Mathematisches Forschungsinstitut Oberwolfach

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Miniworkshop: Least-Squares Finite Element Methods and Applications

June 23rd – June 29th, 2002

This Oberwolfach workshop showed the surprisingly diverse topics currently covered under the common theme of least-squares finite element methods. The first phase of heavy activity in this class of methods actually dates back to the early 1980s. Sadly, one mathematician who was among the first to embrace least-squares finite element methods, George Fix, died before he could attend this workshop. He was deeply missed at the workshop and mentioned almost constantly. Most of the groundwork for the recent gain in interest in least-squares finite element method was done in the 1990's, much of it by participants of this workshop. After this period of intense efforts to develop new least-squares variational formulations for different application problems, the field had reached a mature state.

The presentations given at this workshop were devoted to a new generation of research projects which rest upon the foundations laid in the last two decades. This includes new applications in electrical impedance tomography (Hugh McMillan), for hyperbolic equations (Thomas Manteuffel), engineering problems (Bo-nan Jiang) and to transmission problems in the coupling of finite elements and boundary elements (Ernst Stephan). Least-squares methods for optimization and control were described (Pavel Bochev and Max Gunzburger) as well as solvers especially tailored for nonlinear least-squares problems (Johannes Korsawe). A least-squares based minimal residual scheme was also presented (Ching-Lung Chung). Moreover, the combination of the wavelet methodology with least-squares finite element methods was discussed (Angela Kunoth). The proper treatment of systems with div-dominated or div-curl structure by the construction of appropriate finite element spaces was the subject of a number of talks (Travis Austin, Joe Pasciak, Gerhard Starke). Alternative approaches working with standard finite elements are the so-called discrete least-squares (Zhiqiang Cai) and FOSLL* (Jens Georg Schmidt) methods. The viewpoints about the relationship of these two approaches ranged from "the same" to "completely different". The truth lies somewhere in the middle.

Most importantly, due to the rather small schedule there was plenty of time for individual discussions during the week of the meeting. Also, the Friday was held completely free of talks in order to have a "round-table" discussion future trends and developments in this field. This discussions showed that the following two trends dominate current research on least-squares finite element methods. First, the least-squares finite element methodology seems to be well-suited to complicated systems, in particular, arising from coupled problems. This opens new application areas for these methods. The second focus is currently on the development of re-usable software for least-squares finite element computations.

Abstracts

An approximation technique for div-curl systems

JOE PASCIAK
(joint work with James H. Bramble)

In this talk, I will describe an approximation technique for div-curl systems based in $(L^2(D))^3$ where D is a domain in $\mathbb{R}^3$. Div-curl systems arise, for example, in electromagnetic applications. These systems are troublesome as they appear to be not elliptic and a crude counting indicates that there are more equations than unknowns. We formulate this problem as a general variational problem with different test and trial spaces. The analysis requires the verification of an appropriate inf-sup condition. This results is a very weak formulation where the solution space is $(L^2(D))^3$ and the data resides in various negative norm spaces. The advantages of setting up the problem in such a weak space will be discussed.

Subsequently, we consider finite element approximations based on this weak formulation. We present two possible approaches. The first involves the development of "stable pairs" of discrete test and trial spaces. With this approach, we enlarge the test space so that the discrete inf-sup condition holds and use a least-squares formulation to reduce to a uniquely solvable linear system. The second approach uses a smaller test space and adds terms to the form to stabilize the method. Both methods lead to optimal order estimates for problems with minimal regularity. This is important as it is easy to construct magnetostatic field applications whose solutions have low Sobolev regularity (e.g., $(H^s(D))^3$ with $0 < s < 1/2$).

Least-Squares Methods for Transmission Problem with FEM and BEM

ERNST P. STEPHAN
(joint work with Matthias Maischak)

We analyze a least squares formulation for the numerical solution of second order linear transmission problems in two and three dimensions, which allow jumps on the interface. The second order partial differential equation is rewritten as a first order system in a bounded domain, and the unbounded exterior domain is treated by means of boundary integral equations. The least squares functional is given in terms of negative order as well as half integer Sobolev norms, which are computed by using multilevel preconditioners for second order elliptic problems and for Symm's integral equation. As preconditioners we use both multigrid and BPX algorithms. The flux variable is discretized by using piecewise constant elements, continuous and piecewise linear elements, or Raviart-Thomas elements. The preconditioned system has bounded condition number. Numerical experiments for various combinations of different elements and preconditioners confirm our theoretical results.

FOSLL* for Irregular Boundaries

Jens G. Schmidt

The standard FOSLS approach reformulates an elliptic PDE as a first order system $LU = F$, which is solved in a least-square sense. From both the theoretical and the practical point of view it is of great advantage to use the L^2-norm and the standard H^1 finite element spaces. If the solution of the PDE is not smooth enough (i.e. $U \notin H^1$) these goals can not be met.

For a certain class of non smooth solutions, namely the ones arising from discontinuous coefficients, it is known that solving the dual problem $L^*W = U$ can overcome the above mentioned problems, mainly since $W \in H^1$ holds. This approach is called the FOSLL* method.

For irregular boundaries (e.g. reentrant corners) or irregular boundary conditions (e.g. some types of mixed Dirichlet and Neumann conditions) a straightforward application of FOSLL* may yield a solution W of the dual problem, which is not in H^1 as desired.

In this paper we describe an approach that overcomes this difficulty and therefore allows the use of standard finite element spaces in the discretization process. The efficiency of the improved FOSLL* method is illustrated by several numerical examples.

Robust Iterative Methods for Least-Squares Neutron Transport and Related Applications

Travis Austin

In this talk, we consider a second-order partial differential equation that is dominated by the grad-div operator. A variational form of this equation arises in the context of a formulation of the neutron transport equation using a scaled least-squares formulation. We present a discretization of the variational problem using a cubic-quadratic finite element space which leads to optimal error estimates and a setting for which an optimal multilevel preconditioner can be created. We then present numerical results for the multilevel algorithm. Lastly, we explain the relationship of this second-order equation to the displacement formulation of linear elasticity. Discretization results and multilevel convergence results are presented for linear elasticity using the same cubic-quadratic finite element space.

The Gauss-Newton Multilevel Method for Nonlinear Least-Squares Problems

Johannes Korsawe

This talk is about the solution of a first-order system least-squares ansatz for a nonlinear partial differential equation of second order. A standard way to solve such formulations is the discretization of the solution space H and the application of multilevel methods to the linear systems which arise from Newton-like approaches for the discretized nonlinear problems. In this talk, possibilities are studied to deduce exactness bounds in the solution of the finite-dimensional systems as well as refinement strategies for the discretization in order to ensure convergence at optimal cost. To this end, an overall convergence theory for the minimization of the nonlinear least-squares functional in H is deduced from the extension of inexact Newton methods in $\mathbb{R}^n$ (Eisenstat/Walker) to the infinite-dimensional case, which makes use of two decrease conditions to control the overall convergence. These conditions can be fulfilled by suitably damped descent directions, which can be calculated via the Gauss-Newton method applied to the least-squares functional. The errors from discretization and the only approximate solution of the linear systems then both contribute to the inexactness of the method. As a consequence of the surrounding convergence theory, exactness conditions for the control of the algebraical error and refinement conditions for the transition to the next level can be easily obtained. The application of this method to a realistic water infiltration problem shows the competitiveness of this approach to standard (heuristic) truncation settings.

Discrete First Order System Least-Squares: Second-Order Elliptic Boundary Value Problems

Zhiqiang Cai

An L^2-norm version of first-order system least squares (FOSLS) was developed by Cai, Manteuffel, and McCormick for scalar second-order elliptic partial differential equations in $d = 2$ or 3 dimensions. It was shown that the homogeneous FOSLS functional is equivalent to a $V \times H^1(\Omega)$ norm with $V = H(\mathrm{div}\,;\Omega) \cap H(\mathrm{curl}\, A;\Omega)$ under general assumptions, where A is the diffusion coefficient and Ω is the domain of the underlying problem. Moreover, such a norm was shown to be in fact an $H^1(\Omega)^{d+1}$ norm under the assumption that the original problem is H^2-regular. This product H^1 equivalence means that the minimization process amounts to solving a loosely coupled system of Poisson-like scalar equations. This in turn implies that standard finite element discretization and standard multigrid solution methods admit optimal H^1-like performance.

The limitation of this L^2-norm FOSLS is the requirement of sufficient smoothness of the underlying problem. Such smoothness guarantees the equivalence of norms between V and $H^1(\Omega)^d$ so that it can be approximated by standard continuous finite element spaces. In general, when the domain Ω is not smooth or not convex or the coefficient A is not continuous, these two spaces are not equivalent. In fact, V is equal to $H^1(\Omega)^d$ plus a finite dimensional space which consists of singular functions associated with corners of the boundary and interfaces. Therefore, standard continuous finite element spaces are not good approximation to V in general. In this paper, we will construct an appropriate approximation space for V based on the Helmholtz decomposition. Since our approximation space is discontinuous and is not contained in V, we then modify the FOSLS functional to accommodate such discontinuity and nonconformity of finite element spaces. Under general assumptions, we establish error estimates in the L^2 and H^1 norms for the vector and scalar variables, respectively. Such error estimates are optimal with respect to the required regularity of the solution. Preconditioner for the algebraic system arising from this approach is also considered.

A Direct Minimal Residual Method for the Numerical Solution of Differential Equations

Ching Lung Chang

Since the early 90's, research in numerical solution of partial differential equations yielded many excellent algorithms and error analysis studies for the linear and nonlinear equations by using the least-squares finite element methods. As a result, many problems can be solved much more effectively than before. However, currently it is still very time consuming to solve applied problems with large-scale, nonlinear partial differential equations. During the 1998 SIAM Annual Meeting in Toronto, Canada, several people in their talks estimated that it still requires a modern computer to run continuously for 20 to 60 years in order to solve the large-scale nonlinear Navier-Stokes equations by the least-squares finite element approach. Therefore we have to find a way to reduce the computer time we spend.

The main objective of this research is to study a class of residual-based minimization schemes, called the minimal residual methods, for the numerical solution of some kinds differential equations.

The idea is from the Least-squares FEM, which minimized the norm of $\|Lu - f\|$ if $Lu = f$ has unique solution associate with some boundary or initial conditions. After we generate the grid for the domain then we can define a set with finite element to approximate the solution with the characteristic h. If we also set the step of the coefficients $k = \lambda h$ and set the upper and lower bounds for the solution, then we have a finite number of numerical solution $\sum_{k=1}^{n} C_k \phi_k$. By such idea, to solve a linear or non-linear ODE or PDE have no essential difference of computer time consuming. A preliminary work has been done. we solve the ODE with the form $f(\frac{du}{dt}, u, t) = 0$. Also we solve Laplace PDE in a simple domain as well.

Least-Squares Finite Element Methods for Linear Hyperbolic PDEs

Thomas A. Manteuffel

(joint work with Luke Olson)

In this talk we will present a least-squares formulation of scalar, first-order, linear, hyperbolic equations. A least-squares functional will be presented and coercivity and continuity of the functional will be discussed. The functional includes a weak form of the boundary conditions. Then, a nonconforming functional will be described that involves terms penalizing jumps across cell edges not aligned with the flow. A uniform Poincaré inequality is established for the non-conforming functional. Numerical results on a simple test case with a discontinuous solution will be presented using elements from bi-linear through bi-quartic on quadrilateral grids and triangular grids. The results imply that higher-order elements produced faster convergence per degree of freedom. It will also be shown that the least squares solutions have minimal smearing of the discontinuity and minimal overshoot and oscillations. The nonconforming elements display similar behaviour, and thus, present no apparent advantage over conforming elements. Finally, solution techniques for the resulting linear systems will be discussed. Algebraic multilevel methods show great promise on this class of problems.

First Order System Least-Squares for Electrical Impedance Tomography

Hugh MacMillan

(joint work with Thomas A. Manteuffel)

Electrical impedance tomography (EIT) belongs to a family of imaging techniques that attempt to distinguish spatial variations in an internal electromagnetic parameter. The standard approach to EIT is output least squares (OLS). Given a set of applied normal boundary currents, one minimizes the defect between the measured and computed boundary voltages associated, respectively, with the exact impedance and its approximation. In minimizing a boundary functional, OLS implicitly imposes the governing Poisson equation as an optimization constraint. We introduce a new first-order system least squares (FOSLS) formulation that incorporates the elliptic PDE as an interior functional in a global minimization scheme. We then establish equivalence of our functional to OLS and to an existing least-squares interior functional due to Kohn and Vogelius. That the latter may be viewed as a FOSLL* formulation suggests FOSLS as a unifying framework for EIT.

The limited capacity for resolution in EIT, due to the necessarily finite set of inexact boundary data and the diffusive nature of current flow into the interior, traditionally leads to the conclusion that reconstructing the interior impedance is an ill-posed problem. EIT inherits this difficulty from the simplified inverse problem of reconstructing the electrical conductivity. Since quantifying the limited capacity is the focus of our theory, we begin with the static assumption and consider the reconstruction of conductivity, leaving that of the impedance as future work. We show that each functional in the FOSLS framework is equivalent to a natural norm on the error of the approximate conductivity. We analyze the topology induced by this norm to reveal the qualities of the exact conductivity that we should, in practise, expect to recover. Finally, we present preliminary numerical results for the FOSLS formulation and observe that they are faithful to our theory.

Our approach represents a significant departure from convention in that we do not rely on a generic regularization term. Rather, we accept and incorporate the underlying physics, albeit inhibiting. Problem-specific information, which otherwise might be used to "regularize" the "ill-posed" problem, can be included by either introducing an additional term to the functional or supplementing the space of admissible conductivity.

Wavelet Least-Squares Methods for Boundary Value Problems

Angela Kunoth

(joint work with Wolfgang Dahmen, Reinhold Schneider)

For the numerical solution of stationary operator equations, least squares methods will be considered. The primary focus is the combination of the following conceptual issues: the selection of appropriate least square functionals, their numerical evaluation in the context of wavelet methods and a natural way of preconditioning the resulting systems of linear equations.

First the problem is formulated in a general setting to bring out the essential driving mechanisms. Special cases that fit into this framework are a transmission problem that involves differential and integral operators, and saddle point problems where an elliptic partial differential equations is to be solved subject to side conditions.

One primary motivation has been the well-known fact that a major obstacle in the context of least squares methods based on finite element discretizations is the evaluation of certain norms such as the H^{-1}–norm. In this regard the fact that weighted sequence norms of wavelet coefficients are equivalent to relevant function norms arising in the least squares context are exploited. Truncating the (infinite) wavelet series appropriately leads to stable Galerkin schemes.

Some New Applications of the Least-Squares Finite Element Method

Bo-nan Jiang

It has become standard practise that different numerical schemes are employed for each type of differential equations. In this talk I will I show that without any special treatments by using only one formulation the LSFEM is able to simulate almost all kinds of problems in fluid dynamics and electromagnetics. New examples from solid mechanics and magnetohydrodynamics (MHD) will be given to support my opinion. The LSFEM is able to give simultaneous solutions for displacements, drilling rotation and stresses in elasticity including incompressible materials, and for deflection, slopes, moments and shear forces in plate bending with an optimal rate of convergence for all variables. Without the use of complicated flux-splitting for shock-capturing and an expensive Poisson solver for correcting magnetic field the simple LSFEM can capture shocks and complex flow patterns in compressible MHD.

Least-Squares Finite Element Methods for the Stress-Displacement Formulation of Elasticity

Gerhard Starke
(joint work with Zhiqiang Cai)

A least-squares finite element method for linear elasticity is developed. The least-squares functional is based on the stress-displacement formulation with the symmetry condition of the stress tensor imposed in the first-order system. Using the $H(\text{div})$-conforming Raviart-Thomas spaces for the stress components and nonconforming finite elements for the displacements, this method is shown to be optimal in the $H(\text{div})$ and the (broken) H^1 norm, respectively, uniformly in the incompressible limit. The local evaluation of the least-squares functional therefore represents an a posteriori error estimator. Computational results obtained with an adaptive refinement strategy based on this estimator are presented for a benchmark test problem. Moreover, the least-squares formulation is extended to geometrically nonlinear elasticity where a Gauss-Newton method is described for solving the nonlinear least-squares problems. Finally, an extension to a coupled problem associated with fluid flow in deformable porous media is presented.

Least-squares finite element methods for optimization and control problems for linear partial differential equations (Part 1)

Pavel Bochev
(joint work with Max Gunzburger)

For many years, optimization and control problems for systems governed by partial differential equations have been, in many applications, a subject of interest to experimentalists. For example, boundary layer control in fluid mechanics was studied by Prandtl as early as 1904. These problems also been a subject of theoretical interest and, for almost as long as computers have been around, of computational interest as well. Most of the efforts in the latter direction have employed elementary optimization strategies. For example, a popular "brute force" strategy has been, in problems for which one wishes to minimize a cost or performance functional, to evaluate that functional for several values of the control variables or design parameters and then to simply select those values which result in the smallest value for the functional.

More recently, mathematicians, scientists, and engineers have turned to the application of sophisticated optimization strategies for solving optimization and control problems for systems governed by partial differential equations. On the mathematical side, one may credit J.-L. Lions and D. Russell for helping popularize and foment such approaches. Today, many different local and global optimization strategies, e.g., Lagrange multiplier methods, sensitivity or adjoint-based gradient methods, quasi-Newton methods, evolutionary algorithms, etc., are in common use.

The problems that we will discuss fall into the class of *constrained optimization and control problems.* The four ingredients that a define a problem in this class are:

- a set of *state variables* which describe the physical system of interest;
- a set of *control variables or design paramaters* which are at our disposal in order to effect the optimization;
- a *cost, or performance, or objective functional* which depends on the state and/or control variables and whose minimization is the object of control; and
- a system of partial differential equations along with boundary and initial conditions which act as *constraints* that candidate state and control variables must satisfy.

Several popular approaches to solving such optimization and control problems for systems governed by partial differential equations are based, one way or another, on optimality systems deduced from the application of the Lagrange multiplier rule. This may not be surprising since the Lagrange multiplier rule is, of course, a standard approach to solving finite-dimensional optimization problems. Perhaps more surprising is that penalty methods, which are another popular approach for the latter setting, have not engendered anywhere near as much interest for the infinite-dimensional problems which are of interest here. In this talk, we will see why naively defined penalty methods may not be practical and, using methodologies associated with modern least-squares finite element methods, we will also see how practical penalty methods can be defined. Moreover, we will see how penalty methods offer certain efficiency-related advantages compared to methods based on the Lagrange multiplier rule.

Least-Squares finite element methods for optimization and control problems for linear partial differential equations (Part 2)

Max Gunzburger
(joint work with Pavel Bochev)

(same abstract as Part 1)

Edited by Gerhard Starke

Participants

Dr. Travis Austin
austint73@yahoo.com
Institut für Angewandte Mathematik
Universität Hannover
Welfengarten 1
D–30167 Hannover

Dr. Markus Berndt
berndt@lanl.gov
Los Alamos National Laboratory
Group T7
Mail Stop 284
Los Alamos, NM 87545 - USA

Prof. Dr. Pavel Bochev
pbboche@sandia.gov
Applied Mathematics Division
Sandia National Laboratories
Albuquerque, NM 87185 - USA

Prof. Dr. Zhiqiang Cai
zcai@math.purdue.edu
Dept. of Mathematics
Purdue University
West Lafayette, IN 47907-1395 - USA

Prof. Dr. Ching-Lung Chang
c.chang@csuohio.edu
Dept. of Mathematics
Cleveland State University
Cleveland, OH 44115 - USA

Prof. Dr. Max D. Gunzburger
gunzburg@iastate.edu
Dept. of Mathematics
Iowa State University
400 Carver Hall
Ames, IA 50011 - USA

Prof. Dr. Bo-nan Jiang
bnjiang@yahoo.com
Department of Mathematical Science
Oakland University
Rochester, MI 48309-4401 - USA

Dr. Johannes Korsawe
jkorsawe@ifam.uni-hannover.de
Institut für Angewandte Mathematik
Universität Hannover
Welfengarten 1
D–30167 Hannover

Prof. Dr. Angela Kunoth
kunoth@iam.uni-bonn.de
Institut für Angewandte Mathematik
Universität Bonn
Wegelerstr. 6
D–53115 Bonn

Dr. Hugh Macmillan
hmacmill@McCammon.ucsed.edu
Department of Chemistry and
Biochemistry, University of
California at San Diego
La Jolla CA 92093-0365 - USA

Prof. Dr. Tom A. Manteuffel
tmanteuf@boulder.colorado.edu
Program in Applied Mathematics
University of Colorado at Boulder
Campus Box 526
Boulder, CO 80309-0526 - USA

Prof. Dr. Seymour V. Parter
parter@cs.wisc.edu
Computer Sciences Department
University of Wisconsin-Madison
1210 West Dayton St.
Madison, WI 53706-1685 - USA

Prof. Dr. Joseph E.P. Pasciak
pasciak@math.tamu.edu
Department of Mathematics
Texas A & M University
College Station, TX 77843-3368 - USA

Dr. Jens Georg Schmidt
schorsch@colorado.edu
Dept. of Applied Mathematics
University of Colorado at Boulder
Campus Box 526
Boulder, CO 80309-0526 - USA

Prof. Dr. Gerhard Starke
starke@ifam.uni-hannover.de
Institut für Angewandte Mathematik
Universität Hannover
Postfach 6009
D–30060 Hannover

Prof. Dr. Ernst P. Stephan
stephan@ifa.uni-hannover.de
Institut für Angewandte Mathematik
Universität Hannover
Postfach 6009
D–30060 Hannover