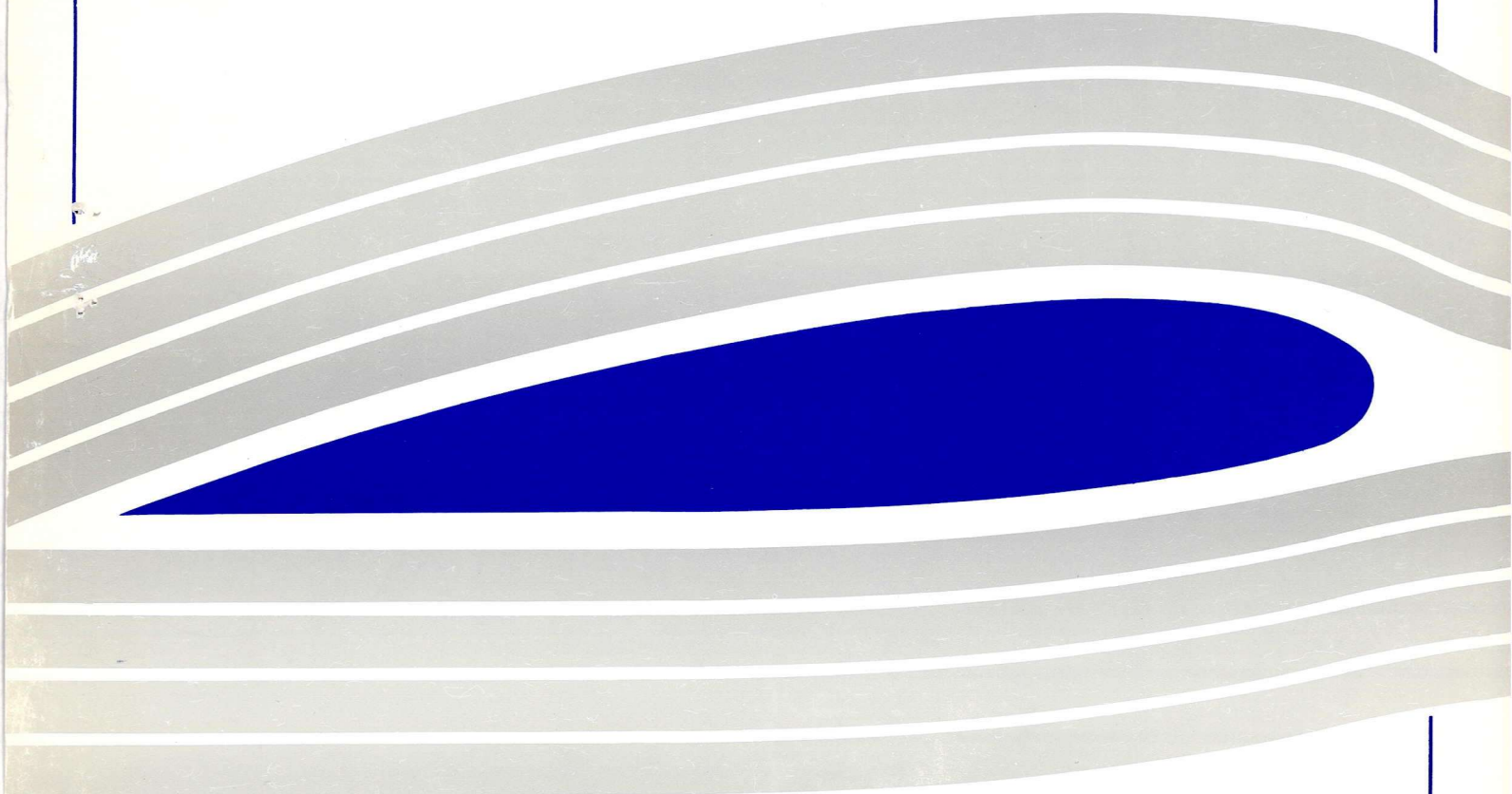
University of Glasgow
DEPARTMENT OF
AEROSPACE
ENGINEERING

SFDN-α-GMRES and SQN-α-GMRES Methods for Fast High Resolution N-S Simulations

N.QIN, X.XU and Bryan E. RICHARDS

G.U. Aero Report 9230



SFDN-α-GMRES and SQN-α-GMRES Methods for Fast High Resolution N-S Simulations

N.QIN, X.XU and Bryan E. RICHARDS

G.U. Aero Report 9230

Department of Aerospace Engineering
University of Glasgow
GLASGOW G12 8QQ

To be published in the Proceedings of the Numerical Methods for Fluid Dynamics, Reading, May 1992. Oxford University Press, Oxford, 1992

SFDN–α-GMRES and SQN–α-GMRES methods for fast high resolution N-S simulations

N. Qin, X. Xu and B. E. Richards

Department of Aerospace Engineering, University of Glasgow, Scotland, U.K.

1. Introduction

The existence of strong shock waves, thin shear layers and their interaction in hypersonic viscous flows requires the use of a high resolution scheme for an accurate numerical simulation. Through an extensive study (Qin et al. 1991) of different flux formulae on their capabilities of capturing both shock waves and shear layers, the Osher flux difference splitting scheme has been found to be satisfactory. However, high resolution schemes usually involve more complicated formulation and thus longer computation time per iteration as compared to the simpler central differencing scheme. Therefore, the acceleration of the convergence for high resolution schemes becomes an increasingly important issue.

In this paper, we will present a new iterative approach for fast steady state solution of Navier-Stokes equations. The approach is illustrated by its application to hypersonic viscous flows over a cone at high angle of attack in which the Osher flux difference splitting high resolution scheme is used for capturing both shock waves and shear layers in the flowfield.

2. The high resolution discretisation

Corresponding to the test case presented in Section 4, the governing equations are the locally conical Navier-Stokes equations, which can be written as

$$\frac{\partial \overline{\mathbf{F}}}{\partial \eta} + \frac{\partial \overline{\mathbf{G}}}{\partial \zeta} + \mathbf{H} = 0 \qquad (2.1)$$

where **H** is the source term resulting from the locally conical approximation. In the cell centred finite difference or finite volume formulation, the state variables are evaluated at cell centres and represent cell-averaged values. The fluxes are evaluated at cell interfaces. The spatial derivatives are then represented as a flux balance across a cell. The convective interface flux is determined from a local one-dimensional model of wave interactions normal to the cell interfaces. With the flux difference splitting (FDS) model developed by Osher and Chakravarthy (1983), the convective interface flux can be written as

$$\tilde{\mathbf{F}}_i = \frac{1}{2}\left[\overline{\mathbf{F}}_i(\mathbf{Q}^L) + \overline{\mathbf{F}}_i(\mathbf{Q}^R) - \int_{\mathbf{Q}^L}^{\mathbf{Q}^R} \left|\frac{\partial \overline{\mathbf{F}}_i}{\partial \mathbf{Q}}\right| d\mathbf{Q} \right] \tag{2.2}$$

where the integral in the state variable domain is carried out along a path piecewise parallel to the eigenvectors of $\partial\overline{\mathbf{F}}_i/\partial\mathbf{Q}$.

The state-variable interpolations determine the resulting accuracy of the scheme. A κ-parameter family of higher-order schemes can be written as

$$\begin{aligned} \mathbf{q}^L_{j+\frac{1}{2},\,k} &= \mathbf{q}_{j,\,k} + \{(\tfrac{s}{4})[(1-\kappa s)\Delta_- + (1+\kappa s)\Delta_+]\mathbf{q}\}_{j,\,k} \\ \mathbf{q}^R_{j+\frac{1}{2},\,k} &= \mathbf{q}_{j+1,\,k} - \{(\tfrac{s}{4})[(1+\kappa s)\Delta_- + (1-\kappa s)\Delta_+]\mathbf{q}\}_{j+1,\,k} \end{aligned} \tag{2.3}$$

where Δ_+ and Δ_- denote forward and backward difference operators, respectively, in the η direction. The parameter κ determines the spatial accuracy of the difference approximation. We choose $\kappa = 1/3$ for a third order upwind-biased scheme. The parameter s serves to limit higher-order terms in the interpolation in order to avoid oscillations at discontinuities such as shock waves in the solutions. The limiting is implemented by locally modifying the difference values in the interpolation to ensure monotone interpolation as

$$s = \frac{2\Delta_+\mathbf{q}\Delta_-\mathbf{q} + \varepsilon}{(\Delta_+\mathbf{q})^2 + (\Delta_-\mathbf{q})^2 + \varepsilon} \tag{2.4}$$

where ε is a small number preventing division by zero in regions of null gradients.

The diffusive fluxes are calculated at cell interfaces using a central differencing scheme.

After the above discretisation and proper treatment at the domain boundaries, a large sparse nonlinear system results, which we denote as

$$\mathbf{R}(\mathbf{Q})=0 \tag{2.5}$$

3. The SFDN–α-GMRES and SQN–α-GMRES methods

3.1 Discussion

For steady state problems, a time dependent approach is often employed, which can be written as

$$\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{R}(\mathbf{Q}) = 0 \tag{3.1}$$

Using a fully implicit method, e.g. the backward Euler implicit method,

$$\left[\frac{1}{\Delta t}\mathrm{I} + \left(\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right)^{n}\right]\Delta \mathbf{Q}^{n} = -\mathbf{R}(\mathbf{Q}^{n}) \tag{3.2}$$

unconditional stability can be achieved and as the time step approaches infinity the method approaches the Newton method

$$\left(\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right)^{n}\Delta \mathbf{Q}^{n} = -\mathbf{R}(\mathbf{Q}^{n}) \tag{3.3}$$

for the solution of the nonlinear system (2.5). In practical applications to CFD problems, however, it is very difficult (1) to get the analytical Jacobian of the nonlinear system for a high order high resolution scheme for viscous flows (it is almost impossible if turbulence or chemical reactions are involved) and (2) to solve the resulting large sparse nonsymmetric linear system efficiently. Previous researchers in CFD have tried to avoid these two difficulties in the following ways respectively: (1) to construct simplified implicit operators, e.g. to use only first order inviscid implicit operators; (2) to use approximate factorization for the multidimensional implicit operator so that the resulting linear systems can be solved easily. Both of these naturally negate the advantages of the fully implicit scheme. Therefore the time step size is still limited due to the inconsistency of the implicit operator and the right hand side (the nonlinear system) and the factorization error which increases with the time step. Simplified implicit methods will thus obviously not approach a Newton iterative method as the time step approaches infinity.

3.2 The SFDN and SQN nonlinear iterative methods

Instead of avoiding the difficulties for a fully implicit method, Qin and Richards (1988, 1990) tried to tackle the problem directly in order to achieve fast convergence for the steady state solution. The discretisation of the Navier-Stokes equations results in a large sparse nonlinear system to be solved, which can be considered as a fully implicit scheme with an infinite time step. Viewing the Navier-Stokes solution as the solution of a large sparse nonlinear system, we derived a fast convergence algorithm which is general and robust.

The algorithm is based on the Newton iterative method. Due to the complexity of the nonlinear system, an analytical expression for the Jacobian matrix is usually not obtainable. Therefore, we took the following two approaches: (1) the sparse finite difference Newton method (SFDN) (Curtis et al. 1974); and (2) the sparse quasi-Newton method (SQN) (Schubert 1970).

The SFDN method calculates numerically the Jacobian of the nonlinear system. Making use of its structured sparsity, Qin and Richards (1988) devised a practical way of calculating the Jacobian using finite differences. If we take the present 2-D as an example, the above higher order spatial discretisation will result in a 13-point stencil (Fig.1). In the calculation of the Jacobian, we can minimize the number of calculations of $\mathbf{R}(\mathbf{Q})$ in the following way. Because the discretisation has a 13-point stencil, we can perturb one of the five state variables by a local increment $h^l_{i,j}$ at every 5 points in both coordinate directions in one evaluation of $\mathbf{R}(\mathbf{Q})$, i.e. we calculate

$$\mathbf{R}(\mathbf{Q} + \sum_{\substack{i=m,I,5 \\ j=n,J,5}} h^l_{i,j}\mathbf{e}^l_{i,j}), \quad l=1,5;\ m=1,5;\ n=1,5 \tag{3.4}$$

where $\mathbf{e}^l_{i,j}$ is the unit vector at point (i,j) for the lth component of the state. Therefore we can get the finite difference approximation of the Jacobian column by column through a total number of 125 evaluations of $\mathbf{R}(\mathbf{Q})$. If the increments are properly chosen according to machine zero and the rounding errors in calculating $\mathbf{R}(\mathbf{Q})$, the SFDN method can still give a quadratic convergence rate as has been shown by Dennis and Schnabel (1983).

The SQN method updates an approximation to the Jacobian from the solution of the linear system and the value of $\mathbf{R}(\mathbf{Q})$ available. It is an extension of the quasi-Newton method to nonlinear systems with sparse Jacobians. To keep the sparsity structure of the Jacobian, only those non-zero elements are updated through a projection operator $\mathbf{P}_J$ The updating procedure can be written as

$$\begin{aligned} A^n\Delta\mathbf{Q}^n &= -\mathbf{R}(\mathbf{Q}^n) \\ \mathbf{Y}^n &= \mathbf{R}(\mathbf{Q}^{n+1}) - \mathbf{R}(\mathbf{Q}^n) \\ \Delta A^n &= \mathbf{P}_J[D^+(\mathbf{Y}^n - A^n\Delta\mathbf{Q}^n)(\Delta\mathbf{Q}^n)^T] \\ A^{n+1} &= A^n + \Delta A^n \end{aligned} \tag{3.5}$$

where D^+ is a diagonal matrix which is determined from the linear solution $\Delta\mathbf{Q}^n$ and the sparsity structure of the Jacobian matrix. One can see that there is no extra evaluation of $\mathbf{R}(\mathbf{Q})$ involved in updating the approximation. It has been proved that the SQN method has a superlinear convergence rate (Dennis and Schnabel 1983). Qin and Richards (1988, 1990) formulated its application to nonlinear systems with sparse block structured Jacobian matrices arising from Euler and Navier-Stokes solutions.

It is obvious that the SFDN method requires much more computing time in generating the Jacobian approximation as compared to the SQN method in which the computing time for generating the Jacobian approximation is negligible. On the other

hand, the difference between quadratic convergence and superlinear convergence can be significant in practical applications because a large amount of computing time has to be spent in solving the large sparse nonsymmetric linear system at each iteration.

3.3 The α-GMRES linear solver

After the linearization of the nonlinear system, a large sparse nonsymmetric linear system results, either (3.3) for the SFDN method or (3.5) for the SQN method, which we denote as

$$A\mathbf{x}=\mathbf{b} \tag{3.6}$$

For a 2-D case, A is a block 13-point diagonal structured sparse matrix as shown in Fig.2.

Xu et al. (1991) proposed a new efficient multilevel iterative method, the α-GMRES (Generalized Minimal RESidual) method for the solution of the sparse nonsymmetric linear system. The matrix is first preconditioned by the inverse of its block diagonal matrix and a parameter α ($0<\alpha<1$) is added to the diagonal to further improve the matrix property for a successful application of GMRES method. Thus a multi-level iterative solver results, which are written as

$$(\alpha I + D^{-1}A)\,\mathbf{x}^{k+1} = D^{-1}\mathbf{b} + \alpha\mathbf{x}^{k} \tag{3.7}$$

where D is the block diagonal matrix of A. We have proved the existence of such an α ($0<\alpha<1$) that the above iterative procedure will converge (Xu et al. 1991). In practical application, the parameter α is determined by a balanced convergence of the GMRES inner loop and the outer loop, which is around 0.1 for the test cases.

Combining the α-GMRES linear solver with the nonlinear SQN and SFDN methods, we have thus devised fast convergent solvers for Navier-Stokes solutions, which we have named the SFDN-α-GMRES and SQN-α-GMRES methods respectively.

4. Numerical examples

The test case chosen is a hypersonic viscous flow around a sharp cone at high angle of attack. The flow is modelled by the Locally Conical Navier-Stokes equations, which is discretised using the Osher flux difference splitting scheme for the inviscid fluxes and a central differencing scheme for the viscous terms. The resulting nonlinear system is then solved by the SQN-α-GMRES method or the SFDN-α-GMRES method. In the present tests, we choose $\alpha=0.1$ and the Krylov subspace dimension in the GMRES method as 30 and 50 for 33×33 or 66×66 girds respectively. To produce a starting solution suitable for an effective application, we use a time dependent approach for the

initial phase, in which a Runge-Kutta method with local time stepping is employed. The computation was carried out on the IBM RISC System/6000 320H workstation.

Fig.3 shows the flow conditions and the crosssectional view of the solved flowfield, in which the strong bow shock wave on the windward side and the separated shear layer on the leeward side can clearly been seen.

Fig.4 plots the convergence against computing time for calculations using the SQN-α-GMRES method or the SFDN-α-GMRES method on a 33×33 grid. As can be seen, the convergence for the explicit scheme is typically slow even though local time stepping has already been employed for efficiency. After switching to the SFDN-α-GMRES method or the SQN-α-GMRES method, the solutions converges quadratically or superlinearly respectively and the residuals reduce to machine zero in 4 or 8 iterations. For this particular case, the two methods produce similar efficiency but the SQN-α-GMRES method is expected to be more promising for problems involving more complicated physics when the expense in evaluating **R(Q)** is much higher.

In Fig. 5, we show a test on a 66×66 grid using different convergence criteria for the iterative linear solver. We do not need to solve the linear systems (3.7) using the GMRES method or (3.6) using the α-GMRES method to a high accuracy as long as a reasonable convergence in the nonlinear iteration can be achieved. In Fig. 5, e1 and e2 represent the convergence criteria for the solution of (3.7) and (3.6) respectively. As can be seen, a larger convergence criterion can save computing time in the linear solver and it will also degrade the convergence rate of the outer nonlinear iteration. An optimum choice can be made through numerical experiments.

5. Conclusions

The SFDN–α-GMRES and SQN–α-GMRES methods presented in this paper have provided a new approach for fast steady state Navier-Stokes solutions, when complexity from using high resolution schemes produces slow convergence using conventional time-dependent approach and when the analytical Jacobian is difficult to obtain. In comparison, both of the methods produce similar improvement over the corresponding explicit method in computing time for the test case. They are to be investigated further in parallel when applied to more complicated cases including turbulent modelling and/or real gas effects.

Acknowledgements

This work was supported by SERC Grant GR/E89056 (NQ and BER), a Glasgow University Research Scholarship and an ORS award (XX).

References

Curtis, A., Powell, M.J.D and Reid, J.K. (1974). On the estimation of sparse Jacobian Matrices. *J. Inst. Maths. Applics.* 13:117-120.

Dennis, J. E. and Schnabel, R. B. (1983). *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*. Prentice Hall, Englewood Cliffs, N.Y.

Osher, S. and Chakravarthy, S. R. (1983). Upwind schemes and boundary conditions with applications to Euler equations in general coordinates. *J. Comp. Phys.* 50:447-481.

Qin, N. and Richards B. E. (1988). Sparse quasi-Newton method for high resolution schemes. *Notes in Numerical Fluid Mechanics*, 20:310-317.

Qin, N. and Richards B. E. (1990). Sparse quasi-Newton method for Navier-Stokes solutions. *Notes in Numerical Fluid Mechanics*, 29:474-483.

Qin, N., Scriba, K. W. and Richards, B. E. (1991). Shock-shock, shock-vortex interaction and aerodynamic heating in hypersonic corner flow. *Aeronautical J.* 945:152-160.

Saad, Y. and Schultz, M.H. (1986) GMRES: A general minimal residual algorithm for solving nonsymmetric linear systems. *SIAM J. Stat. Comp.* 7:856-869.

Schubert, L.K. (1970). Modification of quasi-Newton method for nonlinear equations with a sparse Jacobian. *Math. Comp.* 24:27-30.

Xu, X., Qin, N. and Richards, B.E. (1991). α-GMRES: A new parallelizable iterative solver for large sparse nonsymmetric linear systems arising from CFD. *GU Aero Report* 9110 also *Int. J. Numer. Meths. Fluids*. To appear in 1992.

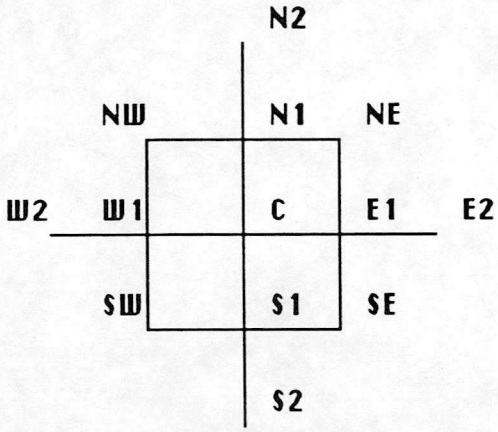


Fig. 1: Discretisation stencil using the high resolution scheme

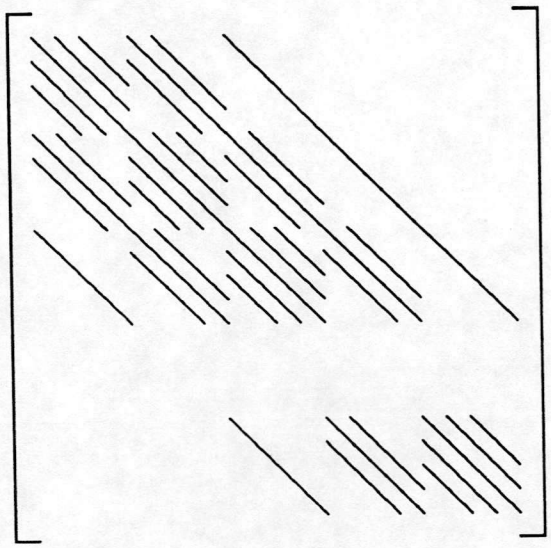


Fig. 2: Sparsity pattern of the Jacobian matrix

10° Cone

AoA = 24°

$M_\infty = 7.95$

$T_\infty = 55.4$ K

$T_w = 309.8$ K

$Re_\infty = 4.1 \times 10^6$

r = 0.1 m

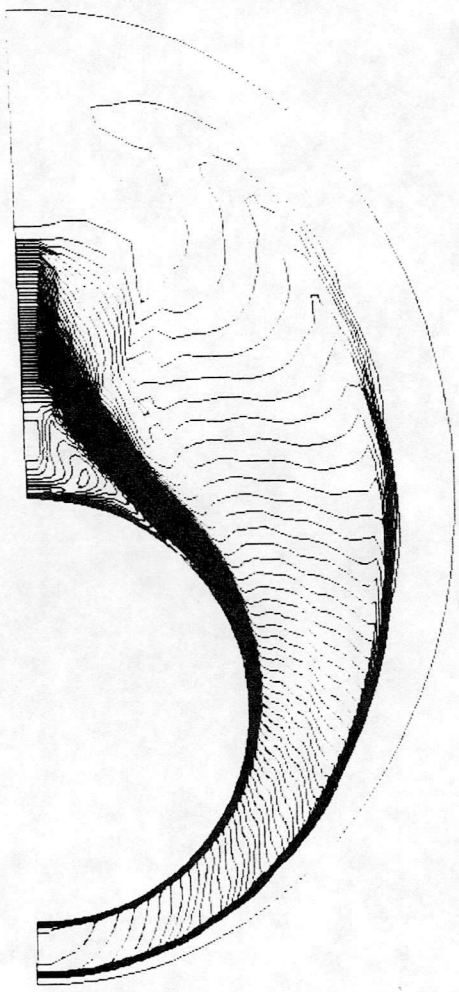


Fig. 3: Crossflow temperature contours of the test case

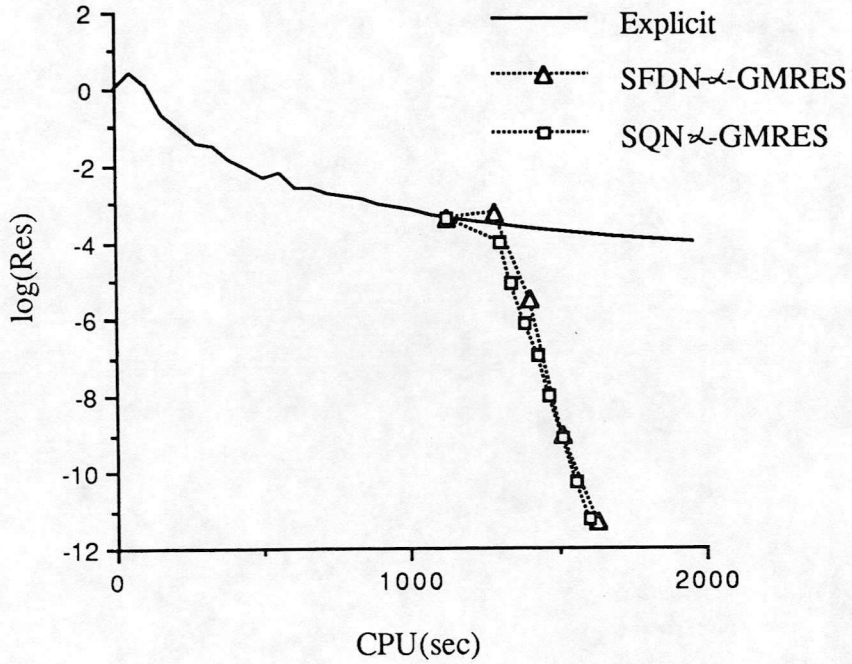


Fig. 4: Convergence of the SFDN–α-GMRES and SQN–α-GMRES methods as compared with the Runge-Kutta explicit method (grid 33×33)

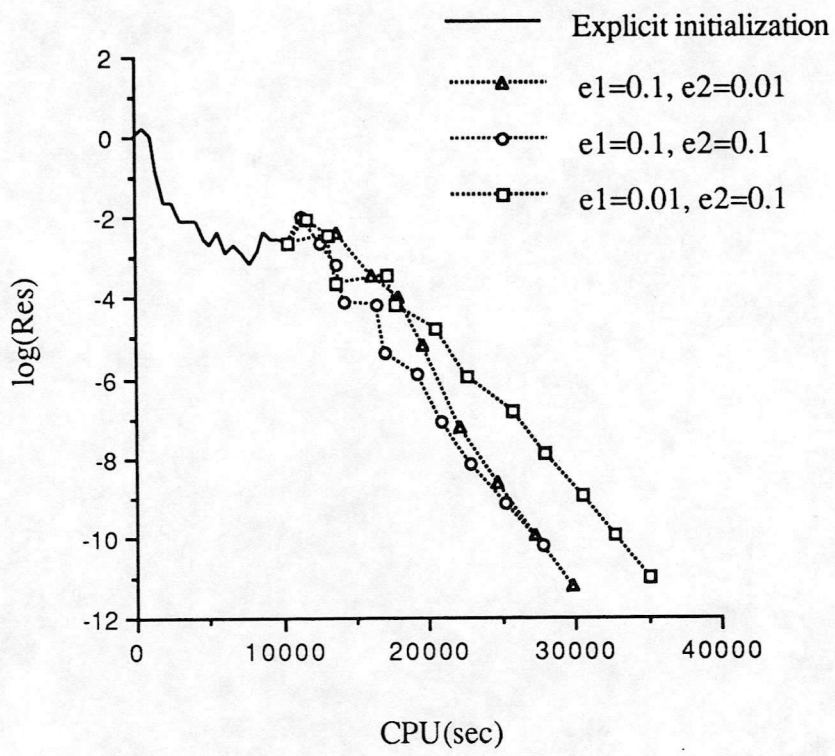


Fig.5 Parameter tests for the SFDN–α-GMRES method (grid 66×66).