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Contents

Abstract.
The recent research of the author and his collaborators on multiscale computational methods is reported, emphasizing main ideas and inter-relations between various fields, and listing the relevant bibliography. The reported areas include: top-efficiency multigrid methods in fluid dynamics; atmospheric data assimilation; PDE solvers on unbounded domains; wave/ray methods for highly indefinite equations; many-eigenfunction problems and ab-initio quantum chemistry; fast evaluation of integral transforms on adaptive grids; multigrid Dirac solvers; fast inverse-matrix and determinant updates; multiscale Monte-Carlo methods in statistical physics; molecular mechanics (including fast force summation, fast macromolecular energy minimization, Monte-Carlo methods at equilibrium and the combination of small-scale equilibrium with large-scale dynamics); image processing (edge detection and segmentation); and tomography.

Key words. scientific computation, multiscale, multi-resolution, multigrid, fluid dynamics, atmospheric flows, data assimilation, wave problems, Dirac equations, inverse matrix, Schrödinger operator, Monte-Carlo algorithms, critical slowing down, molecular mechanics, fast force summation, energy minimization, integro-differential equations, tomography, image processing, edge detection, segmentation.

AMS(MOS) subject classification. 34A50, 35A40, 44–04, 45–04, 65C05, 65F10, 65F15, 65F40, 65K10, 65M30, 65M50, 65M55,65N22, 65N25, 65N38, 65N55, 65R10, 65R20, 65Y05, 68U10, 70-08, 76-04, 76M20, 81-08, 81T80, 82-08, 82B80, 82C80, 92E99.

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Forward References.

Abstract. We establish an a-posteriori error estimate, with corresponding bounds, that is valid for any FOSLS L^2-minimization problem. Such estimates follow almost immediately from the FOSLS formulation, but they are usually difficult to establish for other methodologies. We present some numerical examples to support our theoretical results. We also establish a local a-priori lower error bound that is useful for indicating when refinement is necessary and for determining the initial grid. Finally, we obtain a sharp theoretical error estimate under certain assumptions on the refinement region and show how this provides the basis for an effective refinement strategy. The local a-priori lower error bound and the sharp theoretical error estimate both appear to be unique to the least-squares approach.

Key words. adaptive mesh refinement, a-posteriori error estimates, first-order system least-squares.

44   Experiences with negative norm least–square methods for the Navier–Stokes equations. *P. Bochev*

Abstract. This paper is concerned with the implementation and numerical study of a discrete negative norm least-squares method for the Navier-Stokes equations proposed in [2] and [3]. The main focus of the paper is on the algorithmic development and computational analysis of this method, including design of efficient preconditioners, numerical estimates of convergence rates, etc. Our experiments indicate that the negative norm method yields results that are in agreement with the theoretical error estimates of [3] and compare favorably with the benchmark studies of [11].

63   A multigrid algorithm for higher order finite elements on sparse grids. *Hans-Joachim Bungartz.*

Abstract. For most types of problems in numerical mathematics, efficient discretization techniques are of crucial importance. This holds for tasks like how to define sets of points to approximate, interpolate, or integrate certain classes of functions as accurate as possible as well as for the numerical solution of differential equations. Introduced by Zenger in 1990 and based on hierarchical tensor product approximation spaces, sparse grids have turned out to be a very efficient approach in order to improve the ratio of invested storage and computing time to the achieved accuracy for many problems in the areas mentioned above.
Concerning the sparse grid finite element discretization of elliptic partial differential equations, recently, the class of problems that can be tackled has been enlarged significantly. First, the tensor product approach led to the formulation of unidirectional algorithms which are essentially independent of the number d of dimensions. Second, techniques for the treatment of the general linear elliptic differential operator of second order have been developed, which, with the help of domain transformation, enable us to deal with more complicated geometries, too. Finally, the development of hierarchical polynomial bases of piecewise arbitrary degree p has opened the way to a further improvement of the order of approximation.
In this paper, we discuss the construction and the main properties of a class of hierarchical polynomial bases and present a symmetric and an asymmetric finite element method on sparse grids, using the hierarchical polynomial bases for both the approximation and the test spaces or for the approximation space only, resp., with standard piecewise multilinear hierarchical test functions. In both cases, the storage requirement at a grid point does not depend on the local polynomial degree p, and p and the resulting representations of the basis functions can be handled in an efficient and adaptive way. An advantage of the latter approach, however, is the fact that it allows

the straightforward implementation of a multigrid solver for the resulting system which is discussed, too.

78   The analysis of intergrid transfer operators and multigrid methods for nonconforming finite elements *Zhangxin Chen.*

Abstract. In this paper we first analyze intergrid transfer operators and their iterates for some nonconforming finite elements used for discretizations of second- and fourth-order elliptic problems. Then two classes of multigrid methods using these elements are considered. The first class is the usual one, which uses discrete equations on all levels which are defined by the same discretization, while the second one is based on the Galerkin approach where quadratic forms over coarse grids are constructed from the quadratic form on the finest grid and the iterates of intergrid transfer operators, which we call the Galerkin multigrid method. The properties of these intergrid transfer operators are utilized for the analysis of the first class, while the properties of their iterates are exploited for the second one. Convergence results available for these two classes of multigrid methods are summarized here.

97   Semicoarsening multgrid for systems. *J. E. Dendy.*

Abstract. Previously we examined the black box multigrid approach to systems of equations. The approach was a direct extension of the methodology used for scalar equations; that is, interpolation and residual weighting were operator induced, and coarsening employed a Galerkin strategy. The application was to standard coarsening of the unknowns. In this paper we consider a semicoarsening approach and find that there are a few differences in what is generally effective.

106   Multigrid algorithm for the non-aligned sonic flow. *Boris Diskin.*

Abstract. A multigrid approach using conditional coarsening in constructing solvers for non-elliptic equations on a rectangular grid is presented. Such an approach permits the achievement of a full multigrid efficiency even in the case where the equation characteristics do not align with the grid. The 2D sonic-flow equation linearized

over a constant velocity field has been chosen as the model problem. An efficient FMG solver for the problem is demonstrated.

Key words. multigrid methods, conditional coarsening, sonic flow, non-alignment.

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120   A comparison of multilevel adaptive methods for hurricane track prediction. *Scott R. Fulton.*

Abstract. Adaptive multilevel methods are described and tested for the problem of predicting the path of a moving hurricane. The physical model consists of conservation of vorticity in a two-dimensional incompressible fluid; the discrete model uses conservative second-order finite differences. The methods described are the Berger-Oliger (BO) algorithm, with the Poisson problem for the streamfunction solved by standard multigrid techniques, and a full approximation scheme multigrid (MG) algorithm which incorporates more complete interaction between the computational grids. Numerical results are presented demonstrating the conservation properties, convergence, accuracy, and efficiency of the methods. Adaptive mesh refinement produces speedup factors of 10–20 compared to using uniform resolution. Differences between the performance of the BO and MG methods are slight.

Key words. multigrid, multilevel, adaptive, incompressible, hurricane.

AMS(MOS) subject classification. 65M50, 65M55, 76C15, 86A10.

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Forward References.

133   Multigrid method for $H(\mathrm{div})$ in three dimensions *R. Hiptmair.*

Abstract. We are concerned with the design and analysis of a multigrid algorithm for $\mathbf{H}(\mathrm{div};\Omega)$–elliptic linear variational problems. The discretization is based on $\mathbf{H}(\mathrm{div};\Omega)$–conforming Raviart–Thomas elements. A thorough examination of the relevant bilinear form reveals that a separate treatment of vector fields in the kernel of the divergence operator and its complement is paramount. We exploit the representation of discrete solenoidal vector fields as **curl**s of finite element functions in so-called Nédélec spaces. It turns out that a combined nodal multilevel decomposition of both the Raviart–Thomas and Nédélec finite element spaces provides the foundation for a viable multigrid method. Its Gauß–Seidel smoother involves an extra stage where solenoidal error components are tackled. By means of elaborate duality techniques we can show the asymptotic optimality in the case of uniform refinement. Numerical experiments confirm that the typical multigrid efficiency is actually achieved for model problems.

Key words. multigrid, Raviart–Thomas finite elements, Nédélec's finite elements, multilevel, mixed finite elements.

AMS(MOS) subject classification. 65N55, 65N30.

Files. vol.6.1997/pp133-152.dir/pp133-152.ps; vol.6.1997/pp133-152.dir/pp133-152.pdf.

Forward References.

153   Asymptotic stability of a 9-Point multigrid algorithm for convection-diffusion equations. *Jules Kouatchou.*

Abstract. We consider the solution of the convection-diffusion equation in two dimensions by a compact high-order 9-point discretization formula combined with multigrid algorithm. We prove the ϵ-asymptotic stability of the coarse-grid operators. Two strategies are examined. A method to compute the asymptotic convergence is described and applied to the multigrid algorithm.

Key words. multigrid method, high-order discretization, asymptotic stability, convection-diffusion equation.

AMS(MOS) subject classification. 65F10, 65N06, 65N22, 65N55, 76D07.

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Forward References.

162   Wave-ray multigrid method for standing wave equations. *A. Brandt and I. Livshits.*

Abstract. Multigrid methods are known for their high efficiency in the solution of definite elliptic problems. However, difficulties that appear in highly indefinite problems, such as standing wave equations, cause a total loss of efficiency in the standard multigrid solver. The aim of this paper is to isolate these difficulties, analyze them, suggest how to deal with them, and then test the suggestions with numerical experiments. The modified multigrid methods introduced here exhibit the same high convergence rates as usually obtained for definite elliptic problems, for nearly the same cost. They also yield a very efficient treatment of the radiation boundary conditions.

Key words. Helmholtz equations, multigrid methods, wave-ray approach, radiation boundary conditions.

AMS(MOS) subject classification. 65N55, 65N06, 65N22, 65B99.

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182   Directional coarsening and smoothing for anisotropic Navier-Stokes problems. *Dimitri J. Mavriplis.*

Abstract. Unstructured multigrid techniques for relieving the stiffness associated with high-Reynolds number viscous flow simulations on extremely stretched grids are investigated. One approach consists of employing a semi-coarsening or directional-coarsening technique, based on the directions of strong coupling within the mesh, in order to construct more optimal coarse grid levels. An alternate approach is developed which employs directional implicit smoothing with regular fully coarsened multigrid levels. The directional implicit smoothing is obtained by constructing implicit lines in the unstructured mesh based on the directions of strong coupling. Both approaches yield large increases in convergence rates over the traditional explicit full-coarsening multigrid algorithm. However, maximum benefits are achieved by combining the two approaches in a coupled manner into a single algorithm. An order of magnitude increase in convergence rate over the traditional explicit full-coarsening algorithm is demonstrated, and convergence rates for high-Reynolds number viscous flows which are independent of the grid aspect ratio are obtained.

Forward References.

198 A two-level discretization method for the stationary MHD equations. *W. J. Layton, A. J. Meir, and P. G. Schmidt.*

Abstract. We describe and analyze a two-level finite-element method for discretizing the equations of stationary, viscous, incompressible magnetohydrodynamics (or MHD). These equations, which model the flow of electrically conducting fluids in the presence of electromagnetic fields, arise in plasma physics and liquid-metal technology as well as in geophysics and astronomy. We treat the equations under physically realistic ("nonideal") boundary conditions that account for the electromagnetic interaction of the fluid with the surrounding media.
The suggested algorithm involves solving a small, nonlinear problem on a coarse mesh and then one large, linear problem on a fine mesh. We prove well-posedness of the algorithm and optimal error estimates under a small-data assumption.

Forward References.

211 A stable multigrid strategy for convection-diffusion using high order compact discretization. *Anand L. Pardhanani, William F. Spotz, and Graham F. Carey.*

Abstract. Multigrid schemes based on high order compact discretization are developed for convection-diffusion problems. These multigrid schemes circumvent numerical oscillations and instability, while also yielding higher accuracy. These instabilities are typically exacerbated by the coarser grids in multigrid calculations. Our approach incorporates a 4th order compact formulation for the discretization, while also constructing a consistent multigrid restriction scheme to preserve the accuracy of the fine-to-coarse grid projections. Numerical results demonstrating the higher accuracy and robustness of this approach are presented for representative 2D convection-diffusion problems. These calculations also confirm that our numerical algorithms exhibit the typical multigrid efficiency and mesh-independent convergence properties.

Forward References.

224 A parallel multigrid method using the full domain partition. *William F. Mitchell.*

Abstract. The combination of adaptive refinement, multigrid and parallel computing for solving partial differential equations is considered. In the full domain

partition approach, each processor contains a partition of the grid plus the minimum number of additional coarse elements required to cover the whole domain. A parallel multigrid algorithm using the full domain partition is presented. Multigrid rates of convergence have been observed while communicating between processors only twice per V-cycle. Numerical computations on a network of up to 32 workstations show that parallel efficiency rates of 50% to 90% can be obtained.

Key words. grid partitioning, multigrid, parallel algorithms.

AMS(MOS) subject classification. 65N30, 65N55, 65Y05, 65N50.

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Forward References.

234   A multigrid smoother for high Reynolds number flows. *Erik Sterner.*

Abstract. The linearized Navier–Stokes equations are solved in two space dimensions using a multigrid method where a semi-implicit Runge–Kutta scheme is the smoother. Explicit time-integration in the streamwise direction is combined with implicit integration in the body-normal direction. Thereby the stiffness of the equations due to the disparate scales in the boundary layer is removed. Reynolds number independent convergence is demonstrated in analysis as well as in numerical experiments.

Key words. Navier-Stokes equations, semi-implicit, multigrid, convergence acceleration.

AMS(MOS) subject classification. 65L06, 65M12, 76N20.

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Forward References.

246   Fast solution of MSC/NASTRAN sparse matrix problems using a multilevel approach. *C.-A. Thole, S. Mayer.*

Abstract. As part of the European Esprit project EUROPORT, 38 commercial and industrial simulation codes were parallelized for distributed memory architectures. During the project, sparse matrix solvers turned out to be a major obstacle for high scalability of the parallel version of several codes. The European Commission therefore launched the PARASOL project to develop fast parallel direct solvers and to test parallel iterative solvers on their applicability and robustness in an industrial framework.

This paper presents initial results using a special multilevel method as preconditioner for matrices resulting from MSC/NASTRAN linear static analysis of solid structures. P-elements in MSC/NASTRAN allow the polynomial degree of the base functions to be specified either globally or for each element. Solution dependent adaptive "refinement" of the p-level can be selected. Discretisations with lower p-level can therefore be used as coarser grids for a multilevel method.

Tests have been performed using such a method as preconditioner for a regular cube and a complicated industrial part, which were modelled by tetrahedrons and hexagonal elements. Preliminary performance comparisons on small test cases (about 10000 degrees of freedom) indicate that the multilevel approach is at least as fast as the currently available fastest iterative MSC/NASTRAN solver. Substantial performance improvements are expected for full-size industrial problems.

255 A comparison of multilevel methods for total variation regularization. *P.S. Vassilevski andJ.G. Wade* .

Abstract. We consider numerical methods for solving problems involving total variation (TV) regularization for semidefinite quadratic minimization problems $\min_u \|\mathcal{K}u - z\|_2^2$ arising from illposed inverse problems. Here $\mathcal{K}$ is a compact linear operator, and z is data containing inexact or partial information about the "true" u. TV regularization entails adding to the objective function a penalty term which is a scalar multiple of the total variation of u; this term formally appears as (a scalar times) the L^1 norm of the gradient of u. The advantage of this regularization is that it improves the conditioning of the optimization problem while *not penalizing discontinuities* in the reconstructed image. This approach has enjoyed significant success in image denoising and deblurring, laser interferometry, electrical tomography, and estimation of permeabilities in porus media flow models.
The Euler equation for the regularized objective functional is a quasilinear elliptic equation of the form $\left[\mathcal{K}^*\mathcal{K} + A(u)\right]u = -\mathcal{K}^*z$. Here, $A(u)$ is a standard self-adjoint second order elliptic operator in which the coefficient κ depends on u, by $[\kappa(u)](x) = 1/|\nabla u(x)|$. Following the literature, we approach the Euler equation by means of fixed point iterations, resulting in a sequence of linear subproblems.
In this paper we present results from numerical experiments in which we use the preconditioned conjugate gradient method on the linear subproblems, with various multilevel iterative methods used as preconditioners.

271 Krylov subspace acceleration for nonlinear multigrid schemes. *T. Washio and C. W. Oosterlee.*

Abstract. In this paper we present a Krylov acceleration technique for nonlinear PDEs. As a 'preconditioner' we use nonlinear multigrid schemes such as the Full Approximation Scheme (FAS) [1]. The benefits of nonlinear multigrid used in combination with the new accelerator are illustrated by difficult nonlinear elliptic scalar problems, such as the Bratu problem, and for systems of nonlinear equations, such as the Navier-Stokes equations.