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ROBUST SEMIDIRECT FINITE DIFFERENCE METHODS FOR SOLVING THE NAVIER–STOKES AND ENERGY EQUATIONS

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SUMMARY

Semidirect solution techniques can be an effective alternative to the more conventional iterative approaches used in many finite difference methods. This paper summarizes several semidirect techniques which generally have not been applied to the Navier–Stokes and energy equations in finite difference form. The methods presented use both successive substitution and Jacobian-based updates as well as two variations of Broyden's full matrix update. A hybrid method is also presented, as is a norm-reducing search technique that can be used to enhance the convergence characteristics of any semidirect approach. These methods have been compared with the well known iterative methods SIMPLE and SIMPLER. The comparison was performed on the natural convection and driven cavity problems. The semidirect methods proved to be reliably convergent without the need for *a priori* specification of variable under-relaxation factors, which was necessary with the iterative methods. Natural convection and driven cavity solutions have been readily obtained with the proposed methods for Rayleigh and Reynolds numbers up to 10^9 and 10^6 respectively. Of the semidirect techniques, the hybrid approach was the most robust. From an arbitrary zero initial guess this method was able to obtain a solution to the natural convection problem for Rayleigh numbers three orders of magnitude larger than was possible with the Newton–Raphson update. The computational effort required by the semidirect methods is comparable to that required by the iterative methods; however, the memory requirements can be significantly greater.

KEY WORDS Semidirect methods Finite difference formulation Robust solutions Navier–Stokes and energy equations

INTRODUCTION

The intent of this report is to show how certain semidirect and iterative methods compare when applied to the fluid dynamics equations in finite difference form. The performance of each method depends not only on the solution strategy but also on the discretization practice selected. A detailed description and analysis of several current discretization practices is given by Nieckele.[1] The power law scheme as described by Patankar[2] was used in all of the methods presented in this

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paper. Although selection of the particular discretization practice is important, attention here is focused primarily on the solution method. It is important to note, however, that since the performance of a method does depend on the particular discretization strategy, a direct comparison between the solution techniques presented here and those published elsewhere would require similar discretization practices.

The fundamental difference between iterative and semidirect methods is that with the latter the residual or error is exactly equal (except for round-off errors) to zero for the entire calculation domain at the end of an iteration, whereas in the former the residual is only locally reduced at each iteration. Therefore the iterations required for convergence with semidirect methods are fairly insensitive to the number of unknowns or grid mesh, and for linear problems no iterations are required. The computational effort, however, does increase dramatically as the number of unknowns is increased, owing to the fact that all unknowns are solved for simultaneously. With many iterative approaches, including both SIMPLE and SIMPLER, the iterations required for convergence are strongly dependent on the number of unknowns, and hence the computational effort also increases dramatically as the grids are refined. There are, however, some iterative methods that do not exhibit this strong iteration dependence on grid refinement. One such method is the multigrid strategy first put forth by Brandt.[3] In this approach a series of grids is used to enhance residual reduction. Thus the multigrid strategy attempts a more global residual reduction than is typical with many iterative methods.

An important difference between the iterative and semidirect methods is the role the initial guess plays in the solution process. Semidirect methods tend to be more sensitive to the choice of the initial guess than the iterative methods. Since iterative methods are relatively insensitive to the initial guess, solutions can be obtained quite systematically for various degrees of non-linearities for the same initial guess. Unfortunately, as the non-linearity becomes large, use of a previous solution at a milder non-linearity as an initial guess usually does not help the solution process significantly. With the semidirect methods, almost the opposite is true. Use of a previous solution as an initial guess will greatly facilitate the solution process for strongly non-linear problems.

From the authors' perspective, the most desirable feature of the semidirect approach is the elimination of the need to prescribe under-relaxation factors and hence the potential to obtain a solution in a more systematic fashion than is typical with many iterative methods. Another desirable feature of the semidirect approach is the ability to eliminate residuals completely from the entire calculation domain. Thus, if a discrete solution can be obtained, machine precision accuracy for each field variable is possible. The most serious limitations of the semidirect methods are the memory requirements and the computational effort required as the number of unknowns becomes large.

Before presenting results of the comparison, a brief discussion of the various methods used will be given. Since the iterative methods SIMPLE and SIMPLER are well known and described in detail in Reference 2, only the semidirect methods will be presented. These methods have been constructed by combining desirable features of several techniques from various applications reported in the literature. A few of the more pertinent articles relating to semidirect solution techniques as applied here are given below, followed by a section summarizing the implementation of the semidirect methods constructed for use in the comparison.

EXISTING SOLUTION TECHNIQUES

Two of the most pertinent semidirect finite difference methods investigated were those due to Vanka and Leaf[4] and Braaten.[5] In each of these studies the methods were tested on a driven cavity and sudden expansion problem. In the first semidirect method of Vanka and Leaf the finite

difference primitive variable formulation was solved in a fully coupled manner by sparse matrix techniques. The discrete continuity and momentum equations were solved in their original form using a Newton–Raphson linearization technique.

In a later paper Vanka[6] tried to extend the approach to turbulent flows. The fully coupled solution of the momentum equations was followed by the fully coupled solution of the turbulence equations arising from the K–E model. Because of the source terms in the k–ε model, the Newton–Raphson technique was unable to yield a semidirect solution to the turbulence equations for the generation and dissipation rates encountered.

In the work of Braaten[5] three semidirect methods were developed. The first was a primitive variable formulation very similar to that of Vanka and Leaf. The only differences were that in Braaten's formulation no Newton–Raphson linearization was employed and small non-zero elements were placed on the diagonal of the coefficient matrix to eliminate the need for reordering the momentum and continuity equations. In Braaten's second and third methods pressure was eliminated from the calculation by a penalty function formulation. The penalty function approach is common in finite element methods and is described by Thomasset.[7] Direct solutions of the resulting set of equations were implemented by using a successive substitution scheme in one instance and a Newton–Raphson scheme similar to Vanka's in another. All methods were implemented using sparse matrix techniques.

Unlike finite difference formulations, applications of semidirect methods to finite element formulations are extremely common because these formulations result in a set of algebraic equations that are not diagonally dominant. General approaches are given by Bergan *et al.*[8] and Matthies and Strang,[9] and a review of some promising methods is given by Sticklin *et al.*[10] and Bathe.[11] A particularly interesting paper by Bathe and Cimento[12] describes a procedure for enhancing the convergence characteristic of their semidirect approach. In fact, the ideas put forth by Bathe and Cimento[12] have been applied by Engleman *et al.*[13] to solve the driven cavity recirculation problem. Although it was obvious that his discretizatios were not tailored for fluid mechanics (convergence problems were encountered for Reynolds numbers greater than 500), the applicability of this method for non-symmetric sparse matrices was illustrated.

In addition to the more conventional approaches used with finite difference and finite element formulations, alternative approaches were investigated with the hope of constructing more robust methods. This effort was concentrated in three areas. In the first two areas methods that extend the radius of convergence were investigated. These methods include hybrid methods, which incorporate multiple linearization algorithms into the solution strategy (see Levenberg,[14] Marquardt,[15] Powell[16] and Blue[17]), and parameter methods (see Bryson and Ho[18]), which seek to increase the radius of convergence directly by modifying the path of the solution process with a suitably chosen parameter. The third area dealt with the reduction of computational effort by using superlinear methods based on orthogonalization techniques. This approach is described by Broyden[19, 20] and Broyden *et al.*[21].

FORMULATION AND IMPLEMENTATION

The next few paragraphs illustrate the approach used to formulate and implement the semidirect solution techniques. The formulation is accomplished by first discretizing the governing elliptic equations and then structuring the resulting coupled non-linear algebraic equations in a suitable vector representation.

The general form of the governing equations to be discretized is given by

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) + S. \tag{1}$$

Equation (1) is composed of an unsteady term and a convection, diffusion and source term. The particular values of ϕ, Γ and S are determined directly from the transport equations governing the problem of interest. For this study only steady state solutions are considered; therefore the first term in equation (1) is ignored.

The discretization practice chosen here utilizes a control volume formulation and a staggered grid. Equation (1) is integrated over each of the control volumes for the continuity equation ($\phi = 1$) and for each of the dependent variables to yield a set of coupled algebraic equations.

The discretization equations can be conveniently cast into vector form by defining a suitable state vector. For this study the state vector is defined by

$$\mathbf{x} = (u_1, \ldots u_{N^d}, v_1, \ldots v_{N^d}, p_1, \ldots p_{N^d}, T_1, \ldots T_{N^d})^T, \tag{2}$$

where $_{N^d}$ is the number of grid points for each dependent variable. Using the definitions given by equation (2), the discretization equations can be written in vector notation as

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b}, \tag{3}$$

where $\mathbf{x}$ is the N-dimensional state vector, $\mathbf{A}$ is the $(N \times N)$-dimensional coefficient matrix and $\mathbf{b}$ is the N-dimensional source vector. The form of equation (3) and the related $\mathbf{A}$-matrix is given in Figure 1. The elements of $\mathbf{A}$-matrix are the coefficients of the discretization equations. These coefficients are a function of the local convective and diffusive fluxes and are evaluated by the power law scheme described by Patankar.[2]

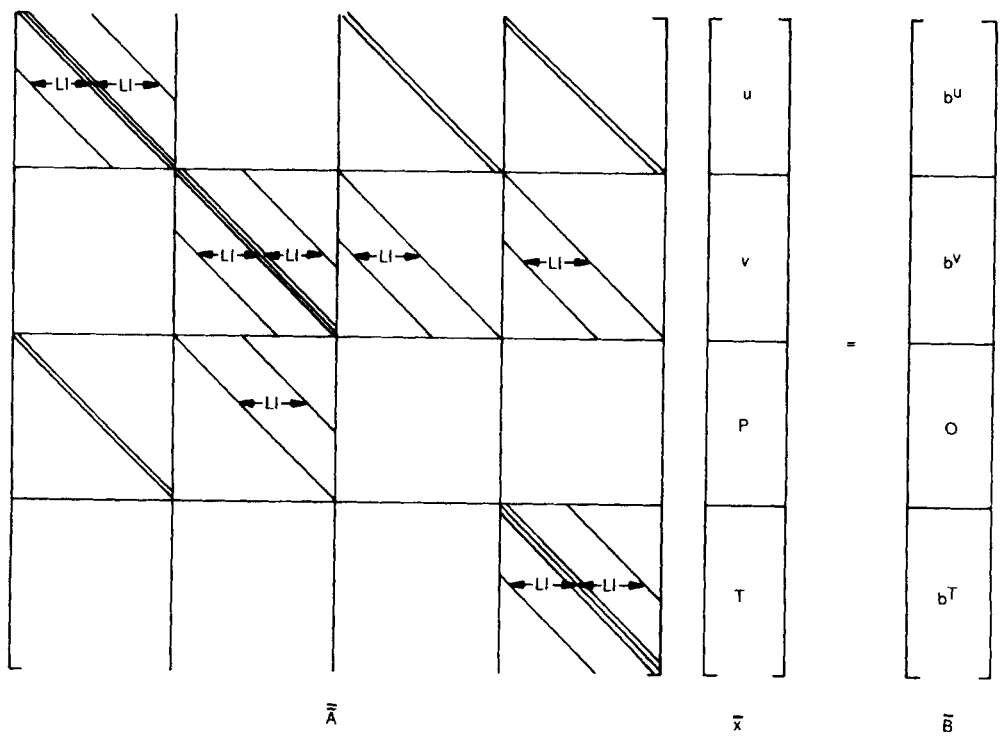

Figure 1. System representation

It is the goal of the solution process to solve for $\mathbf{x}$ such that the residual vector given by

$$\mathbf{R} \equiv \mathbf{b} - \mathbf{A} \cdot \mathbf{x} \tag{4}$$

is identically equal to zero.

All of the semidirect approaches used in this paper have been implemented by using a fixed point iterative scheme in vector form. The form of the general vector update is given by

$$\mathbf{x}_{i+1} = \mathbf{x}_i + t\mathbf{P}(\mathbf{x}_i), \tag{5}$$

where $\mathbf{P}$ is the direction vector and t is a scalar multiplier that can be set equal to one or can be determined by a search procedure. When a search is used, this scalar multiplier serves to select the appropriate length of the direction vector such that the updated state vector will minimize or reduce the residual relative to a full step update (i.e. $t = 1$). An expression for the direction vector that results in a zero residual vector at the end of an iterative step is given by

$$\mathbf{P} = \mathbf{H}^{-1} \cdot \mathbf{R}. \tag{6}$$

In equation (6) $\mathbf{H}$ is the generalized coefficient matrix, which takes on different forms depending on the particular solution method.

All of the semidirect techniques described in this paper can be represented compactly in terms of equation (5) by a suitable choice of the direction vector and the corresponding search parameter. The semidirect methods, along with each associated direction vector and search parameter, are summarized in Table I. The forms of the direction vector used for each of these methods are given in Table II. In Table I the undetermined parameters are ε, t^* and δ. Selection of δ is based on t^*. Selection of ε and t^* is done by performing a search. ε is generally some small value, while t^* generally ranges between zero and two. The value of t^* is determined by solving the following auxiliary minimization problem:

$$\partial y / \partial t = 0, \tag{7}$$

where

$$y \equiv \mathbf{R}(\mathbf{x}_i + t\mathbf{P}_i) \cdot \mathbf{R}(\mathbf{x}_i + t\mathbf{P}_i). \tag{8}$$

Equation (8) illustrates that y can be interpreted as the square of the Euclidean norm of the residual vector; therefore the solution of equation (7) for $t = t^*$ results in a strict norm minimization update. It is often more effective to perform norm reduction rather than strict minimization. A norm reduction strategy has been used in this study by relaxing the equality

Table I. Summary of methods developed

Method	Direction vector	Search parameter
A-matrix or successive substitution (SS)	$\mathbf{P}_i = \mathbf{P}_i^A$	$t = 1$
Newton–Raphson (NR)	$\mathbf{P}_i = \mathbf{P}_i^J$	$t = 1$
Modified Broyden (MB)	$\mathbf{P}_i = \mathbf{P}_i^B$	$t = 1$
Recursive Broyden (RB)	$\mathbf{P}_i = \mathbf{P}_i^R$	$t = 1$
Steepest descent (SD)	$\mathbf{P}_i = \mathbf{P}_i^S$	$t = \varepsilon$
Search with A-matrix update (SA)	$\mathbf{P}_i = \mathbf{P}_i^A$	$t = t^*$
Search with Jacobian update (SJ)	$\mathbf{P}_i = \mathbf{P}_i^J$	$t = t^*$
Search with Broyden update (SB)	$\mathbf{P}_i = \mathbf{P}_i^B$	$t = t^*$
Hybrid scheme (HS)	$\mathbf{P}_i = \delta \mathbf{P}_i^A + (1-\delta)\mathbf{P}_i^J$	$t = t^*$

Table II. Summary of direction vectors

Update	Form of direction vector
A-matrix	$\mathbf{P}_i^A = \mathbf{A}^{-1} \cdot \mathbf{R}$ where $\mathbf{A}$ is the matrix of a coefficients
Jacobian	$\mathbf{P}_i^J = \mathbf{J}^{-1} \cdot \mathbf{R}$ $\mathbf{J} \equiv \partial \mathbf{R} / \partial \mathbf{x}\|_{\mathbf{x}_i}$
Modified Broyden	$\mathbf{P}_i^B = \mathbf{q}_i - \rho_i(\mathbf{d}_i + \mathbf{r}_i)\mathbf{d}_i \cdot \mathbf{q}_i$ where $\mathbf{q}_i = -\mathbf{J}_0^{-1} \cdot \mathbf{R}_i$ $\mathbf{d}_i = t_{i-1}\mathbf{P}_{i-1}^B$ $\mathbf{r}_i = \mathbf{q}_i - \mathbf{P}_{i-1}^B$ $\rho_i = 1/(\mathbf{d}_i \cdot \mathbf{r}_i)$
Recursive Broyden	$\mathbf{P}_i^R = \mathbf{q}_i - \rho_i(\mathbf{d}_i + \mathbf{r}_i)\mathbf{d}_i \cdot \mathbf{q}_i$ where $\mathbf{q}_{j+1} = \mathbf{q}_j - \rho_j(\mathbf{d}_j + \mathbf{r}_j)\mathbf{d}_j \cdot \mathbf{q}_j;\ j = 1, i-1$ $\mathbf{q}_1 = -\mathbf{J}_0^{-1} \cdot \mathbf{R}_i$ $\mathbf{d}_i = t_{i-1}\mathbf{P}_{i-1}^R$ $\mathbf{r}_i = \mathbf{q}_i - \mathbf{P}_{i-1}^R$ $\rho_i = 1/(\mathbf{d}_i \cdot \mathbf{r}_i)$
Steepest descent	$\mathbf{P}_i^S = -\mathbf{R} \cdot \mathbf{J}$

constraint given in equation (7). The strategy chosen is particuarly effective since it results in less computational effort than strict minimization and for all practical purposes the same t^*. It does not, however, require a monotonic reduction in the norm at each and every iteration since the search parameter results in a norm that only approximates the minimum. As illustrated in Table I, the search has been used with all of the basic updates summarized in Table II. A detailed description of these updates as applied to the fluid dynamics equations in finite difference form is given in Reference 22.

In each of the basic updates the discretization equations are solved simultaneously and the non-linearities are resolved by iteration. The A-matrix update is a successive substitution formulation in which the generalized coefficient matrix contains only the coefficients appearing in the original discretization equations. In contrast to this formulation, the Jacobian update (which when used without a search is the well-known Newton–Raphson method) utilizes a generalized coefficient matrix composed not only of the original coefficients but also of additional terms that serve to accelerate convergence as the solution is approached. These terms are the direct result of the differentiation of the residual vector with respect to the state vector and in this implementation are determined analytically.

With the Broyden-based methods the fundamental idea is to reduce computational effort by performing approximate Jacobian updates. In Broyden's original method neither the Jacobian nor its inverse was required once the algorithm was started. Unfortunately the original approach is not directly applicable to large systems since it entails full matrix manipulations. For the methods used here, Broyden's original approach has been approximated by modifying his full matrix update. This approximation retains the essence of the original method but requires that the Jacobian and its factorization be evaluated at least on selected iterations. Two versions of the vector updates have been implemented. In the first the Jacobian and its factorization are evaluated

on alternate iterations. In the second a pseudo-direction vector, which is also based on a Broyden update, is used to better approximate the original approach. The latter update requires the user to specify how many steps are to be taken before the algorithm is to be restarted. Note that this is the only semidirect method that requires *a priori* parameter specification.

With the hybrid approach the goal is to enhance robustness by using a first-order type of linearization when the procedure is far from the solution and then switch to a second-order linearization as the solution is approached. Initially this was implemented by using a combination of steepest descent and Jacobian updates. The steepest descent algorithm was chosen because of its simplicity and the fact that factorization is not required. This algorithm forces the state vector to move in the direction of maximum change. Unfortunately the residual vector is not guaranteed to be equal to zero at the end of any iteration with this update. Performance of the steepest descent algorithm, even with a search, was not as robust as originally desired. To improve the robustness of the overall hybrid method, the steepest descent algorithm was discarded and replaced with an **A**-matrix update.

Use of any of the proposed methods requires determination of the direction vector, the general form of which is given by equation (6). Thus it can be seen that the direct methods require the evaluation of $\mathbf{H}^{-1}\cdot\mathbf{R}$, where **H** is large, non-symmetric and sparse. In actual practice the coefficient matrix is never inverted; rather the evaluation of the direction vector is performed by using a form of Gaussian elimination. For this study the Yale sparse matrix package (YSMP) (Eisenstat *et al.*[23]), which uses an efficient LU decomposition, was used to evaluate the direction vectors.

The final information needed to implement the various methods is the specification of the boundary conditions. This information may be incorporated through the source term or by treating the boundary variables in the same manner as all other dependent variables. This latter treatment facilitates the general implementation of either prescribed or gradient-type conditions, the latter of which requires the calculation of the dependent variable on the boundary.

Treatment of a prescribed value of ϕ, whether on the boundaries or anywhere in the calculation domain, is handled by initializing the appropriate state with the prescribed value of ϕ, setting the residual equal to zero, and in the corresponding row of the coefficient matrix setting the off-diagonal elements equal to zero and the diagonal element equal to one.

Evaluation of the pressure field requires two special features. When the normal velocities are prescribed on all boundaries, the pressure must be prescribed at one point in the calculation domain. The value of the pressure, which is immaterial since only pressure differences appear in the discretized equations, is prescribed as stated above. The second feature is necessary since pressure does not appear explicitly in the continuity equation, hence the main diagonal of the coefficient matrix corresponding to pressure is zero (see Figure 1). The treatment taken here is to insert a small non-zero value of 10^{-10} on the diagonal and require that the residual vector satisfy the original continuity equation.

RESULTS

The methods outlined in this paper have been used to solve both the natural convection and driven cavity problems. The square cavity problems were solved using a 30×30 irregularly spaced grid. The non-uniformity of this grid was generated in an exponential fashion with the refined grids along the boundaries. The accuracy of this grid mesh has been established by comparing results with those given by the benchmark paper of De Vahl Davis.[24] In his paper a systematic analysis of computation errors was presented. The results generated in the work presented here are within 0·5% of the benchmark solution over the range of Rayleigh numbers given by De Vahl

Davis. In this work the same grid was used for all Rayleigh numbers; thus the results at the largest Rayleigh number would be less accurate than those at or below 10^6 (the maximum value presented in the De Vahl Davis paper). The same grid was also used for the driven cavity problem. Results for the natural convection problem will be given first, followed by those of the driven cavity problem.

Natural convection problem

To solve this problem in the same form as given by others,[25] the Boussinesq approximation was invoked. The governing equations are

$$\frac{\partial U}{\partial X}+\frac{\partial V}{\partial Y}=0 \tag{9}$$

$$U\frac{\partial U}{\partial X}+V\frac{\partial U}{\partial Y}=-\frac{\partial P}{\partial X}+\frac{\partial^2 U}{\partial X^2}+\frac{\partial^2 U}{\partial Y^2}+Gr\,\theta\sin\phi, \tag{10}$$

$$U\frac{\partial V}{\partial X}+V\frac{\partial V}{\partial Y}=-\frac{\partial P}{\partial Y}+\frac{\partial^2 V}{\partial X^2}+\frac{\partial^2 V}{\partial Y^2}+Gr\,\theta\cos\phi, \tag{11}$$

$$U\frac{\partial \theta}{\partial X}+V\frac{\partial \theta}{\partial Y}=\frac{1}{Pr}\left(\frac{\partial^2\theta}{\partial X^2}+\frac{\partial^2\theta}{\partial Y^2}\right), \tag{12}$$

Subject to the following boundary conditions:

$$\theta=0; \quad X=0, \qquad \theta=1; \quad X=1,$$
$$\partial\theta/\partial Y=0; \quad Y=0, \qquad \partial\theta/\partial Y=0; \quad Y=1$$
$$U=V=0; \quad \text{all boundaries.}$$

Results are presented in terms of the Rayleigh number, which is $Ra=GrPr$. All results are given for $Pr=0{\cdot}71$. Hence large Rayleigh numbers correspond to large Grashof numbers. Results for the various methods are summarized in Table III. This table shows the number of iterations required for convergence and execution times (in seconds on the CRAY-1 computer) for each of the methods for various Rayleigh numbers. The results were generated using a zero initial guess and full factorization.

Table III. Iterations and (time) required for the direct solution of the natural convection problem (initial guess $\mathbf{x}(0)=\mathbf{0}$, full factorization)

$Ra=$ Method	10^4	10^5	10^6	10^7
Hybrid (HS)	6 (26·4)	7 (28·5)	11 (42·7)	21 (70·6)
Jacobian search (SJ)	6 (26·4)	10 (44·2)	19 (85·1)	—
Newton–Raphson (NR)	6 (25·8)	11 (44·9)	—	—
Broyden search (SB)	8 (20·2)	11 (29·7)	—	—
Recursive search (SR)	8 (16·6)	14 (24·2)	—	—
A-matrix search (SA)	9 (21·6)	25 (62·3)	—	—
Modified Broyden (MB)	8 (18·9)	—	—	—
Recursive Broyden (RB)	16 (13·3)	—	—	—

Note: no entry implies that the method failed to converge after 30 iterations or, as in the case of the Newton–Raphson method, diverged.

It was the original intent in the construction of this table to include SIMPLE and SIMPLER. However, solution of the natural convection problem by the iterative methods over the range of Rayleigh numbers illustrated in the table proved more difficult than originally anticipated. The difficulty was due to the fact that the iterative methods require the selection of a set of suitable under-relaxation factors. Hence several runs were required for each Rayleigh number. These results will be presented shortly; however, first the highlights of the semidirect methods summarized in Table III will be discussed.

Since the Newton–Raphson method is the most commonly used semidirect method, it is convenient to compare the other techniques to this approach. Table III illustrates that with the Newton–Raphson method solutions were obtained from a zero initial guess for $Ra \leqslant 10^5$. This same result has been reported by Stevens[25] and Taylor and Ijam.[26] Inspection of the table shows that the Newton–Raphson scheme is superior to two of the proposed strategies. It also shows that there are two methods that are as robust as the Newton–Raphson method and two that are significantly more robust.

Use of the modified and recursive Broyden methods without a search is not advised for problems with substantial non-linearities. When used with a search, however, they can be as robust as the Newton–Raphson method yet require only half the computational effort. The search with the A-matrix update, although capable of obtaining a solution for the same degree of non-linearity as the Newton–Raphson method, requires significantly more iterations than the latter. The successive substitution method, which is the same as the A-matrix update without the search, does not appear. This method, although effective for solving the driven cavity problem, as will be illustrated shortly, required more than 30 iterations to obtain a solution to the natural convection problem, even for $Ra = 10^4$.

Table III illustrates the superiority of the hybrid scheme. The method is in fact even more robust than indicated here since no results have been reported for situations that require more than 30 iterations. By removing this restriction, the hybrid method was capable of obtaining a solution from a zero initial guess for $Ra = 10^8$. Figure 2 illustrates the performance of the hybrid method as a function of the Rayleigh number. The performance of this method represents a significant improvement over existing semidirect techniques.

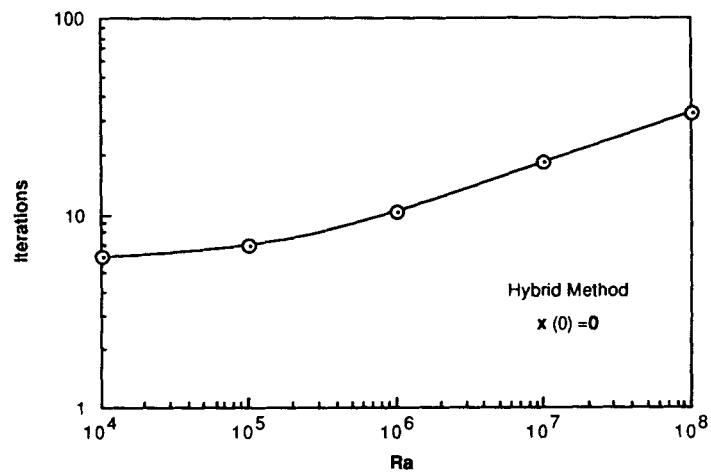

Figure 2. Performance of hybrid method as a function of the Rayleigh number

A comparison between the most promising semidirect methods and the well known iterative methods SIMPLE and SIMPLER is given in Table IV. The semidirect methods have been run with reduced factorization and initial guesses from previous solutions where appropriate. The iterative methods have been run with optimum or near-optimum under-relaxation factors. The under-relaxation factors were determined by trial and error, and this effort is *not* included in the table; hence the results for the iterative methods assume that the optimum under-relaxation factors are known *a priori*. The total iterations are given first, along with the number of iterations performed with reduced factorization for the semidirect methods. When previous solutions are used as an initial guess, the iterations refer to the sum of the total iterations required to obtain the converged solution. Time in seconds required to obtain a converged solution is shown in parentheses.

With the iterative methods SIMPLE and SIMPLER solutions were obtained for Rayleigh numbers up to 10^7. Based on results at $Ra = 10^7$, three new combinations of under-relaxation factors were tried for $Ra = 10^8$, and each run was made with a minimum of 1000 iterations. The runs were performed both with and without the initial guess from the solutions of $Ra = 10^7$. The norm could only be reduced to 10^9 for the best case. Although this does not imply that solutions are impossible, they are difficult. No solution was attempted for $Ra = 10^9$.

Compared to the iterative methods, the semidirect techniques are shown to be significantly more robust. Solutions have been readily obtained for Rayleigh numbers up to 10^9. Although no attempt was made to obtain a solution for $Ra > 10^9$, it is believed that this could be accomplished without significant difficulty. For the cases where the iterative methods converged, the relative computational effort between the iterative and semidirect approaches is shown to be comparable. Note, however, that if the optimum under-relaxation factors are not known in advance, the required execution times can be expected to increase by approximately two to three times.

Use of the previous solution as an initial guess did not help significantly with the iterative methods. Comparison of Tables III and IV shows that for the direct methods the impact can be substantial. An interesting feature of using results from previous solutions is that the full capability of the more robust methods is not as apparent as with the zero initial guess. The reason is that use of a previous solution results in a less difficult problem and the advantages of the more robust methods are diminished.

At $Ra = 10^9$ solutions were not obtained with the Newton–Raphson method and the search with Broyden update using solutions from $Ra = 10^8$. Instead Ra increments of 0·25 and $0{\cdot}5 \times 10^9$ were used, which resulted in rapidly convergent solutions for these methods. The highly robust nature of the hybrid method and the search with Jacobian update was evident at $Ra = 10^9$ since solutions could be obtained directly using results from $Ra = 10^8$. These solutions, however, were

Table IV. Comparison of direct and iterative methods in terms of iterations and (time)

$Ra =$ Method	10^4	10^5	10^6	10^7	10^8	10^9
HS	6–2 (19·21)	7–1 (24·89)	11–2 (35·95)	19–5 (59·755)	28–8 (87·76)	53–15 (171·37)
SJ	6–2 (19·21)	13–6 (34·15)	20–9 (53·96)	28–12 (77·99)	35–15 (106·0)	62–22 (189·67)
SB	8–1 (16·57)	11–2 (22·44)	19–2 (39·14)	33–5 (61·47)	62–8 (124·95)	116–13 (245–35)
NR	6–1 (22·17)	14–6 (34·84)	21–9 (53·66)	27–12 (76·26)	36–15 (102·73)	63–24 (182·10)
SIMPLE	289 (29·23)	441 (44·56)	350 (35·20)	533 (53·27)	—	—
SIMPLER	84 (8·99)	284 (30·40)	217 (23·12)	665 (71·33)	—	—

Note: no entry implies that no solution was obtained.

not as efficient as those obtained by the Ra increments used with the Newton–Raphson and Broyden search methods. Since these increments result in fewer iterations and lower execution times, the data presented in the table for $Ra=10^9$ are based on these increments.

Driven cavity problem

In this problem the bottom wall of the cavity moves with unit velocity and the solution of the energy equations is not required. Assuming constant properties, the governing equations are

$$\frac{\partial U}{\partial X}+\frac{\partial V}{\partial Y}=0, \tag{13}$$

$$U\frac{\partial U}{\partial X}+V\frac{\partial U}{\partial Y}=-\frac{\partial P}{\partial X}+\frac{1}{Re}\left(\frac{\partial^2 U}{\partial X^2}+\frac{\partial^2 U}{\partial Y^2}\right), \tag{14}$$

$$U\frac{\partial V}{\partial X}+V\frac{\partial V}{\partial Y}=-\frac{\partial P}{\partial Y}+\frac{1}{Re}\left(\frac{\partial^2 V}{\partial X^2}+\frac{\partial^2 V}{\partial Y^2}\right), \tag{15}$$

with

$$U=1; \qquad Y=0, \qquad U=V=0; \quad \text{all other boundaries.}$$

This problem has also been studied in semidirect finite difference form by Vanka and Leaf[4] and by Braaten.[5] In both of these previous studies the discretization practice was identical to that used here. The Reynolds number range over which the driven cavity problem was solved previously was 0·1 to 10^3. In this study the driven cavity problem has been solved for Reynolds numbers ranging from 10^{-1} to 10^6. A detailed investigation has been performed for Reynolds numbers between 10 and 10^3. A summary of this investigation in terms of the most suitable semidirect methods of this paper is given in Table V. The 30×30 irregular grid used in the previous problem was used here also. The results given in Table V show the iterations and times required to obtain a solution with full factorization. The nature of this problem is such that the highly robust methods are not actually required to obtain a rapidly convergent solution, at least not for the Reynolds numbers indicated.

For the range of Reynolds numbers shown in Table V even the iterative methods were well behaved; that is, no adjustments to the under-relaxation factors were necessary to obtain convergence. A comparison between the semidirect and iterative methods is given in Table VI. These results illustrate that the semidirect methods are rapidly convergent and are approximately two to three times more efficient than SIMPLE and SIMPLER. A notable exception is the solution for $Re=10^3$. Here SIMPLER requires less computational effort than the semidirect methods. It should also be noted that the successive substitution approach gives results essentially identical to those obtained by Braaten[5] with his UVP method.

Table V. Driven cavity results in terms of iterations and (time) for direct methods using full factorization

$Re=$ Method	10	10^2	10^3
Broyden search (SB)	3 (3·17)	5 (4·98)	9 (8·92)
Hybrid (HS)	3 (4·79)	4 (5·94)	6 (10·05)
Newton–Raphson (NR)	3 (4·64)	4 (5·72)	8 (10·21)
Successive substitution (SS)	3 (4·79)	7 (9·63)	13 (16·86)

Table VI Comparison of direct and iterative methods for the driven cavity problem in terms of iterations and (time) with reduced factorization

$Re=$ Method	10	10^2	10^3
Successive substitution (SS)	3–1 (3·71)	7·4 (5·28)	12–8 (6·95)
Broyden search (SB)	3–1 (2·73)	6–1 (4·10)	14–4 (7·45)
Newton–Raphson (NR)	3–1 (3·66)	4–1 (4·72)	8–3 (7·23)
Hybrid (HS)	3–1 (3·80)	4–1 (4·96)	8–4 (8·32)
SIMPLE	368 (27·51)	390 (29·15)	295 (21·86)
SIMPLER	98 (8·19)	105 (8·79)	71 (5·95)

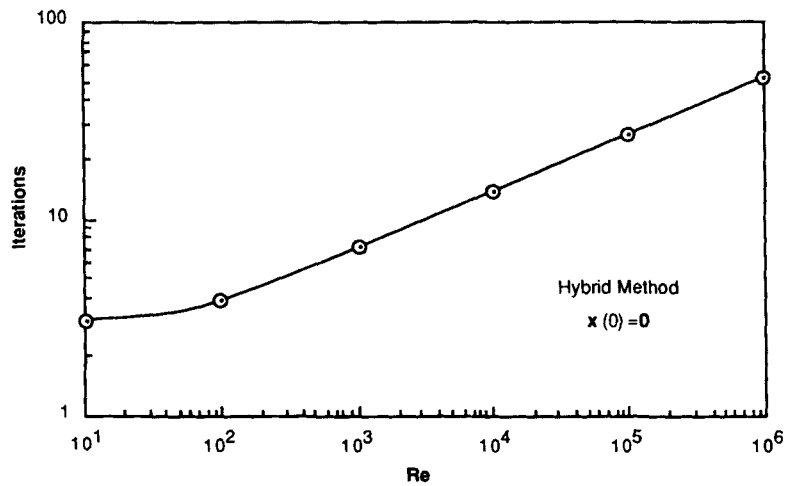

Figure 3. Performance of the hybrid method as a function of the Reynolds number

As a final exercise, the hybrid method was used to see if any problems would be encountered at significantly larger Reynolds numbers. The range of Reynolds numbers investigated was 10 to 10^6. The results for this test are illustrated in Figure 3 in terms of iterations as a function of Reynolds number. This figure illustrates performance similar to that shown for the natural convection problem in Figure 2. These figures illustrate that the performance of the hybrid method on both the natural convection and driven cavity problems is very encouraging.

Effect of grid on performance

As stated previously, the semidirect methods require substantial memory. Although it is felt that with virtual memory machines this limitation is not severe, it is still significant. The total core requirements as a function of grid subdivision for the basic methods used in the comparison are illustrated in Figure 4. This figure shows that the memory requirements of the semidirect methods are significant. The search with recursive Broyden update with a 15-iteration restart window on a 30×30 grid is approaching the maximum internal memory of the CRAY-1 computer (1 M word).

Changing the refinement of the grid will affect the accuracy of the results as well as the performance of the individual methods. For this study the non-uniformity of the grid was selected

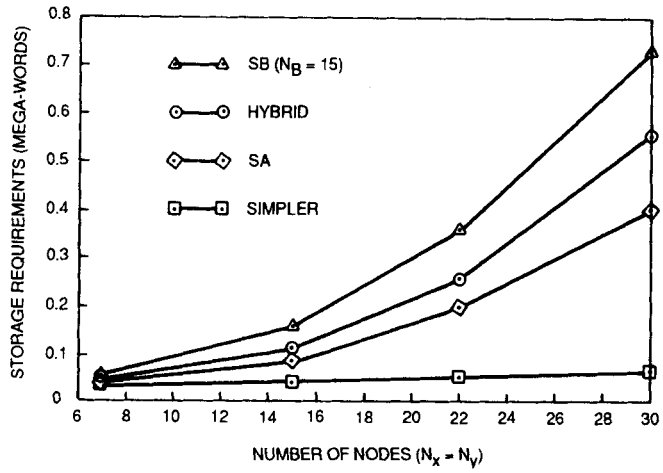

Figure 4. Storage requirements as a function of grid subdivision

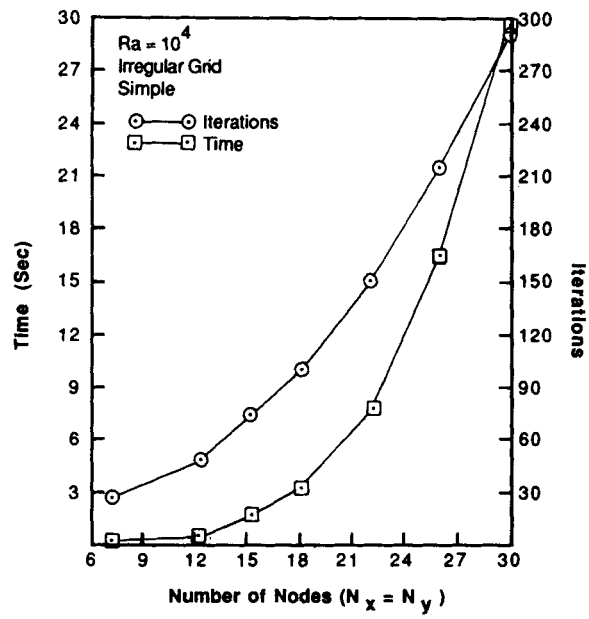

Figure 5. Effect of grid subdivision on the performance of SIMPLE

such that the 30×30 mesh would yield meaningful results for the natural convection problem (i.e. local and average Nusselt numbers within 0·5% of those given by DeVahl Davis[24]). Typical performances of the iterative and semidirect methods as a function of the grid mesh for non-uniform grids are shown in Figures 5 and 6 respectively.

These figures illustrate the exponential increase in computational effort as the grid is refined. With the iterative methods the computational effort per iteration increases in a linear fashion as the number of unknowns increases. However, owing to the sequential solution procedure, the rate

of propagation of boundary information into the interior of the calculation domain diminishes significantly as the grid is refined. Hence the iterations required for convergence increase in a non-linear fashion. With the semidirect methods boundary information is transmitted instantaneously; therefore the iterations are fairly insensitive to the number of unknowns. Unfortunately the operation count per iteration increases exponentially with these methods.

While the techniques put forth in this paper can be effective, it is apparent from these figures that as stand-alone procedures they are not well suited for fine grids. An interesting approach to alleviate the problem encountered with fine grids yet maintain robustness is to incorporate the semidirect solution procedure into a multigrid algorithm.

An important aspect of the multigrid technique is the choice of an efficient solution procedure. This topic has received considerable attention over the past several years. Typically some form of coupled implicit relaxation procedure is used. For example, Ghia *et al.*[27] have used a coupled strongly implicit procedure. As an alternate approach Vanka[28] has used a local block implicit technique that may be considered a symmetrically coupled Gauss–Seidel procedure. More recently, Kelkar and Patankar[29] have implemented a correction scheme that incorporates a semidirect solution on the coarse correction grid and an iterative solution on the fine grid. Their work has shown that semidirect approaches can be effective, even for fine grid resolution, when applied in a multigrid scheme.

CONCLUDING REMARKS

In this article several semidirect finite difference methods have been used to solve the natural convection and driven cavity problems. It has been demonstrated that semidirect formulations can be an effective alternative to the more conventional iterative approaches SIMPLE and SIMPLER. The search with Jacobian update and the hybrid approach were the most robust

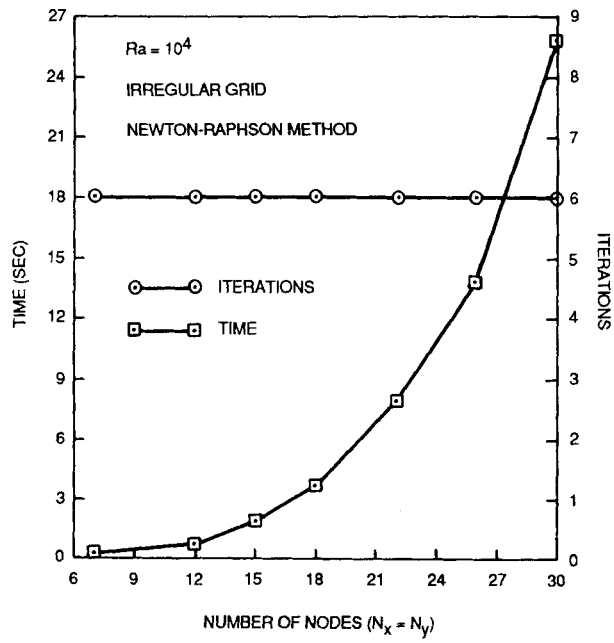

Figure 6. Effect of grid subdivision on the performance of the Newton–Raphson method

methods studied. The search with the modified Broyden update, although somewhat less robust than these methods, was generally more computationally efficient. The convergence characteristics of semidirect methods can be enhanced considerably by incorporating a norm-reducing search. Although stand-alone semidirect methods are not well suited for fine grid resolution, they can be used to enhance the overall robustness algorithms better suited for these applications.

APPENDIX: NOMENCLATURE

$\mathbf{A}$	matrix containing the coefficients of algebraic transport equations
$\mathbf{b}$	vector of source terms
$\mathbf{d}$	delay direction vector
Gr	Grashof number
$\mathbf{H}$	general coefficient matrix
$\mathbf{J}$	Jacobian matrix
Nu	Nusselt number
p	pressure
P	dimensionless pressure
Pr	Prandtl number
$\mathbf{P}$	direction vector
$\mathbf{q}$	pseudo-direction vector
R	residual
$\mathbf{R}$	residual vector
$\mathbf{r}$	auxiliary vector
Ra	Rayleigh number
T	Temperature
t	scalar search parameter
U	dimensionless u-velocity
V	dimensionless v-velocity
X	dimensionless distance in x-direction
$\mathbf{x}$	state vector
y	square of Euclidean norm
Y	dimensionless distance in y-direction

Greek symbols

ε	scalar search parameter
θ	dimensionless temperature
ρ	density
ϕ	general dependent variable
Γ	diffusion coefficient

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