Splitting methods for high order solution of the incompressible Navier–Stokes equations in 3D

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SUMMARY

The incompressible Navier–Stokes equations are discretized in space by a hybrid method and integrated in time by the method of lines. The solution is determined on a staggered curvilinear grid in two space dimensions and by a Fourier expansion in the third dimension. The space derivatives are approximated by a compact finite difference scheme of fourth-order on the grid. The solution is advanced in time by a semi-implicit method. In each time step, systems of linear equations have to be solved for the velocity and the pressure. The iterations are split into one outer iteration and three inner iterations. The accuracy and efficiency of the method are demonstrated in a numerical experiment with rotated Poiseuille flow perturbed by Orr–Sommerfeld modes in a channel. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: finite difference method; high order; 3D incompressible flow; iterative solution

1. INTRODUCTION

The multiscale nature of turbulent flow requires highly accurate and efficient numerical solution techniques. Higher order approaches offer flexibility concerning the geometry at only slightly reduced accuracy compared to a spectral method. The advantage over low-order discretizations is that the same accuracy is achieved with fewer grid points, or the solution has better accuracy on the same grid. Reviews of recent developments are given in References [1, 8].

In this paper, we propose a hybrid method of fourth-order accuracy in two space dimensions (2D), of spectral accuracy in the third dimension, and of second-order in time for solution of

Contract/grant sponsor: The Swedish Research Council

Received 27 April 2004 Revised 13 September 2004 Accepted 22 September 2004

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the incompressible Navier–Stokes equations. In References [1, 2] a finite difference method of fourth-order in space for curvilinear grids in two dimensions is described, and its accuracy is confirmed in numerical experiments including complex geometries. The method is extended here to three-dimensional problems with a periodic third dimension by expanding the solution in a Fourier series. With this discretization, our approach has potential for higher efficiency than 3D difference methods and will still allow for simulation of relevant turbulent flow cases in complex 2D geometries such as diffuser flow or flow over a swept airfoil.

The solution in curvilinear body-fitted coordinates in 2D is obtained by a mapping of the equations to a rectangular grid where the derivatives are approximated by a compact scheme [6]. No filtering or artificial viscosity is needed since spurious oscillations are suppressed by solving the equations in primitive variables on a staggered grid with local velocity components. Another key feature is the formulation of the boundary conditions. They are derived by analysis of the linearized equations, are proved to be stable in Reference [4] and remove the singularity in the system matrix resulting from the discretization.

The equations are advanced in time by a semi-implicit scheme. The space operator is split so that the viscous term and the pressure gradient are treated implicitly resulting in a system of linear equations to solve for the velocity and the pressure in each time step. Stability issues for the time-integration are addressed in Reference [5]. It is shown that in the turbulent boundary layer, the time step is limited by the accuracy and not by the stability of the method. The novel solution algorithm uses an approximate factorization of the system matrix in an outer iterative loop and involves a suitable formulation of the boundary conditions as described in Reference [1]. By the approximate factorization, a solution procedure is obtained similar to the ones in time split methods [7], but no boundary conditions for intermediate values of velocities or the pressure are required in our method. Corrections to the velocity and the pressure are computed from three linear systems with iterative techniques.

In a numerical example, the accuracy and efficiency of the method are tested in the solution of rotated Poiseuille flow in a straight channel perturbed with Orr–Sommerfeld modes. The results are in very good agreement with data computed with spectral accuracy according to Reference [9] and the order of accuracy in space is as expected in the numerical experiments. The grid is Cartesian in this example but the code is developed for curvilinear grids in a plane and is thoroughly verified for such problems in 2D [1].

2. DISCRETIZATION

The Navier–Stokes equations for incompressible flow are solved in the primitive variables. Let u, v and w be the velocity components in the x-, y- and z-directions, respectively, p the pressure, and v the kinematic viscosity. Then the Reynolds number is $R = u_b \ell / v$ for some characteristic length ℓ and characteristic speed u_b . Let $\mathbf{U} = (u \ v \ w)^T$ and introduce the non-linear and linear terms

$$\mathcal{N}(\mathbf{U}) = (\mathbf{U} \cdot \nabla)\mathbf{U}, \quad \mathscr{L}(\mathbf{U}, p) = \nabla p - R^{-1}\Delta \mathbf{U}$$

Then the equations in three dimensions are

$$\partial_t \mathbf{U} + \mathcal{N}(\mathbf{U}) + \mathscr{L}(\mathbf{U}, p) = 0 \tag{1}$$

$$\mathscr{D}\mathbf{U} = \nabla \cdot \mathbf{U} = 0 \tag{2}$$

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Int. J. Numer. Meth. Fluids 2005; 47:1157-1163

The space discretizations of \mathcal{N} and \mathcal{L} in (1) are written \mathcal{N}_h and \mathcal{L}_h and the discretization of the continuity equation (2) is $\mathcal{D}_h \mathbf{U} = \mathbf{0}$.

The variables u, v, w and p are expanded in a Fourier series in the spanwise z-dimension. For u at a grid point (x_i, y_k) in the 2D plane and z_i in the spanwise direction, we have

$$u(x_{j}, y_{k}, z_{l}) = \sum_{m=-n_{z}/2}^{n_{z}/2-1} \hat{u}_{m}(x_{j}, y_{k}) \exp(i\beta_{m}\ell_{z}l/n_{z})$$

where ℓ_z is the length of the computational domain in the z-direction, $z_l = \ell_z l/n_z$, and $\beta_m = 2\pi m/\ell_z$ is the *m*th wave number. The discrete variables \hat{u}_{jkm} , \hat{v}_{jkm} , and \hat{p}_{jkm} are located in a staggered grid in the usual manner and \hat{w}_{jkm} has the same position as the pressure.

An orthogonal curvilinear grid is generated in the (x, y)-plane. The solution is assumed to be periodic in the z-direction. A mapping is introduced from the physical coordinates (x, y)to the variables (ξ, η) in a rectangular computational domain. The derivatives in the x and y variables are approximated by compact finite difference formulas of fourth-order accuracy in the (ξ, η) domain [1, 6]. The z-derivative in Fourier space is exactly $i\beta_m \hat{u}_m$ for the *m*th wave number. The non-linear convection term \mathcal{N}_h^n at t^n is evaluated in physical space as follows. First, the inverse Fourier transform is applied to \hat{u}^n, \hat{v}^n , and \hat{w}^n and the difference approximations in the ξ and η directions. Then, \mathcal{N}_h^n is determined and finally the Fourier transform brings \mathcal{N}_h^n back to Fourier space to become $\hat{\mathcal{N}}_h^n$. The boundary conditions are of Dirichlet or Neumann type including an integral of the pressure for $\beta = 0$ to remove the ambiguity in the pressure level.

The time integration to time t^{n+1} is performed with a semi-implicit method of second-order. First, $\hat{\mathcal{N}}_h$ is extrapolated from t^{n-1} and t^n with a second-order formula to t^{n+1} and then the second-order backward differentiation formula (BDF-2) approximates $\partial_t \mathbf{U}$ at $t^{n+1} = t^n + \Delta t$ to arrive at

$$\frac{3}{2}\hat{\mathbf{U}}^{n+1} + \Delta t \hat{\mathscr{L}}_{h}(\hat{\mathbf{U}}^{n+1}, \hat{p}^{n+1}) = 2\hat{\mathbf{U}}^{n} - \frac{1}{2}\hat{\mathbf{U}}^{n-1} - \Delta t(2\hat{\mathscr{N}}_{h}^{n} - \hat{\mathscr{N}}_{h}^{n-1})$$
(3)

$$\hat{\mathscr{D}}_h \hat{\mathbf{U}}^{n+1} = 0 \tag{4}$$

The unknown variables \hat{U}^{n+1} and \hat{p}^{n+1} satisfy a system of linear equations. How this system is solved in each time step is described in the next section. The convergence rate of the iterative solvers is improved for wave numbers different from 0 if the system is solved in the Fourier components as in (3) and (4).

3. ITERATIVE SOLUTION

After eliminating boundary values of the variables, the resulting system of linear equations to solve for each $\beta = \beta_m$ for the velocities $\hat{\mathbf{U}}_1 = (\hat{u}, \hat{v})^T, \hat{w}$, and \hat{p} at t^{n+1} is

$$\begin{pmatrix} A_1 & 0 & \Delta tG \\ 0 & A_w & i\beta\Delta tI \\ D & i\beta D_w & E \end{pmatrix} \begin{pmatrix} \hat{\mathbf{U}}_1^{n+1} \\ \hat{w}^{n+1} \\ \hat{p}^{n+1} \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ b_w \\ b_D \end{pmatrix}$$
(5)

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Int. J. Numer. Meth. Fluids 2005; 47:1157-1163

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All submatrices A_1, A_w, G, D, D_w , and E in (5) are real. The right-hand side depends on old values of the solution and the boundary conditions. The structure of A_1 and A_w is

$$A = 1.5I + \Delta t R^{-1} (I\beta^2 - L_2)$$

where L_2 approximates the Laplace operator in 2D. The diagonal elements of A increase as the wave number increases. The matrix E is 0 for $\beta \neq 0$ and is sparse and depends on the boundary conditions for $\beta = 0$. Without E, the system matrix would be singular for such a β . The submatrices in (5) are dense matrices and not known explicitly due to the compact difference approximation. However, in the iterations below we need only the submatrix multiplying a vector. This is easily computed by solving a few tridiagonal systems. See Reference [1] for details.

A matrix \tilde{M} is constructed approximating the system matrix M in (5). The LU decomposition of \tilde{M} is simple and explicitly available. The factors L and U are

$$L = \begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_w & 0 \\ D & i\beta D_w & I \end{pmatrix}, \quad U = \begin{pmatrix} I & 0 & \gamma \Delta t G \\ 0 & I & \gamma i\beta \Delta t I \\ 0 & 0 & Q \end{pmatrix}$$
(6)

where $\gamma = 1/(1.5 + \Delta t R^{-1} \beta^2)$ and

$$Q = E - \gamma \Delta t (DG - \beta^2 D_w) \tag{7}$$

The last part of Q resembles a discretization of the Laplace operator since D and G approximate the divergence and the gradient and D_w is close to an identity matrix. Rewrite (5) as

$$Mx = \mathbf{b}$$

Then, solve it by fixed point iteration using the approximate factorization

$$\tilde{M} \delta x^{(k)} = LU \delta x^{(k)} = r^{(k)} = \mathbf{b} - M x^{(k)}$$

$$x^{(k+1)} = x^{(k)} + \delta x^{(k)}$$
(8)

In each outer iteration (8), the following six steps are taken

1. Solve
$$A_1 \mathbf{y}_1 = \mathbf{b}_1$$
.
2. Solve $A_w y_w = b_w$.
3. $y_2 = -D\mathbf{y}_1 - i\beta D_w y_w$.
4. Solve $Q\delta \hat{p} = y_2$.
5. $\delta \hat{w} = y_w - i\beta \gamma \Delta t \delta \hat{p}$.
6. $\delta \hat{\mathbf{U}}_1 = \mathbf{y}_1 - \gamma \Delta t G \delta \hat{p}$.

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Int. J. Numer. Meth. Fluids 2005; 47:1157-1163

The equations are solved for the real part and the imaginary part of the right-hand sides separately. Since the submatrices are real, we obtain the real and imaginary parts of the solutions in this way without introducing complex arithmetic. The solutions in steps 1 and 2 are computed by fixed point iteration as in (8) with a diagonal scaling as preconditioner. The residual in (8) quantifies the iteration error in the discretization of the Navier–Stokes equation in each time step and stops the iterations as the residual drops below a specified tolerance. The correction in \hat{p} in step 4 is obtained by iterations with the Krylov subspace method BiCGSTAB with the matrix preconditioned by an incomplete LU factorization depending on β [3]. This is the most time consuming part of the solution process. Since E in (7) is sparse and has low rank, we have essentially a Poisson equation to solve for $\delta \hat{p}$ in step 4.

4. NUMERICAL RESULTS IN 3D

Several examples in Reference [1] demonstrate fourth-order accuracy in space and secondorder accuracy in time for u, v, and p with our discretization in 2D. One particular case with a curvilinear grid is a constricting channel.

In the numerical example here, we study eigensolutions, i.e. modes of Orr–Sommerfeld type, to the linearized form of the Navier–Stokes equations, see Reference [9], in order to validate the proposed numerical method in 3D. In Reference [9] a solution algorithm is provided which computes the corresponding eigenfunctions with spectral accuracy. In plane Poiseuille flow, the eigenmode is of the form

$$\tilde{u}_j = \tilde{u}_j(y) e^{\mathbf{i}(\alpha x - \omega t)}, \quad j = 1, 2$$
(9)

with the streamwise wave number α and $\omega = \alpha c = \alpha(c_r + ic_i)$ is the eigenvalue. The imaginary part c_i of c determines if the amplitude of the mode is growing or decaying in time. Since Orr–Sommerfeld modes result from linear stability theory, we implement them as a perturbation to Poiseuille base flow in the domain $[0 \ 4\pi] \times [-1 \ 1] \times [0 \ 4\pi]$ as follows:

$$u = 1 - y^2 + \varepsilon \tilde{u}_1(y) e^{i(\alpha x - \omega t)}, \quad v = \varepsilon \tilde{u}_2(y) e^{i(\alpha x - \omega t)}$$
(10)

In order to make the problem three-dimensional, the mode is rotated around the y-axis by $\pi/6$. The flow is then periodic in the z-dimension, which covers one wavelength of the eigenmode.

The experimentally obtained constants $c_{i,exp}$ with our code are compared to the spectrally computed value. The values are determined by computing the decay in kinetic energy in the components. Table I summarizes the results and the relative errors for each of the three velocity components. The numerical simulation involves $n_x \times n_y \times n_z = 61 \times 81 \times 16$ nodes on a Cartesian grid. The mode investigated here is stable and computed with spectral accuracy as in Reference [9] at R = 2000 with $c_r = 0.3121$ and $c_i = -0.0197987$. By letting $\varepsilon = 10^{-5}$ in (10), we can neglect non-linear interactions. No slip conditions are applied at the upper and lower walls and Dirichlet conditions are specified at the in- and outflow boundaries. The simulation is run at a constant time step $\Delta t = 0.01$ until time T = 10. The convergence tolerance is set to 10^{-10} in both the inner and outer iteration loops.

Convergence statistics for the iterative solvers in the inner iteration are summarized in Table II for the tolerance 10^{-10} and $\Delta t = 0.01$ as above. The numbers of iterations in the solver for the real part of the solution are shown for the first four Fourier modes in the

Component	$C_{i,\exp}$	Rel. error	
u	-0.019731	3.42e - 3	
v	-0.019719	4.01e - 3	
W	-0.019716	4.18e - 3	

Table I. Orr–Sommerfeld solutions for plane Poiseuille flow. Numerically obtained decay constants at T = 10 and the relative difference in the constants between a value computed with a spectral method and our method.

Table II. Orr–Sommerfeld solutions for plane Poiseuille flow. The average number of iterations over 1000 time steps for the first four Fourier modes for the two *A*-systems and the *Q*-system.

Wave number	β_0	β_1	β_2	β_3
$\overline{A_1}$	4.0	2.0	1.0	1.0
A_w	4.0	2.0	1.0	1.0
Q	1.6	2.0	0.2	0.2

Table III. Orr–Sommerfeld solutions for plane Poiseuille flow. The error norms on a coarse grid (e_c), a medium grid (e_m), and a fine grid (e_f) and spatial convergence rates in parentheses for u, v, and w after 1000, 2000 and 3000 time steps. $\Delta t = 10^{-5}$, $\varepsilon = 10^{-7}$.

Time step	1000	2000	3000
$\overline{e_{\rm c}(u)}$	2.98e - 10	2.95e - 10	2.93e - 10
$e_{\rm m}(u)$	1.17e - 11(4.7)	1.16e - 11(4.7)	1.17e - 11(4.7)
$e_{\rm f}(u)$	5.38e - 13(4.6)	6.72e - 13(4.4)	8.74e - 13(4.2)
$e_{\rm c}(v)$	6.67e - 10	6.70e - 10	6.73e - 10
$e_{\rm m}(v)$	2.80e - 11(4.6)	2.83e - 11(4.6)	2.86e - 11(4.6)
$e_{\rm f}(v)$	1.24e - 12(4.5)	1.27e - 12(4.5)	1.31e - 12(4.5)
$e_{\rm c}(w)$	1.57e - 10	1.60e - 10	1.63e - 10
$e_{\rm m}(w)$	7.40e - 12(4.4)	7.30e - 12(4.5)	7.31e - 12(4.5)
$e_{\rm f}(w)$	3.32e - 13(4.4)	3.66e - 13(4.4)	4.35e - 13(4.3)

two A-systems (steps 1 and 2) and the Q-system (step 4) needed to fulfil the convergence criterion. The number of iterations for the imaginary part is similar for wave numbers $\beta \neq 0$. In general, fewer iterations are needed for higher wave numbers. Only one outer iteration was required for every β .

The theoretically expected fourth-order convergence in space is achieved in the second numerical experiment summarized in Table III. Three simulations are run at three different resolutions with $n_x \times n_y \times n_z = 16 \times 21 \times 8$, $31 \times 41 \times 16$ and $61 \times 81 \times 32$ cells. The numerically obtained results are compared to the Orr–Sommerfeld reference solutions and the errors are measured in an x-y plane in the l_2 norm. The error norms of the u, v and w components and the obtained spatial order of accuracy are displayed in Table III.

ACKNOWLEDGEMENTS

We have benefited from many discussions with Professors Dan Henningson and Arne Johansson.

REFERENCES

- Brüger A, Gustafsson B, Lötstedt P, Nilsson J. High order accurate solution of the incompressible Navier–Stokes equations. Journal of Computational Physics 2005; 203:49–71. Available at http://www.it.uu.se/research/reports/.
- 2. Brüger A, Nilsson J, Kress W. A compact higher order finite difference method for the incompressible Navier–Stokes equations. *Journal of Scientific Computing* 2002; **17**:551–560.
- 3. Greenbaum A. Iterative Methods for Solving Linear Systems. SIAM: Philadelphia, 1997.
- 4. Gustafsson B, Nilsson J. Fourth order methods for the Stokes and Navier–Stokes equations on staggered grids. In *Frontiers of Computational Fluid Dynamics*—2002, Caughey DA, Hafez MM (eds). World Scientific Publishing: Singapore, 2002; 165–179.
- Kress W, Lötstedt P. Time step restrictions using semi-implicit methods for the incompressible Navier–Stokes equations. *Technical Report 2004-030*, Department of Information Technology, Uppsala University, Uppsala, Sweden, 2004. Available at http://www.it.uu.se/research/reports/.
- 6. Lele SK. Compact finite difference schemes with spectral-like resolution. *Journal of Computational Physics* 1992; **103**:16–42.
- 7. Perot JB. An analysis of the fractional step method. Journal of Computational Physics 1993; 108:51-58.
- 8. Piller M, Stalio E. Finite-volume compact schemes on staggered grids. *Journal of Computational Physics* 2004; **197**:299–340.
- 9. Schmid PJ, Henningson DS. Stability and Transition in Shear Flows. Springer: New York, 1999.