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Abstracts

Modifying CLJP Coarse Grid Selection to Attain Lower Complexities

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To build an efficient parallel algebraic multigrid (AMG) solver both the setup phase and the solve phase need to be implemented with parallel algorithms. Parallelizing the latter is straightforward because of the similarities between the AMG solve phase and geometric multigrid. However, parallelizing the original Ruge-Stüben (RS) setup phase presents difficulties. The RS coarse grid selection algorithm uses a breadth first search for its first pass which makes the algorithm inherently sequential. Parallel coarse grid selection algorithms had to be designed in order to make a parallel setup phase.

Of those algorithms which select coarse grids for use with RS interpolation, Cleary-Luby-Jones-Plassmann (CLJP) is unique because it produces the same coarse grid regardless of the number of processors on which the coarsening algorithm is run. Additionally, CLJP is able to coarsen the grid to a single node. Both of these properties have positive implications in the design of a parallel setup phase. Unfortunately, CLJP tends to select coarse grids which lead to high operator complexities on many problems and especially high complexities on problems in three dimensions.

This talk discusses methods to modify CLJP in order to produce grid hierarchies which lead to lower operator complexities. In particular, methods to modify the maximal independent set algorithm on which CLJP is based are examined. By modifying this algorithm, CLJP can be made to produce results with more evenly distributed coarse nodes. Experimental results show that these changes lead to lower operator complexities. The eventual goal is to create CLJP-based algorithms with performance close to that of the Falgout hybrid algorithm while retaining the positive aspects of the original CLJP.

Toward an efficient nonlinear solver for an mesh smoothing problem

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The problem of unstructured mesh smoothing can be approached by solving a set of Laplace-Beltrami equations that are discretized using finite elements. The resulting discrete problem is non-linear and a Newton-Krylov type

procedure can be employed to solve it. We will report on our efforts to speed up the solution of this problem using an AMG based preconditioner in the Krylov step.

Efficient parallelisation of a multigrid multilevel integration EHL solver

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The numerical solution of large scale elastohydrodynamic lubrication (EHL) problems is only computationally realistic on fine meshes by making using using multilevel techniques. In this work we show how the parallelisation of both multigrid and multilevel multi-integration for these problems may be accomplished without damaging solution quality. A parallel performance model of the implemented algorithm is described and analyzed using the Isoefficiency and Isomemory metrics for distributed memory architectures. Results are shown with good speed-ups and excellent scalability.

Parallelisation of scientific engineering codes, such as the EHL code considered here, has proved to be particularly useful whenever either results are needed quickly or the memory requirements are too large to be handled in serial. In the case of solvers for the important engineering problem of elastohydrodynamic lubrication both these situations can arise. The EHL regime occurs in journal bearings and gears, where, under severe loads in the presence of a lubricant, there may be a very large pressure exerted on a very small area, often up to 3 GPa. This causes the shape of the contacting surfaces to deform and flatten out at the centre of the contact. There are also significant changes in the behavior of the lubricant in this area, for example it may take on glass-like properties.

The computational challenge in solving such problems is considerable. The equations to be solved consist of a nonlinear differential equation which is elliptic/hyperbolic and defined in terms of pressure film thickness values and a coupled integral equation which defines the film thickness in terms of all the spatial pressures. The efficient serial solution of these problems is achieved by using a multigrid solver for the differential equation coupled to a multilevel multi-integration method for the film thickness calculation. Although the time dependent partial differential and integral equations apply only in one or two space dimensions, they have a dense sparsity pattern and are highly nonlinear. Full details of both the EHL problem and the serial solution methods used are described in the book by Venner and Lubrecht and with details specific to the discussion here given by the thesis of Goodyer.

One of the EHL problems of current interest is to calculate the frictional characteristics of measured surface roughness profiles. This has been successfully undertaken for one dimensional line contact cases. Tackling the more realistic 2-D case has been recognized as one of the immediate challenges in tribology. In order to do this spatial meshes of $10^6 \times 10^6$ points may be needed. This means that 10^{12} dense nonlinear equations need to be solved. This challenge is beyond a single workstation at present and requires the use of parallel computers.

In order to describe the parallel solution techniques the numerical problem to be solved and the serial algorithm will first be described. The multigrid and multilevel techniques used will be highlighted, along with the reasons why they make effective parallelisation such a communication intensive process. The parallel approaches we have taken are then explained and a careful performance model constructed using the isomemory and isoefficiency metrics. This analysis will show how a demanding numerical problem, which is both highly intensive in terms of communication, and requires global knowledge, has been successfully parallelised. Use of MPI has meant this implementation is portable between both shared and distributed memory architectures. Communication costs have been limited through use of non-blocking local directives, and the memory requirements per process

have been significantly reduced. The computational results show the overall speed-up of the code is excellent, especially on higher grid resolutions. The scalability has been shown to be similarly impressive with comparable results when increasing the problem size and number of processors whilst utilising the same coarsest multi-level multi-integration level. The paper concludes by considering future directions in terms of solving still larger problems.

A new prolongator for multigrid for the curlcurl equation

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We consider algebraic multigrid methods for the numerical solution of curlcurl systems in computational electromagnetics. Existing prolongation schemes for the curlcurl equation are often based on the Reitzinger-Schöberl prolongator presented in [1]. There, a piecewise constant edge prolongator P_e is derived from a piecewise constant nodal prolongator P_n, such that the commutation property is satisfied. This prolongation scheme can be improved by applying ideas of smoothed aggregation multigrid to it ([2], [3]).

We will present an alternative prolongation scheme that takes as a starting point an arbitrary partition of unity nodal prolongator P_n. We will show that it is possible to associate with the set of coarse nodal elements (the columns of P_n) a set of coarse edge elements. The link between both sets is the analytical formula for edge elements on triangular/tetrahedral meshes

$$E_{ij} = N_i \nabla(N_j) - N_j \nabla(N_i)$$

We will show that in the coarse setting, this formula has an exact discrete counterpart, which satisfies the commutation property. This prolongation schema contains the Reitzinger-Schöberl edge prolongator as the special case for a piecewise constant nodal prolongator P_n.

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Adaptive Algebraic Multigrid Preconditioners in Quantum Chromodynamics

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Standard algebraic multigrid methods assume explicit knowledge of so-called algebraically-smooth or near-kernel components, which loosely speaking are errors that give relatively small residuals. Tyically, these methods automatically generate a sequence of coarse problems under the assumption that the near-kernel is locally constant. The difficulty in applying algebraic multigrid to lattice QCD is that the near-kernel components can be far from constant, often exhibiting little or no apparent smoothness. In fact, the local character of these components appears to be random, depending on the randomness of the so-called "gauge" group. Hence, no a priori knowledge of the local character of the near-kernel is readily available.

This talk proposes adaptive algebraic multigrid (AMG) preconditioners suitable for the linear systems arising in lattice QCD. These methods recover good convergence properties in situations where explicit knowledge of the near-kernel components may not be available. This is accomplished using the method itself to determine near-kernel components automatically, by applying it carefully to the homogeneous matrix equation, $Ax = 0$. The coarsening process is modified to use and improve the computed components. Preliminary results with model 2D QCD problems suggest that this approach yields optimal multigrid-like performance that is uniform in matrix dimension and gauge-group randomness.

Multigrid Algorithms for C^0 Interior Penalty Methods for Fourth Order Problems

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Multigrid algorithms for C^0 interior penalty methods (which are discontinuous Galerkin methods) for fourth order problems will be discussed. We will show that the convergence behavior of the multigrid algorithms is similar to that for second order problems, provided that we use a smoothing scheme involving a Poisson solve as a preconditioner. Such a preconditioner can be easily implemented because the C^0 finite element spaces are standard spaces for second order problems.

Application of the Adaptive Smoothed Aggregation to Problems with Nonsmooth Kernels

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The success of multigrid methods relies on complementarity between the relaxation processs and the coarse-grid correction. Multigrid methods are usually designed based on the assumption that the error that needs to be eliminated by the coarse-grid correction possesses smoothness.

We discuss several applications of practical interest where these assumptions are violated, so standard approaches cannot be successfully applied. We describe the recently developed extension of the smoothed aggregation method, designed to identify the critical error components and to incorporate them into the coarse space design. The presented numerical experiments demonstrate that the method can be used to achieve good convergence.

Algebraic Multigrid Schemes

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Considerable efforts in recent multigrid research have concentrated on algebraic multigrid schemes. A vital aspect of this work is uncovering algebraically smooth error modes in order to construct effective multigrid components. Many existing algebraic multigrid algorithms rely on assumptions regarding the nature of algebraic smoothness. For example, a common assumption is that smooth error is essentially constant along 'strong connections'. Performance can degrade as smooth error for a problem differs from this assumption. Through tests on the homogeneous problem ($\boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}$) adaptive multigrid methods expose algebraically smooth error.

The method presented in this talk uses relaxation and subcycling on complementary grids as an evaluative tool in correcting multigrid cycling. Each complementary grid is constructed with the intent of dampening a subset of the basis of algebraically smooth error. The particular implementation of this framework manages smooth error in a manner analogous to spectral AMGe. Numerical results will be included.

Effective adaptive multigrid for strongly anisotropic problems with Krylov smoothers

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We consider the parallel solution of strongly anisotropic diffusion problems on adaptive grids by multigrid methods. The standard multigrid methods with pointwise relaxation and standard coarsening have problems because smoothers are not effective. To improve multigrid, the common ways are to use semicoarsening or line smoothers. However, neither of these techniques is suitable for parallel adaptive grids environment. Moreover, both techniques require that the anisotropy aligned with the grid, which may not be the case for realistic problems. In this talk, we will discuss a robust and easy-to-parallelize smoother for multigrid which can deal with strongly anisotropic problems on adaptive grids effectively. This method remains effective even if the anisotropy is not aligned with the grid.

We use multilevel adaptive technique (MLAT). The main idea of MLAT is to perform smoothing sweeps only on locally refined grids, and use the full approximation scheme (FAS) to generate the error correction cycle. We propose to use Krylov subspace methods as smoothers. Our numerical experiments show that they reduce oscillatory error components effectively. Therefore with such smoothers, multigrid achieves fast convergence rate. Moreover, parallelizing Krylov methods is straightforward since only matrix vector products and vector inner products need communication.

Convergence rate analysis for multigrid on adaptive grids can be simplified to analysis on uniform grids, since with properly chosen interpolation and prolongation operators, convergence rate on adaptive grids is almost identical to that on uniform grids. Standard analytic tools such as Local Fourier Analysis (LFA) fail for Krylov smoothers because they require the smoothing operators to be linear. In addition, Krylov methods are not "strict" smoothers. Their smoothing effect for high frequency modes may deteriorate when large smooth error components are present. In our work, we use a slightly different approach. Assume the coarse grid correction operator (including interpolation and restriction) satisfies certain requirements, we derive the level-independent upper bound for convergence rate of Krylov methods. This rate is used to estimate multigrid convergence rate. This explains why level-independent convergence rate of multigrid is achieved. The numerical experiments verify our statement. Our approach of quantitative analysis can be applied to more general problems and may be useful for other multigrid practitioners.

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A Robust Multigrid Method with Cell-Based Coarsening

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Generally robust multigrid codes, like BoxMG, employ Galerkin coarsening to form the coarse grid operators. That is, if the fine grid operator is A, then the coarse grid operator is RAP, where P is the interpolation operator from the coarse grid to the fine grid, and R is the restriction operator from the fine grid to the coarse grid. In BoxMG, R is chosen as the transpose of P. This choice minimizes the error in the range of interpolation. Also, in BoxMG, interpolation is operator-induced, thereby approximately preserving the continuity of the normal component of the flux across interfaces. Cell-centered discretizations on a logically structured grids are readily treated with BoxMG by associating them with the corresponding dual grid. However, this approach does not preserve the cell based structure on coarser levels. Although this structure may not be important in some applications, in the case of patch- or cell-based mesh refinement, it is very desirable.

Several multigrid methods have been proposed to coarsen by cells, but these methods have been either too costly or not robust with respect to fine-scale discontinuous coefficients. For example coarsening by cells, using an operator-induced piecewise bilinear interpolation for P, the transpose of P for R, and forming the coarse grid operator as RAP leads to unacceptable stencil growth. In contrast, Wesseling has investigated a method that coarsens by cells, in which R is not the transpose of P, yet under certain conditions RAP is symmetric; however, his use of a non-operator-dependent P yields a method that is not as robust as BoxMG. In this paper we explore the use of multiple dual-meshes on a logically structured two-dimensional grid in conjunction with the variational framework of BoxMG to create a robust method that coarsens by cells while maintaining a 9-point coarse-grid operator on all levels. This approach readily extends to the cases of patch- and cell-based refinement.

Study of Aggressive Coarsening and Multipass Interpolation in Algebraic Multigrid

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Algebraic multigrid is a very efficent algorithm for solving large linear systems on unstructured grids. Use of coarsening schemes such as parallel variants of the standard coarsening algorithm by Ruge and Stueben [1] or CLJP coarsening [2], a method based on parallel maximal independent set algorithms, can lead to high complexities with regard to memory usage as well as computation time, which adversely affect scalability. In recent work [3], we have proposed two new parallel AMG coarsening schemes, that are based on solely enforcing a maximum independent set property, resulting in sparser coarse grids. The new coarsening techniques remedy memory and execution time complexity growth for various large three-dimensional (3D) problems. If used within AMG as a preconditioner for Krylov subspace methods, the resulting iterative methods tend to converge fast. For some difficult problems, however, these methods still produce complexities that are too high, or don't converge well enough, and further remedies in terms of coarsening and interpolation need to be found in order to obtain scalable methods. In this paper we describe the combination of these various coarsening

methods with "aggressive coarsening" techniques, which require long range "multipass" interpolation [4], and empirically study complexity and convergence properties of the resulting iterative methods. The resulting AMG methods, implemented in the hypre solver library [5], are applied to first-order system least-squares (FOSLS) discretizations of elliptic PDE systems. Parallel scalability of the combined FOSLS-AMG method is investigated for large-scale three-dimensional applications.

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Dynamic Data-Driven Application Simulations (DDDAS)

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DDDAS is a new paradigm in which data dynamically controls almost all aspects of long term simulations. Rather than run many simulations using static data as initial conditions, a very small number of simulations are run with additional data injected as it becomes available. Most candidate problems for the DDDAS paradigm involve solving a nonlinear time dependent partial differential equation of the form $F(x+Dx(t)) = 0$ by iteratively choosing a new approximate solution x based on the time dependent perturbation $Dx(t)$.

In practice, the data streaming in may have errors and therefore may not be completely accurate or reliable (for example, in reservoir data sets, a 15% error in the data is common). As a result, perhaps one does not need to solve the nonlinear equation precisely at each step. This can expedite the execution.

At each iterative step, the following three issues may need to be addressed:

1. Incomplete solves of a sequence of related models must be understood.
2. The effects of perturbations, either in the data and/or the model, need to be resolved and kept within acceptable limits.

3. Nontraditional convergence issues have to be understood and resolved.

Consequently, there will be a high premium on developing quick approximate direction choices, such as, lower rank updates and continuation methods, and understanding their behavior are important issues. Fault tolerant algorithms have a premium.

The dynamic data is used to determine

1. Whether or not a warm restart is necessary due to unacceptable errors building up in parts of the domain.
2. If a rollback in time is required.
3. If the simulation is running with acceptable errors.

Ideally, there does not have to be a human in the control loop throughout a simulation.

Using the data appropriately lets the physical and mathematical models, the discretization, and the scales of interesting parts of the computations become parameters that can be changed during the course of the simulation. In addition, error propagation is of particular interest in nonlinear time dependent simulations.

DDDAS offers interesting computational and mathematically unsolved problems, such as, how do you analyze the properties of a generalized PDE when you do not know either where or what the local boundary conditions are at any given moment in the simulation in advance?

Sharpening the Predictive Properties of Compatible Relaxation

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The notion of compatible relaxation (CR) was introduced by Brandt in [1] as a modified relaxation scheme that keeps the coarse-level variables invariant. Brandt stated that the convergence rate of CR is a general measure for the quality of the set of coarse variables. A supporting theory for these ideas was presented in [2], from which we developed a CR-based algebraic coarsening algorithm for use in algebraic multigrid (AMG) methods. In [3], a new sharp convergence theory was developed for AMG. The form of this new theory bears a striking resemblance to its predecessor and suggests the possibility of improving the CR measure.

In this talk, we will use the relationship between these two theories to motivate a new approach for CR, one that has the potential of being a sharper measure of coarse grid quality and a better predictor of AMG convergence (one specific version of this method was suggested by Livne [4]). We will discuss the theoretical properties of the new method, provide some numerical results, and discuss open questions and future directions.

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p-Multigrid Solution of High-Order Discontinuous Galerkin Discretizations of the Euler and Compressible Navier-Stokes Equations

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In this talk, we focus on a p-multigrid solution algorithm for high-order discontinuous Galerkin (DG) finite element discretizations of the Euler and compressible Navier-Stokes equations. p-Multigrid, or multi-order, solution strategies have been studied by other authors, including Helenbrook, Mavriplis, and most recently Bassi and Rebay. Common features of this method for high-order DG include ease of implementation and order-independent convergence rates. A key aspect of our p-multigrid implementation is the use of an element-line Jacobi smoother instead of the standard element-Jacobi. The element-line Jacobi smoother consists of solving implicitly on lines of elements formed using coupling based on a $p = 0$ discretization of the scalar convection-diffusion equation. This choice of elemental coupling allows for the removal of stiffness associated with strong convection or regions of high grid anisotropy frequently required in viscous layers. A line creation algorithm is presented for general unstructured meshes, showing how unique lines can be obtained in two and three dimensions for a given elemental coupling.

Using Fourier analysis for scalar convection-diffusion, we demonstrate that the higher-order DG discretizations can be stably marched for all orders with element Jacobi and element-line Jacobi schemes without the use of multi-stage iterations. p-Multigrid is then applied with the element-line smoother to inviscid and viscous test cases, in two and three dimensions. Results demonstrate optimal order of accuracy of the discretization, as well as p-independent multigrid convergence rates. h-dependence is observed, although it is not found to be strong for many practical problems. Finally, for the smooth problems considered, p-refinement outperforms h-refinement in terms of the time required to reach a desired high accuracy level.

Multigrid Solvers on Spherical Geodesic Grids

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Spherical geodesic grids offer several attractive features for geophysical fluid dynamics modeling: quasi-isotropic discretizations and quasi-uniform resolution (which eliminates the pole problem of conventional latitude-longitude grids). Modeling fluid flow on such a grid results in various elliptic problems which must be solved efficiently, e.g., the Poisson problem relating stream function to vorticity and modified Helmholtz problems with variable coefficients arising in semi-implicit time integration.

Heikes and Randall (1995) introduced a multigrid algorithm for the two-dimensional Poisson problem on a spherical geodesic grid. In this paper we: (1) provide a smoothing analysis for this method and discuss possible algorithmic improvements, (2) extend the algorithm to variable-coefficient problems in two and three dimensions (using an isentropic vertical coordinate), and (3) provide numerical experiments showing performance consistent with the analysis. We also illustrate the use of these multigrid solvers in a three-dimensional dynamical core for a climate model.

Nonlinear Nearly Matrix-Free Algebraic Multigrid for Solid Mechanics

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The increasing demands of large-scale complex solid mechanics simulations are placing greater emphasis on the challenges associated with the efficient solution of the set of nonlinear equations. Here, the solution of large systems of equations with material and geometric nonlinearities in a parallel framework is addressed.

Instead of applying widely used Newton- or Newton-Krylov type methods that involve the derivation of a stiffness matrix and a sequence of linear solves, the presented work details the implementation of a (nearly) matrix-free nonlinear algebraic multigrid algorithm applied to solve this set of nonlinear equations.

As a basic iterative method, a nonlinear conjugate gradient algorithm (nlnCG) using the Polak-Ribiere formula and a secant method for the step size is applied. It has the advantage of being a completely matrix-free method eliminating the need to form a stiffness matrix. Preconditioned nonlinear CG is then applied as a smoother/coarse solver in a classical full approximation scheme (FAS) nonlinear multigrid cycle. Transfer operators are constructed by an aggregation approach operating on the graph of the fine level problem. The preconditioners to the nlnCG on all levels are obtained by multicolor finite differencing and are chosen to be either simple Jacobi or a direct solve on the coarsest level. For Jacobi-preconditioned nonlinear CG, only the main diagonal of a Jacobian matrix needs to be formed involving a distance-1 graph coloring algorithm and an inexpensive modified colored finite difference scheme.

The algorithm is implemented within Sandia National Laboratories' freely available parallel 'Trilinos' linear algebra framework and makes use of its smoothed aggregation multigrid library 'ML' and its nonlinear solver

library 'NOX'. The outline of the algorithm and implementation are given together with examples demonstrating the advantages of this new approach. Several variants of the algorithm will be discussed and compared.

Using parallel algebraic multi-grid preconditioner in an industrial reservoir simulation software

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As full field reservoir simulations require a large amounts of computing resources, the trend is to use parallel computing to overcome hardware limitations. This paper presents the linear solvers and the preconditioning techniques applied to solve very large scale problems in the reservoir simulation software developed at IFP, software which has been specially designed for Linux clusters. We discuss on the choice of different efficient preconditioners. We report the scalability of the parallel simulator and numerical stability of underlying algorithms calculated from a test campaign on either synthetical or real industrial study case.

The reservoir simulator is based on a system of partial differential equations with algebraic closure laws discretized with a finite volume scheme in space and a fully implicit or semi-implicit time integration. After a Newton type linearization of the non linear system, we are left, at each Newton iteration, with the solution of a large, ill conditioned linear system coupling several unknowns of mixed parabolic and hyperbolic type. Progress of computer performances now allows to better take into account physical phenomenon like strong and very strong rock heterogeneities and anisotropies in reservoir modeling so that the complexity of reservoir simulations keeps on increasing with larger meshes, and more difficult problems. This in turn urges the need to design more efficient and more scalable preconditioned iterative solvers, adapted to the new parallel architectures, in order to fully benefit from the computers performances on such complex cases.

Due to the high condition number of the linear system, the convergence of the Newton algorithm can be very sensitive to the choice of the preconditioner, to the linear system stopping criteria and even to the number of processors in parallel implementations. In such cases, the accuracy of the solver is critical to ensure parallel performance as the cumulative number of steps (solver resolution, Newton loops, time loops) can be very dependent on the number of domains and as the cost of a run depends on this cumulative number of steps. This shows the importance of choosing a stable numerical scheme, good solver options and robust parallel preconditioner to have a numerically stable simulation. This difficulty emphasizes the special importance of using very stable numerical schemes during parallel simulation. Solver options may have important influence on convergence criteria, and the choice of a good parallel preconditioner can help to have stable convergence iteration numbers.

In the standard sequential simulator, linear systems are efficiently solved by the Bi Conjugated Gradient Stabilised with an incomplete ILU0 preconditioner. This preconditioner, well known to be efficient for standard case is not naturally parallel as its algorithm is recursive.

We have developed a new parallel ILU0 preconditioner which turns to be a good scalable preconditioner. However, it can encounter difficulties on complex industrial cases with very complex geometry and physical models. ILU0 is not scalable with respect to the size of the mesh and the jumps of the permeability field. Multigrid methods are known to be scalable for scalar convection diffusion problems but it is also known that they are not adapted to systems coupling unknowns of mixed types. Our approach is to define a pressure block that will concentrate most of the bad conditioning and ellipticity of the system, and for which we shall used a multigrid preconditioner.

The definition of this block is obtained by linear combination of the rows and columns in order to reduce the coupling with the other variables (compositions and concentrations). For the remaining variables and equations we use a block Gauss Seidel approach. In some cases, this approach does not ensure a sufficient coupling of the variables, and it needs to be combined mutiplicatively with a global ILU0 preconditioner.

In reservoir modeling, the linear systems couple a pressure unknown of elliptic or parabolic type to concentrations or saturations unknowns of hyperbolic type. In some industrial cases, especially when there are a lot of heterogeneities and anisotropies, we have noticed that the variations of saturation are very sensitive to pressure gradient so that having a robust preconditioner for the pressure is very important. As a consequence, Algebraic Multigrid Methods have to be considered as good candidates for preconditioning. Thus, we have developed 2 AMG based preconditioners . The first approach is a Block Aggregation AMG. It aims at taking advantage of the natural block structure of the system when the unknowns pressure and saturation are grouped cell by cell. This strategy turns out to be effective when a block ILU0 smoother is used in the multigrid cycle. The second approach called "Two level AMG" combines an algebraic multigrid method on pressure unknowns with a more traditional parallel method on other variables (ILU0, Block ILU0, polynomial). This results in a new method which is robust, parallel and efficient

We have tested these methods (Parallel ILU0, Two level AMG and Block Aggregation AMG) and studied their influence on the performance and on the numerical stability of the reservoir simulator for different study case. We discussed the results obtained on a synthetical study case, the Tenth SPE Comparative Solution Project, Model 2 and on some real industrial customer study cases.

On Recursive Multiscale Trust-Region Algorithms for Unconstrained Minimization

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A large class of large-scale finite-dimensional minimization programs arises from the discretization of infinite-dimensional problems, such as optimal-control problems defined in terms of either ordinary or partial differential equations. We report here on a potentially efficient new class of algorithms using this structure and briefly discuss a first set of numerical experiments. A simple first approach that we refer to as mesh refinement, is to use coarser grids in order to compute approximate solutions which can then be used as starting points for the optimization problem on a finer grid (see [2], [3] or [8], for instance). However, potentially more efficient techniques are inspired from the multigrid paradigm in the solution of partial differential equations and associated systems of linear algebraic equations (see, for example, [4] or [5]). The work presented here was in particular motivated by the "generalized truncated Newton algorithm" presented in Fisher [7], a talk by Moré [10], the contribution by Nash and Lewis [9] and the computational success of the low/high-fidelity model management techniques of Alexandrov, Lewis and co-authors [1].

We aim at minimizing the cost function $f(x)$, $x \in \mathbf{R}^n$, and assume that we know a collection of functions f_0, $\ldots$, f_r, such that each f_i is a twice-continuously differentiable function from $\mathbf{R}^{n_i}$ to $\mathbf{R}$ (with $n_i \geq n_{i-1}$), the connection with our original problem being that $n_r = n$ and $f_r(x) = f(x)$ for all x in $\mathbf{R}^n$. We also assume that, for each i=1, $\ldots$,r, f_i is "more costly" to minimize than f_{i-1}. This may be because f_i has more variables than f_{i-1} (as would typically be the case if f_i represent increasingly finer discretizations of the same infinite-dimensional objective), or because the structure (in terms of partial separability, sparsity or eigenstructure) of f_i is more complex than that of f_{i-1}, or for any other reason. Our algorithm generates at each level i a sequence of

iterates using either a recursive call to a coarser level (lower level iteration) or an iteration at level i (same level iteration). A condition for function f_{i-1} to be useful in minimizing f_i is provided in terms of gradient of these functions prolongated in suitable spaces. If this condition does not hold, a same level iteration is performed. The same level iterations fall into two classes: smoothing iterations aim at decreasing high-frequency components of the gradients and damping iterations, which decrease their low-frequency components. A multilevel trust region mechanism is implemented that ensures a global convergence of the algorithm to first order critical points, under some classical assumptions, such as the sufficient decrease condition (in the sense of the Cauchy condition) [6].

We present a numerical applications for one of the possible implementations. We provide details on the mechanisms ensuring that the convergence conditions are met. Other implementation questions are concerned with the form of the recursive iterations, ranging from free form (where the optimization at lower levels is governed purely by accuracy requirements) to fixed cycles (such as the V and W cycles inspired by multigrid techniques). Demonstration of the efficiency of the method when compared to mesh refinement is done on a minimum surface problem with highly oscillatory boundary conditions and on the Dirichlet-to-Newman transfer problem. Problems involving up to 1.1 million variables were solved by the new algorithm in MATLAB on a laptop PC (Pentium 4 Mobile, 1.6 GHz).

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A new Rayleigh quotient minimization algorithm based on algebraic multigrid

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Mandel and McCormick [2] introduced the RQMG method, which approximately minimizes the Rayleigh quotient over a sequence of grids. In this talk, we will present an algebraic extension. We replace the geometric mesh information with the algebraic information defined by an AMG preconditioner. At each level, we improve the smoother to accelerate the convergence. With a series of numerical experiments, we assess the efficiency of this new algorithm to compute several eigenpairs.

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Tools for Analyzing Multigrid Performance

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In this talk we discuss a variety of practical tools that we have developed to analyze and correct parallel multigrid performance. These include visualization capabilities for assessing aggregate quality, run time tools for analyzing the convergence of existing multigrid methods, rebalancing schemes to improve parallel communication patterns, and an adaptive multigrid method based on that outlined in "Adaptive Smoothed Aggregation (αSA)" by Brezina, Falgout, MacLachlan, et. al. We conclude with some examples from Sandia applications where these tools have been applied.

Multigrid Methods for Pricing American Options under Stochastic Volatility

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We study numerical methods for pricing American put options with Heston's stochastic volatility model. This model leads to a two dimensional parabolic partial differential equation with an early exercise constraint. We perform the space discretization using a finite difference method with a seven point stencil. Implicit time discretizations lead to a sequence of linear complementarity problems (LCPs).

We consider two approaches employing multigrid methods. The first approach uses an operator splitting method [4]. The idea is to decouple the system of linear equations and the early exercise constraint into separate fractional time steps. In the first fractional step, a convection diffusion type problem with a second-order cross derivative is solve. In a multigrid method we use an alternating direction smoother proposed by Oosterlee in [5]. In the second fractional step, a simple update is performed so that the solution satisfies the early exercise constraint.

The second approach is to solve the LCPs using a multigrid based on a projected full approximation scheme (PFAS) proposed by Brandt and Cryer in [1]. The papers [3,5] consider such multigrids for pricing American options. We study the use of the Brennan and Schwartz algorithm [2] in the line smoothing in these multigrids.

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Parallel Multigrid on a Beowulf Cluster

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In this talk we discuss the performance of parallel multigrid codes of the 48 nodes Beowulf parallel computer at Florida Tech. In particular, we discuss how the relative communication and computation speeds impact the parallel performance of multigrid solvers.

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p-Multigrid for the Nodal Discontinuous Galerkin Approximation

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The Discontinuous Galerkin (DG) Method is increasingly used nowadays to solve advection-dominated problems. Its most attractive features, namely the high accuracy obtained without the use of an extended stencil and the inherent parallelization, have turned it into a method of choice for Computational Fluid Dynamics problems (see the recent review in [Cockburn,Karniadakis,Shu (2001)]). The early formulation of the DG method by Cockburn and Shu (1989) uses as degrees of freedom the coefficients of the solution in a polynomial basis expansion (Legendre polynomials being used in one dimension to take advantage of their orthogonality). This modal formulation seems more intuitive, but has a large drawback for nonlinear problems: to compute nonlinear fluxes, one needs to first compute the value of the solution by evaluating the polynomial expansion at the flux integration points, then evaluate the fluxes. Researchers realized later that this translation from modal space into physical space can be avoided through a collocation (nodal) formulation. In the latter framework the degrees of freedom are the values of the solution at the collocation points, so the flux values can be evaluated easily, in particular if the collocation points are chosen to coincide with the integration points [Stanescu,Hussaini,Farassat (2003)], [Kopriva,Woodruff,Hussaini (2001)].

In the context of multigrid methods, the modal DG formulation again is more intuitive: the polynomial-type basis functions can be made hierarchical, and a p-multigrid approach is natural (the restriction operator for example just neglects extra modes); see recent research in this direction [Helenbrook,Mavriplis,Atkins (2003)], [Fidkowski,Darmofal (2003)]. Due to the advantage of the nodal approach for nonlinear problems, we want to investigate the feasibility of a p-type multigrid method in this latter formulation. It seems that such an investigation has not been reported yet in the literature. The use of an acceleration technique such as multigrid may reduce the difference in cost between the two approaches; however, this is very likely to be problem dependent, hence arguably a nodal DG p-multigrid method may lead to savings in computer time.

For a preliminary numerical result, we solve the one-dimensional nonlinear Euler equations and compare the performance (CPU time, MG cycles) of a nodal DG p-multigrid with a modal DG p-multigrid. Figure 1 shows the accuracy versus the number of MG cycles:

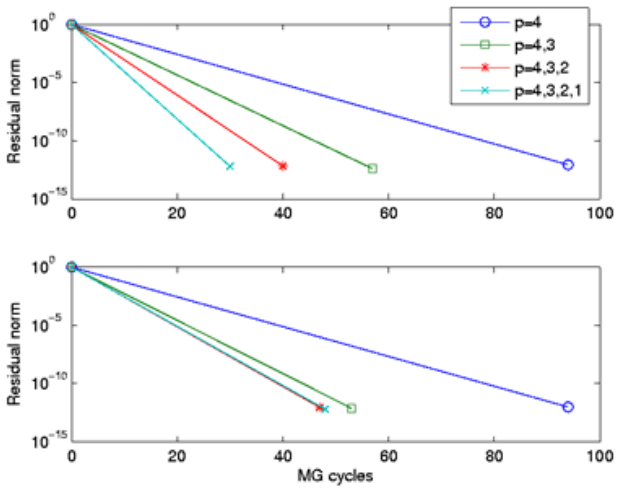
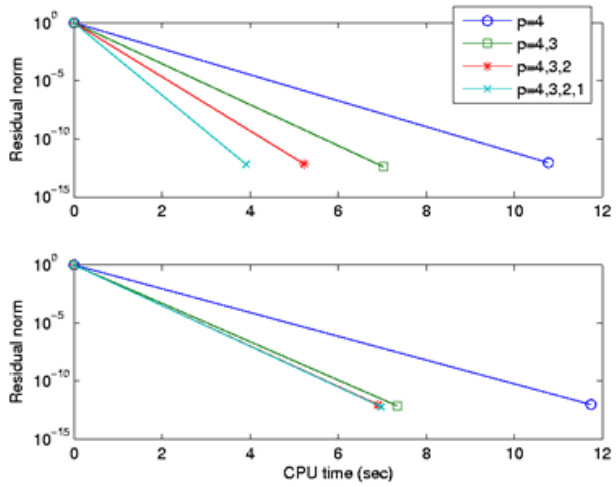


Figure 2 shows the accuracy versus CPU time:



A preconditioner on high-order finite element methods

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Even if the high-order finite element method has many advantages for solving a uniformly self adjoint elliptic operator such as

$$Lu := -\nabla \cdot \mathbf{A}\nabla \mathbf{u} + \mathbf{c_0 u} \quad \text{in} \quad \Omega = [-\mathbf{1}, \mathbf{1}] \times [-\mathbf{1}, \mathbf{1}]$$

with boundary conditions ($\Gamma_L = \Gamma_D(L) \cup \Gamma_N(L)$)

$$u = 0 \quad \text{on} \quad \Gamma_D(L), \quad \mathbf{n} \cdot \mathbf{A}\nabla \mathbf{u} = \mathbf{0} \quad \text{on} \quad \Gamma_{\mathbf{N}}(\mathbf{L}),$$

one may have a difficulty controlling condition numbers occurred from spectral element discretizations which makes it uneasy to use iterative methods. In order to alleviate such a situation, we take a lower order finite element preconditioner operator corresponding to

$$Bv := -\nabla \cdot \nabla u + b_0 u \quad \text{in} \quad \Omega$$

with boundary conditions ($\Gamma_B = \Gamma_D(B) \cup \Gamma_N(B)$)

$$v = 0 \quad \text{on} \quad \Gamma_D(B), \quad \mathbf{n} \cdot \nabla \mathbf{v} = \mathbf{0} \quad \text{on} \quad \Gamma_{\mathbf{N}}(\mathbf{B}).$$

Let $\{\eta_k\}_{k=0}^N$ be the standard Legendre-Gauss-Lobatto (=:LGL) points in $[-1, 1]$. By translations from I to a j^{th} subinterval $I_j := [x_{j-1}, x_j]$ we denote $\{\xi_k^j\}_{k=0}^N$ as the $k^{th}-$ LGL points in each subinterval I_j for $j = 1, 2, \cdots, M$. Let $\mathcal{P}_N^h$ be the subspace of $C[-1, 1]$ which consists of piecewise polynomials with support $I_j = [x_{j-1}, x_j]$ whose degree is less than or equal to N. For the space $\mathcal{P}_N^h$, we choose a *piecewise Lagrange polynomial basis functions* denoted as $\{\phi_k^j(x)\}$ supported in I_j for $j = 1, \cdots, M$. Let $\mathcal{V}_N^h$ be the space of all *piecewise Lagrange linear functions* $\psi_k^i(x)$. Define an interpolation operator $\mathcal{I}_N^h : C[-1, 1] \to \mathcal{P}_N^h(I)$ such that

$$(\mathcal{I}_N^h v)(\xi_\mu) = v(\xi_\mu), \quad v \in C[-1, 1].$$

First, we set up the following relations for $v \in \mathcal{V}_N^h$

$$c\|v\| \leq \|\mathcal{I}_N^h v\| \leq C\|v\|, \quad c\|v\|_1 \leq \|\mathcal{I}_N^h v\|_1 \leq C\|v\|_1,$$

where two positive constants c and C do not independent of the mesh size $h_j = x_j - x_{j-1}$ and the degree N of piecewise polynomial. Let $(\hat{\mathrm{L}}_N^h)$ and $\hat{\mathbf{B}}_N^h$ be finite element stiffness matrices corresponding to L and B respectively . Then we will show the preconditioned system

$$(\hat{\mathbf{B}}_N^h)^{-1}\hat{L}_N^h$$

has positive eigenvalues which are independent of the mesh size $h_j = x_j - x_{j-1}$ and the degree N of piecewise polynomial.

Implementation of An Overlapping Balancing Domain Decomposition Method for Elliptic PDEs on Unstructured Meshes

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A new type of overlapping Domain Decomposition algorithm, Overlapping Balancing Domain Decomposition (OBDD) algorithms, has been recently presented by M. Sarkis and J.H. Kimn. This new algorithm can be considered as an extension of the Balancing Domain Decomposition algorithms to overlapping subdomains. This approach can be applied to structured and unstructured meshes and relies on Partition of Unity function to construct a sparse matrix for coarse space.

In this talk, we will discuss several aspects of the practical parallel implementation of this method. We will show numerical results for large unstructured meshes.

Experiments with Adaptive Element Agglomeration Algebraic Multigrid for H(div) and H(curl).

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In this talk we combine the element agglomeration AMGe (from [2]) and the adaptive AMG (from [1]). The former method is used to generate an initial V-cycle that coarsens only the null space of the respective H(div) or H(curl) form, whereas the second method is used to gradually augment the current coarse grids and interpolation matrices. The numerical tests indicate that 3 to 5 adaptive cycles are sufficient in order to achieve an efficient

AMG solver. A main tool in the adaptation process is the hierarchical construction of the modified interpolation matrices, see [3], which is based on solving local constrained minimization problems, fitting one "algebraically smooth" vector at a time.

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Preconditioned eigensolvers in Hypre and PETSc

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We present preliminary results of an ongoing project to develop codes of the Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) method for symmetric eigenvalue problems for Hypre and PETSc software packages. Hypre and PETSc packages provide high quality multigrid and domain decomposition preconditioning on parallel clusters with distributed or shared memory architecture. 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. However, the only publicly available at present LOBPCG implementation remains our implementation for Hypre, which is already included in Hypre 1.8.2 release. We describe the current state of the LOBPCG software for Hypre and PETSc, developed by our group and demonstrate initial scalability results.

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A Multilevel Time Parallelization Algorithm

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Parallel methods are usually not applied to the time domain because of the inherit sequentialness of time evolution. But for many evolutionary problems, computer simulation can benefit substantially from time parallelization methods. In this talk, we present several such multilevel algorithms that actually exploit the sequential nature of time evolution through a predictor-corrector procedure. This sequentialness ensures convergence of a parallel predictor corrector procedure within a fixed number of iterations. The performance of these novel algorithms which can be derived from the classical alternating Schwarz method, are illustrated through several examples from reservoir simulation.

A Multilevel Adaptive Solver for the Density-Gradient Equation

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Continuing advances in the miniaturization of integrated circuits have imposed new challenges to designers of semiconductor devices, as traditional circuit analysis tools are no longer applicable. In this study, we focus on the gate region of MOSFET devices with an oxide thickness of order 4-6 nanometers. For oxide layers of this width, quantum effects start to become noticeable and the standard equations of semiconductor physics require quantum corrections. The Density-Gradient equation [1], [2] is a means of calculating approximate quantum corrections to existing formulae without solving the full Poisson-Schrödinger system.

We use a one-dimensional approximation to reduce the D-G equations to a set of singularly perturbed ODEs [3]. These equations have interior layer solutions, which compromise the numerical treatment of the problem if care is not taken to resolve the large gradients in the solution within the layer correctly. Several approaches have been proposed to resolve the boundary layer region including nonlinear discretization schemes [4], [5]. However, these methods have difficulty resolving interior layers [6]; therefore, we propose a multilevel adaptive scheme to solve the model equations. The method is akin to multigrid, but utilizes high-order inter-grid operators, which preserve a nested space structure throughout the various resolution levels, similar to the methods described by Goedecker [7] and Warming & Beam [8]. This multilevel method has several advantages over the previous discretization schemes, the most important being that it adapts dynamically to interior layers without a priori knowledge of the location or geometry of the layer.

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Multilevel eigenbasis for Schrödinger eigenvalue problems

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In this talk we discuss AMG algorithms for eigenbasis approximation for Schrödinger eigenvalue problems with variable potential. The algorithms employ the multilevel eigenvalue structure suggested by Livne and Brandt, and are used to solve one-dimensional (at $O(N \log N)$ operations) and two-dimensional problems (at somewhat comparable costs). Also to be addressed is the issue of the quality of the approximated eigenbasis, such as its fullness and independence of the eigenfunctions. Numerical results for both one- and two-dimensional problems will be discussed.

Fully Adaptive AMG

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Numerical simulation of physical processes is often constrained by our ability to solve the complex linear systems at the core of the computation. Classical geometric and algebraic multigrid methods rely on (implicit) assumptions about the character of these matrices in order to develop appropriately complementary coarse-grid correction processes for a given relaxation scheme. The aim of the adaptive multigrid framework is to reduce the restrictions imposed by such assumptions, thus allowing for efficient black-box multigrid solution of a wider class of problems.

There are, however, many challenges in altogether removing the reliance on assumptions about the errors left after relaxation. In this talk, we discuss work to date on a fully adaptive AMG algorithm that chooses all components of

the coarse-grid correction based on automated analysis of the performance of relaxation. Fundamental measures of the need for and quality of a coarse-grid correction will be discussed, along with related techniques for choosing coarse grids and interpolation operators. We will also discuss the (lack of) computability of these ideal measures, and suggest cost-efficient alternatives.

This research has been performed in collaboration with James Brannick, Marian Brezina, Tom Manteuffel, Steve McCormick, and John Ruge at CU-Boulder. It has been supported by an NSF SciDAC grant (TOPS), as well as Lawrence Livermore and Los Alamos National Laboratories.

Block Preconditioners with Algebraic Multigrid Block Solve in Stratigraphic Modeling for oil exploration

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Stratigraphic models simulate the erosion and sedimentation of sedimentary basins at geological time scales given the sea level variations, the tectonics displacements of the basement, and the sediments fluxes at the boundary of the basin. We consider in this talk a sediments transport model coupling three main processes: a gravity driven transport of the sediments for which the fluxes are proportional to the gradient of the topography, a weather limited transport taking into account the disymmetry between erosion and sedimentation, and a fluvial transport model for which the sediments fluxes are proportional to the water discharge. The main variables of the problem are the sediment thickness, a flux limitor, and the L sediments concentrations in basic lithologies such as sand or shale or carbonates. Such model is applied in oil exploration for a better prediction of potential reservoirs location. The model is derived writing the mass conservation of each lithology leading to a system of mixed parabolic hyperbolic type. It is discretized by a finite volume scheme in space and a fully implicit time integration, leading to the solution at each time step of a non linear systems of $L+2$ variables on the 2D mesh.

After Newton type linearization, we are left with the solution of an ill conditioned linear system with sharp jumps in the diffusion coefficients and coupling $L+2$ variables of mixed types. These linear systems are solved using an iterative solver and a block approach for the preconditioner in order to separate the different variables. In a first step, a mixture equation is obtained by linear combinations of the rows that should concentrate the ellipticity of the system and as much as possible decouple the first two variables (sediment thickness and flux limitor) from the L concentrations variables. Then the overall system is solved using a block Gauss Seidel preconditioner. The First block (sediment thickness and flux limitor variables) is preconditioned either by a direct sparse solver or by an ILU0 incomplete factorization, or by a vcycle of an algebraic multigrid solver (AMG1R5 from Ruge and Stueben) on the sediment thickness sub-block only in order to avoid non diagonal dominance. The remaining blocks are solve using a gauss seidel sweep in topographical order leading to an exact inversion of these blocks. These block preconditioners are compared with a sparse direct solver and an ILU0 incomplete factorization on the overall system. The comparison is made in terms of CPU time, and scalability with respect to the mesh size and the jump of the diffusion coefficients on two real test cases: the Paris basin and a Rift test case with water discharge. It shows that the block approach combined with a multigrid preconditioning of the the sediment thickness sub-block is a very efficient method, nearly scalable for this problem.

Multigrid solution of the lattice Boltzmann equation

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The last decade has seen rapid progress in the theoretical understanding, algorithmic development, and use of lattice Boltzmann methods (LBM). As opposed to traditional computational fluid dynamics approaches, which compute macroscopic fluid dynamic properties by discretizing the continuum governing equations, the independent variables in a lattice Boltzmann approach consist of particle distribution functions in phase space, from which macroscopic continuum fluid properties can be recovered. Historically, LBM methods have been derived from lattice gas automata (LGA) methods. LGA methods model macroscopic fluid motion through the evolution of a set of discrete particles on a regular lattice (cartesian grid). Many of the deficiencies of LGA methods in reproducing accurate macroscopic behavior were resolved by the LBM approach, by neglecting individual particle motion, and adopting a particle distribution function approach. However, LBM methods have retained this conceptual link to particle methods such as LGA, which has inhibited the use of more sophisticated numerical techniques.

In this work, we first describe the lattice Boltzmann method as a particular finite-difference discretization in space and time of the Boltzmann equation. The LBM time-step is then shown to be equivalent to a first-order explicit time step (forward Euler), which is also equivalent to a Jacobi iteration for the steady-state form of the LBM equations. It is then shown how this iteration strategy may be used as a solver for the steady-state lattice Boltzmann equation, or as a solver for an implicit time-integration strategy. Finally, it is shown how these problems may be solved more efficiently using the Jacobi iteration as a smoother in a multigrid scheme for the steady-state lattice Boltzmann equation. This requires under-relaxation of the iteration scheme to achieve good high-frequency damping properties, and a careful matching of the LBM discretizations on the coarse grid levels, in order to ensure consistent coarse and fine grid problems. The final result is a multigrid solver which can make use of a pre-existing LBM routine in a modular fashion, by invoking the LBM routine on each grid level. Convergence rates which are independent of the mesh resolution are demonstrated for the driven cavity problem on a cartesian grid, although the convergence rates degrade with increasing Reynolds number.

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A cache-oblivious self-adaptive full multigrid method

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In many implementations of modern solvers for partial differential equations, the use of multigrid methods in particular in combination with dynamically adaptive grids causes a non-negligible loss of efficiency in data access and storage usage: As multilevel data on adaptively refined grids are typically organized in trees and stored with the help of pointer structures, the evaluation of difference stencils, restrictions and interpolations generate jumps within the physical memory space and, thus, prevent an efficient usage of cache-hierarchies and prefetching strategies. In addition, the storage of pointers to neighbors, fathers and sons of each grid cell is required. Our algorithm overcomes these inefficiencies by a linearization of all data with the help of space-trees and space-filling curves. Space-filling curves are well known as an efficient tool for parallelization strategies on space-tree grids as they define a linear ordering of all grid cells and, thus, allow a simple partitioning of data. Space-tree grids are structured grids but, at the same time, permit arbitrary local refinement (The only exception are unisotropic refinements. The realization of such refinements is subject of our current studies.).

In our algorithm, we associate the degrees of freedom of the unknown function(s) to the vertices of the grid cells and - as a first step towards cache-optimality - we replace the common pointwise operator evaluation - that is the complete computation of the operator value at a grid point necessitating access to data of neighboring points and, thus, causing a part of the jumps within the physical memory space. We use an elementwise operator evaluation instead: We decompose the pointwise difference stencils in parts only incorporating vertex data of the actual cell and get the overall operator value by accumulation over all cells involved. From the algorithmic point of view, the consequence is a cellwise instead of pointwise processing of the space-tree grid during the iterations of our solver.

The second and crucial step on our way to cache-optimality is to construct suitable data structures with minimal storage overhead and strictly local access properties. If we use the discrete iterates of the Peano-curve, a self-similar recursively defined space-filling curve, to define a top-down-depth-first processing order of the grid cells (on all levels), we can derive a storage concept with a fixed, small and constant number of stacks as the only kind of data structures [1,2,3,4]: Due to the dimension-recursivity of the Peano-curve, this traversal order leads to a to-and-fro-processing of vertex data on certain sub-manifolds of the domain which exactly fits the properties of stacks: Stacks are very simple data structures allowing only the two basic operations push and pop (push puts data on top of a pile and pop takes data from the top of a pile). Due to this, the locality of data access is inherently very high which makes data access very fast - even faster than the common access of non-hierarchical data stored in matrices - and, in particular, reduces cache misses considerably. In addition, we can define locally deterministic rules for pushing and poping data to/from the set of stacks. Thus, also the storage overhead for administrational information is minimal. Each cell only has to carry one bit for geometrical and one bit for refinement information.

Dynamical adaptivity can be realized in a very natural way in this concept by definition of data sources and sinks at interface to the input and output stacks of a solver iteration. Based on the algorithmic concepts described above, we implemented an adaptive Full Multigrid method for the three-dimensional Poisson equation with several adaptivity criteria like shape of the domain, error estimators for the global error and dual approaches to handle local accuracy requirements. In addition, the Multigrid method was combined with a tau-extrapolation scheme to achieve a fourth order discretization [5,6]. Thus, we considerably enhanced the numerical efficiency without loosing cache-efficiency compared to a simple non-adaptive one-level solver. In all case studies, the number of actual cache misses is only about ten percent higher than the unavoidable minimum of cache misses caused by the first loading of data points to the cache.

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The Action-Dependent Wave Function Problem: Well Posedness and Efficient Numerical Solutions

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We describe some results for a mixed (elliptic-hyperbolic) partial differential equation and an efficient multigrid algorithm for its numerical solution. The problem models an equation which arises in atomic physics and describes a new object: an "action-dependent wave function."

Multilevel Upscaling: Multigrid's Lost Twin

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In many applications, homogenization (or upscaling) techniques are necessary to develop computationally feasible models on scales coarser than the variation of the coefficients of the continuum model. The accuracy of such techniques depends dramatically on assumptions that underlie the particular upscaling methodology used. For

example, decoupling of fine- and coarse-scale effects in the underlying medium may utilize artificial internal boundary conditions on sub-cell problems. Such assumptions, however, may be at odds with the true, fine-scale solution, yielding coarse-scale errors that may be unbounded.

In this work, we present an efficient multilevel upscaling (MLUPS) procedure for single-phase saturated flow through porous media. Coarse-scale models are explicitly created from a given fine-scale model through the application of standard operator-induced variational coarsening techniques. Such coarsenings, which originated with robust multigrid solvers, have been shown to accurately capture the influence of fine-scale heterogeneity over the complete hierarchy of resulting coarse-scale models. Moreover, implicit in this hierarchy is the construction of interpolation operators that provide a natural and complete multiscale basis for the fine-scale problem. Thus, this new multilevel upscaling methodology is similar to the Multiscale Finite Element Method (MSFEM) and, indeed, we show that it attains similar accuracy on a variety of problems. While MSFEM is based on a two-scale approach, MLUPS generates a complete hierarchy of coarse-scale models, resulting in a speed-up factor of approximately 15. In addition, we demonstrate that this new upscaling methodology can use both structured coarsening algorithms, such as Dendy's BoxMG, and fully algebraic algorithms, such as Ruge's AMG.

High-Order Spectral *hp*-Multigrid Methods on Unstructured Grids

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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. Herein we extend the spectral multigrid approach described in [1] to the two-dimensional steady-state Euler equations, and couple the spectral p-multigrid approach with a more traditional agglomeration h-multigrid method for unstructured meshes. The investigation of efficient smoothers to be used at each level of the multigrid algorithm is also pursued, and comparisons between linear and non-linear solver strategies are made as well [2]. 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 computational domain is partitioned into an ensemble of non-overlapping unstructured elements and within each element the solution is approximated by a truncated polynomial expansion. The semi-discrete formulation employs a local discontinuous Galerkin formulation in spatial variables within each element. Thus, the solution approximation is local, discontinuous, and doubled valued on each elemental interface. Monotone numerical fluxes are used to resolve the discontinuity, providing the means of communication between adjacent elements and specification of the boundary conditions. An approximate Riemann solver is used to compute the flux at inter-element boundaries. The discrete form of the local discontinuous Galerkin formulation is defined by the particular choice of the set of basis functions. Hereby a set of hierarchical basis functions is used in order to simplify our subsequent spectral multigrid implementation. The full description of the basis function set is given in [3]. The resulting set of equations is solved in the modal space and the integrals are evaluated by Gaussian quadrature rules.

The spectral p-multigrid approach is based on the same concepts as a traditional h-multigrid method, but makes use of "coarser" levels which are constructed by reducing the order of accuracy of the discretization, rather than using physically coarser grids with fewer elements. Furthermore, the formulation of the interpolation operators, between fine and coarse grid levels, is greatly simplified when a hierarchical basis set is employed for the solution approximation. The main advantage is due to the fact that the lower order basis functions are a subset of the higher order basis (i.e. hierarchical) and the restriction and prolongation operators become simple projection operators into a lower and higher order space, respectively [4]. For pure p-multigrid methods, the recursive application of lower order discretizations ends with the $p = 0$ discretization on the same grid as the fine level problem. For relatively fine meshes, the (exact) solution of this $p = 0$ problem at each multigrid cycle can become expensive, and may impede the h-independence property of the multigrid strategy. The $p = 0$ problem can either be solved approximately by employing the same number of smoothing cycles on this level as on the finer p-levels, or it can be solved more accurately by performing a larger number of smoothing cycles at each visit to this coarsest level. In either case, the convergence efficiency will be compromised, either due to inadequate coarse level convergence, or due to excessive coarse level solution cost. An alternative is to employ an h-multigrid procedure to solve the coarse level problem at each multigrid cycle. In this scenario, the p-multigrid scheme reverts to an agglomeration multigrid scheme once the $p = 0$ level has been reached, making use of a complete sequence of physically coarser agglomerated grids, thus the designation hp-multigrid. First-order accurate (p=0) agglomeration multigrid methods for unstructured meshes are well established [5] and deliver near optimal convergence rates. Therefore, this procedure has the potential of resulting in a truly h- and p-independent solution strategy for high-order accurate discontinuous Galerkin discretizations.

At each h- or p-multigrid level an element-Jacobi type scheme is used as a smoother. The element-Jacobi scheme can be viewed as an approximate Newton scheme where the full Jacobian matrix is replaced by the block diagonal entries representing the coupling between all modes within each element, [D], thus neglecting the coupling between neighboring element modes, which arises through the inter-element flux evaluations. The [D] blocks represent small dense matrices associated with each grid element. A second variant of this solver is denoted as the "linearized" element-Jacobi method. In this approach, the full Jacobian matrix is retained, but is decomposed into block diagonal [D] and off-diagonal [O] components. Note that the linearized element Jacobi scheme involves a dual iteration strategy, where each nth outer non-linear iteration entails "k" inner linear iterations. The advantage of this formulation is that the non-linear residual and the Jacobian entries, [D] and [O], are held constant during the linear iterations. This can significantly reduce the required computational time per cycle for expensive non-linear residual constructions. Because this scheme represents an exact linearization of the element-Jacobi scheme both approaches can be expected to converge asymptotically at the same rates per cycle [6]. The convergence can be further accelerated by using a Gauss-Seidel strategy where the off-diagonal matrices are split into lower, [L], and upper, [U] contributions (i.e. [O]=[L]+[U]). This last solver variant, again, involves a dual iteration strategy, but follows an ordered sweep across the elements using latest available neighboring information in the Gauss-Seidel sense. In this work, we employ a frontal sweep along the elements which begins near the inner boundary and proceeds toward the outer boundary, using the numbering assigned to the grid elements from an advancing front mesh generation technique.

The resulting hp-multigrid scheme demonstrates p-independent and nearly h-independent convergence rates. The coupling of p- and h-multigrid procedures, through the use of agglomerated coarse levels for unstructured meshes, increases the overall solution efficiency compared to a p-alone multigrid procedure, and the benefits of the hp-multigrid approach can be expected to increase for finer meshes. The multigrid procedure can itself be applied as a non-linear solver (FAS), or as a linear solver (CGC) for a Newton scheme applied to the non-linear problem. The linear multigrid approach demonstrates superior overall efficiency, provided a suitable linear iteration termination strategy is employed. Results are presented for compressible flow over a bump in a channel and for flow over a four element airfoil in two dimensions.

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Multilevel Preconditioners in Thermohaline Ocean Circulation

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The numerical continuation of steady states in thermohaline ocean circulation requires the solution of large systems. The (linearized) equations describing the thermohaline ocean circulation (for a detailed description of these equations see [5]) can be split into equations for velocities in longitudinal and latitudinal direction (x_{uv}), velocity in vertical direction (x_w), pressure (x_p) and salinity and temperature (x_{ST}). The equations are coupled in the following way,

$$\begin{pmatrix} A_{uv} & 0 & G_{uv} & 0 \\ 0 & 0 & G_w & B_{ST} \\ D_{uv} & D_w & 0 & 0 \\ B_{uv} & B_w & 0 & A_{ST} \end{pmatrix} \begin{pmatrix} x_{uv} \\ x_w \\ x_p \\ x_{ST} \end{pmatrix} = \begin{pmatrix} b_{uv} \\ b_w \\ b_p \\ b_{ST} \end{pmatrix}$$

where $G*$ represents the discrete gradient operator and $D*$ the discrete divergence operator. We assume that $G* T = D*$, i.e. the discrete operators are each others transpose. Furthermore, A_{ST} is a convection-diffusion matrix, A_{uv} is also a convection-diffusion matrix, but includes a Coriolis force. Respectively the four equations describe conservation of momentum (in longitudinal and latitudinal direction), the hydrostatic pressure, conservation of mass and conservation of salt and heat.

Due to the size of the systems they are solved via a Krylov subspace method using a preconditioner to speed up the convergence. In general there are two ways to obtain a preconditioner for the matrix in the equation. One could try to exploit the structure of the system or apply a general black-box preconditioning method like an incomplete LU factorization. We will do both and compare the results.

In the current code for numerical simulation of thermohaline ocean circulation (THCM, see [5], the systems are solved with the MRILU [1] preconditioner. MRILU is a multilevel ILU method containing ideas similar to algebraic multigrid methods. However MRILU doesn't need any smoothing steps, because of sophisticated dropping- and lumping criteria. In THCM MRILU is applied to the clustered equations, that is the six unknowns (u,v,w,p,T,S), that belong to one and the same cell, are treated as one unknown. The method is able to construct a good factorization and the Krylov subspace method converges fast. Unfortunately the preconditioner requires a lot of construction time and memory, which becomes a problem if the size of the problem is increased.

In order to reduce the memory usage, we developed an alternative preconditioner that exploits the structure. The ingredients are: a splitting of the pressure in a depth-averaged pressure and a component perpendicular to that;

a non-symmetric reordering of the matrix; dropping the block B_{ST}. This together gives a block-Gauss-Seidel preconditioner, that requires some matrix-vector products and the solution of three relatively easy systems: (i) a depth-averaged saddle point system based on A_{uv}, G_{uv} and D_{uv}, (ii) a convection-diffusion-Coriolis equation involving A_{uv} and (iii) a convection-diffusion equation involving A_{ST}. The last two problems can be handled very well by MRILU. For the saddle point system we can apply any of the preconditioners from literature [3,4] or the ones we developed ourselves based on artificial compressibility and grad-div-stabilization [2] respectively.

A comparison of the structured preconditioner with MRILU applied to the subsystems and MRILU applied to the clustered matrix at once shows that the required amount of memory is reduced with almost a factor 10. We have to pay for that in an increase of the number of iterations in the Krylov subspace method, but this factor is at most 2. Overall we see a serious speed up.

On the conference we will describe the block-Gauss-Seidel preconditioner and show the results of a comparison using both MRILU and an algebraic multigrid method as a subsolver in the preconditioner.

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AMG Preconditioned Conjugate Gradient Type Methods for Nonsymmetric Eigenproblems

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When we need to compute the eigenvalues of a large sparse matrix numerically, the projection method such as the Lanczos type or the Davidson type methods has been the most orthodox choice. However, recent studies revealed that the conjugate gradient method combined with appropriate preconditioners can compute a few eigenpairs of such problems quite efficiently. For large scale nonsymmetric eigenproblems, we expand this approach to the conjugate residual and the bi-conjugate gradient type methods, and evaluate the combination with the AMG preconditioner.

Algebraic Multigrid (AMG) for Higher-Order Finite Elements

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In this talk we consider two related approaches for solving linear systems that arise from a higher-order finite element discretization of elliptic partial differential equations. The first approach explores direct application of an algebraic-based multigrid method (AMG) to iteratively solve the linear systems that result from higher-order discretizations. While the choice of basis used on the discretization has a significant impact on the performance of the solver, results indicate that AMG is capable of solving operators from both Poisson's equation and a first-order system least-squares (FOSLS) formulation of Stoke's equation in a scalable manner, nearly independent of basis order, p. The second approach incorporates preconditioning based on a bilinear finite element mesh overlaying the entire set of degrees of freedom in the higher-order scheme. AMG is applied to the operator based on the bilinear finite element discretization and is used as a preconditioner in a conjugate gradient (CG) iteration to solve the algebraic system derived from the high-order discretization. This approach is also nearly independent of p. We present several numerical examples that support each method and discuss the computational advantages of the preconditioning implementation.

Multigrid for a segregated version of the poroelasticity system

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Poroelasticity has a wide range of applications in biology, filtration, tissue engineering and soil sciences. It represents a model for problems where an elastic porous solid is saturated by a viscous fluid. The poroelasticity equations were derived by Biot in 1941, studying the consolidation of soils. In this talk we will present an efficient solution method for the poroelasticity system. A staggered grid discretization is adopted from incompressible flow and modified for the poroelasticity system. Standard finite elements (or finite differences) do not lead to stable solutions without additional stabilization. The staggered grid discretization leads to a natural stable discretization. In contrast to our previous work, where we provided multigrid solvers for the whole system of poroelasticity equations, here we first split the system into scalar equations. This splitting can be interpreted as a segregated solution approach, similarly to pressure-correction methods in incompressible fluid flow simulation. In fact, we just reverse loops as compared to our previous work: The distributive smoothing method from now acts as the "outer loop" in the solution process. The method can also be seen as a form of preconditioning of the original poroelasticity system. Next to a right- we also present the left-preconditioned system and corresponding results. In the segregated framework we need to solve for scalar equations only, thus enabling the solution of three-dimensional problems on relatively fine grids. Highly efficient multigrid schemes are used to solve the resulting scalar equations. Next to numerical experiments and analysis results we will present some theoretical convergence results for the approach adopted.

A Fully Coupled Implicit Method for A Magnetohydrodynamics Problem

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In this talk we discuss a parallel fully implicit Newton-Krylov-Schwarz algorithm for the numerical solution of the unsteady magnetic reconnection problem described by the system of the reduced magnetohydrodynamics (MHD) equations in two-dimensional space. In the MHD formalism plasma is treated as conducting fluid and behaves according to the fluid dynamics equations, coupled with the system of Maxwells equations. One of the intrinsic features of MHD is the formation of singular current density sheets, which is believed to be linked to the reconnecting of magnetic fields. A robust solver is required for handling the high nonlinearity associated with the simulation of magnetic reconnection phenomena. The near singular behavior of the solution of the system often limits the usable time step size required by explicit schemes thus making implicit methods potentially more attractive. We employ a stream function approach to enforce the divergence-free conditions on the magnetic and velocity fields, and solve the resulting fully coupled current-vorticity system of equations with a fully implicit time integration using Newton-Krylov techniques with an one-level additive Schwarz preconditioning. In this work we study the parallel convergence of the implicit algorithm and compare our results with those obtained by an explicit method.

The convergence of V-cycle multigrid algorithms for axisymmetric Laplace and Maxwell equations

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We investigate some simple finite element discretizations for the axisymmetric Laplace equation and the azimuthal component of the axisymmetric Maxwell equations as well as multigrid algorithms for these discretizations. Our main result is that the standard V-cycle with point smoothing converges at a rate independent of the number of unknowns. This is contrary to suggestions in the existing literature that line relaxations and semicoarsening are needed in multigrid algorithms to overcome difficulties caused by the singularities in axisymmetric problems. Our multigrid analysis proceeds by applying the well known regularity based multigrid theory. In order to apply this theory, we prove regularity results for the axisymmetric Laplace and Maxwell equations in certain weighted Sobolev spaces. These, together with some new finite element error estimates in certain weighted Sobolev norms, are the main ingredients of our analysis.

Space-Time Adaptive Finite Difference Method for European Multi-Asset Options

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We are interested in the numerical solution of the multi-dimensional Black-Scholes equation to determine the arbitrage free price $F(t, x)$ of an option. We will consider European call basket options on several underlying assets (e.g. stocks). This problem can e.g. be solved by finding a numerical solution to a multi-dimensional PDE. This way to determine the arbitrage free price was introduced independently by F. Black and M. Scholes (who gave name to the PDE) and R.C. Merton in 1973.

In a previous paper an adaptive finite difference method was developed with full control of the local discretization errors. The method was shown to be very efficient. In this paper we develop a space-time adaptive FD-method with control of the global error.

The Black-Scholes equation is discretized by second order accurate finite difference stencils on a Cartesian grid. An error equation is derived for the global error $E(t, x)$ in the solution. The driving right hand side in the error equation is the discretization error in the original PDE. This error is estimated a posteriori and the grid is adapted so that the Cartesian structure of the grid is maintained and the time step is adapted in every time step. The step sizes are chosen so that a linear functional of the solution error at maturity of the option satisfies an accuracy constraint. This means that the integral over the error, $E(x, t)$ times a function $g(x)$ is smaller than some positive constant.

The time step is adjusted to comply with the bound on the local error and the space grid is changed at a few pre-specified time points. The weights for the local error bounds in each time interval are solutions of the adjoint equation of the multidimensional Black-Scholes PDE. The growth of the error in the intervals between the grid adaptations is estimated a priori by the maximum principle for parabolic equations. In the same manner estimates of the solution of the adjoint equation is bounded.

The advantage with our procedure is that we obtain estimates of the numerical errors and we have an algorithm to choose the computational grid so that bounds like the functional explained above on the errors are satisfied also for multi-dimensional equations. For more dimensions than five (or so), the solution with finite difference approximations on a grid suffers severely from the 'curse of dimensionality' with an exponential growth in the number of grid points and other alternatives must be considered.

Performance of FAC Preconditioners for Multi-Material Equilibrium Radiation Diffusion on Adaptively Refined Grids

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Radiation transport plays an important role in numerous fields of study, including astrophysics, laser fusion, and combustion applications such as modeling of coal-fired power generation systems and wildfire spread. A diffusion approximation provides a reasonably accurate description of penetration of radiation from a hot source to a cold medium in materials with short mean free paths. This approximation features a nonlinear conduction coefficient that leads to formation of a sharply defined thermal front, or Marshak wave, in which the solution can vary several orders of magnitude over a very short distance. Resolving these localized features with adaptive mesh refinement (AMR) concentrates computational effort by increasing spatial resolution only locally. Previously we have demonstrated the effectiveness of combining AMR with implicit time integration to solve these highly nonlinear time-dependent problems. The key to this approach has been the use of effective multilevel preconditioners that exploit the hierarchical structure of AMR grids.

Our previous work used the Fast Adaptive Grid (FAC) method which is multiplicative in nature. While extremely robust FAC does impose sequential processing of levels in an AMR hierarchy. The additive variants of FAC, namely AFAC and AFACx, provide the opportunity to overlap communication and computation. However, little is known about their performance as preconditioners for difficult problems. We report on efforts to solve multimaterial equilibrium radiation diffusion problems using structured AMR and the Newton-Krylov method preconditioned by FAC, AFAC, or AFACx. We describe our FAC, AFAC, and AFACx solvers and report on their performance.

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Modeling Jaw and Teeth Mechanics

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To get a better understanding of forces acting on teeth and the temporo-mandibular joint (TMJ) during the mastication process, we are developing accurate finite element models for parts of the human musculo-skeletal system. While the ultimate goal is to obtain models guided by active electrical muscle activation, we focus in a first step on large displacement deformations of the muscles of mastication. The deformation of these muscles is dictated by their material properties and the movement of the mandible. A motion tracking system is used to track the movements of the mandible during a chewing cycle. This allows us to prescribe the displacements at the attachment points of the muscles to the bone.

Three dimensional high-order (cubic Hermite) elements are used to construct accurate meshes for the anatomically based geometries. Taking into account the complexity (and desired accuracy) of the geometry, the high-order discretizations, and the kinematics and kinetic of the mandible, it is clear that fast, efficient and accurate iterative solvers, such as an (algebraic) multigrid method, are inevitable. In this talk, we discuss the applications, introduce the model creation for bone, teeth, and muscles, and present first numerical results.

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A robust multigrid solver for the Euler-Lagrange equations with non-smooth coefficients

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Optical flow and non-rigid registration of medical data sets lead to a variational minimization problem that requires robust and efficient numerical solvers. Existing multigrid solvers for these problems depend highly on the smoothness of the given image data. Therefore the images are often smoothed before the computations. This can lead to difficulties, e.g., when one tries to detect the motion of very small objects. In order to handle non-smoothed image data we apply several multigrid techniques, such as Galerkin coarsening and matrix-dependent transfer operators. Further improvements can be obtained by developing suitable line-wise and block-smoothers. Our synthetic and real world results demonstrate that we can relax the restrictions on the smoothness of the image data without loosing the fast multigrid convergence rate. For high resolution 3D data it is necessary to parallelize the algorithms.

On the Use of Algebraic Multigrid inside a Non-Linear Finite Element Method for Maxillo-Facial Surgery Simulations

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In this paper we will present a computational tool chain for simulating the outcome of the ostheogenetic distraction process of a maxillo-facial surgery.

The main tool of this tool chain is a parallel Finite Element code for non-linear, viscoelastic elasticity (FEBiNA), that has been developed at the C+C Labs.

The Finite Element meshes used for this maxillo-facial surgery simulation are based on patient specific tomography data and their geometry is highly complicated. In addition to that the material parameters for bony structures, like skull and teeth, differ by several orders of magnitude from those for the soft tissues of the human head. Finally, the latter materials are nearly incompressible.

Due to those difficulties, the systems of linear equations that have to be solved during the simulation process are severely malconditioned. Our tests show that given our hardware environment, only multigrid methods can handle those systems within a reasonable solution time.

Nevertheless, the algebraic multigrid solvers we are using do not always show satisfying behavior. We will show some numerical experiments and point out the arising problems we encountered during the linear solution phase.

By doing so, we hope to nurture a fruitful discussion on the use of algebraic multigrid methods for these kinds of problems.

Fourier-mode analysis of a multigrid method for PDEs with random parameters

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We consider the numerical solution of elliptic and parabolic partial differential equations with stochastic coefficients. Such equations appear, e.g., in reliability problems. Various approaches exist for dealing with such 'uncertainty propagation' models: Monte Carlo methods, perturbation techniques, variance propagation, etc. Here, we deal with the stochastic finite element method (SFEM) [1]. This method transforms a system of PDEs with stochastic parameters into a stochastic linear system by means of a finite element Galerkin discretization. The stochastic solution vector of this system is approximated by a linear combination of deterministic vectors; the coefficients are orthogonal polynomials in the random variables. Unlike commonly used methods such as the perturbation method, the SFEM gives a result that contains all stochastic characteristics of the solution. It also improves Monte Carlo methods significantly because sampling can be done after solving the system of PDEs.

In order to solve the discretized stochastic system that appears in the SFEM, stochastic versions of iterative methods can be applied, and their convergence can be accelerated by implementing them in a multigrid context [2]. In the work we present here, the convergence properties of these stochastic iterative methods and multigrid methods are investigated theoretically: deterministic (local) Fourier-mode analysis techniques are extended to the stochastic case by taking the eigenstructure into account of a matrix that depends on the random structure of the problem. This is equivalent to choosing an alternative set of polynomial basis functions in the random variables, which results in a decoupling of the original stochastic problem into a very large number of deterministic problems of the same type. The theoretical convergence rates that we obtain predict the results of numerical experiments very well, and the results of the analysis can also be used to design optimal stochastic multigrid algorithms.

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Optimized Preconditioners for High-Order Finite-Elements

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Semi-implicit time discretization of the atmospheric primitive equations results in a modified Helmholtz equation for the pressure. Eigen-mode decomposition of the vertical structure matrix then gives rise to independent problems for each vertical coordinate level. Second-order finite differences are employed in the vertical and high-order finite-elements in the horizontal direction. The independent linear systems on each level are solved using Krylov iteration. Several preconditioning strategies are investigated. An optimized Schwarz method is compared to a new scheme related to the cell discretization algorithm of Greenstadt. The latter yields dramatically improved convergence rates and a reduction in computation time by eliminating communication in matrix-vector products. The link with penalty and discontinuous Galerkin methods for elliptic problems is established.

AMR for Turbulent Buoyant Plumes

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Numerical simulation of turbulent buoyancy driven plumes is characterized by two distinct length and time scales. Buoyancy induces large scale mixing of air and other species, forming a plume which can persist as an organized structure over large length scales. These large scale vortical structures have a puffing frequency that is inversely proportional to the square root of the length scales of these structures. The small scales tend to reduce the buoyant force by local mixing phenomena. Global refinement to capture the details at smaller length scales is not practical in many applications. Local mesh refinement provides an efficient alternative to global refinement. Motivation to simulate buoyant plumes and capture the salient flow features in the regions where small scale mixing occurs led us to develop a code with the capability of Adaptive Mesh Refinement (AMR). The coupled AMR, Large Eddy Simulation (LES) procedure allows us to capture the information at the scales of the large structures with a higher fidelity and also the details which require a sub grid scale LES model.

Our approach uses a filtered form for the variable density incompressible flow equations that conserves both mass and momentum. We use a collocated grid for our computations. The projection formulation used avoids any velocity pressure decoupling. The method is based on a projection formulation for momentum equations in which we first solve the advection diffusion equations to predict intermediate velocities. We then project the velocities after interpolating them on to the faces to enforce the continuity constraint. This projection method successfully handles “large density” variations of ten to one observed in buoyant plume applications. This approach is implemented in SAMRAI (Structured Adaptive Mesh Refinement Application Infrastructure), an AMR framework from Lawrence Livermore National Laboratory (LLNL) developed for structured hierarchical grids. For solving the pressure poisson equation on a composite mesh, we use Fast Adaptive Composite (FAC) solver in SAMRAI, which is a multilevel solver. The FAC solver interfaces with HYPRE [developed at LLNL] linear solvers on the coarsest level. The time integration algorithm is a recursive procedure for each level of refinement. For this study, the criteria used for grid refinement is the gradient of the mass fraction of a specie.

Verification and Validation of our method is done to assess its accuracy and reliability. Verification tests are carried out by using the analytical solutions for Eulers equation and Navier Stokes equations on a periodic box. These test examples demonstrate the accuracy and convergence properties of the algorithm. Validation of the code is carried out by demonstrating the performance of the method on a more relevant problem, in which a jet of light density fluid like Helium mixes in ambient air in the computational domain.

Analysis of a two-level time-parallel time-integration method for ordinary and partial differential equations

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During the last twenty years several algorithms have been suggested for solving time dependent problems parallel in time. In such algorithms parts of the solution later in time are approximated simultaneously to parts of the solution earlier in time. A very recent method was presented in 2001 by Lions, Maday and Turinici, who called their algorithm the parareal algorithm [1]. The name parareal was chosen for the iterative algorithm to indicate that it is well suited for parallel real time computations of evolution problems whose solution can not be obtained in real time using one processor only.

The method is not meant as a method to be used on a one processor computer. One iteration of the method costs already as much as the sequential solution of the entire problem, when used on one processor only. If however several processors are used, then the algorithm can lead to an approximate solution in less time than the time needed to compute the solution sequentially; hence parallel speedup is possible with the parareal algorithm.

The parareal algorithm has received a lot of attention over the past few years and extensive experiments have been done for fluid and structure problems [2,3,4]. In this talk, we will show that the parareal algorithm can be reformulated as a two-level space-time multigrid method with an aggressive semi-coarsening in the time-dimension. The method can also be seen as a multiple shooting method with a coarse grid Jacobian approximation. These equivalences have opened up new paths for the convergence analysis of the algorithm, which is the topic of the second part of this talk.

First, we will show a sharp linear, and a new superlinear convergence result for the parareal algorithm applied to ordinary differential equations. We then use Fourier analysis to derive convergence results for the parareal algorithm applied to partial differential equations. We show that the algorithm converges superlinearly on bounded time intervals, both for parabolic and hyperbolic problems. On long time intervals the algorithm converges linearly for parabolic PDEs. For hyperbolic problems however there is no such convergence estimate on long time intervals.

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Implicit Solution of High-Order Accurate Discontinuous Galerkin Discretizations of the Unsteady Wave Equation Using Spectral Multigrid

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The use of high-order accurate spatial discretizations for simulating steady and unsteady fluid flows has become more widespread over the last decade, For unsteady simulations using high-order spatial discretizations with a wide disparity between temporal and spatial scales, higher-order implicit time-integration approaches are desirable. However, such approaches require the efficient solution of a non-linear problem at each time-step in order to remain competitive. In this work, we investigate the use of spectral multigrid methods for driving implicit time-integration schemes of high-order discontinuous Galerkin discretizations, using the linear two-dimensional wave equation as a model problem.

The method of lines is employed, in which the wave equation is first discretized in space, resulting in a large set of coupled ordinary differential equations, which are then discretized and integrated in time. The Discontinuous Galerkin (DG) method represents a spatial discretization approach based on a finite-element method, which makes use of element based basis functions which are discontinuous across element interfaces [1]. In this approach, the computational domain is partitioned into an ensemble of non-overlapping elements and within each element the solution is approximately by a truncated polynomial expansion. The solution is thus determined by the modal coefficients of the expansion in terms of the basis functions within each element. Because the resulting solution representation is discontinuous across element interfaces, an upwind numerical flux function is used to resolve the discontinuity at element interfaces. The current implementation uses a set of hierarchical basis functions on triangles [2], enabling solutions from 1st order ($p = 0$), up to 4th order ($p = 3$) spatial accuracy.

In order to solve the time-dependent problem, the resulting spatially discretized equations must be integrated in time. Although explicit time-integration schemes have been widely used for DG discretizations, in this work we concentrate on the use of implicit time-integration schemes, which are not restricted by the stability limit of explicit methods, and are more suitable for stiff problems. The implicit time-integration schemes employed in this work range from first to fourth-order accurate in time, including both first and second order accurate multistep backward difference formulas(BDF1, BDF2) and a fourth-order accurate implicit multistage Runge-Kutta scheme. The use of implicit Runge-Kutta schemes represents an attempt to balance the spatial and temporal orders of accuracy. Moreover, even for second-order accurate finite-volume schemes, fourth-order implicit Runge-Kutta schemes have been found to outperform BDF2 schemes for engineering accuracy levels [3].

At each time-step, implicit time-integration methods require the solution of one or more non-linear problems. Efficient non-linear solvers are required for this task in order to result in an overall competitive approach. Our approach consists of using a spectral multigrid strategy [4,5] for solving the implicit system at each time step. The spectral or p-multigrid approach consists of a multigrid method where the coarser levels are constructed by reducing the order of accuracy (p-coarsening) while keeping the spatial grid resolution fixed (as opposed to h-coarsening). Thus, for a $p = 3$ (fourth-order accurate) spatial discretization, three coarser multigrid levels are employed, consisting of $p = 2$, $p = 1$, and $p = 0$ at the coarsest level. At each p-multigrid level, an

element-Jacobi scheme is used as a smoother. The element Jacobi smoother can be viewed as an approximate Newton method, where only the Jacobian entries corresponding to the modal coupling within an element are retained, and all other entries are discarded, resulting in a block diagonal matrix, which is easily inverted using Gaussian elimination at the block level. When used as a single grid solver, this smoother is shown to produce p-independent convergence rates, with strong h-dependence. When used as a smoother within the p-multigrid scheme, both h and p independent convergence rates are obtained.

In the paper, we show both p and h independent convergence rates for the implicit systems arising from the various time discretizations using the element Jacobi driven spectral multigrid solver. The overall efficiency and accuracy of the various time-integration schemes are compared by examining the error as a function of time for various time step sizes, where the design accuracy of the respective time-integration schemes is demonstrated. Further work will focus on extending this approach to the unsteady Euler and Navier-Stokes equations.

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Multilevel two-dimensional phase unwrapping

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Two-dimensional phase unwrapping is the problem of deducing unambiguous "phase" from values known only modulo 2π. Many authors agree that the objective of phase unwrapping should be to find a weighted minimum of the number of places where adjacent (discrete) phase values differ by more than π. This NP-hard problem is of considerable practical interest, largely due to its importance in interpreting data acquired with synthetic aperture radar (SAR) interferometry. Consequently, many heuristic algorithms have been proposed. In this talk we shall present a novel multi-level graph algorithm for the approximate solution of this problem via an equivalent problem: minimal residue cut in the dual graph.