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SOME RECENT TOPICS IN COMPUTATIONAL MATHEMATICS — FINITE ELEMENT METHODS

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Abstract. The objective of numerical analysis is to devise and analyze efficient algorithms or numerical methods for equations arising in mathematical modeling for science and engineering. In this article, we present some recent topics in computational mathematics, specially in the finite element method and overview the development of the mixed finite element method in the context of second order elliptic and parabolic problems. Multiscale methods such as MsFEM, HMM, and VMsM are included.

1. Introduction

The basic mathematical models of science and engineering often take the form of differential equations, typically expressing laws of physics such as conservation of mass or momentum enhanced with various constitutive relations between state variables and fluxes such as Hooke's law, Fourier's law, Stokes' law or Darcy's law, etc. By determining the solution of differential equations for given data, we may obtain desired information concerning the physical process being modeled. Exact solutions may sometimes be determined through symbolic computation by hand or using software, but in most cases this is not possible, and the alternative is to approximate solutions with numerical computations using a computer. Although massive computational effort is often needed, the cost of computation is rapidly decreasing and new possibilities are quickly being opened. The objective of numerical analysis is to devise

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and analyze efficient algorithms or numerical methods for equations of mathematical models.

In this note, we present some recent topics in numerical analysis, specially in the finite element method (FEM) and overview the development of the mixed finite element method in the context of second order elliptic and parabolic problems. In the end, we include interesting results of the survey conducted by I. Babuška [35]. We have made no attempt to list exhaustive topics in numerical analysis.

2. FEM and Mixed FEM

The theory of the finite element method has been developed during the last fifty years. The discovery of the FEM is usually attributed to R. Courant. Nevertheless, there are some older references to finite element-like methods [35]. The notion *element* was introduced in the 1950's by aerospace engineers performing elasticity computations. The notion *finite element* was introduced by mathematicians later, in the 1960's.

In principle, a finite element method can only be considered in relation with a variational principle and a function space in which it is posed. Each choice of these leads to a different finite element approximation. So far, a great deal of progress has been made in FEM software. The whole computational processes can be essentially automated including the following steps:

preprocessing of input data, generation of triangulations, assembling FE-matrices, solving discrete problems, postprocessing of output data, a posteriori error estimates, graphical illustration of results.

Nevertheless, many theoretical questions, related to the foundations of the method and being born by practical problems and their needs, are still open.

The mixed finite element method was designed to compute both the state variable and the flux simultaneously with comparable accuracy, be it directly or through post-processing. In many applications, it seems to yield better results than standard finite element methods when an accurate approximation for the flux variable is needed.

In 1974, Brezzi [7] published his celebrated paper providing a theoretical background for mixed finite element methods. His theory is based on two major assumptions, Z-ellipticity and the inf-sup condition, known as LBB condition.

In 1977, Raviart and Thomas [24] constructed, for the first time, a finite element space satisfying the discrete LBB condition through the construction of a projection, known as the Raviart-Thomas projection, to approximate the Dirichlet problem for the Laplacian operator in planar domain. The underlying Hilbert spaces are $\mathbf{V} = H(\,\mathrm{div}\,;\Omega)$, $W = L^2(\Omega)$. Their finite elements are conforming (requiring $\mathbf{V}_h \subset \mathbf{V}$, $W_h \subset W$). While the requirement $W_h \subset W$ does not represent any constraint, the inclusion $\mathbf{V}_h \subset \mathbf{V}$ implies some regularity on the elements of $\mathbf{V}_h$, more precisely, the normal components of vectors in $\mathbf{V}_h$ must be continuous across the interelement boundaries. Applying Brezzi's general theory, Raviart and Thomas obtained explicit error estimates. Then, in 1980, this Raviart-Thomas element was generalized and extended to the three-dimensional case by Nedelec [21]. There Nedelec also developed approximation spaces of $H(\,\mathrm{curl}\,;\Omega)$ and gave some application to Maxwell's equations and the equations of elasticity.

In 1980 Falk and Osborn [13] provided an abstract approach to the analysis of mixed methods for elliptic boundary value problems. They obtained quasi-optimal error estimates in the usual Sobolev norms.

Raviart-Thomas-Nedelec(RTN) elements received a considerable attention and provided a source for many applications. In 1981, Johnson and Thomée [16] studied mixed methods for second order elliptic and parabolic problems.

Douglas and Roberts in 1985 [10] gave global error estimates in $L^2(\Omega)$, $L^\infty(\Omega)$, and $H^{-s}(\Omega)$ for Dirichlet problems for the elliptic operator,

$$Lp = -\,\mathrm{div}\,(a\nabla p + \mathbf{b}p) + cp,$$

based on the RTN elements of index $k \geq 0$. However, their technique does not lead to an $L^\infty(\Omega)$-error bound for the vector unknown. Scholtz [27] derived an estimate in $L^\infty(\Omega)$ for $\mathbf{u} - \mathbf{u}_h$ which is optimal modulo a factor of $|log\, h|$ for $k \geq 1$.

In 1985, Milner in his thesis [19] extended Douglas' and Roberts' results [10] to

$$Lp = -\,\mathrm{div}\,(a(p)\nabla p + \mathbf{b}(p)) + c(p).$$

Kwon and Milner [18] have derived, for the whole range of indexes k in RTN, a quasi-optimal order estimate in $L^\infty(\Omega)$ for $\mathbf{u} - \mathbf{u}_h$ in the semi-linear case using weighted L^2-norms. Durán [11] derived, using the known properties of Ritz projection, sharp L^q-error estimates ($1 \leq q \leq \infty$) when $Lp = -\operatorname{div}(a(p)\nabla p)$.

In 1989, Gastaldi and Nochetto [14] derived sharp asymptotic $L^\infty(\Omega)$ error estimates for both the scalar and vector unknowns for linear second order elliptic problems in an abstract setting satisfying the commuting diagram property.

In 1995, Milner and Park [20] developed mixed methods for $Lp = -\operatorname{div}\mathbf{a}(\nabla p)$ and the minimal surface equation was treated as an application.

Park [22] in the same year extended the results to fully nonlinear elliptic problems in divergence form:

$$Lp = -\operatorname{div}\mathbf{a}(p, \nabla p) + b(p, \nabla p),$$

using RTN elements for $k \geq 1$. Newton's method was presented and analyzed to solve the nonlinear algebraic equations resulting from mixed finite element equations. Quadratic convergence of the algorithm was proved.

However, the lowest order case ($k = 0$) was not covered in the paper [22] and still remains open.

Fully nonlinear parabolic problems in divergence form are treated for the first time in [17] and applications to some flow problems in porous media are given in [23].

Many issues arise in actual implementation of the numerical methods. Standard fully discrete schemes for nonlinear second order time dependent problems would generate large, nonlinear systems of equations for each time level t^n. Since the different systems arise from an evolution process, the approximate solution at time level t^n will be a good initial guess for the nonlinear system produced at time level t^{n+1}. Clearly, the smaller we take the time steps, the better these initial guesses are. With good initial guesses, a Newton-Raphson linearization of the nonlinear systems will converge quadratically. We see our efficiency trade-off. The smaller the time steps the faster the Newton-convergence, but the larger the total number of nonlinear systems that must be solved to reach a specified time level.

The next point to note is that the construction of the Jacobian and its evaluation for each iteration is a very large and time-consuming process.

We are thus led to consideration of inexact or quasi-Newton linearizations which allow cheaper updates at the expense of possibly slower convergence rates. The study of partial or efficient updates for Newton-like methods is a major area of research interests [12].

In any of the linearization methods mentioned, a new large, symmetric/nonsymmetric linear system must be solved at each iteration and for each time step. The fill-in that would result from direct solutions of each linear system for large, three dimensional applications would swamp the computational effort. Therefore *iterative procedures* for these large symmetric/nonsymmetric systems must be considered.

Since this linear solution is a part of the Newton iteration, it is natural to consider how the choices of the tolerances for the linear, inner iteration and the Newton outer iteration can be chosen to minimize computational effort. Again the size of the time-step should also be considered since an even larger outer time loop is in operation. The optimal choice of a combination of time-step and iteration tolerances to minimize computational time is an important research topic.

Of course, the convergence rates for the iterative process described are heavily dependent upon the conditioning of the matrices involved. In general, the matrices arising from these partial differential equations are highly ill-conditioned with the condition number growing as the reciprocal of the square of the spatial discretization grid size. Therefore, efficient *preconditioners* are essential for these applications.

Recently, in [31] we studied mixed finite element approximation of reaction-diffusion equations. To linearize the mixed-method equations, we used a two-grid scheme that relegates all of the Newton-like iterations to grids much coarser than the original one, with no loss in order of accuracy. The use of a multigrid-based solver for the indefinite linear systems that arise at each iteration, as well as for the similar system that arises on the fine grid, allows for even greater efficiency.

We mention [8, 25] for general account of mixed FEM. See Ciarlet [9] for finite element methods for elliptic problems and the recent book by V. Thomée [29] for parabolic problems.

3. Some Recent Topics

In this section we mention only a few topics and start with a posteriori error estimate.

• A Posteriori Error Estimates: A priori error estimates have been an ingredient of finite element analysis from the outset, but a posteriori error estimates have really only emerged over the past decade to take their natural place alongside a priori estimates. A posteriori error estimators provide quantitative estimates for the actual error (as opposed to estimates for the rate of convergence) and give base on adaptive refinement strategy to optimize the computational work needed to reach a certain accuracy. In this direction, we cite the first monograph on the subject [30].

• Preconditioning: The convergence of a matrix iteration depends on the properties of the matrix– the eigenvalues, the singular values, or sometimes other information. The problem of interest can be transformed so that the properties of the matrix are improved drastically. This process of "preconditioning" is essential to most successful applications of iterative methods. We list a number of preconditioners: *Diagonal scaling or Jacobi, Incomplete Cholesky or LU factorization, Coarse-grid approximation (multigrid iteration), Local approximation, Block preconditioners and domain decomposition, Lower-order discretization, Constant-coefficient or symmetric approximation, Splitting of a multi-term operator, Dimensional splitting or ADI, One step of a classical iterative method, Periodic or convolution approximation, Unstable direct method, Polynomial preconditioners.* The reader is referred to [1, 26] for summaries of the current state of the art. See also [15, 28] for more topics in numerical linear algebra.

• Multiscale Methods: Multiscale modelling and computation is a rapidly evolving area of research in computational science and engineering such as material science, chemistry, fluid dynamics and biology. For example, natural porous media has extreme heterogeneity which requires multiscale modelling and computation.

Several different but related mathematical frameworks for multiscale computation have been proposed, including Multiscale finite element method (MsFEM) [48], Heterogeneous multiscale method (HMM) [43], and Variational multiscale method (VMS/VMM) [51].

In the classical finite element method there is a missing information in the numerical solution with the reasonable mesh size. The MsFEM is based on the construction of local basis which captures a fine scale nature. The MsFEM traces back to Babuska *et al* who defined the generalized FEM using non-polynomial basis functions in the one dimensional case [36] and extended to 2-D case in [35]. Recently, T. Hou et al [48] improved and proposed a multiscale finite element method. Main idea is an introduction of so called oversampling. In oversampling, one defines a basis function on a larger domain to capture more of fine scale nature such as heterogeneity. The resulting scheme is of non-conforming type since the basis functions do not piece together continuously at the interfaces. An error analysis has been given in [49]. Chen and Hou [41] extended this idea to mixed finite element method. Much progress has been made more recently. For example, monlinear problem, numerical homogenization, applications to parabolic problems and random media are vigorously studied [45, 46, 50, 57].

On the other hand, in 1995 and 1998, Hughes et al [51, 52] developed a variational multiscale formulation (VMsM). In 1999, Brezzi [40] independently developed a similar framework. VMsM provides a framework that allows formally scale separation from coarse scale and subgrid (fine grid). This kind of two scale seperation seems natural from a computational point of view since discetization introduces one scale. This idea has been successfully applied to convection-dominated diffusion equations and turbulent flow models [53]. Arbogast [33, 34] developed a VMsM in the context of mixed formulation.

The heterogeneous multiscale method (HMM) recently introduced by W. E and B. Engquist [43] draws a lot of attention. The HMM allows a general framework for efficient numerical computation of problems with multi-scales and multi-physics on multi-grids. The method relies on an efficient coupling between the macroscopic and microscopic models. In case the macroscopic model is not explicitly available or is invalid in part of the domain, the microscopic model is used to supply the necessary data for the macroscopic model. Applications of the method include homogenization, molecular dynamics, kinetic models and interfacial dynamics, among others. Error analysis has been given in [44]. Finite difference HMM is studied in [32].

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