Principles of Systematic Upscaling (SU)

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Abstract:

Partly motivated by algebraic multigrid and renormalization group methods, systematic multiscale procedures are described for solving or simulating very large systems, with computations at each fine scale being confined to just small parts of the entire domain. Applicable to nonlinear, deterministic or stochastic, autonomous systems with strong interscale interactions. Examples from molecular dynamics to turbulent flows.

Analysis and Convergent Adaptive Solution of the Einstein Constraint Equations

Professor Michael Holst
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Abstract:

There is currently tremendous interest in geometric PDE, due in part to the geometric flow program used recently to solve the Poincare conjecture. Geometric PDE also play an expanding role in many other applications, such as understanding the gravitational wave models of Einstein. The need to validate these models has led to the construction of gravitational wave detectors in the last several years, such as the NSF-funded LIGO project. In this lecture, we consider the coupled nonlinear elliptic constraints in the Einstein equations, a geometric flow which describes the propagation of gravitational waves generated by collisions of massive objects such as black holes. The constraint equations must be solved numerically to produce initial data for gravitational wave simulations, and to enforce the constraints during dynamical simulations. In the first part of the lecture, we consider a thirty-year-old open question involving existence of solutions to the constraint equations on space-like hyper-surfaces with arbitrarily prescribed mean extrinsic curvature, and we give a partial answer using a priori estimates and a new type of topological fixed-point argument.

In the second part of this lecture, we develop some adaptive numerical methods for which we can prove a number of useful results on convergence, optimality, and scalability. Based on the a priori estimates developed in the first part of the talk, we first establish some critical discrete estimates. We then derive error estimates for Galerkin approximations, and describe a class of nonlinear approximation algorithms based on adaptive finite element methods (AFEM). We establish some new AFEM convergence and optimality results for geometric PDE problems with non-monotone nonlinearities such as the Einstein constraints. We then describe an overlapping domain decomposition algorithm based on the chart structure of the underlying domain manifold, and we outline a framework for establishing convergence of the algorithm.

We finish by illustrating the algorithms with some examples using the Finite Element ToolKit (FETK).

Adaptive Multilevel Primal-Dual Interior-Point Methods in PDE Constrained Optimization

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Abstract:

We are concerned with structural optimization problems in CFD, life and material sciences where the state variables are supposed to satisfy a linear or nonlinear PDE and the design variables are subject to bilateral pointwise constraints. Within a primal-dual setting, we suggest an all-at-once approach based on interior-point methods. Coupling the inequality constraints by logarithmic barrier functions involving a barrier parameter and the PDE by Lagrange multipliers, the KKT conditions for the resulting saddle point problem represent a parameter dependent nonlinear system. The efficient numerical solution relies on multilevel path-following predictor-corrector techniques with an adaptive choice of the continuation parameter where the discretization is taken care of by finite elements with respect to nested hierarchies of simplicial triangulations of the computational domain. In particular, the predictor is a nested iteration type tangent continuation, whereas the corrector is a multilevel inexact Newton method featuring transforming null space iterations. We also discuss the application of model reduction techniques based on a decomposition of the computational domain.

As applications, we consider optimal shape designs of microfluidic biochips, electrorheological shock absorbers, and microstructured biomorphic ceramics.

Domain decomposition and electronic structure calculations: a new approach

Claude Le Bris

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Abstract:

Electronic structure calculations are a well known challenging problem of computational chemistry. Such calculations consist in nonlinear eigenvalue problems of large size, which have several specificities in comparison with other eigenvalue problems arising in other engineering sciences. The talk will first introduce the context, and point out the peculiarities of the problem under consideration. Then, a recently developed approach, based on the domain decomposition paradigm, will be presented.

The talk is based upon joint works with Maxime Barrault, Guy Bencteux (Electricite de France), Eric Cances (ENPC-INRIA) and William Hager (University of Florida). References include:

*Journal of Computational Physics, Volume 222, March 2007, pp~86-109,
*Parallel Computing, to appear,
*SIAM Numerical Analysis, submitted, http://hal.inria.fr/inria-00169080/

From Domain Decomposition to Homogeneisation in the Numerical Modelling of Materials

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Abstract:

Problems where there is a significant separation of scales between the global macroscopic problem and the local heterogeneities governing the response of the constitutive materials. They are based on the notion of representative volume elements (RVE), which are microscopic samples of the system under study. Each sample is solved at a microscopic scale taking as boundary conditions uniform or periodic displacement data deduced from the solution observed at macroscopic scale.

The talk will review some of these techniques and explain how to adapt mortar elements techniques as introduced in domain decomposition techniques to the construction of aposteriori error estimates in numerical homogeneization. The domain decomposition strategies turn out also to be useful for developing several approximate strategies for the numerical solution or the iterative coupling of the microscopic problems.

Variational scale separation methods

Jan Martin Nordbotten
University of Bergen and Princeton

Abstract:

Many applications in the physical sciences require a detailed understanding of the interaction of processes on multiple scales. This has led to the development of countless analytical and numerical approaches, varying in generality and robustness. In this talk, we discuss and extend of some of the methods for dealing with multiple scales, seen from the context of potential driven conservation equations. These equations are relevant in modeling of e.g. heat transfer and stress-strain calculations for elastic materials; however, we will focus on the application to flow in porous media.

We will pay particular attention to the so-called multi-scale mixed finite elements, the mortar mixed finite elements, variational sub-grid upscaling, and their relationship to numerical linear algebra schemes such as balancing domain decomposition applied to the finest scale. This allows us to highlight desirable properties of the different methods, and ask the question: Can the best of these methods be combined?

We present an extension of the variational sub-grid upscaling method, which provides a general framework within which we discuss the remaining methods. While the development is given for the continuous problem, we nevertheless are able to construct a family of discrete multi-scale methods, within which existing methods appear as special cases.

We conclude the talk by comparing some of the discussed methods on example problems, in particular focusing on compressible two-phase flow in porous media. We address questions of accuracy, adaptivity, multiple scales, and computational cost.

Plane wave discontinuous Galerkin methods

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Abstract:

The oscillatory behavior of solutions to time harmonic wave problems, along with numerical dispersion, renders standard finite element methods inefficient already in medium-frequency regimes. As an alternative, several ways to incorporate information from the equation into the discretization spaces have been proposed in the literature, giving rise to methods based on shape functions which are solutions to either the primal or the dual problem, among them the so-called "ultra weak variational formulation" (UWVF) introduced by Despres for the Helmholtz equation in the early 1990's.
The UWVF is based on a domain decomposition approach and on the use of discontinuous piecewise plane wave basis functions. This method, which was numerically proved to be effective, has received a new interest very recently (see, e.g., papers by Huttunen, Kaipio, Malinen and Monk). From a theoretical point of view, the UWVF has been analyzed by Cessenat and Despres in 1998: they proved that the discrete solutions converge to the impedance trace of the analytical solution on the domain boundary. On the other hand, numerical results showed that convergence is achieved not only at the boundary, but in the whole domain.

In this talk, a priori convergence estimates in L2 and energy norms for the h-version of UWVF will be presented. The analysis is based on recasting the UWVF in the discontinuous Galerkin framework (a similar approach has been used very recently by Buffa and Monk for the derivation of L2 norm error estimates), and on new inverse and approximation estimates for plane waves in two dimensions, used in the context of duality techniques. Asymptotic optimality of the method in a mesh dependent energy norm and in the L2 norm are established. However, these estimates require a minimal resolution of the mesh to resolve the wavelength. Numerical evidence shows that this requirement which reflects the presence of numerical dispersion, cannot be dispensed with.

These results have been obtained in a joint work with Claude Gittelson and Ralf Hiptmair, Seminar for Applied Mathematics, ETH Zurich.

Numerical Zoom for Multi-Scale Problems

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Abstract:

The safety assessment of a nuclear waste repository underground in a clay layer is by nature a multiscale problem for which, in principle it is not possible to obtain a numerical solution without extensive computer resources [3].

However if the solution is needed only in some small restricted region of space then a multiscale decomposition is possible which, when combine with a numerical zoom or domain decomposition, allows optimal precision with much less computer memory and cpu time.

The domain is decomposed into a large one where the simulations may not be precise and a small one where precision is required and the process can be iterated. A similar approach has been used before in Steger's Chimera method [5]. In Brezzi et al [1] it was shown to be a particular implementation of Schwarz' method and of Lions' Hilbert space decomposition method [4]. Error estimates in the context of numerical zoom have been obtained by Wagner et al[6] and we will present here a better version for convergence of the iterative algorithm.

References:
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[4] Lions, J.L., Pironneau, O. (1999): Domain decomposition methods for CAD. C.R.A.S., 328 73-80
[5] Steger J.L. (1991): The Chimera method of flow simulation. Workshop on applied CFD, Univ. of Tennessee Space Institute
[6] Wagner J. : FEM with Patches and Appl. Thesis 3478, EPFL, March 2006.

Domain Decomposition methods: industrial experience at Hutchinson

François-Xavier Roux
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Abstract:

In this presentation the unique experience of industrial utilisation of the FETI methods at Hutchinson will be presented. In fact, after the theoretical basis of the method was established at the end of the eighties, an industrialisation, i.e. integration in a real finite element code was done in the framework of several European projects. In this very early stage of the development, the method was adopted by Hutchinson SA for its numerical simulation activities. Hutchinson is a world leader in manufacturing of rubber products for automotive, aerospace and other industries. Design of sophisticated components requires complex nonlinear simulations involving very large and ill conditioned models. In the middle of the nineties, the computer hardware available for Hutchinson was unable to tackle the models neither in term of speed, nor of storage. The only solution was to switch to a distributed computing environment, making the domain decomposition approach conjugated with clusters of PC as a good candidate for a breaking technology solution. Since then, the FETI method has proven itself as an extremely efficient simulation tool in real industrial environment. Currently, dozens of parallel jobs are run on a daily basis at Hutchinson Research Center and in several Hutchinson Departments. Static and dynamic rigidity, stress distribution in time or frequency domain, and other engineering quantities are computed for advanced metal-rubber components subject to large deformations and complex boundary conditions, such as contact with friction. Today, Hutchinson in-house finite element code contains several variants of one- and two-Lagrange Multiplier FETI solvers. During the presentation, several real industrial applications will be shown; problems of usage in industrial environment will be analyzed, and perspectives for both usage and code development will be outlined.

The balancing domain decomposition methods by constraints (BDDC)

Professor Xuemin TU
University of California, Berkeley

Abstract:

The balancing domain decomposition methods by constraints (BDDC) are non overlapping iterative substructuring domain decomposition methods for the solution of large sparse linear algebraic systems arising from the discretization of elliptic boundary value problems.

In this talk, the BDDC algorithms will be presented to solve a class of symmetric indefinite system of linear equations, which arises from the finite element discretization of the Helmholtz equation of time-harmonic wave propagation in a bound interior domain.

The proposed BDDC algorithm is closely related to the dual-primal finite element tearing and interconnecting algorithm for solving Helmholtz equations (FETI-DPH). The BDDC algorithms will also be presented to solve a class of non symmetric, positive definite linear systems resulting from the finite element discretization of advection-diffusion equations. In addition to the standard ubdomain vertex and edge/face average continuity constraints, certain flux average constraints across the subdomain interface, which depend on the coefficient of the first order term of the problems, will be introduced to improve the convergence.

The convergence rate estimate for the BDDC preconditioned GMRES iterations will be established and some numerical experiments will be discussed for both cases.

This talk is based on a joint work with Professor Jing Li at Kent State University, U.S.A.

Accomodating Irregular Subdomains in Domain Decomposition Theory

Olof Widlund

Abstract:

In the theory for domain decomposition methods, we have previously often assumed that each subdomain is the union of a small set of coarse shape-regular triangles or tetrahedra. In this study, we discuss recent progress which makes it possible to analyze cases with irregular subdomains such as those provided by mesh partitioners

Our goal is to extend our analytic tools to problems on subdomains that might not even be Lipschitz and to characterize the rates of convergence of our methods in terms of a few, easy to understand, geometric parameters of the subregions. For two dimensions, we have already obtained some best possible results for scalar elliptic and linear elasticity problems: the subdomains should be John or Jones domains and the rate of convergence is determined using the parameters that define such domains and that of an isoparametric inequality. Progress on three dimensions will also be reported.

New results have also recently been obtained concerning variants of classical two-level additive Schwarz preconditioners. Our family of overlapping Schwarz methods borrows and extends coarse spaces from older iterative substructuring methods, i.e., methods based on non-overlapping subdomains. The local components of these preconditioners, on the other hand ,are based on Dirichlet problems defined on a set of overlapping subdomains which cover the original domain.

Our methods are robust even in the presence of large changes ,between subdomains ,of the materials being modeled in the finite element models. An extra attraction is that our methods can be applied directly to problems where the stiffness matrix is available only in its fully assembled form .

We will also discuss several applications of the new tools.
They include new results on almost incompressible elasticity and mixed finite elementsusing spaces of discontinuous pressures. We will also touch on recent work on Maxwell's equations in two dimensions.

Our work has been carried out in close collaboration with Clark R. Dohrmann of theSandia National Laboratories, Albuquerque, NM and Axel Klawonn and Oliver Rheinbach of the University of Duisburg-Essen, Germany.

Robust Iterative Methods for Singular and Nearly Singular Systems of Equations

Professor Jinchao XU

Penn. State University.

Abstract:

After giving a basic criterion for designing robust iterative methods (including multigrid and domain decomposition methods) based on space decomposition and subspace corrections, I will report a number of recent results on singular and nearly singular algebraic systems arising from the discretization of various (parameter- dependent) partial differential equations including elliptic equations with strongly discontinuous jumps, Maxwell equations, nearly incompressible linear elasticity, Stokes equations, Darcy's law and coupling of Stokes and Darcy.