FINAL SCIENTIFIC REPORT

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Title: Computational Fluid Dynamics at the ICMA

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The first project dealt with the computation of stationary Navier-Stokes solutions using continuation methods. Error estimates for certain finite element solutions of the Navier-Stokes operator were investigated. Numerical methods for the detection of Hopf bifurcation were studied.

The second project involved the construction, analysis and implementation of efficient computer algorithms for the finite difference and finite element-dual variable discretization of the two-dimensional Navier-Stokes problems. Particular attention was given to solving...
ITEM #19, ABSTRACT, CONTINUED: to finite element and finite difference discretizations of such problems that arise in combustor modeling.

The third project sought to extend the dual variable reduction technique to various fluid models. This required the construction of a network analogue for the discrete difference equations along with an analysis of the fundamental matrix and dual variable transformation involved.
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I. ACCOMPLISHMENTS

Included below is a brief summary of the accomplishments under Grant AFOSR-80-0176.

A. Dual Variable Method and Navier-Stokes Problems

Many natural implicit discretizations of the Navier-Stokes equations can, with the proper identification, be regarded as systems defining flows on associated networks. A set of network variables (the "dual variables") is introduced which significantly reduces the size of the original system and hence, economizes on its solution. The method avoids the need to compute pressures, and produces velocities that are exactly discretely divergence free. Details for transient problems can be found in:


The extension of the dual variable method to finite element discretizations was also investigated. Such discretizations of the Navier-Stokes problem yield systems of nonlinear ordinary differential equations with constraints of the generic form
\[ M \frac{d\vec{U}}{dt} + Q(\vec{U})\vec{U} + A^T \vec{P} = \vec{B} \]  

(1)

\[ A\vec{U} = \vec{S} \]  

(2)

for velocities \( \vec{U} \) and pressures \( \vec{P} \). The dual variable method consists of the following steps:

(i) Construct a basis \( \{\phi_i\}_{i=1}^d \) for the null space of \( A \) and define the matrix \( C = [\phi_1 \cdots \phi_d] \).

(ii) Construct a particular solution \( \vec{U}_p \) to (2) then

\[ \vec{U} = \vec{U}_p + C \vec{\gamma} \]  

(3)

for some vector \( \vec{\gamma} \) (the dual variables).

(iii) Multiply (1) by \( C^T \) (this eliminates \( \vec{P} \) from (1)) and use (3) to get

\[ C^T M C \frac{d\vec{U}}{dt} + C^T Q(\vec{U})C \vec{\gamma} = \vec{B}' . \]  

(4)

(iv) Solve (4) for the dual variables \( \vec{\gamma} \) and use (3) and (1) to recover the velocities \( \vec{U} \) and pressures \( \vec{P} \).

Research centered on the investigation of \( \text{NS}(A) \), the null space of the finite element analogue \( A \) of the divergence operator. What is \( d \), the dimension of \( \text{NS}(A) \)? How can a basis for \( \text{NS}(A) \), i.e. \( C \), be efficiently constructed?

If the above scheme is to be computationally efficient then the construction of \( C \) must be cheap. In the context of finite differences, the
matrix $C$ was the fundamental matrix of an associated network and its "construction" was trivial.

The finite element investigation was carried out in the context of the 4-node quadrilateral element for approximating velocity and the constant quadrilateral element for approximating pressures.

For virtually arbitrary unions of rectangular elements an algorithm was devised for the construction of $C$ which does not require the solution of any linear system. The number of columns of $C$, i.e. the $\dim \NS(A)$, is determined by the following theorem:

**Theorem:** Let $A$ be the discrete divergence operator associated with the combination of 4-node bilinear velocity elements and constant pressure elements. If the domain is admissibly decomposed into a union of $N$ rectangular elements and there are $M$ interior nodes then:

(i) $A$ is $N \times 2M$,

(ii) $\dim \NS(A) = 2M - N + 2$.

Note that (1) and (2) is a system of $2M$ ODES with $N$ algebraic constraints while (4) is a system of $2M - N + 2$ ($\sim N$) ODES.

For virtually arbitrary unions of quadrilaterals another algorithm has been devised for the construction of $C$ which requires the solution of a sequence of relatively small linear systems. The work is contained in:

The dual variable method has also been extended to transient compressible fluid flow problems. The complication now is the introduction of the pressure into the continuity equation (density is now a function of pressure). It is still possible to regard implicit finite difference discretizations of compressible flow problems as systems defining "flows" on networks. A set of network variables (dual variables) is introduced which reduces, by a factor of two, the size of the linear system which must be solved at each time step. A report on this extension authored by J. Burkardt, C. Hall and T. Porsching will be issued in the near future. See also


B. Discretization Error for Parametrized Nonlinear Equations

Steady-state flow problems are governed by nonlinear parameter-dependent equations of the general form

\[ F(z,\lambda) = 0. \quad (5) \]

Here, as well as in many other applications, \( F \) is a nonlinear Fredholm mapping from a Banach space \( X = Z \times \Lambda \) to a Banach space \( Y \), \( Z \) represents a state space (usually infinite-dimensional), and \( \Lambda \) an \( m \)-dimensional parameter space. In the case of flow problems, \( F \) is generated by the Navier-Stokes equations and the given boundary conditions, \( z \) represents
the state variables characterizing the flow problem (usually the components of the velocity vector, the pressure, and so on), and \( \lambda \) is an \( m \)-dimensional vector of intrinsic parameters (for instance, the Reynolds number or any other dimensionless numbers characterizing the flow).

For practical flow problems, it is rarely of interest to compute only some solutions of (5) for a few given parameter vectors. Instead, interest centers on such concerns as the variation of solutions under specified changes of the parameters and their stability properties. For this purpose, the equilibrium states of the flow problem should be considered as points \((z, \lambda)\) in the product space \( X = Z \times \Lambda \), and the set of solutions \((z, \lambda) \in Z \times \Lambda\) of (5) constitutes an \( m \)-dimensional manifold in \( Z \times \Lambda \). The problem then is to analyze computationally the characteristic features of this equilibrium manifold.

Work on this topic has addressed three principal subareas. The first involves a comprehensive study of the discretization errors arising when the original problem (5) is replaced by an equation between finite-dimensional spaces. A theory of a priori discretization errors for problems of the form (5), which generalizes the results of previous studies in two important ways, has been developed. In particular, the theory covers a broader class of problems than the mildly nonlinear problems to which other approaches are restricted, and the results are valid for the general case of an \( m \)-dimensional parameter space for any \( m > 1 \). Details of this on-going study appear in the following publications:


The second subarea concerns a study of computational methods for analyzing solution manifolds of problems of the form (5) and the development of library-grade software for such methods. Included in this study are the application of the continuation package PITCON, developed by W. Rheinboldt and J. Burkardt at ICMA, to steady-state flow problems and the use of techniques for reducing the sizes of the systems arising in typical flow problems. Special emphasis was placed on the reduced-basis technique. Details of this work may be found in the following publications:


The third subarea consists of a study of the computational detection
and analysis of singularities on solution manifolds. Such singularities include bifurcation phenomena of practical flow problems. Based on the general theory of discretization mentioned above, augmented equations and computationally accessible coordinate systems on solution manifolds of parametrized equations have been studied with special emphasis on singularities. Computational algorithms for the efficient determination of singularities on a solution manifold are also being investigated. The development of these algorithms stems from earlier work by W. Rheinboldt. The results of this study are contained in the following publications:


Included here for reference are some earlier publications on this topic:


C. Mixed Finite Element Methods for Stationary Navier-Stokes Problems

Conforming mixed finite element methods for incompressible viscous flow problems were examined. Preliminary work consisted of studying linearized Navier-Stokes equations such as the Oseen equations. This work culminated in a report entitled

\begin{itemize}
  \item "On Conforming Mixed Finite Element Methods for Incompressible Viscous Flow Problems", M. D. Gunzburger (University of Tennessee), R. A. Nicolaides (Carnegie-Mellon University) and J. S. Peterson (University of Pittsburgh), Comp. & Maths. with Appl. 8 (1982), 167.
\end{itemize}

In this paper the asymptotic rates of convergence are given for four finite element discretizations.

This work has been extended to the inhomogeneous stationary (nonlinear) Navier-Stokes equation with inhomogeneous boundary data. Specifically, the problem considered is to find \( u \) and \( p \) satisfying

\begin{equation}
-v \Delta u + u_j \frac{\partial u}{\partial x_j} + \text{grad} \, p = f \quad \text{in} \quad \Omega \tag{6}
\end{equation}

\begin{equation}
\text{div} \, u = g \quad \text{in} \quad \Omega \tag{7}
\end{equation}

\begin{equation}
u \vert_{\Gamma} = q \tag{8}
\end{equation}

for given \( f \in H^{-1}(\Omega) \) , \( g \in L_2(\Omega) \) and \( q \in H^{1/2}(\Omega) \) such that
\[ \int_{\Omega} g = \int_{\Gamma} q \cdot n \]

where \( \Gamma \) is the boundary of \( \Omega \). Here \( H^r(\Omega) \) for \( r > 0 \) denotes the \( r \)-th order Sobolev space associated with the set \( \Omega \); \( H^{-r}(\Omega) \) denotes the dual space of \( H^r(\Omega) \); and \( L_2(\Omega) \) represents the space of functions which are square integrable in \( \Omega \). For the particular weak formulation of (6)-(8) considered, it is possible to show existence and uniqueness of the solution under certain conditions on the data. In addition, optimal error estimates for the velocity measured in the \( H^1(\Omega) \) norm and for the pressure measured in the \( L^2(\Omega) \) norm for the Galerkin approximation to the weak problem are derived. Since the discretization process leads to a system of nonlinear algebraic equations, iterative techniques (simple iteration, Newton iteration and Modified-Newton iteration) are used to solve this system. Rates of convergence for each scheme are derived. Numerical examples which use an efficient choice of finite element spaces are also provided. This work is presented in the following report:


An additional area of interest for the Navier-Stokes problem is to determine the error in the velocity measured in the \( L^2(\Omega) \)-norm. To obtain such a result it was first necessary to improve upon the existing theory of the approximation of boundary value problems with inhomogeneous essential boundary conditions such as the inhomogeneous Dirichlet problem for second order elliptic partial differential equations. An optimal error obtained in the \( L^2(\Omega) \)-norm was then obtained for the (nonlinear) stationary Navier-Stokes equations. This analysis of the finite element method for problems
with inhomogeneous essential boundary conditions, along with numerical examples for problems posed on polyhedral domains, is presented in the report.


The work described above deals with the Navier-Stokes equations in primitive variable formulation. Also of interest is the streamfunction-vorticity formulation of the Stokes and Navier-Stokes equations. Finite element algorithms have been derived which require low continuity finite element spaces and do not require any artificial specification of the vorticity at solid boundaries. In addition, methods for handling multiply connected domains have been analyzed both theoretically and computationally. This work is presented in the paper:


D. Krzhivitski-Ladyzhenskaya Finite Difference Equations

In 1966, Krzhivitski and Ladyzhenskaya presented a finite difference discretization of the Navier-Stokes problem for which they prove unconditional stability in the discrete $L^2$-norm. Their scheme also generates approximations which converge to a weak solution of the continuous problem as the discretization parameters tend to zero. Their analysis required homogeneous boundary data.

Under this grant the analysis of the K & L difference scheme was
extended in two respects:

(i) Existence and uniqueness theorems for solutions of the stationary K & L equations were established for both homogeneous and inhomogeneous boundary conditions. The results for the homogeneous boundary conditions were announced in the paper and Ph.D. thesis


(ii) As a step towards handling curved domains consideration was given to extensions of the K & L difference scheme to a differential system that arises when the Navier-Stokes system is transformed through the introduction of a curvilinear coordinate system. This required the derivation and analysis of a new class of finite difference approximations. A new 7 point stencil was derived and was proven to be unconditionally stable. For a given mesh gauge $h$, a piecewise bilinear function $u_h$ was constructed which interpolates to the finite difference solution, and it has been shown that as $h \to 0$, $u_h$ converges to the weak solution of the continuous problem.

Details of this work are contained in:

E. Binary Gas Mixture Flow Through Combustors

In an attempt to reduce the development cycle costs associated with design of gas turbine engine combustors, mathematical combustor models are being employed to provide information about performance trends and to predict velocity, pressure and thermodynamic property profiles in simulated practical combustion environments. It has been demonstrated that the dual variable method can be applied to the predictive model of the fluid dynamics associated with an axially symmetric centerbody combustor being studied at WPAFB. This was discussed in the report


A cooperative effort between ICMA and the Aero Propulsion Laboratory, WPAFB is underway to incorporate the dual variable reduction technique into their combustion modelling program TEACH-T.

F. Numerical Solution of Convection-Conduction Problems

The convection-conduction equation arises in fluid dynamics as the vorticity transport equation. In convection dominated situations (high Reynolds number) numerical solutions may contain severe nonphysical oscillations. Upwind finite difference methods and finite element methods have been developed over the years to prevent such spatial oscillations. Upwind finite element schemes were developed under this grant which lead to diagonally dominant systems of positive type:

This guarantees, for example, that the solution satisfies a maximum principle, a property which is not shared by all finite element discretizations as shown in


II. LIST OF PAPERS AND REPORTS (AFOSR-80-0176)


III. PROFESSIONAL PERSONNEL

Investigators:

1. Ian Christie  
   Assistant Professor of Mathematics

2. James P. Fink  
   Associate Professor of Mathematics

3. Charles A. Hall  
   Professor of Mathematics and  
   Executive Director, ICMA

4. Janet S. Peterson  
   Assistant Professor of Mathematics

5. Thomas A. Porsching  
   Professor of Mathematics

6. Werner C. Rheinboldt  
   Andrew W. Mellon Professor  
   of Mathematics

Scientific Programmer:

1. John Burkardt

2. Addison Frey

Graduate Research Assistants

1. Anna Cha (Ph.D., December 1982)

2. So-Hsiang Chou (Ph.D., expected 1984)

3. John Ellison (Ph.D., August 1982)

4. Gary Hart (Ph.D. candidate)

5. Timothy Holmes

6. George Mesina (Ph.D. candidate)

7. Frank Sledge (Ph.D., August 1983)
IV. INTERACTIONS


2. Contacted Dr. W. Roquemore, AFWAL-WPAFB in January, 1982 concerning combustor modelling and the possibility of using the dual variable method to economize on the numerical solution of such problems.

3. Visited Dr. W. Roquemore, AFWAL-WPAFB in September, 1982, made presentation and exchanged research information. AFWAL provided us with a copy of the TEACH fluids code in which we implemented the dual variable method.

4. Participated in the AFOSR Supercomputing Meeting at Kirtland AFB, Albuquerque, NM on April 4-6, 1984.
11. TITLE (Include Security Classification)

COMPUTATIONAL FLUID DYNAMICS AT THE ICMA

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16. ABSTRACT (Continue on reverse if necessary and identify by block number)

This research concerned three independent projects of ICMA (Institute of Computational Mathematics and Applications) personnel, each belonging to the general area of computational fluid dynamics.

The first project dealt with the computation of stationary Navier-Stokes solutions using continuation methods. Error estimates for certain finite element solutions of continuation problems were derived and extensions to more general operators including the Navier-Stokes operator were investigated. Numerical methods for the detection of Hopf bifurcation were studied.

The second project involved the construction, analysis and implementation of efficient computer algorithms for the finite difference and finite element-dual variable discretization of the two-dimensional Navier-Stokes problems. Particular attention was given (CONT.)