and the cost of the preconditioner varies.

This is joint work with Sue Dollar, Nick Gould and Wil Schilders

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Converging in the right norm

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For PDE problems, Numerical Analysts would always wish to establish error estimates in 'natural' norms for a given problem. In the context of iterative solution methods there is similarly the issue of the right norm for convergence: discrete norms are equivalent, but measuring a convergence tolerance in a norm in which half of the variables are scaled by h^{-5} or h^5 is definitely not the right thing to do in general!

In particular this issue arises when preconditioning with minimum residual methods because then monotonic residual reduction occurs in a norm based on the preconditioner. (For SPD problems and Conjugate Gradients it is well known that any SPD preconditioning does not affect the relevant norm).

In this talk we will discuss this issue in the context of models of incompressible flow — Poisson, Stokes, Advection-Diffusion and Navier-Stokes problems — and show how the optimal block preconditioners developed by Silvester and the author for the Stokes problem give convergence in the right norm; comments will also be made regarding Navier-Stokes preconditioning.

This is joint work with Howard Elman and David Silvester

A least-squares finite element method for viscoelastic flow

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The equations describing viscoelastic fluid flow are inherently nonlinear and pose a continuing challenge to most numerical approximation methods. Even the addition of a small component of elastic behavior to Newtonian fluid can introduce instabilities. In this talk we present progress toward a multilevel least-squares finite element method for steady viscoelastic fluid flow of Oldroyd-B type. Our approach is to combine an outer iteration consisting of linearization steps on a nested sequence of grids with an inner iteration of a least-squares finite element discretization and algebraic multigrid linear solver. One of the challenges arising from this system is in treating the convective nature of the constitutive equation. We discuss an analogous, but simplified, problem that illustrates the difficulties, and suggest a strategy for least-squares discretizations to treat equations with strong convective terms.

An embedding method for simulation of immobilized enzyme kinetics and transport in sessile hydrogel drops

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We present a new numerical method, termed the embedding method, to solve a system of nonlinear PDEs for multi-phase problems in asymmetric 3-D domains. The main feature of this method is its ability to perform interface

calculation and account for conditions relating solution properties across phase interface using a finite difference / volume-fraction-based front-capturing hybrid technique.

The approach begins by considering the computational domain as physically separated phases. A finite difference method with a Cartesian grid is employed on the whole domain while modifications are applied to correct boundary conditions at the interfaces. The volume-fraction-based front-capturing algorithm is used to capture each interface in terms of the volume fraction in each cell. The major aspect of this method is its implementation simplicity, which results in code generation that can be highly optimized. To highlight this method, an application is presented for simulation and investigation of enzyme reactions within a sessile hydrogel drop, where the Michaelis-Menten kinetics is used to model the reaction mechanism.

An algorithmic framework for convex mixed integer nonlinear programs

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We present a hybrid framework for convex mixed-integer nonlinear programming. In one extreme case, the method becomes the branch-and-bound approach, where a nonlinear optimization problem is solved in each node of the enumeration tree, and in the other extreme it reduces to the polyhedral outer approximation algorithm, which alternates between the solution of a nonlinear optimization problem and a mixed-integer linear program.

Numerical results are presented, using an open source software implementation available on http://www.coin-or.org.

This work results from an on-going research collaboration between IBM and CMU.

Optimal solvers for H(curl) and H(div) systems in terms of Poisson solvers

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A new class of optimal solvers will be presented for H (curl) and H(div) systems in terms of Poisson Solvers. As a direct application, optimal AMG solvers can be obtained for H(curl) and H (div) systems whenever optimal AMG solvers are available for Poisson equations. Both theoretical and numerical examples will be given. This work is in joint with Ralf Hiptmair.

A multilevel Newton's method for a two phase mixture model with nonlinear discontinuous degenerate diffusion coefficient

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The traditional Newton's method requires certain smoothness of the coefficients of partial differential equations to get local convergence. In this paper, a multilevel Newton's method is developed for a two phase model with nonlinear discontinuous degenerate diffusion coefficient arising in fuel cell applications. A major finding is that the discrete algebraic function after using linear finite element method is Lipschitz continuous. Numerical example shows the robustness of this method.

A constrained minimization algorithm for solving nonlinear eigenvalue problems in electronic structure calculation

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One of the fundamental problems in electronic structure calculation is to determine electron orbitals associated with the minimum total energy of large atomistic systems. The total energy minimization problem is often formulated as a nonlinear eigenvalue problem and solved by an iterative scheme called Self Consistent Field (SCF) iteration. In this talk, a new direct constrained optimization algorithm for minimizing the Kohn-Sham (KS) total energy functional is presented.

The key ingredients of this algorithm involve projecting the total energy functional into a sequences of subspaces of small dimensions and seeking the minimizer of total energy functional within each subspace. The minimizer of

the projected energy functional not only provides a search direction along which the KS total energy functional decreases but also gives an optimal "step-length" to move along this search direction. Due to the small dimension of the projected problem, the minimizer of the projected energy functional can be computed by several different methods. These methods will be examined and compared in this talk. Numerical examples will be provided to demonstrate that this new direct constrained optimization algorithm can be more efficient and robust than the SCF iteration.

On parallel algebraic multigrid preconditioners for systems of PDEs

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Algebraic multigrid (AMG) is a very efficient, scalable algorithm for solving large linear systems on unstructured grids. When solving linear systems derived from systems of partial differential equations (PDEs) often a different approach is required than for those derived from a scalar PDE. There are mainly two approaches, the function approach (also known as the "unknown" approach), and the nodal or "point" approach. The function approach defines coarsening and interpolation separately for each function. The nodal approach uses AMG in a block manner, where all variables that correspond to the same grid node are coarsened, interpolated and relaxed together. While the function approach is much easier to implement and often more efficient, there are problems for which this approach is not sufficient and the more expensive nodal approach is needed.

Several parallel implementations of both approaches using various coarsening schemes and interpolation operators are investigated. Advantages and disadvantages of both approaches are discussed, and numerical results are presented.

New algorithms for vector quantization

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Vector quantization is the classical problem of representing continuum with only a finite number of representatives or representing an initially rich amount of discrete data with a lesser amount of representatives. This problem has numerous applications. The objective of achieving a quantization with minimal distortion leads to a hard non-convex optimization problem, typically with many local minima. The main problem is thus to find an initial approximation that is close to a "good" local minimum. Once such an approximation is found, the well-known Lloyd-Max iterative algorithm may be used to converge to the nearby a local minimum. In this talk we will describe the problem and present two new approaches to its approximate solution.

Finite-difference solution of the 3D EM problem using integral equation type preconditioners

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The electromagnetic prospecting problem requires fine gridding to account for sea bottom and to model complicated targets. This results in large computational costs using conventional finite-difference solvers. To circumvent these problems, we employ a volume integral equation approach for preconditioning and to eliminate the background, thus significantly reducing the condition number and dimensionality of the problem. Since the problem should be solved in unbounded domain we use so-called optimal grids to truncate error of approximation at infinity. Special averaging procedure is proposed to account for inhomogenuity. Theory and numerical results will be presented.

On multigrid methods for generalized finite element methods on unstructured grids

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We consider the symmetric positive semi-definite problems arising from generalized finite element discretizations on unstructured grids. The focus will be on a simple two level approach, in which the coarse grid problem corresponds to the space spanned by the partition of unity functions. We characterize the kernel components of the stiffness matrix for GFEM discretizations in two and three spatial dimensions. With this characterization in hand, we can derive a stable decomposition of the underlying GFEM space, using as an auxiliary coarse space the piece-wise linear and continuous functions and prove a uniform convergence result for the resulting two level method.
