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FINAL REPORT

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PARALLEL ALGORITHMS IN THE FINITE ELEMENT APPROXIMATION OF FLOW PROBLEMS

Submitted on May 29, 1988 by

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This is the final report for AFOSR Grant Number 83-0101. We discuss a portion of the research which has been carried out during the past few years under AFOSR sponsorship. This includes work on finite element methods for a Ladyzhenskaya model of viscous incompressible flow, hyperbolic partial differential equations, exterior problems, algebraic turbulence models, streamfunction-vorticity formulations of viscous flows and first order elliptic systems of partial differential equations, and on substructuring methods for the approximate solution of partial differential equations. For the sake of brevity, we will not go into great detail in this discussion. Further information concerning these topics can be gained from the appropriate references listed at the end of the report.

1 - Analysis and approximation of a Ladyzhenskaya model for viscous flow

The Navier-Stokes equations are the most commonly used mathematical model describing the motion of viscous incompressible fluids. Although this model is generally accepted and is even thought by many to be valid for turbulent flows, it does have some shortcomings. Of the latter, the most important one is that it is not known, nor is it believed, that three dimensional solutions are globally, in time, unique.

Among the other models proposed for viscous incompressible flows are some formulated by Ladyzhenskaya. Her models differ from the Navier-Stokes model only in the constitutive relations used. Whereas the Navier-Stokes equations are derived using a linear constitutive model, Ladyzhenskaya introduces nonlinear ones. One advantage shared by all of her models is that one can show,

in both two and three dimensions, that solutions are globally unique in time.

One particular set of Ladyzhenskaya equations is given by

$$\operatorname{div} u = 0$$

and

$$\frac{\partial u}{\partial t} - \operatorname{div} \left[A(u) \left(\operatorname{grad} u + (\operatorname{grad} u)^T \right) \right] + u \cdot \operatorname{grad} u + \operatorname{grad} p = f$$

over some domain Ω , where u is the velocity, p the pressure, f the given body force and

$$A(\nabla) = \gamma_0 + \gamma_1 |\nabla|^{r-2}, \quad r \geq 2.$$

The Navier-Stokes model corresponds to $\gamma_1=0$. Ladyzhenskaya herself has shown that these equations, with suitable boundary conditions, have a unique solution whenever $\gamma_1 > 0$. We have derived some new *a priori* inequalities for this model which we then use to show that solutions of the Ladyzhenskaya equations converge to those of the Navier-Stokes equations as $\gamma_1 \rightarrow 0$.

Ladyzhenskaya also showed that the stationary version of these equations possesses a solution for any value of the Reynolds number. However, she did not explore the uniqueness question with respect to the stationary equations. It is well known that one can show that the Navier-Stokes equations have a unique solution whenever

$$N \|f\|_{-1} / \gamma_0^2 \leq 1$$

where N is a constant such that

$$\int_{\Omega} \mathbf{w} \cdot \text{grad} u \cdot \nabla \leq M \|u\|_1 \|\nabla\|_1 \|\mathbf{w}\|_1 \quad \text{for all } u, v, \mathbf{w} \in H_0^1(\Omega) .$$

For the Ladyzhenskaya equations we have obtained an improved uniqueness condition in the sense that her equations can be shown to have a unique solution for "larger" values of the data \mathbf{f} . This result is of interest because usually the uniqueness condition for the Navier-Stokes equations is overly pessimistic, i.e., there are many known stationary flows which are uniquely determined for values of the Reynolds number for which the uniqueness condition is not valid. Thus our uniqueness condition for the Ladyzhenskaya equations is, from a physical point of view, less pessimistic than the one for the Navier-Stokes equations.

We have also studied finite element approximations of the Ladyzhenskaya model. We have shown that one may use the same finite element spaces for the velocity and pressure as are used for Navier-Stokes calculations. Furthermore, we have obtained error estimates for finite element approximations which are identical, with respect to rates of convergence, as those available for finite element approximations for the Navier-Stokes equations. This result remains valid even when one uses approximate quadrature rules in determining the discretized equations, in spite of the presence of the additional nonlinear viscous term. We have also investigated the performance of iterative methods for the solution of the discrete equations. For example, we have shown the local quadratic convergence of Newton's method.

A code has been written which implements a Taylor-Hood method for the Ladyzhenskaya model. The code demonstrates the theoretical results mentioned in the previous paragraph. In particular, it shows how existing Navier-Stokes codes can be amended in a trivial manner to handle the Ladyzhenskaya equations.

2 - Finite element methods for the streamfunction-vorticity equations

An extensive study of finite element methods for the streamfunction-vorticity formulation of viscous incompressible flows has been completed. We have developed algorithms which can account for various type of boundary conditions encountered in practical situations. These include boundary conditions which may be used at inflows, outflows, solid walls and to match with inviscid flows. The basis for the algorithms is a particular Galerkin weak formulation. The resulting finite element algorithms are of a considerably greater generality than existing methods, including those based on finite difference discretizations. We also note that the algorithms which we have developed do not require the imposition of artificial boundary conditions on the vorticity at solid walls.

Likewise, we have investigated, in a systematic and rigorous manner, the treatment of multiply connected domains. Our methodology does not suffer from the usual *ad hoc* decisions necessary in finite difference methods. The difficulty here is, of course, that the streamfunction-vorticity equations admit many solutions, and therefore auxiliary conditions, i.e., the continuity of the pressure, must be enforced in order to extract the correct physical solution. We have considered two different classes of methods for handling multiply connected domains. The first class enforces the required auxiliary conditions in a direct manner, i.e., the finite element spaces are chosen so that this requirement is satisfied automatically. This technique leads to certain inefficiencies in the solution of the discrete system. Therefore, we have developed and analyzed a second type of method wherein a sequence of problems similar to simply connected domain discretizations (insofar as their

complexity is concerned) is solved. Analytical and numerical comparisons of the two approaches have been carried out, showing, for the most part, the superiority of the second approach.

Once the streamfunction and vorticity have been determined, the recovery of the primitive variables, especially the pressure, is often carried out using some dubious assumptions, e.g., applying the normal momentum equation at the boundary. We have developed and rigorously analyzed a method for obtaining the pressure which requires no such assumptions. The method is based on well known algorithms for the finite element approximation of the primitive variable formulation. We show how one should choose the pressure approximating spaces according to the choices made for the streamfunction and vorticity spaces, and with such a proper choice, that the pressure can be approximated as well as the vorticity.

The use of piecewise linear finite element spaces is of interest because it results in the simplest algorithm for the discretization of the Galerkin weak form of the streamfunction-vorticity equations. On the other hand there are serious questions regarding the stability of discretizations by such low order elements and therefore a theoretical and computational study of these is important. We have shown that although there is in general a loss of accuracy in the vorticity approximations, the derivatives of the streamfunction and therefore the velocity field are optimally approximated. Thus in many settings, linear elements can be used to great advantage. In addition, error estimates have been derived and computational experiments have been performed using higher order elements.

3 - Finite element methods for first order elliptic systems

We have devised, analyzed and implemented a new finite element algorithm for the approximate solution of Petrovski elliptic systems in the plane. This class of equations arise in a variety of settings such as the Maxwell equations of electromagnetics, the vorticity and continuity equations of fluid mechanics, and in certain problems in elasticity. Existing finite element methods are based on the discretization of least squares type variational principles corresponding to the given system of partial differential equations. Our new method, which we dub a *subdomain collocation/least squares method*, directly discretizes the partial differential equation system using a Galerkin type approach; subsequently the resulting system of linear algebraic equations is solved by an algebraic least squares technique. Note that the old approach applies least squares principles to the differential equations and then discretizes while our approach reverses the sequence, i.e., we discretize first and then apply a least squares technique. We show that our method, as does the older one, produces optimally accurate approximations; indeed both approaches yield the same rates of convergence. However, at least for some model problems, the new method seems to involve smaller constants and thus, for practical grids, may be more efficient.

What is certainly true about the new method is that it is simple to implement and has the promise to yield to parallel computation in a natural and efficient manner. These advantages result from the fact that the discretization is an element wise process, i.e., a particular discrete equation is determined completely within a single element. Briefly, the test functions of the Galerkin method are chosen to have support on a single element of the triangulation of

the given domain; this not only uncouples the assembly process but also enables the use of solution algorithms which have a great deal of inherent parallelism.

Another aspect of this study is the treatment of similar problems in three dimensions. Here more serious difficulties arise even in simple settings such as $\text{div}u=f$ and $\text{curl}u=g$. In two dimensions these represent two equations in the two components of u , but in three dimensions these represent four equations in three unknowns. The redundancy is due to the fact that for a solution u to exist one must have that $\text{div}g=0$. We show, in a rigorous manner, how to effectively treat such problems by both the older least squares methods and by our new method. In particular, we obtain the same type of optimal error estimates as we obtained in the two dimensional setting.

4 - Parallel computation of flow problems

This effort has been largely directed at the solution of stationary incompressible flow problems, i.e., the Navier-Stokes equations. The discretization of these equations is accomplished by finite element techniques which are known to yield stable and optimally accurate approximations, at least for moderate values of the Reynolds number. The nonlinear system of discrete equations are solved by a combination of a fixed point iteration/Newton's method algorithm. The bulk of the computational time is taken by the assembly and especially the subsequent solution of a linear system of equations at each step of the nonlinear iteration process. It is the parallel computation of these tasks which we addressed. In both cases, a substructuring algorithm was employed. Substructuring is an old idea which is in general use in solving structural mechanics problems, but which presents special problems when applied

to the Navier-Stokes equations. In the following we will briefly describe the idea, state the problems encountered, and indicate how we were able to take care of them.

The substructuring idea is very simple. We divide the (computational) flow region Ω into subregions $\Omega_1, \Omega_2, \Omega_3, \dots$. We denote by Γ_{ij} the interface between subregions Ω_i and Ω_j . (Of course, such an interface may not exist if the regions are not contiguous.) We assume that the interfaces Γ_{ij} coincide with sides of the triangles used in the triangulation of the region Ω i.e., the interfaces do not cut through the interior of any triangle. All of these tasks are easily accomplished. We now label by the vector \mathbf{x}_i all unknowns (velocity and pressure) associated with the interior of Ω_i or with $\Gamma \cap \bar{\Omega}_i$, where Γ denotes the boundary of Ω . The unknowns associated with the interfaces Γ_{ij} are collected in the vector \mathbf{y} . Then it is easily seen that the linear system of equations to be solved can be ordered in such a way so that it takes on the block form

$$\begin{array}{ccccccc}
 A_1 & & & & B_1 & \mathbf{x}_1 & \mathbf{f}_1 \\
 & A_2 & & & B_2 & \mathbf{x}_2 & \mathbf{f}_2 \\
 & & \cdot & & \vdots & \vdots & \vdots \\
 & & & A_m & B_m & \mathbf{x}_m & \mathbf{f}_m \\
 C_1 & C_2 & \cdot & C_m & D & \mathbf{y} & \mathbf{g}
 \end{array} =$$

where m is the number of subregions.

The parallelism in the assembly process is evident. Each of the sets $(A_i, B_i, C_i, \mathbf{f}_i)$ may be independently assembled. In addition, the matrix D and vector \mathbf{g} may be expressed in the form

$$D = \sum_{i=1}^n D_i \quad \text{and} \quad \mathbf{g} = \sum_{i=1}^n \mathbf{g}_i$$

where each of the sets (D_i, \mathbf{g}_i) may be independently assembled. Thus, except for the concatenations needed to compute D and \mathbf{g} from the D_i 's and \mathbf{g}_i 's, the whole assembly procedure may be parallelized, e.g., by assigning to each of m processors the task of assembling one of the sets $(A_i, B_i, C_i, \mathbf{f}_i, D_i, \mathbf{g}_i)$. Note that this assembly can be carried out without the need for processors to communicate, except at the end with perhaps a host processor which carries out the sums needed to compute D and \mathbf{g} .

At first glance, it seems that the solution of systems such as the one above can exhibit large degrees of parallelism, say by a block elimination technique. Indeed for problems arising in elasticity, such is indeed the case since the coefficient matrix is positive definite. However, in the Navier-Stokes case, and for some choices of finite element spaces, one finds that the matrices A_i are singular, precluding the use of a naive block elimination procedure. This is the case, for example, if one uses piecewise constant pressure approximating spaces. For other choices of finite element spaces, e.g., Taylor-Hood, one is stymied because the final system for \mathbf{y} is singular. Of course, any attempt at pivoting in order to circumvent these difficulties destroys the chances for parallelism in the computations.

We have developed an easily implementable algorithm which can perform the block elimination procedure in spite of these difficulties. In fact, this algorithm is a special case of a general algorithm we have devised for solving general linear systems problems, including singular and rectangular ones, through an elimination procedure which does not require pivoting. In the context of the above linear system, our method does require, for instance, the computation of the null spaces of the A_i 's. However, we have shown how the bulk

of the computations can be done in parallel using elimination procedures. Codes have been written implementing the method and have been used to demonstrate its effectiveness.

5 - Finite element methods for hyperbolic systems

We have studied various finite element methods for first order hyperbolic systems of partial differential equations in several space variables. We considered equations of the positive symmetric type, i.e., of the Friedrichs type. Such equations arise in many applications, e.g., fluid mechanics and electromagnetics. Standard finite element methods for these type equations are not optimally accurate in the sense that the error in the finite element approximation does not converge at the same rate as the error in the best approximation, out of the finite element space employed, to the solution of the differential equation.

We study a nonstandard finite element method which yields better accuracy in the H^1 -norm and, for sufficiently regular solutions, in the L^2 -norm as well. The method, which was employed by other authors in simpler settings, may be viewed as a combined Galerkin and least squares method.

If we symbolically denote the hyperbolic system by

$$\partial u / \partial t + L(u) = 0$$

for some unknown function u , the method is based on the weak formulation

$$\left(\partial u / \partial t + L(u) , Gv + \delta GL_0(v) \right) = 0$$

where $L_0(\cdot)$ is an operator related to the principal part of $L(\cdot)$ and δ is a parameter related to the grid size. The matrix G is chosen to enhance the stability of the scheme in the presence of boundaries. One great advantage of the method is that the test functions v may be chosen in the same space in which the solution u is sought. This should be contrasted with other finite element methods for which different test and trial spaces must be used in order to obtain stable approximations. We show that by properly choosing the parameter δ improved accuracy may be obtained. Specifically, with $\delta=O(h)$, where h is a discretization parameter related to the grid size, we obtain error estimates which show that the nonstandard method we consider is more accurate by a factor of $O(h^{1/2})$ than are standard finite element methods.

6 - The approximation of viscous flows in exterior domains

We have studied the approximation of the Stokes equations in an exterior domain. Specifically, we have considered the problem

$$-\Delta u + \text{grad} p = f \quad \text{in } \Omega$$

$$\text{div} u = 0 \quad \text{in } \Omega$$

$$u = 0 \quad \text{on } \Gamma$$

where Ω is the complement of a closed bounded set in R^3 and where Γ represents the boundary of Ω . In addition, one must impose appropriate decay conditions at infinity.

The first task accomplished was to show that the above problem possesses a unique solution. The key feature of this analysis was the use of the weighted Sobolev spaces of Hanouzet. Not only did this enable us to prove the existence and uniqueness of the solution of the above equations, but in the subsequent analyses of a truncated problem and of finite element approximations, it enabled us to derive error estimates containing constants independent of the distance from the origin.

The above problem, being posed on an unbounded domain, is difficult to approximate directly. Therefore, we also consider the truncated domain problem

$$-\Delta u_R + \text{grad} p_R = \mathbf{f}_R \quad \text{in } \Omega_R$$

$$\text{div} u_R = 0 \quad \text{in } \Omega_R$$

$$u_R = 0 \quad \text{on } \Gamma$$

$$\mathfrak{B}(u_R, p_R) = 0 \quad \text{on } \Gamma_R$$

where Γ_R is a bounded surface which encloses Γ , e.g., Γ_R could be a sphere of sufficiently large radius R , and Ω_R is the open bounded set between the surfaces Γ and Γ_R . Also \mathbf{f}_R is an approximation to \mathbf{f} . For example, if \mathbf{f} is of bounded support, then we may take $\mathbf{f}_R = \mathbf{f}$. Finally, $\mathfrak{B}(\cdot, \cdot)$ is a linear artificial boundary operator introduced in order to close the problem.

It is possible to choose the boundary operator $\mathfrak{B}(\cdot, \cdot)$ so that the solutions of the two problems above coincide on Ω_R . Such an operator is necessarily non-local, i.e., it involves integrals of u_R over Γ_R . This leads to a coupled finite element/boundary integral discretization. We have fully analyzed this

approach, but for the sake of brevity, say no more about it here.

Instead we report on the use of local artificial boundary conditions. Specifically, we employ a series of boundary conditions of increasing accuracy and which preserve the self-adjointness of the problem. The price to be paid for increasing the accuracy of the boundary condition is that higher derivatives of the solution must be used on the boundary. Using these artificial local boundary conditions, we have proved the existence and uniqueness of solutions to the truncated domain problem and derived error estimates for the differences $(u-u_R)$ and $(p-p_R)$. These take the form

$$\|u-u_R\|_1 + \|p-p_R\|_0 \leq C/R^\alpha$$

where α increases with the accuracy of the boundary condition used and where the constant C depends on \mathbf{f} but not on R .

Once the truncated problem has been set up using the bounded domain Ω_R , it may be discretized by standard techniques. We were able to derive optimal error estimates for the differences (u^h-u_R) and (p^h-p_R) where u^h and p^h denote the approximate velocity and pressure, respectively. These error estimates are with respect to a discretization parameter h and again, through the use of the weighted Sobolev spaces of Hanouzet, involve constants which are independent of the truncation parameter R .

Having derived estimates for $(u-u_R)$ and $(p-p_R)$ and for (u^h-u_R) and (p^h-p_R) it only requires a trivial application of the triangle inequality to derive error estimates for (u^h-u) and (p^h-p) . These last estimates depend on two parameters, namely h and R . These dependencies may be balanced to obtain an optimal set of parameters for a given desired accuracy.

We note that a quasi-uniform triangulation of Ω_R will in general yield an

inefficient algorithm, i.e., one that requires too many degrees of freedom. Fortunately, one may take advantage of the fact that u and p decay as $|\mathbf{x}| \rightarrow \infty$ to introduce a mesh grading technique wherein the mesh size increases with $|\mathbf{x}|$. By properly choosing the mesh grading, the accuracy of the approximations is preserved while at the same time using relatively few degrees of freedom.

7 - Finite element methods for algebraic turbulence models

The goal of this effort was to devise and rigorously analyze finite element methods for a particular, but typical, algebraic model of turbulence. The importance of such an endeavor is that often when examining turbulence calculations it is difficult to separate modelling errors from numerical errors. Therefore we wanted to put existing turbulence models on a firm numerical footing so that these models may be safely studied to determine their physical validity without worrying about questions of numerical accuracy and stability.

The particular model chosen was a popular algebraic (or eddy viscosity or zero equation model). Here the time averaged Navier-Stokes equations are closed by assuming that the Reynolds stresses may be replaced by ordinary stresses but with a viscosity coefficient which is in some sense proportional to the shear stresses themselves. This introduces new nonlinearities into the differential equations which are not present in the Navier-Stokes equations. Therefore the first task at hand was to study these partial differential equations. We have obtained existence, uniqueness and regularity results analogous to those in the literature for the Navier-Stokes equations.

Having obtained results concerning the partial differential equations, a

finite element algorithm was devised and analyzed. In the algorithm the nonlinear eddy viscosity is lagged so that an iteration is set up between the velocity field and the eddy viscosity. Of course, the former itself requires the solution of a nonlinear system of equations similar to that resulting from discretizations of the Navier-Stokes equations, while the latter is simply an algebraic function of the derivatives of the velocity field (hence the terminology *algebraic model*). This algorithm may be easily extended to more complicated models, e.g., the $k-\epsilon$ equations. The finite element algorithm applied to the algebraic model was rigorously analyzed in conjunction with a Newton method solution technique for the discrete system. The convergence of the method for sufficiently good initial guesses was proved.

8 - Other relevant information concerning AFOSR sponsored research

In addition to the work described above, we have also been involved in various other projects. These include studies of finite element approximations of problems with inhomogeneous essential boundary conditions, finite element methods for the inhomogeneous Navier-Stokes equations, boundary condition treatments in finite difference and finite element methods for hyperbolic systems, higher order, e.g., spectral methods, for the approximate solution of differential equations, etc.

In addition to the Principal Investigator, one Visiting Associate Professor at Carnegie Mellon University (William Layton) and a number of past and present Ph.D. students have been supported by AFOSR through previous grants.

Every year we report some of our results at professional meetings, often in the guise of invited talks. For example, last year (1987), we have given

invited talks at the *AMS Meeting* held at Kent State University, at the meeting on *Advances in Computer Methods for Partial Differential Equations* held in Lehigh, at the *International Symposium on Numerical Methods for Laminar and Turbulent Flow* held in Montreal, and at a minisymposium within the *SIAM National Meeting* in Denver.

9 - Selected papers published as a result of AFOSR sponsored research

We list some of the papers which have resulted from research supported by AFOSR. We confine ourselves to papers which are to appear or which have appeared in the last three years.

1. On the approximation of the exterior Stokes problem in three dimensions; *Proc. 5-th Intern. Symposium on Finite Elements and Flow Problems*; U. of Texas at Austin, 1984, 149-154; with G. Guirguis.
2. Mixed finite element approximations for the biharmonic equation; *Proc. 5-th Intern. Symposium on Finite Elements and Flow Problems*; U. of Texas at Austin, 1984, 281-286; with G. Fix, R. Nicolaides and J. Peterson.
3. On the finite element approximation of the streamfunction vorticity equations; *Advances in Computer Methods for Partial Differential Equations V*, IMACS, 1984, 47-56; with J. Peterson.
4. Issues in the implementation of substructuring algorithms for the Navier-Stokes equations; *Advances in Computer Methods for Partial Differential Equations V*, IMACS, 1984, 57-63; with R. Nicolaides.
5. Some aspects of finite element approximations of incompressible viscous flows; *Computational Methods in Viscous Flows*, Pineridge, 1984, 173-189; with R. Nicolaides.
6. Elimination with noninvertible pivots; *Linear Algebra Appl.* 64, 1985, 183-189; with R. Nicolaides.
7. Algorithmic and theoretical results on computation of incompressible viscous flows by finite element methods; *Comput. Fluids* 13, 1985, 361-373; with C. Liu and R. Nicolaides.

8. On substructuring algorithms and solution techniques for the numerical approximation of partial differential equations; *Appl. Numer. Methods.* 2, 1986, 243-256; with R. Nicolaides.
9. A non-standard finite element method of higher accuracy for hyperbolic systems in several space variables; *Advances in Computer Methods for Partial Differential Equations VI*, IMACS, 1987, 92-97; with Q. Du and W. Layton.
10. Error estimates and implementation issues for artificial boundary condition methods for exterior problems; *Advances in Computer Methods for Partial Differential Equations VI*, IMACS, 1987, 338-345; with G. Guirguis.
11. Finite element methods for a Ladyzhenskaya model of incompressible viscous flow; *Numerical Methods in Laminar and Turbulent Flow*, Pineridge, 1987, 161-169; with Q. Du.
12. Finite element methods for vorticity formulations of incompressible viscous flows; *Numerical Methods in Laminar and Turbulent Flow*, Pineridge, 1987, 170-181; with J. Peterson.
13. A finite element method for first order elliptic systems in three dimensions; *Applied Math. Comp.* 23, 1987, 171-184; with C. Chang.
14. On the approximation of the exterior Stokes problem in three dimensions; *Math. Model. Numer. Anal.* 21, 1987, 445-464; with G. Guirguis.
15. Mathematical aspects of finite element methods for incompressible viscous flows; to appear in a Springer book on finite element methods.
16. Finite element methods for the streamfunction-vorticity equations: boundary condition treatments and multiply connected domains; to appear in *SIAM J. Sci. Stat. Comput.*; with J. Peterson.
17. A subdomain collocation/least squares method for first order elliptic systems in the plane; to appear in *SIAM J. Numer. Anal.*; with C. Chang.
18. Finite element methods for a zero-equation model of turbulence; to appear in *Comput. Math. Appl.*; with J. Turner.
19. A low dispersion, high accuracy finite element method for first order hyperbolic systems in several space variables; to appear in *Comp. Math. Appl.*; with Q. Du and W. Layton.