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Contract No. NAS1-17070
May 1985

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Operated by the Universities Space Research Association
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Abstract

A new splitting scheme is proposed for the numerical solution of the time-dependent, incompressible Navier-Stokes equations by spectral methods. A staggered grid is used for the pressure, improved intermediate boundary conditions are employed in the split step for the velocity, and spectral multigrid techniques are used for the solution of the implicit equations.

Research for the second author was supported by the National Aeronautics and Space Administration under NASA Contract No. NAS1-17070 while he was in residence at ICASE, NASA Langley Research Center, Hampton, VA 23665.
I. INTRODUCTION

Numerical simulations of transition and turbulence are playing an increasingly important role in the investigation of the basic physics of these strongly nonlinear, three-dimensional phenomena. The most efficient direct simulation codes are those which use spectral methods in simple geometries such as the periodic box ([1], [2]), the channel ([3] - [7]), the pipe ([8], [9]), the parallel boundary layer ([7], [8], [10]), and the region between two infinite, concentric cylinders [11]. All of these algorithms require periodic boundary conditions in at least two directions and thus are unsuitable for such more realistic problems as the true, non-parallel boundary layer and the flow between two finite, concentric cylinders. Moreover, in most applications the viscosity must be treated implicitly, at least in the non-periodic directions, and these algorithms are quite limited in the nature of the viscosity that they can handle. The most flexible of these algorithms [7] can treat implicitly a viscosity which varies in time and in the one non-periodic direction.

The limitation to at most one non-periodic direction arises from the solution schemes used for the implicit systems of equations in the algorithms, typically a Poisson equation for the pressure and Helmholtz equations for the velocity components. These are usually solved by direct methods which first diagonalize the equations in the periodic directions and then resort to special efficient solution procedures which apply only when there is at most one non-periodic direction. These spectral methods invariably use Fourier series in the periodic directions and Chebyshev or some other Jacobi polynomials in the non-periodic directions. The Fast Fourier Transform (FFT) can be used to diagonalize the equations in the periodic directions provided
that the viscosity (or at least the part of it which is treated implicitly) is independent of the periodic coordinates. In a limited number of cases an efficient solution procedure exists for the remaining, non-periodic direction. Thus, in addition to the obvious need for new, more general spectral algorithms for problems with more than one non-periodic coordinate, there is also a need for new algorithms even for fully periodic problems with strongly position-dependent viscosity.

The way to achieve greater generality is to abandon direct solution techniques in favor of iterative methods. The algorithm described in [7] does use iterative techniques, but only in one of the directions. This method does not use splitting and the implicit equations are solved together as a system. A preconditioned iterative scheme is at the core of this method. The effective iteration matrix has complex eigenvalues. The extension of this method to the more general cases of interest here is not straightforward. The use of splitting would lead to implicit equations which are positive definite and much more straightforward to solve by iterative methods. However, Marcus [11] has clearly pointed out serious errors that can arise in splitting methods. In this paper we describe a new type of splitting in which these errors are absent. Moreover, we discuss efficient iterative solution of the implicit systems by spectral multigrid techniques ([12] - [16]).
II. SPLITTING SCHEME

The incompressible Navier-Stokes equations can be written

\[ \frac{\partial \mathbf{u}}{\partial t} = \mathbf{u} \times \mathbf{\omega} + \nabla \cdot (\mu \nabla \mathbf{u}) - \nabla p \quad \text{in } \Omega \]

\[ \nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \]

\[ \mathbf{u} = \mathbf{g} \quad \text{on } \partial \Omega \]

\[ \mathbf{u}(x,0) = \mathbf{u}_0(x) \quad \text{in } \Omega, \]

where \( \mathbf{u} = (u,v,w) \) denotes the velocity, \( \mathbf{\omega} = \nabla \times \mathbf{u} \) the vorticity, \( p = p + \frac{1}{2} |\mathbf{u}|^2 \) the total pressure, \( \mu \) the viscosity, \( \Omega \) the interior of the domain, and \( \partial \Omega \) its boundary. In some problems the above system should be supplemented with an equation for the temperature, and the viscosity may depend upon position \( \mathbf{x} \) and time \( t \). An empirical formula for the viscosity is given in [17] (and repeated in [7]) in terms of the temperature. A complete description of the equations governing the parallel boundary layer is given in [7].

The solution algorithm is based upon the following splitting scheme for advancing from \( t = t_n \) to \( t = t_{n+1} \):

\[ \frac{\partial \mathbf{u}^*}{\partial t} = \mathbf{u}^* \times \mathbf{\omega}^* + \nabla \cdot (\mu \nabla \mathbf{u}^*) \quad \text{in } \Omega \]

\[ \mathbf{u}^* = \mathbf{g}^* \quad \text{on } \partial \Omega \]

\[ \mathbf{u}^*(x,t_n) = \mathbf{u}(x,t_n) \quad \text{in } \Omega, \]
\[
\begin{align*}
\mathbf{u}_t &= - \nabla \mathbf{p} \quad \text{in } \Omega \\
\nabla \cdot \mathbf{u} &= 0 \quad \text{in } \Omega \\
\mathbf{u} \cdot \hat{n} &= \mathbf{g} \cdot \hat{n} \quad \text{on } \partial \Omega \quad (3) \\
\mathbf{u}_t \cdot \hat{\tau} &= - \nabla \cdot \mathbf{p} \cdot \hat{\tau} \quad \text{on } \partial \Omega \\
\mathbf{u}^*(x,t^*) &= \mathbf{u}^*(x,t^*) \quad \text{in } \Omega,
\end{align*}
\]

where Eq. (2) is integrated from \( t_n \) to the intermediate time \( t^* \); then Eq. (3) is integrated from \( t^* \) to \( t_{n+1} \) and \( \mathbf{u}(x,t_{n+1}) \) is identified with \( \mathbf{u}^*(x,t_{n+1}) \). Here \( \hat{n} \) denotes the unit normal to the boundary and \( \hat{\tau} \) a unit tangent vector at the boundary. Note that in the velocity step all of the velocity components are specified at the boundary, whereas in the pressure step only the normal velocity component is specified on the boundary, and the differential equation itself is used for the tangential velocity components there. The boundary conditions for each step are determined by the condition that the individual step be well-posed. At the end of a full step the flow will be divergence-free, but there will be a slip velocity at the boundary. If the boundary conditions on the intermediate, velocity step are \( \mathbf{u}^* = \mathbf{g}^n \) or \( \mathbf{u}^* = \mathbf{g}^{n+1} \), then the slip velocity at the end of the full step will be \( O(\Delta t) \). This can be reduced by resorting to intermediate boundary conditions of the type suggested in [18]. We set,
\[ \mathbf{u}^* \cdot \hat{\mathbf{r}} = (\mathbf{g}^n + \Delta t (\mathbf{g}_t^n + \nabla \mathbf{P}^n)) \cdot \hat{\mathbf{r}} \]

\[ \mathbf{u}^* \cdot \hat{\mathbf{n}} = (\mathbf{g}^n + \Delta t \mathbf{g}_t^n) \cdot \hat{\mathbf{n}}. \]

This reduces the final slip velocity to \( O(\Delta t^2) \). Higher-order corrections are also possible.

There are two key elements of this splitting scheme which distinguish it from the standard splitting scheme for spectral algorithms [3], whose problems have been documented by Marcus [11]. The first is the use of a staggered grid for the pressure [7], and the second is the use of intermediate boundary conditions, i.e., \( \mathbf{g}^* \), which are not the desired boundary conditions on \( \mathbf{u} \), i.e., \( \mathbf{g} \), but rather are derived from the principles developed by LeVeque and Oliger [18] and applied by Kim and Moin [19] to a two-dimensional finite difference algorithm.

The advantages of the staggered grid for finite difference and finite element schemes are well-known. Principal among them is that the pressure step does not require any numerical boundary conditions on the pressure. The usual procedure on a non-staggered grid is to reduce Eq. (3) to a Poisson equation for the pressure and to use the normal momentum equation to obtain a Neumann boundary condition on \( \mathbf{P} \). However, the incompressible Navier-Stokes equations with boundary conditions solely on the velocity form a well-posed mathematical problem. The imposition of pressure boundary conditions is an overspecification of the problem and can lead to numerical instability or inconsistent results. Such difficulties are far more likely to be observed in solutions obtained via spectral methods rather than via finite difference methods. The former are notoriously sensitive to boundary conditions--see
Figure 2 of [20] for a dramatic example of instability arising in a spectral calculation with overspecified boundary conditions—and produce solutions that are sufficiently accurate so that even minor inconsistencies are noticeable—see [11] for an example of a spectral calculation which gives an incorrect result because of the pressure boundary conditions. Kleiser and Schumann [4] and Marcus [11] have devised a method for imposing a consistent pressure boundary condition on the Poisson equation, but this applies only to incompressible flow with constant viscosity, and not to the more general problems of interest here.

III. DISCRETIZATION

For simplicity we will describe the spectral discretization for a two-dimensional channel flow problem with periodic boundary conditions in $x$ and no-slip boundary conditions in $y$ on $\Omega = [0,2\pi] \times (-1,1)$. The spectral method is based upon Fourier series in $x$ and Chebyshev polynomials in $y$. The collocation points in these directions are

$$x_i = \frac{2\pi i}{N_x} \quad i = 0,1,\ldots,N_x-1$$

$$y_j = \cos \frac{\pi j}{N_y} \quad j = 0,1,\ldots,N_y$$

$$y_{j+1/2} = \cos \frac{\pi (j+1/2)}{N_y} \quad j = 0,1,\ldots,N_y-1.$$  \hspace{1cm} (5)

The velocity is defined at $(x_i,y_j)$ and the pressure at $(x_i,y_{j+1/2})$. The momentum equation is enforced at the interior velocity nodes (cell edges) and the continuity equation at the pressure nodes (cell centers).
The velocity step is discretized in the usual spectral collocation manner. A Fourier transform in \( x \) simplifies the pressure step. Define the Fourier components by

\[
\hat{u}_k(y_j) = \frac{1}{N_x} \sum_{\ell=0}^{N_x-1} u(x_\ell, y_j) e^{-ikx_\ell},
\]

for \( k = -N_x/2, -N_x/2+1, \ldots, N_x/2-1 \). Let \( C_0 \) and \( C_+ \) be the matrices which represent the operations of computing Chebyshev coefficients from function values at the velocity nodes and the pressure nodes, respectively; let \( D \) represent the differentiation operator in terms of the Chebyshev coefficients, and let \( iK \) represent the differentiation operator in terms of the Fourier coefficients. (\( K \) is a real diagonal matrix and \( D \) is a real, strictly upper triangular matrix.)

The discrete divergence operator is

\[
\mathcal{D}_u = (C_0^{-1} C_0)(iKu + C_0^{-1} D C_0 \hat{v}).
\]

(The operator \( C_0^{-1} C_0 \) represents interpolation from the cell edges to the cell centers.) This may be decomposed into a part which depends on the normal velocity component at the boundary, denoted by \( B_u \) and the remaining part, denoted by \( (D - B)\hat{u} \). The discrete gradient operator is

\[
\mathcal{G}_p = (C_0^{-1} C_+)(iKp, C_+ D p).
\]

Letting \( \hat{Q} = \Delta t \hat{p} \), the fully discrete version of Eq. (3) is
\[ \hat{u}^{n+1} = \hat{u}^* - G \hat{Q} \]  

at interior cell edges

\[ \begin{align*}
\hat{u}^{n+1} &= \hat{u}^* - (G \hat{Q})_x \\
\hat{v}^{n+1} &= (G^{n+1})_y
\end{align*} \]  

at \( y = \pm 1 \)

\[ \nabla \hat{u}^{n+1} = 0 \]  

at cell centers.

These combine to yield

\[ \nabla \hat{u}^{n+1} = (\nabla - B)(\hat{u}^* - G \hat{Q}) + B \hat{g}^{n+1} = 0 \]  

(11)

or

\[ \hat{L} \hat{Q} = \hat{F} \]  

(12)

with

\[ \hat{L} \hat{Q} = -\hat{k}^2 \hat{Q} + C_+^{-1} \text{DC}_+^{-1} C_0^{-1} \text{DC}_+ \hat{Q} \]  

(13)

\[ \hat{F} = \nabla \hat{u}^* + B (\hat{g}^{n+1} - \hat{u}^*) \]  

(14)

where \( C_i \) is \( C_0 \) with its first and last rows replaced with zeroes. The pressure is computed from Eq. (12) and the velocities are then adjusted via Eq. (9). The equation for the pressure is diagonal in the wavenumbers \( k \). It is singular for \( k = 0 \), but this merely reflects the indeterminacy of the pressure to within an additive constant. Note that no pressure boundary
condition is included in Eq. (12). The right-hand side, however, contains the desired boundary conditions on the normal velocity.

Traditional time discretizations for the Navier-Stokes equations use explicit Adams-Bashforth or Runge-Kutta methods for the explicit terms and Crank-Nicolson for the implicit terms. We use the low-storage, third-order Runge-Kutta/Crank-Nicolson scheme detailed in [7] for the velocity step, with a backward Euler pressure correction applied after each stage of the Runge-Kutta method.

The velocity step contains Helmholtz equations for the velocity components. If the viscous term in the periodic directions is explicit, this equation will have the form (in Fourier space)

\[ (-2\Delta t)\hat{u}_k + \frac{\partial}{\partial y} \left( \bar{u}(y,t) \frac{\partial \hat{u}_k}{\partial y} \right) = \hat{f}_k, \]  

(15)

if it is semi-implicit,

\[ (-2\Delta t)\hat{u}_k - k^2 \bar{u}(y,t)\hat{u}_k + \frac{\partial}{\partial y} \left( \bar{u}(y,t) \frac{\partial \hat{u}_k}{\partial y} \right) = \hat{f}_k \]  

(16)

and if it is fully implicit, it will have the form (in physical space)

\[ (-2\Delta t)\mu + \frac{\partial}{\partial x} \left( \mu(x,y,t) \frac{\partial \mu}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu(x,y,t) \frac{\partial \mu}{\partial y} \right) = f, \]  

(17)

where

\[ \bar{\mu}(y,t) = \frac{1}{N_x} \sum_{i=0}^{N_x-1} \mu(x_i,y,t). \]
Further details on spectral collocation for a similar, but unsplit method are available in [7]. The z direction is treated in a manner analogous to the x or y directions here, depending upon whether the boundary conditions in the third direction are periodic or non-periodic. Of course, if the y direction is periodic as well, then it is treated the same as the x direction. Spectral collocation methods are readily applied in conjunction with mappings. In particular, for the parallel boundary layer problem the y direction is semi-infinite. Both algebraic [7] and exponential [10] mappings are feasible.

IV. MULTIGRID ASPECTS

The role of spectral multigrid (SMG) methods in this spectral collocation algorithm for the incompressible Navier-Stokes equations is to accelerate the iterative solution of Eq. (12) and either Eq. (15), Eq. (16), or Eq. (17) at each time step. We refer the reader to [12] and [13] for the fundamentals of SMG and to [21] for a general background on multigrid methods. The trigonometric interpolation techniques described in [13] for the prolongation and restriction operators apply directly to the current problems. As usual, the relaxation procedures must be tailored to the specific problem.

In some fully periodic problems, the relaxation may be explicit, but in most cases it is essential to precondition the relaxation with a finite difference approximation to the differential equation [22]. If the preconditioning is used in only one coordinate direction, then multigrid methods are not really necessary, for the finite difference approximation may be inverted quickly and relaxation on a single grid has a spectral radius
independent of the size of the problem. However, if preconditioning is used in more than one direction, multigrid methods are important because they allow incomplete solutions of the finite difference operator to serve as effective and efficient preconditioners.

Since the FFT may be used for both Fourier series and Chebyshev polynomial manipulations, the asymptotic operation count for evaluating the explicit terms in both the velocity and pressure steps is $O(N_x N_y \log(N_x N_y))$ in two dimensions. A single iteration on the implicit systems costs $O(N_x N_y \log(N_x N_y))$ operations for the residual evaluation plus whatever work is required to invert the finite difference preconditioning operator. A complete inversion of the finite difference operator has an operation count which is generally of larger order than that for the residual evaluation, whereas an incomplete inversion costs $O(N_x N_y)$. The most desirable situation would be to have the number of iterations required for an acceptable solution to the implicit equations be independent of $N_x$ and $N_y$ while using incomplete inversions of the finite difference operator. This is not achievable for single-grid iterative schemes ([13], [15]). With SMG methods, however, the ideal situation is nearly achievable, with the number of iterations growing as some small fractional power of $N_x N_y$.

SMG methods have yet to be applied to fully three-dimensional Poisson problems. We anticipate that as in two dimensions, successful smoothing and grid coarsening strategies for three-dimensional SMG methods will be the appropriate modifications of strategies for three-dimensional finite difference multigrid methods (FDMG). On the more difficult three-dimensional problems FDMG methods have had to resort to alternating plane relaxation (with coarsening in all three directions) or to alternating line relaxation (with coarsening in only two directions).
Fully Periodic Problems

For this class of problems the pressure equation is quite simple, and it can be solved easily by a direct method since it is a diagonal system in Fourier space. The Fourier SMG techniques developed in [12] and refined in [16] will solve even Eq. (17) very efficiently. As long as the grid size is the same in all directions, Richardson relaxation combined with residual averaging and position-dependent relaxation parameters will achieve an order of magnitude reduction in the residual per fine grid relaxation [16]. On more general grids, SMG is best applied in conjunction with incomplete finite difference preconditioning. Brandt, et al. [16], have demonstrated that alternating direction Zebra relaxation using the finite difference preconditioner is effective on a vector processor.

Problems with One Non-Periodic Direction

In this case as well, the pressure equation can be solved efficiently on a single grid, since a complete inversion of the preconditioning operator requires just the solution of independent tridiagonal systems. Simple estimates of the type used by Orszag [22] suggest that the condition numbers of the preconditioned systems, i.e., the ratios of the largest to the smallest eigenvalues of the effective iteration matrices, should be a decreasing function of the Fourier wavenumber, with a maximum of 2.5 for \( k = 0 \) and a minimum of 1 as \( k \to \infty \). A residual reduction by at least a factor of 3 is easy to achieve, e.g., by a Chebyshev semi-iterative scheme [22]. The minimum residual scheme used in [7] is nearly as effective and requires no relaxation parameters.
For the velocity step, only the fully implicit viscous time discretization requires SMG. Both Eqs. (15) and (16) can be solved efficiently by the same techniques used for the pressure equation. For Eq. (17), however, SMG is practically a necessity, especially for large problems. Preconditioners for Fourier-Chebyshev SMG methods are already available, e.g., ADI relaxation [13] as well as incomplete LU decomposition and various Zebra schemes (T. Phillips, private communication).

Problems with Two Non-Periodic Directions

Here SMG methods are advisable for all the implicit equations because of the rapid increase in expense of direct methods for inverting the preconditioning operator. Incomplete LU decomposition combined with non-stationary Richardson relaxation has already proven successful for problems with two Chebyshev directions [13] as have ADI methods [14]. Although the smoothing rates of the ADI schemes are not as fast as those of the incomplete LU schemes, the ADI methods may nonetheless be superior on current supercomputers because they vectorize better and require less auxiliary storage.

V. NUMERICAL EXPERIENCE

The novel aspects of the proposed spectral algorithm are the staggered grid in a splitting scheme, the intermediate boundary conditions given in Eq. (4), and the SMG solution of the pressure equation. The remaining components of this algorithm have been tested extensively elsewhere.
The results of the unsplit spectral collocation algorithm described in [7] will be used to check the soundness of the present discretization. The first test problem will be one of the examples used in [7] to verify the unsplit algorithm for channel flow at a Reynolds number of 5000, namely the three-dimensional Tollmein-Schlichting wall mode listed there in Table I. Periodic boundary conditions are applied in x and z and no-slip boundary conditions in y. The grid is $4 \times 48 \times 4$ and the time-step $\Delta t = 0.10$. The initial condition consists of the mean flow plus a very small multiple of the linear eigenfunction—it disturbs the mean flow by at most 0.001% in the x direction. The criterion is how well the computed growth rate matches the linear growth rate at $t = 50$.

The results appear in Table I. The linear growth rate is -0.076227. Note the extremely high accuracy of the unsplit code—even after more than two full periods of the Tollmein-Schlichting wave, there is more than five-digit accuracy. Results are given in the table for the split code under two different boundary conditions. The zero-order boundary conditions are that $g^* = 0$, and the first-order boundary conditions are given by Eq. (4). The first-order boundary conditions produce much better results than the zero-order boundary conditions. Indeed, the unsplit code performs only slightly better than the split code with first-order boundary conditions.

A second comparison of the split and unsplit codes was performed for a Reynolds number of 1500 on a $32 \times 64 \times 32$ grid. The initial conditions were essentially the same as those used in reference 23. The time history of the energy in several of the horizontal Fourier harmonics is provided in Figure 1. The shear component $\partial u / \partial y$ is given in Figure 2 at $t = 15$ for the plane $z = 0$. The two calculations agree to better than 0.1%.
It might appear preferable to use the same intermediate boundary conditions on the normal velocity component as are used for the tangential velocity. However, calculations performed with such first-order boundary conditions prove to be unstable. This channel flow problem is yet another example of the great sensitivity of spectral methods to the boundary conditions. Calculations performed with a similar split code which uses finite differences rather than Chebyshev polynomials in the normal direction display no problems with first-order boundary conditions on all three-velocity components. Indeed, calculations performed with the split Fourier-finite difference code exhibit a substantial improvement when the full first-order intermediate velocity boundary conditions are used in place of the usual zero-order ones: for a calculation similar to the one shown in Figure 12 of [7], but on a \(16 \times 100 \times 16\) grid, the split code agrees with the corresponding unsplit code at \(t = 30\) to five significant digits with the first-order intermediate boundary conditions, whereas only three-digit agreement is achieved with the zero-order ones.

Several alternative intermediate boundary conditions on the normal velocity are possible, and these are currently under investigation to determine their accuracy and stability for the fully spectral algorithm.

As noted above, the pressure equation for this problem may be solved acceptably fast with a single-grid relaxation scheme such as the minimum residual method. Some preliminary calculations have been made with a SMG scheme employing minimum residual relaxation. They do indicate that the fine grid relaxations are more effective when combined with coarse grid relaxations, e.g., upon returning to the fine grid the residual is initially reduced at over twice the rate that it would have been had the calculation simply remained on the fine grid.
VI. CONCLUDING REMARKS

The techniques discussed here allow spectral methods to be applied reliably and efficiently to a wider range of time-dependent Navier-Stokes calculations than heretofore possible. They allow solutions of fully periodic problems of greater generality than even those covered by the algorithm presented in [2]. They appear to be just as efficient as the best available algorithms for parallel channel flow. Together with [7] this is the only spectral algorithm suitable for the heated, parallel boundary layer, as well as the only spectral algorithm for the usual parallel boundary layer and the infinite concentric cylinder problem with an asymptotic operation count as low as $O(N_x N_y N_z \log(N_x N_y N_z))$. Moreover, the iterative schemes employed in this algorithm are more robust than those in [7].

This algorithm is directly applicable to the finite concentric cylinder problem. The collocation points will be automatically clustered near the boundaries, where the most resolution is required. It can also be applied to the non-parallel boundary layer. Some modifications are desirable because the usual collocation points are not well-suited to the resolution requirements in the streamwise direction. This difficulty can be alleviated to some extent by a streamwise coordinate mapping. A more desirable approach appears to be a combination of the best aspects of this method with those of the spectral element method ([24], [25]), which in its current form still relies on direct solution techniques for the implicit equations.

Acknowledgment

Discussions with C. Canuto, R. LeVeque, and T. Phillips have contributed to our views on some of the details of this algorithm.
REFERENCES


Table I.
Effect of Intermediate Boundary Conditions

| Code     | $\omega_i|_{\text{calc.}}$ | $\omega_i|_{\text{error}}$ |
|----------|--------------------------|---------------------------|
| Unsplit  | -.076234                 | -.000007                  |
| Zeroth-order Split | -.075849  | .000378                   |
| First-order Split   | -.076244         | -.000017                  |
Figure 1. Harmonic histories for two channel flow simulations. The harmonics are labelled by their respective streamwise (x) and spanwise (z) wavenumbers; (a) unsplit code; (b) split code.
Figure 2. Vertical shear $\partial u / \partial y$ at $t = 15$ in the plane $z = 0$; (a) unsplit code; (b) split code.
A new splitting scheme is proposed for the numerical solution of the time-dependent, incompressible Navier-Stokes equations by spectral methods. A staggered grid is used for the pressure, improved intermediate boundary conditions are employed in the split step for the velocity, and spectral multigrid techniques are used for the solution of the implicit equations.
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