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A New Finite Element Formulation for Incompressible Flow

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Abstract

A basic objective in computational fluid dynamics is the efficient solution of nonlinear systems of equations that arise in finite element modeling of convective-diffusive flow. The use of implicit Newton-like schemes to solve the coupled system of Navier-Stokes and continuity equations enables rapid convergence, although the well-known difficulty of indirect pressure linkage requires attention when forming the Jacobian matrices. Traditional approaches for overcoming this obstacle include reordering strategies, modification of diagonal terms, and changes of variables. In contrast, we develop a primitive variable finite element formulation which employs an auxiliary pressure equation derived from the Navier-Stokes and continuity equations. This formulation extends the work of Rice and Schnipke, where a similar equation was developed in the context of a segregated solution method. Approximate Newton methods using the new finite element formulation are evaluated in terms of accuracy, convergence rate, and overall efficiency for flow problems with varying degrees of nonlinearity.

1 Introduction

The efficient solution of nonlinear systems of equations that arise in finite element modeling of convective-diffusive flow is a basic objective in computational fluid dynamics. One commonly used approach is to employ implicit Newton-like schemes to solve the coupled system of Navier-Stokes and continuity equations, where the difficulty of indirect specification of pressure necessitates consideration. Specifically, if the primitive variables of velocity and pressure are used in direct discretization of the problem, zero terms are produced on the diagonal of the Jacobian matrix. To remedy this situation, researchers have devoted much effort to the development of reorderings and modification of the diagonal terms. Alternatively, we develop a primitive variable formulation that overcomes the difficulty of indirect pressure linkage and its detrimental effects on the Jacobian matrix by incorporating an auxiliary pressure equation derived from the Navier-Stokes and continuity equations. We consider explicit formation of the Jacobian matrix both analytically and with the use of finite differencing approximations.

Development of the subsidiary pressure equation extends the finite element work of Rice and Schnipke [1], which is itself based on the SIMPLER finite difference technique of Patankar [2], where similar equations are derived within the context of a segregated solution approach. As described, for example, by Chorin [3], a distinguishing characteristic of segregated solution methods is that the governing partial differential equations are repeatedly solved in sequence rather than concurrently. This feature offers the advantage of relatively modest memory requirements, since the coefficient matrix for only one linearized system

must be stored at a given time. However, segregated solvers sometimes cannot adequately handle strong coupling because of the approximations that produce the linearized systems. In addition, since the segregated solution approach reduces the residual only locally at each step, the number of iterations required for convergence and the computational effort tend to increase significantly as grids are refined (see, e.g., [4]).

We maintain the favorable features of the Rice-Schnipke finite element formulation and incorporate the benefits of solving a fully coupled nonlinear system in which the residual is reduced globally at each iteration. The resulting discretized pressure equation is symmetric positive definite, and equal-order interpolation functions can be employed for all variables instead of the usual lower-order interpolation for pressure. As shown by Rice and Schnipke [1], the segregated solution variant of this problem formulation eliminates spurious pressure modes that often arise for simple multilinear elements when constant pressures would be required to satisfy the Babuska-Brezzi stability condition.

We evaluate the effectiveness of the new velocity-pressure-temperature formulation in the context of approximate Newton methods for solving flow problems with varying degrees of nonlinearity. Numerical results are presented for several standard test problems, including developing duct flow, flow over a backward-facing step, and natural convection. The Newton-like methods are compared with the corresponding segregated solution technique in terms of solution accuracy, rate of convergence, and overall efficiency.

2 Problem Formulation

In this section we define the class of problems under consideration, namely, those arising in the modeling of incompressible, laminar, Newtonian fluid flow. The finite element discretization of the governing partial differential equations is presented, and the subsidiary pressure equation is derived.

2.1 Governing Partial Differential Equations

We consider the three-dimensional steady-state partial differential equations that govern incompressible, laminar, Newtonian fluid flow. The conservation of mass equation, or continuity equation, is given by

$$\nabla \cdot \rho \boldsymbol{u} = 0, \tag{2.1}$$

where ρ and $\boldsymbol{u} = [u_1, u_2, u_3]^t$ respectively denote density and velocity, with the superscript t indicating the vector transpose. The continuity equation is coupled with the Navier-Stokes equations and the thermal energy equation with no heat generation, which in the Cartesian coordinate system are given respectively by

$$\rho \boldsymbol{u} \cdot \nabla u_j = \nabla \cdot (\mu \nabla u_j) + \rho \hat{g}_j - \frac{\partial p}{\partial x_j}, \quad j = 1,\ 2,\ 3, \tag{2.2}$$

and

$$\rho c_p \boldsymbol{u} \cdot \nabla T = \nabla \cdot (k \nabla T). \tag{2.3}$$

Here T, $\hat{g}$, μ, k, and c_p respectively denote temperature, gravitational force, viscosity, thermal conductivity, and specific heat, where the last three variables are known functions of temperature and pressure. All fluid properties are assumed to be constant within an element, so that $\nabla \cdot \boldsymbol{u} = 0$ on an element basis.

While the density, ρ, is usually removed from (2.1) for incompressible flow, we retain it to ensure conservation of mass for nonisothermal flows, where density may vary according to a particular constitutive equation.

To discuss derivation of the auxiliary pressure equation, we focus first on the coupling of the steady-state continuity and incompressible Navier-Stokes equations. Thus, we initially consider two-dimensional isothermal flow, for which the temperature and density variables remain constant, to discuss the problem formulation. This form can then easily be extended to include the additional velocity, temperature, and density variables for three-dimensional nonisothermal flow. The corresponding boundary value problem is as follows: Given the bounded spatial domain $\Omega \subset \Re^2$, with a smooth boundary Γ and unit outward normal $\boldsymbol{n}$, find $\boldsymbol{u}(\boldsymbol{x})$ and $p(\boldsymbol{x})$ satisfying (2.1) and (2.2) as well as the appropriate well-posed boundary conditions. Typical Dirichlet and diffusive-flux Neumann boundary conditions for velocity are expressed by

$$\boldsymbol{u} = \boldsymbol{g}(\boldsymbol{x}), \;\; \boldsymbol{x} \in \Gamma_g \qquad \text{and} \qquad \mu \nabla \boldsymbol{u} \cdot \boldsymbol{n} = h(\boldsymbol{x}), \;\; \boldsymbol{x} \in \Gamma_h, \tag{2.4}$$

where $\boldsymbol{g}$ and h are given functions, and Γ_g and Γ_h are subsets of the boundary Γ such that

$$\overline{\Gamma_g \bigcup \Gamma_h} = \Gamma, \qquad \Gamma_g \cap \Gamma_h \;\; = \emptyset. \tag{2.5}$$

Note that outflow boundary conditions for incompressible flow are subject to different interpretations, as discussed by Gresho [5].

2.2 Finite Element Discretization

Finite element discretization of the flow equations yields a nonlinear system

of the form

$$\boldsymbol{F}(\boldsymbol{w}) = A(\boldsymbol{w})\boldsymbol{w} - \boldsymbol{b}(\boldsymbol{w}) = 0, \tag{2.6}$$

where $\boldsymbol{F} : \Re^2 \rightarrow \Re^2$. Using the primitive variables of velocity and pressure, $\boldsymbol{w}$ can be partitioned accordingly:

$$\boldsymbol{w} = [\boldsymbol{u}_1,\ \boldsymbol{u}_2,\ \boldsymbol{p}]^t. \tag{2.7}$$

The matrix A in (2.6) has block diagonal structure, which for two-dimensional isothermal flow is given by

$$A = \begin{bmatrix} A_{u_1} & & \\ & A_{u_2} & \\ & & A_p \end{bmatrix}, \tag{2.8}$$

where A_{u_1} and A_{u_2} indicate the coefficient matrices corresponding to the momentum equations, and A_p is the coefficient matrix of the auxiliary pressure equation. The contents of these matrices and the corresponding components of $\boldsymbol{b}$ will be discussed in this section.

Consider the application of the finite element method to (2.2), where for simplicity we first discuss the scalar convection-diffusion equation. This equation is restated as follows in terms of the general variable ϕ, denoting either u_1 or u_2:

$$\rho \boldsymbol{u} \cdot \nabla \phi = \nabla \cdot (\mu \nabla \phi) + \rho \hat{g}_j - \frac{\partial p}{\partial x_j}, \tag{2.9}$$

where j denotes the corresponding spatial dimension 1 or 2. We wish to solve the following boundary value problem: Given the bounded domain $\Omega \subset \Re^2$, with smooth boundary Γ such that (2.5) holds and has unit outward normal $\boldsymbol{n}$, find the function ϕ that satisfies (2.9) and the boundary conditions

$$\phi = g(\boldsymbol{x}),\ \boldsymbol{x} \in \Gamma_g \qquad \text{and} \qquad \mu \nabla \phi \cdot \boldsymbol{n} = h(\boldsymbol{x}),\ \boldsymbol{x} \in \Gamma_h\,. \tag{2.10}$$

The variational formulation is determined by taking the weighted average of (2.9), where the spaces of admissible trial and weighting functions are given respectively by

$$S \equiv \{\psi(\boldsymbol{x}) : \ \psi \in H^1(\Omega), \ \psi|_{\Gamma_g} = g\} \tag{2.11}$$

and

$$V \equiv \{\hat{\psi}(\boldsymbol{x}) : \ \hat{\psi} \in H^1(\Omega), \ \hat{\psi}|_{\Gamma_g} = 0\}. \tag{2.12}$$

The variational formulation thus becomes: Find $\phi \in S$ such that for all $\hat{\phi} \in V$

$$a(\phi, \hat{\phi}) = L(\hat{\phi}), \tag{2.13}$$

where the bilinear form $a(\phi, \hat{\phi})$, which is nonsymmetric for the convection-diffusion problem, is given by

$$a(\phi, \hat{\phi}) = \int_\Omega \rho \boldsymbol{u} \cdot \nabla\phi\hat{\phi} d\Omega + \int_\Omega \mu \nabla\phi \cdot \nabla\hat{\phi} d\Omega, \tag{2.14}$$

and the linear form $L(\hat{\phi})$ is given by

$$L(\hat{\phi}) = \int_\Omega (\rho \hat{g}_j - \frac{\partial p}{\partial x_j})\hat{\phi} d\Omega + \int_{\Gamma_h} h\hat{\phi} d\Gamma. \tag{2.15}$$

The streamline upwind Petrov-Galerkin (SUPG) approach of Brooks and Hughes [6], with enhancements by Hughes, Mallet, and Mizukami [7], is incorporated for accurate modeling of convective effects. A modified weighting function is introduced so that a streamline upwind perturbation exists only in the flow direction. An additional term, acting in the direction of the solution gradient, is used to capture discontinuities.

The problem domain Ω is partitioned into E discrete regions Ω_e, where

$$\bar{\Omega} = \bigcup_{e=1}^{E} \bar{\Omega}_e \qquad \text{and} \qquad \bigcap_{e=1}^{E} \Omega_e = \emptyset. \tag{2.16}$$

We employ the finite element analogue of the space S, as given by

$$S^h \equiv \{\psi^h \in C^0(\Omega) : \psi^h|_{\Omega_e} \in \tilde{P}^k(\Omega_e) \,\forall\, \Omega_e \in \gamma^h,\ \psi^h|_{\Gamma_g} = g\}, \tag{2.17}$$

where $\tilde{P}^k(\Omega_e)$ is the space of polynomials of degree $k \geq 0$ on Ω_e, and γ^h denotes the partitioning used for a given problem. There is no continuity requirement across interelement boundaries, so that the weighting function

$$\hat{\phi}_{SUPG} = \hat{\phi} + \hat{w}, \tag{2.18}$$

is contained in W^h, where

$$W^h \equiv \{\hat{\psi}^h \in C^{-1}(\Omega) : \hat{\psi}^h|_{\Omega_e} \in \tilde{P}^k(\Omega_e) \,\forall\, \Omega_e \in \gamma^h,\ \hat{\psi}^h|_{\Gamma_g} = 0\}. \tag{2.19}$$

Here $\hat{\phi} \in C^0$ is the standard Bubnov-Galerkin weighting function (corresponding to the interpolation function) and $\hat{w} \in C^{-1}$ is a discontinuous perturbation of $\hat{\phi}$ which includes weighting functions for upwinding and discontinuity-capturing effects:

$$\hat{w} = \tau_1 \boldsymbol{u} \cdot \nabla \hat{\phi} + \tau_2 \check{\boldsymbol{u}} \cdot \nabla \hat{\phi}. \tag{2.20}$$

The locally defined upwinding and discontinuity-capturing terms, given respectively by τ_1 and τ_2, have the dimension of time, so that $\hat{w}$ is nondimensional. While various techniques have been developed for determining τ_1 and τ_2, which are functions of velocity, material properties, and element parameters, we employ the method given in [7]. Also, $\check{\boldsymbol{u}}$ denotes the projection of $\boldsymbol{u}$ on $\nabla\phi^h$, as given by

$$\check{\boldsymbol{u}} = \begin{cases} \frac{\boldsymbol{u} \cdot \nabla \phi^h}{|\nabla \phi^h|^2} \nabla \phi^h & \text{if } \nabla \phi^h \neq 0 \\ 0 & \text{otherwise.} \end{cases} \tag{2.21}$$

A discrete approximation of the variational problem then becomes: Find $\phi^h \in S^h$ such that for all $\hat{\phi} \in W^h$

$$a_\tau(\phi^h, \hat{\phi}) = L_\tau(\hat{\phi}), \tag{2.22}$$

where

$$a_\tau(\phi^h, \hat{\phi}) = a(\phi^h, \hat{\phi}) + \sum_{e=1}^{E} \int_{\Omega_e} [\rho \boldsymbol{u} \cdot \nabla \phi^h + \nabla \cdot (-\mu \nabla \phi^h)] \, \hat{w} d\Omega, \tag{2.23}$$

and the summation notation indicates that the element quantities are placed in global positions according to the node numbering scheme. The linear form $L_\tau(\hat{\phi})$ is given by

$$L_\tau(\hat{\phi}) = L(\hat{\phi}) + \int_\Omega (\rho \hat{g}_j - \frac{\partial p}{\partial x_j}) \hat{w} d\Omega, \tag{2.24}$$

and $\hat{w}$ is given by (2.20). Because the perturbations introduced by the SUPG formulation are restricted to the element interiors, they affect neither boundary nor continuity conditions.

Note that a_τ cannot be interpreted as a global integral over Ω because of the diffusive term $\nabla \cdot (-\mu \nabla \phi^h) \hat{w}$, which is properly defined only over the elements Ω_e. Hughes and Brooks [8] indicate the circumstances under which this term of (2.23) vanishes: the medium of interest is isotropic, so that $\mu = \mu \delta_{ij}$, multi-linear isoparametric interpolation functions are employed, and the elements are rectangular. This is the case for all problems considered in this work.

2.3 Derivation of the Auxiliary Pressure Equation

We extend the segregated velocity-pressure approach of Rice and Schnipke [1] to derive the new pressure equation. As previously discussed, the method of

weighted residuals is employed to discretize the momentum eqs. (2.2). We next turn to the continuity eq. (2.1), by which pressure is indirectly determined. Specifically, if the correct pressure is substituted in the momentum equations, then the resulting velocity field satisfies the continuity condition. While many techniques attempt to remedy the problem of indirect pressure linkage, most of these produce either unstable or inaccurate solutions. In our method the problem of indirect pressure specification is solved by manipulating the momentum and continuity equations to derive a subsidiary Poisson equation for pressure.

Derivation of the auxiliary pressure equation begins with consideration of the weak form of the element continuity equation,

$$\int_{\Omega_e} \boldsymbol{N} \nabla \cdot \rho \boldsymbol{u} d\Omega = 0, \tag{2.25}$$

where for Galerkin's method of weighted residuals the weighting functions and interpolants are identical. Applying the chain rule and Green's formula to this equation and approximating the velocity components by their interpolated values then produce in the two-dimensional case

$$\int_{\Omega_e} \rho \sum_{k=1}^{2} \frac{\partial \boldsymbol{N}}{\partial x_k} \boldsymbol{N}^t \boldsymbol{u}_k d\Omega = \int_{\Gamma_e} \rho \boldsymbol{N} \sum_{k=1}^{2} u_k n_k d\Gamma, \tag{2.26}$$

where the n_k denote the components of the unit vector normal to Γ, and in this context the $\boldsymbol{u}_k$ are element vectors. Note that the surface integrals are zero everywhere except for the inflow and outflow boundaries, where they represent mass flux crossing the boundaries.

At this point the pressure variable is introduced into the system. First, the form of the discretized system of equations for momentum is modified to

emphasize the pressure variable. These equations become

$$A_{\phi}^{e}\boldsymbol{\phi}^{e} = \hat{\boldsymbol{f}}_{j}^{e} - \int_{\Omega_e} \tilde{\boldsymbol{N}} \frac{\partial p}{\partial x_j} d\Omega, \tag{2.27}$$

where A_{ϕ}^{e} indicates the coefficient matrix corresponding to the bilinear form (2.14) and

$$\hat{\boldsymbol{f}}_{j}^{e} = \int_{\Gamma_e} \boldsymbol{N}\, \mu \nabla\phi \cdot \boldsymbol{n} d\Gamma + \int_{\Omega_e} \tilde{\boldsymbol{N}}\, \rho \hat{g}_j \, d\Omega. \tag{2.28}$$

Note that for SUPG convection modeling

$$\tilde{\boldsymbol{N}} = \boldsymbol{N} + \tau_1 \left(u_1 \frac{\partial \boldsymbol{N}}{\partial x_1} + u_2 \frac{\partial \boldsymbol{N}}{\partial x_2} \right) + \tau_2 \left(\breve{u}_1 \frac{\partial \boldsymbol{N}}{\partial x_1} + \breve{u}_2 \frac{\partial \boldsymbol{N}}{\partial x_2} \right). \tag{2.29}$$

We introduce an approximation by assuming that the pressure gradient remains constant over a given element and thus can be removed from the integral. Hence, the following explicit representation of the velocity results:

$$\boldsymbol{\phi}^{e} = \left[A_{\phi}^{e} \right]^{-1} \left(\hat{\boldsymbol{f}}_{j}^{e} - \int_{\Omega_e} \tilde{\boldsymbol{N}} d\Omega \frac{\partial p}{\partial x_j} \right). \tag{2.30}$$

Next, velocity is expressed in terms of the pressure gradient and is substituted into the continuity equation. We assume that the pressure gradients can be expressed as constants at each node of a given element, as given by the vector $\boldsymbol{c}_{\phi}^{e}$ in the following equation:

$$\boldsymbol{\phi}^{e} = \bar{\boldsymbol{\phi}}^{e} - \boldsymbol{c}_{\phi}^{e} \frac{\partial p}{\partial x_j}, \tag{2.31}$$

where $\bar{\boldsymbol{\phi}}^{e}$ are considered to be partial velocities, as determined by the momentum equations with the effect of pressure removed.

Equating terms that represent the pressure contributions to velocity in the eqs. (2.30) and (2.31) and then assembling the appropriate global systems produce the following set of equations, which can be used to calculate the pressure

coefficients $\boldsymbol{c}_\phi$:

$$A_\phi \boldsymbol{c}_\phi = \boldsymbol{s}, \tag{2.32}$$

where $\boldsymbol{c}_\phi = \sum_{e=1}^{E} \boldsymbol{c}_\phi^e$ and

$$\boldsymbol{s} = \sum_{e=1}^{E} \int_{\Omega_e} \tilde{\boldsymbol{N}}\, d\Omega. \tag{2.33}$$

Instead of solving the linear system (2.32) to obtain the pressure coefficients, these nodal values are approximated by

$$c_i = \frac{s_i}{a_{ii}}, \;\; i = 1, \ldots, n, \tag{2.34}$$

where $A_\phi = [a_{ij}]$, $\boldsymbol{c}_\phi = [c_1, \ldots, c_n]^t$, and n indicates the global system dimension. Note that if ϕ_i is specified as a Dirichlet boundary condition, then (2.31) indicates that $\phi_i = \bar{\phi}_i = \phi_{b.c.}$, so that $c_i = 0$. Next, substitution of (2.31) into (2.26) for the element vectors $\boldsymbol{u}_k$ and interpolation of the pressure gradients enable the element pressure vector, $\boldsymbol{p}$, which is considered constant for a given element, to be placed outside the integrals. The following system results:

$$A_p^e \boldsymbol{p}^e = \boldsymbol{f}_p^e, \tag{2.35}$$

where the coefficient matrix is symmetric positive definite, as given by

$$A_p^e = \int_{\Omega_e} \rho \sum_{k=1}^{2} \boldsymbol{N}^t \boldsymbol{c}_{u_k}^e \left(\frac{\partial \boldsymbol{N}}{\partial x_k} \frac{\partial \boldsymbol{N}}{\partial x_k}^t \right) d\Omega, \tag{2.36}$$

and

$$\boldsymbol{f}_p^e = \int_{\Omega_e} \rho \sum_{k=1}^{2} \left(\frac{\partial \boldsymbol{N}}{\partial x_k} \boldsymbol{N}^t \bar{\boldsymbol{u}}_k \right) d\Omega - \int_{\Gamma_e} \rho \boldsymbol{N} \sum_{k=1}^{2} (u_k n_k)\, d\Gamma. \tag{2.37}$$

We next consider the formation of the partial velocities $\bar{\boldsymbol{u}}_k$, which are used to compute the right-hand-side vector $\boldsymbol{f}_p^e$ of (2.35). The nodal form of (2.30) is

given by

$$\phi_i^e = \frac{1}{a_{ii}} \left(-\sum_{\substack{l=1 \\ l \neq i}}^{n} (a_{il}\phi_l^e) + \hat{f}_{j_i}^e - \int_{\Omega_e} \tilde{N}_i d\Omega \frac{\partial p}{\partial x_j} \right), \ 1, \ldots n, \tag{2.38}$$

where the notation $\hat{f}_{j_i}^e$ indicates the i^{th} component of the vector $\hat{\boldsymbol{f}}_j^e$. The components of the partial velocity $\bar{\boldsymbol{\phi}} = [\bar{\phi}_1, \ldots, \bar{\phi}_n]^t$ can thus be represented by

$$\bar{\phi}_i = \frac{1}{a_{ii}} \left(-\sum_{\substack{l=1 \\ l \neq i}}^{n} (a_{il}\phi_l) + \hat{f}_{j_i} \right), \ i = 1, \ldots, n. \tag{2.39}$$

Note that the algebraic form of the partial velocities developed in the segregated solution approach of Rice and Schnipke [1] is retained, although the intermediate linearized momentum systems are not solved to obtain trial velocities for use in the row sums.

3 Formation of the Jacobian Matrix

We next consider analytic formation of the Jacobian matrix corresponding to (2.6), which is given by

$$\boldsymbol{F}'(\boldsymbol{w}) = A(\boldsymbol{w}) + A'(\boldsymbol{w})\boldsymbol{w} - \boldsymbol{b}'(\boldsymbol{w}), \tag{3.1}$$

where $\boldsymbol{b}'(\boldsymbol{w}) = \left[\frac{\partial b_i}{\partial w_j}\right]$. Note that if the j^{th} column of A is denoted by $\boldsymbol{a}_j(\boldsymbol{w})$, then the matrix-vector product $A(\boldsymbol{w})\boldsymbol{w}$ can be written as

$$A(\boldsymbol{w})\boldsymbol{w} = \sum_{j=1}^{n} w_j \boldsymbol{a}_j(\boldsymbol{w}), \tag{3.2}$$

so that $A'(\boldsymbol{w})\boldsymbol{w}$ can be formed as a linear combination of its columns' Jacobian matrices:

$$A'(\boldsymbol{w})\boldsymbol{w} = \sum_{j=1}^{n} w_j \boldsymbol{a}_j'(\boldsymbol{w}). \tag{3.3}$$

As shown by Curfman [9], the Jacobian contributions corresponding to the momentum equations are formed as expected. We present details only for the auxiliary pressure equation, where (3.3) implies

$$\frac{\partial A_p^e}{\partial \boldsymbol{u}_k}\boldsymbol{p} = \sum_{l=1}^{n_v} p_l \frac{\partial \boldsymbol{a}_l^{p\,e}}{\partial \boldsymbol{u}_k}, \quad k = 1,2, \tag{3.4}$$

and n_v denotes the number of nodes of an element, taken here to be four for the quadrilateral case. The element Jacobian is given by

$$\frac{\partial \boldsymbol{a}_l^{p\,e}}{\partial \boldsymbol{u}_k} = \left[\frac{\partial a_{l_i}^{p\,e}}{\partial u_{k_j}}\right], \quad k = 1,2, \tag{3.5}$$

and the two-dimensional nodal form of (2.36) indicates

$$a_{l_i}^{p\,e} = \int_{\Omega_e} \rho \left(\frac{\partial N_i}{\partial x_1}\frac{\partial N_l}{\partial x_1} \sum_{m=1}^{n_v} \frac{N_m s_m}{a_{mm}^{u_1}} + \frac{\partial N_i}{\partial x_2}\frac{\partial N_l}{\partial x_2} \sum_{m=1}^{n_v} \frac{N_m s_m}{a_{mm}^{u_2}} \right) d\Omega, \tag{3.6}$$

where $\frac{N_m s_m}{a_{mm}^{u_k}}$, $k = 1,2$, is replaced by zero if u_{k_m} is specified as a Dirichlet boundary condition. Partial differentiation of (3.6) produces

$$\begin{aligned} \frac{\partial a_{l_i}^{p\,e}}{\partial u_{k_j}} = \int_{\Omega_e} \rho \Bigg[& \frac{\partial N_i}{\partial x_1}\frac{\partial N_l}{\partial x_1} \sum_{m=1}^{n_v} \left(\frac{-N_m s_m}{(a_{mm}^{u_1})^2} \frac{\partial a_{mm}^{u_1}}{\partial u_{k_j}} + \frac{N_m}{a_{mm}^{u_1}} \frac{\partial s_m}{\partial u_{k_j}} \right) + \\ & + \frac{\partial N_i}{\partial x_2}\frac{\partial N_l}{\partial x_2} \sum_{m=1}^{n_v} \left(\frac{-N_m s_m}{(a_{mm}^{u_2})^2} \frac{\partial a_{mm}^{u_2}}{\partial u_{k_j}} + \frac{N_m}{a_{mm}^{u_2}} \frac{\partial s_m}{\partial u_{k_j}} \right) \Bigg] d\Omega, \end{aligned} \tag{3.7}$$

The term s_m is given by (2.33), so that

$$\frac{\partial s_m}{\partial u_{k_j}} = \sum_{e=1}^{E} \int_{\Omega_e} \frac{\partial \tilde{N}_m}{\partial u_{k_j}} d\Omega, \tag{3.8}$$

where

$$\begin{aligned} \frac{\partial \tilde{N}_m}{\partial u_{k_j}} = & \frac{\partial \tau_1}{\partial u_{k_j}} \left(u_1 \frac{\partial N_m}{\partial x_1} + u_2 \frac{\partial N_m}{\partial x_2} \right) + \tau_1 N_j \frac{\partial N_m}{\partial x_k} \\ & + \frac{\partial \tau_2}{\partial u_{k_j}} \left(\breve{u}_1 \frac{\partial N_m}{\partial x_1} + \breve{u}_2 \frac{\partial N_m}{\partial x_2} \right) + \tau_2 \left(\frac{\partial \breve{u}_1}{\partial u_{k_j}} \frac{\partial N_m}{\partial x_1} + \frac{\partial \breve{u}_2}{\partial u_{k_j}} \frac{\partial N_m}{\partial x_2} \right). \end{aligned} \tag{3.9}$$

Because of the analogous forms of $\frac{\partial \boldsymbol{f}_p}{\partial \boldsymbol{u}_1}$ and $\frac{\partial \boldsymbol{f}_p}{\partial \boldsymbol{u}_2}$, we present only the submatrix $\frac{\partial \boldsymbol{f}_p}{\partial \boldsymbol{u}_1}$:

$$\frac{\partial \boldsymbol{f}_p}{\partial \boldsymbol{u}_1} = \sum_{e=1}^{E} \int_{\Omega_e} \rho \left(\frac{\partial \boldsymbol{N}}{\partial x_1} \boldsymbol{N}^t \frac{\partial \bar{\boldsymbol{u}}_1}{\partial \boldsymbol{u}_1} + \frac{\partial \boldsymbol{N}}{\partial x_2} \boldsymbol{N}^t \frac{\partial \bar{\boldsymbol{u}}_2}{\partial \boldsymbol{u}_1} \right) d\Omega - \sum_{e=1}^{E} \int_{\Gamma_e} \rho \boldsymbol{N} \frac{\partial (u_1 n_1)}{\partial \boldsymbol{u}_1} d\Gamma. \tag{3.10}$$

Differentiation of (2.39) yields

$$\begin{aligned} \frac{\partial \bar{u}_{k_i}}{\partial u_{1_j}} &= \frac{\partial}{\partial u_{1_j}} \left[\frac{1}{a_{ii}^{u_k}} \left(- \sum_{\substack{l=1 \\ l \neq i}}^{n} (a_{il}^{u_k} u_{k_l}) + \hat{f}_{k_i} \right) \right] \qquad (3.11) \\ &= \frac{1}{a_{ii}^{u_k}} \left((\delta_{ij} - 1) \delta_{k1} a_{ij}^{u_k} - \frac{\partial a_{ii}^{u_k}}{\partial u_{1_j}} \bar{u}_i - \sum_{\substack{l=1 \\ l \neq i}}^{n} \frac{\partial a_{il}^{u_k}}{\partial u_{1_j}} u_{k_l} + \frac{\partial \hat{f}_{k_i}}{\partial u_{1_j}} \right), \; k = 1, 2, \end{aligned}$$

where δ_{ij} denotes the Kronecker delta. Note that if u_{k_i} is specified as a Dirichlet boundary condition so that $u_{k_i} = \bar{u}_{k_i}$, then $\frac{\partial \bar{u}_{k_i}}{\partial u_{k_j}} = \delta_{ij}$ and $\frac{\partial \bar{u}_{k_i}}{\partial u_{\hat{k}_j}} = 0$.

4 Numerical Results

The objective of this section is to evaluate the efficiency of the approximate Newton strategies for the solution of convective-diffusive flow problems with varying degrees of nonlinearity when the previously described velocity-pressure formulation is employed. Of particular interest is a comparison between the Newton-like schemes and the segregated solution approach of Rice and Schnipke [1], since the velocity-pressure formulations of the two approaches are closely related. All computational results were generated on a single processor of a CRAY Y-MP at the NASA Langley Research Center.

4.1 Description of Test Problems

We employ three basic test problems: developing flow in a plane channel, flow over a backward-facing step, and natural convection within an enclosed region. Since these cases have been previously examined by numerous other researchers, the accuracy of our solutions can easily be validated. We discretize each of these test problems with a coarse and fine mesh of rectangular elements, and alter the fluid properties to create varying degrees of nonsymmetry and nonlinearity.

We first consider isothermal developing flow in a 1m by 100m rectangular plane channel at Reynolds numbers of 75, 150, 400, 800, and 1600. A uniform velocity profile is specified at the inlet, while zero pressure is imposed at the outlet. No slip boundary conditions are given for the top wall, and a symmetry condition exists at the bottom of the grid. These test cases are similar to cases considered by Rice and Schnipke [1] and Gosman et al. [10] as well as various other researchers, and are presented for benchmark comparisons of flow features. The meshes DUCT1 and DUCT2 are employed, which respectively have the dimensions of 7×61 and 11×181.

We examine isothermal flow over a backward-facing step, where the problem and mesh geometry are adapted from Rice and Schnipke [1] and Gartling [11]. Although the problem geometry is simple, the flow exhibits complex features that are found in many other cases of practical interest. The channel is 10.1mm by 200mm and has fully-developed flow specified at its inlet, $0 \leq x_2 \leq 5.2$mm, so that the channel region upstream of the step is excluded. All solid walls are

assumed to be non-slip, and zero pressure is assumed at the outflow boundary. The inflow is specified by $u_1(x_2) = .222x_2(5.2 - x_2)$ for $0 \leq x_2 \leq 5.2$mm, producing an average inflow velocity of $u_1 = 1$mm/s. Fluid properties are varied to produce flow at Reynolds numbers 100 and 200, which duplicate the experimental conditions of Armaly et al. [12]. Meshes of sizes 25×43 and 35×63 are considered as test cases STEP1 and STEP2.

While the previous flow problems include only the momentum and pressure equations, thermally driven cavity flow with the Boussinesq approximation incorporates the thermal energy equation and a constitutive equation for density. The problem geometry is taken from the comparative study of de Vahl Davis and Jones [13], in which various numerical methods are considered for the natural convection problem of air at a Prandtl number of .71 in a square cavity with differentially heated vertical sides. The walls of the problem domain in the x_1-direction are insulated, while the walls in the x_2-direction are held at temperatures T_1 and T_2, where $T_1 > T_2$. Gravitational force is assumed to act in the $-x_2$ direction. In accordance with the work of Schnipke [14], we analyze the problem on a uniform 25×25 grid, labeled CONV1, for Rayleigh numbers $10^3, 10^4$, and 10^5 and on a uniform 41×41 grid, labeled CONV2, for the Raleigh number 10^6. Our solution accuracy is compared with that of Schnipke [14] as well as with the benchmark solution of de Vahl Davis [15].

Table 1 contains various parameters of the analytically formed Jacobian matrices associated with these test problems, including the mesh dimension, matrix dimension, and approximate number of nonzeros. Note that the Ja-

cobian's nonzero structure tends to vary slightly for a given mesh according to flow parameters and even among different Newton iterations of a particular problem. However, this table provides adequate estimates for our purposes, since the number of nonzeros for an individual grid deviated a maximum of 0.5 percent for all test problems.

4.2 Solution Procedure

We begin by generating an initial approximation for the Newton-like schemes by performing a variable number of iterations of the segregated solution approach. Experimentation has shown that reduction of the relative residual norm, $\frac{\|\boldsymbol{F}\|_2}{\|\boldsymbol{F}_0\|_2} < \epsilon_1$, to less than 0.5 works well for the developing duct flow and natural convection problems, while the slightly larger value of 1.0 is sufficient for the backward-facing step problems.

Analytic formation of the Jacobian matrix proved to be very efficient, requiring only four to five times as long as a single evaluation of the residual vector $\boldsymbol{F}$ for the cases under consideration. Although the residual can be evaluated with little additional effort during the assembly of the Jacobian matrix, we elect to form the residual as the first step of each Newton iteration to monitor convergence and to indicate whether evaluation of the Jacobian is necessary in the Newton process. For all cases under consideration, we form a new Jacobian matrix $\boldsymbol{F}'(\boldsymbol{w}^{k+1})$ only if $\frac{||\boldsymbol{F}(\boldsymbol{w}^k)||_2}{||\boldsymbol{F}(\boldsymbol{w}^{k-1})||_2} > .25$.

In addition to analytic formation of the Jacobian matrix, we consider forward differencing approximations. Both techniques accurately capture the flow field for the test cases; however, even with the use of strategies for minimizing the

number of function evaluations, the differencing approach is much more costly than analytic formation. Since for most flow problems of practical interest, the number of required function evaluations for the differencing approximation significantly exceeds five, the utility of the differencing approach is limited.

The natural ordering of the nodes is used, where all unknowns for a particular grid point are numbered before proceeding to the succeeding node. We solve the linearized Newton systems by banded LU decomposition using LAPACK [16]. While inexact Newton methods that incorporate Krylov projection techniques for the solution of the linear systems are often preferable in terms of storage requirements and computational effort, these methods require appropriate preconditioning strategies and convergence monitoring. Since these issues can complicate the solution process, particularly for nonsymmetric systems, direct solution allows us to focus on the problem formulation without these additional concerns.

4.3 Comparison of Results

Convergence and timing information for the segregated and simultaneous solution approaches are presented in Tables 2, 3, and 4 for developing duct flow, backward-facing step flow, and natural convection, respectively. Iteration counts for the approximate Newton's method are given in the form a/b, where a indicates the number of iterations of the segregated solver needed to generate an appropriate initial approximation, and b denotes the number of Newton iterations. Damping is required within the approximate Newton approach only for solution of the natural convection problem with a Raleigh number of 10^6.

Within the segregated solver a variable-band Cholesky factorization method [17] is used to solve the symmetric pressure equation. In addition, a tridiagonal matrix algorithm [2], [14] is employed for the momentum equations.

Our experiments indicate that for all test problems the approximate Newton method, using the velocity-pressure formulation discussed in Section 2, determines the flow solution both rapidly and accurately. Differences between solutions obtained by the segregated solution technique and the approximate Newton method fluctuate only according to the specified strictness of the convergence criteria. Key flow features agree with those discussed by Rice and Schnipke [1], Gosman et al. [10], and Armaly et al. [12].

The new velocity-pressure-temperature formulation overcomes the difficulty of indirect pressure linkage inherent in the coupled system of Navier-Stokes and continuity equations. The auxiliary pressure equation generates nonzero terms for all diagonal elements of the Jacobian matrix, thereby facilitating the use of rapidly converging Newton-like methods without requiring reordering strategies or modification of the diagonal terms.

This approach is particularly useful for finely discretized problems with high degrees of nonlinearity. As discussed by MacArthur and Patankar [4], since the segregated solver reduces the residual only locally at each step of the solution process, its convergence rate is strongly influenced by the number of unknowns. In addition, the decoupling inherent in the segregated solver causes relatively slow transmission of boundary data throughout the problem domain. In contrast, the Newton-like schemes reduce the residual for the entire domain and

instantaneously propagate boundary data throughout the problem.

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Table 1: **Test Problem Parameters**

Problem Name	**Mesh Dimension**	**Jacobian Dimension**	**Number of Nonzeros**
DUCT1	7×61	1,281	33,750
DUCT2	11×181	5,973	181,355
STEP1	25×43	3,225	105,380
STEP2	35×63	6,615	225,710
CONV1	25×25	3,125	108,600
CONV2	41×41	8,405	291,875

Table 2: **Comparison of Solution Techniques: Problems DUCT1 and DUCT2**

Reyn. #	**Solution Method**	**Problem: DUCT1**			**Problem: DUCT2**		
		# of Iter	**Time (sec)**	$\frac{\|\boldsymbol{F}\|_2}{\|\boldsymbol{F}_0\|_2}$ $(\times 10^{-7})$	**# of Iter**	**Time (sec)**	$\frac{\|\boldsymbol{F}\|_2}{\|\boldsymbol{F}_0\|_2}$ $(\times 10^{-7})$
75	Seg.	43	6.86	7.75	43	31.29	9.16
	Newton	2/4	1.56	0.70	2/5	8.60	3.58
150	Seg.	47	7.50	8.24	51	37.13	8.53
	Newton	2/4	1.56	1.80	3/6	9.17	5.91
400	Seg.	60	9.59	8.43	64	46.85	9.89
	Newton	3/7	1.77	1.78	3/5	11.39	1.44
800	Seg.	73	11.77	8.39	81	59.84	9.67
	Newton	3/5	2.12	0.26	2/6	12.04	4.73
1,600	Seg.	83	13.50	9.55	107	79.76	9.20
	Newton	5/6	2.39	3.41	2/5	15.02	6.10

Seg.: Segregated Solution
Newton: Approximate Newton's Method
Convergence Criterion: $\frac{||\boldsymbol{F}||_2}{||\boldsymbol{F}_0||_2} < 10^{-6}$

Table 3: **Comparison of Solution Techniques: Problems STEP1 and STEP2**

Reyn. #	**Solution Method**	**Problem: STEP1**			**Problem: STEP2**		
		# of Iter	**Time (sec)**	$\frac{\|\boldsymbol{F}_{final}\|_2}{\|\boldsymbol{F}_0\|_2}$ $(\times 10^{-7})$	**# of Iter**	**Time (sec)**	$\frac{\|\boldsymbol{F}_{final}\|_2}{\|\boldsymbol{F}_0\|_2}$ $(\times 10^{-7})$
100	Seg.	127	51.96	9.00	231	191.64	9.87
	Newton	4/8	9.01	6.96	4/7	20.03	2.67
200	Seg.	179	73.02	9.58	306	255.55	9.00
	Newton	4/8	13.37	8.19	4/8	32.74	2.75

Seg.: Segregated Solution
Newton: Approximate Newton's Method
Convergence Criterion: $\frac{||\boldsymbol{F}||_2}{||\boldsymbol{F}_0||_2} < 10^{-6}$

Table 4: **Comparison of Solution Techniques: Problems CONV1 and CONV2**

Problem	**Solution Method**	**# of Iter**	**Time (sec)**	$\frac{\|\boldsymbol{F}_{final}\|_2}{\|\boldsymbol{F}_0\|_2}$ $(\times 10^{-7})$
CONV1-10^3	Seg.	90	41.48	9.93
	Newton	2/6	14.20	2.61
CONV1-10^4	Seg.	120	57.34	9.79
	Newton	3/7	15.67	3.92
CONV1-10^5	Seg.	143	67.01	9.88
	Newton	3/8	19.32	8.81
CONV2-10^6	Seg.	253	152.43	9.39
	Newton	4/10	44.11	5.33

Seg.: Segregated Solution
Newton: Approximate Newton's Method
Convergence Criterion: $\frac{||\boldsymbol{F}||_2}{||\boldsymbol{F}_0||_2} < 10^{-6}$