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A Divergence-Free Chebyshev Collocation Procedure for Incompressible Flows with Two Non-periodic Directions

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The enforcement of divergence-free condition in the interior and on the boundaries of an incompressible flow with two non-periodic directions is discussed for a Chebyshev collocation formulation. An influence matrix technique along with a correction methodology is used to satisfy the continuity equation everywhere in the domain. Details of implementing this procedure in a collocation method are presented. An efficient solution procedure based on matrix diagonalization has been used to solve the resulting full matrices. Two test problems: (a) flow in a driven square cavity, and (b) fully-developed laminar flow in a square duct subject to a three-dimensional perturbation are studied. Run-time statistics (CPU, memory, MFLOPS) of the solution procedure are presented for representative grid sizes. © 1993 Academic Press, Inc.

1. INTRODUCTION

The integration of Navier–Stokes equations with high temporal and spatial accuracies is required in all applications of computational fluid dynamics, more so in direct simulations of turbulent flows (e.g., [1, 2]). In comparison with finite-difference and finite-element methods, spectral discretization of the spatial derivatives where applicable is the preferred approach due to its exponential convergence property. However, because of their global nature, spectral methods are more sensitive to the precise manner in which the conditions at non-periodic boundaries are implemented. In incompressible flows, the continuity equation has no time-derivative terms and pressure becomes a diagnostic variable ensuring that the velocity field remains divergence-free. There has been much discussion in the literature [3–6] on the specification of proper boundary conditions for pressure. Different opinions exist on the proper boundary conditions for the pressure Poisson equation obtained by combining the momentum and continuity equations. While alternate formulations such as those using vector potential and vorticity as dependent variables (e.g., [7, 8]) automatically satisfy the incompressibility constraint, the primitive-variable formulation (with **u** and p) continues to be preferred by most researchers.

The implementation of the divergence-free condition in the interior as well as on the boundaries differs between implicit and explicit schemes. In a purely explicit scheme, the satisfaction of interior and boundary divergences is relatively easy as shown by Ku *et al.* [9, 10]. However, purely explicit formulations impose severe restrictions on the allowable time increment when used with Chebyshev collocation. The explicit treatment of the diffusion terms requires that the stable time increment vary as $1/N^4$, where N is the number of Chebyshev modes. An implicit treatment of the viscous terms leads to momentum equations which are very similar to those for the Stokes problem. The difficulty in solving these momentum equations along with the continuity equation lies in the coupling of the scalar components of the velocity field and the pressure. In problems with only one non-periodic direction, the discrete version of the coupled equations results in a blocked system of linear equations for the velocity and pressure (Moin and Kim [11], Malik *et al.* [12]). A direct inversion of these blocked matrices is computationally expensive in a two- or three-dimensional (2D or 3D) problem. If one resorts to iterative techniques, the poor condition number associated with the spectral second derivative operator requires efficient preconditioners for rapid convergence.

The coupling between the velocity and pressure can be reduced, although not completely eliminated, by solving a Poisson equation for pressure. A simple way to achieve complete decoupling is by time-splitting or operator-splitting technique of Chorin [13]. Here, the momentum equations are first solved without the pressure gradient terms. In the second step, a Poisson equation is solved for a scalar potential and the velocities are corrected to satisfy continuity. Since there are no natural boundary conditions for the intermediate velocity and scalar potential fields, several approximate conditions have been used by various investigators (Ku *et al.* [9], Kim and Moin [14], Streett

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and Hussaini [15]). However, these procedures do not guarantee zero divergence at the boundaries. In addition, small slip velocities are produced at the boundaries. While these errors may be small and harmless to the eventual objective, they are not satisfactory if their effect is unknown.

As an alternative to time-splitting techniques, Kleiser and Schumann [16] proposed an influence matrix method to decouple the pressure Poisson equation from the momentum equations and obtain zero boundary divergence. In this technique, the momentum equations are first solved with an arbitrary boundary pressure distribution and the resulting divergences on the boundary are calculated. Using a predetermined influence matrix, corrections to the boundary pressures are evaluated. These boundary pressures are then used to obtain a new pressure field and the final velocity field is obtained by solving again the momentum equations. Although this method is computationally more expensive than methods using operator-splitting, the solution has the desired divergence-free properties. In principle, the influence matrix approach should give zero boundary and interior divergences at the end of the time step. However, because of the discrete nature of the momentum equations, small but non-zero divergences appear at the interior points. This situation was remedied by Kleiser and Schumann [16] by proposing a "tau correction" to obtain the correct pressure field. Kleiser and Schumann [16] demonstrated this procedure in the spectral-tau context for a flow with one non-periodic direction and two periodic directions. A collocation implementation of this correction for one non-periodic direction was discussed by Canuto *et al.* [17].

The extension of the influence matrix approach to two non-periodic directions in Chebyshev–collocation context was considered by le Quere and de Roquefort [18] and Ku *et al.* [9] but only incompletely without the tau correction. Therefore, its performance was observed to be inferior to time-splitting methods for some model problems. Recently, Tuckerman [19] has extended the "tau correction" to Chebyshev discretizations in two directions. Tuckerman's formulation and solution were primarily in the context of a spectral-tau procedure. However, from an implementation viewpoint, collocation methods are preferred (Canuto *et al.* [17]) despite their larger computational costs over spectral-tau methods. In the present paper, the implementation of the influence matrix approach for two non-periodic directions, including a correction for interior divergences, is demonstrated for a Chebyshev–collocation procedure.

The present study was motiviated by our final objective to study the structure of fully developed turbulence in a duct of square cross section. The contributions of this study are primarily in the implementation and assessment of a Chebyshev–collocation procedure with a correction for interior divergences. We also discuss the added CPU time and memory for this procedure as compared to the time-splitting and without the "collocation correction" procedures. Two applications: (a) flow in a driven square cavity and (b) decay of a 3D perturbation in a fully developed laminar flow are considered for demonstration. In Section 2, the basic solution procedure with the traditional influence matrix approach is described. In Section 3, the "collocation correction" for obtaining zero interior divergences is explained. The applications are presented in Section 4 and the conclusions are given in Section 5.

2. BASIC SOLUTION METHODOLOGY

We begin with the non-dimensionalized Navier–Stokes equations for the conservation of mass and momentum for an incompressible flow with constant properties and no body forces,

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla \tilde{p} + \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{u}, \tag{2}$$

where $\mathbf{u}$, $\tilde{p}$, t, and Re are the velocity, pressure, time, and Reynolds number, respectively. We consider the solution of these equations with the boundary conditions $\mathbf{u}_b = \mathbf{q}$ on x and y boundaries and periodic conditions in the z-direction. Let Ω denote the interior of the domain of interest and $\partial\Omega$ denote its non-periodic boundary. A semi-implicit discretization in time of the governing equations by the Adams–Bashforth scheme for the convection terms and the Crank–Nicolson scheme for the diffusion terms gives

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \left(\frac{3}{2}\mathbf{H}^n - \frac{1}{2}\mathbf{H}^{n-1}\right) = -\nabla \tilde{p}^{n+1} + \frac{1}{2\mathrm{Re}} (\nabla^2 \mathbf{u}^{n+1} + \nabla^2 \mathbf{u}^n) \tag{3}$$

$$\nabla \cdot \mathbf{u}^{n+1} = 0 \tag{4}$$

$$\mathbf{u}_b^{n+1} = \mathbf{q}^{n+1} \qquad \text{on } \partial\Omega, \tag{5}$$

where $\mathbf{H}$ represents the convective terms. Equation (3) can be abbreviated as

$$(\nabla^2 - 2\mathrm{Re}/\Delta t)\, \mathbf{u}^{n+1} - \nabla p^{n+1} = \mathbf{S}, \tag{6}$$

where $p = 2\mathrm{Re}\, \tilde{p}$, and $\mathbf{S}$ includes all the terms evaluated explicitly,

$$\mathbf{S} = -(\nabla^2 + 2\mathrm{Re}/\Delta t)\, \mathbf{u}^n + 2\mathrm{Re}(\tfrac{3}{2}\mathbf{H}^n - \tfrac{1}{2}\mathbf{H}^{n-1}). \tag{7}$$

The momentum equations are thus reduced to the Stokes equations. They are coupled to each other through the pressure gradient term such that the velocity field remains divergence free. In an unsplit decoupled procedure, the momentum equations are solved in conjunction with an equation for pressure. By taking the divergence of the momentum equation, the familiar pressure Poisson equation,

$$\nabla^2 p^{n+1} = -\nabla \cdot \mathbf{S} \tag{8}$$

can be obtained if the following condition is satisfied by the divergence of velocity:

$$(\nabla^2 - 2\text{Re}/\Delta t)\, \nabla \cdot \mathbf{u}^{n+1} = 0 \qquad \text{in } \Omega. \tag{9}$$

From the above equation, it can be seen that $\nabla \cdot \mathbf{u}^{n+1}$ is zero in the interior if and only if $\nabla \cdot \mathbf{u}^{n+1}$ is zero on the boundary. Therefore, if pressure is obtained from Eq. (8) such that $\nabla \cdot \mathbf{u}^{n+1} = 0$ on $\partial\Omega$, then the velocity distribution determined using this pressure distribution in the momentum equations would satisfy the continuity equation in the interior. This coupling between the velocity and pressure fields can be resolved by the influence matrix approach.

2.1. *Influence Matrix Method*

The influence matrix method originally due to Kleiser and Schumann [16] relies on the linearity of the time discretized momentum and pressure equations to combine a series of boundary pressure distributions which will eventually satisfy $\nabla \cdot \mathbf{u}^{n+1} = 0$ in Ω and on $\partial\Omega$. Let the pressure and velocity fields be given by the sum of a particular solution and a complementary solution.

$$p^{n+1} = p_p + p_c \qquad \text{and} \qquad \mathbf{u}^{n+1} = \mathbf{u}_p + \mathbf{u}_c. \tag{10}$$

The particular solutions are obtained with arbitrary (say, zero) pressure boundary conditions and given velocity boundary conditions as

$$\nabla^2 p_p = -\nabla \cdot \mathbf{S} \qquad \text{in } \Omega \text{ with } p_p = 0 \qquad \text{on } \partial\Omega \tag{11}$$

$$(\nabla^2 - 2\text{Re}/\Delta t)\, \mathbf{u}_p - \nabla p_p = \mathbf{S} \qquad \text{in } \Omega \text{ with } \mathbf{u}_p = \mathbf{q} \qquad \text{on } \partial\Omega. \tag{12}$$

The complementary solution in turn is represented as the sum of a series of complementary functions (Green's functions) as

$$p_c = \sum \alpha_i \bar{p}_i, \qquad \mathbf{u}_c = \sum \alpha_i \bar{\mathbf{u}}_i. \tag{13}$$

The summation is over all i, and $i = 1$ to N_b, where N_b is the total number of boundary points excluding the corners. Each complementary function $(\bar{p}_i, \bar{\mathbf{u}}_i)$ is a solution to the governing equations with zero source terms (i.e., $\mathbf{S} = \mathbf{0}$). The pressure field is solved with zero Dirichlet conditions at all but one of the boundary points. Using this pressure field, the momentum equations are solved with homogeneous boundary conditions. Thus, the complementary functions are solutions to the following equations,

$$\nabla^2 \bar{p}_i = 0 \qquad \text{in } \Omega \text{ with } (\bar{p}_i)_j = \delta_{ij} \qquad \text{on } \partial\Omega \tag{14}$$

$$(\nabla^2 - 2\text{Re}/\Delta t)\, \bar{\mathbf{u}}_i - \nabla \bar{p}_i = \mathbf{0} \qquad \text{in } \Omega \text{ with } \bar{\mathbf{u}}_i = \mathbf{0} \qquad \text{on } \partial\Omega, \tag{15}$$

where $(\bar{p}_i)_j$ is the value of the ith complementary pressure at the jth boundary point and $j = 1$ to N_b represents all the boundary points in some sequential manner. The α_i's are in effect the unknown boundary pressures that need to be determined such that the boundary divergence of the final velocity field $(\mathbf{u}_p + \mathbf{u}_c)$ is zero. Therefore, at every jth point on the boundary,

$$\left(\sum \alpha_i \nabla \cdot \bar{\mathbf{u}}_i\right)_j = -(\nabla \cdot \mathbf{u}_p)_j \tag{16}$$

from which α_i's can be determined as

$$[\alpha] = -[\mathbf{A}]^{-1}\, [(\nabla \cdot \mathbf{u}_p)_b], \tag{17}$$

where the subscript b denotes the boundary and $\mathbf{A} = [(\nabla \cdot \bar{\mathbf{u}}_i)_j]$ is the influence matrix. The influence matrix $(\mathbf{A})$ is evaluated and its inverse is stored at the beginning of the entire solution procedure. As it is not feasible to store all the complementary functions except for very small grids, the pressure and momentum equations are solved again with the new boundary conditions. The pressure equation (Eq. (9)) is solved with the boundary condition $p_i = \alpha_i$ on $\partial\Omega$ and the momentum equations are solved using this pressure distribution.

The discretized momentum equations are 3D Helmholtz equations and the pressure equation is a 3D Poisson equation. In our 3D problem of interest, the flow is non-periodic only in two directions (x and y) and periodic in the third (z) direction. Therefore, the flow variables can be expanded in Fourier series in the z-direction, and the Fourier transforms of the momentum and pressure equations yield 2D Helmholtz equations for each wavenumber in the z-direction. Chebyshev polynomials are used to expand flow variables in the two non-periodic directions. The resulting 2D Helmholtz equations for each wavenumber can be solved efficiently using the matrix diagonalization procedure [20, 17] and the reduced matrix method [10]. At first sight, the work involved in the influence matrix method appears to be twice the work of an operator-split method. However, only the momentum equations in the non-periodic directions and the pressure equation need to be solved twice. Also, the nonlinear term (S) needs to be computed only once. Thus, the increase in work is less than a factor of two. In our demonstration calculations, we observe an increase of only 35% over a split method.

The above described method has been used by le Quere and de Roquefort [18] and Ku *et al.* [9]. However, the velocity field obtained from the above procedure is not divergence-free in the interior. This is because, in a discrete sense the momentum equations are not satisfied at the boundaries but are assumed to do so in obtaining the Poisson equation for pressure (Eq. (9)) thereby resulting in small errors. Kleiser and Schumann [16] estimated these errors to be proportional to the Chebyshev coefficients of the two highest modes in the tau method. They also reported that in some applications this led to numerical instability. To obtain exact zero interior divergences, Kleiser and Schumann [16] proposed a correction in the tau context for flows with one non-periodic direction. This correction has been recently extended to two non-periodic directions by Tuckerman [19]. These two formulations have been in the spectral-tau context. A collocation implementation of this correction procedure for one non-periodic direction was discussed by Canuto *et al.* [17]. We present below the details of implementing the "collocation correction" for two non-periodic directions.

3. CORRECTION FOR INTERIOR DIVERGENCES

The reason for the appearance of non-zero interior divergences in the above-described procedure is the discreteness of the spatial operator [16, 19]. Thus, while the influence matrix procedure described in the previous section is sufficient to ensure divergence-free condition everywhere in the domain in a continuous formulation, the discrete spatial representation of the equations (which is unavoidable in any numerical procedure) leads to interior divergences. This is because the discrete momentum equations are not satisfied on the boundaries and consequently the estimation of the pressure field is in error. However, if these boundary momentum residuals are included in the procedure, the interior divergences can be made zero.

The discrete momentum equations that are actually solved can be expressed as

$$(\nabla^2 - 2\mathrm{Re}/\Delta t)\,\mathbf{u}^{n+1} - \nabla p^{n+1} = \mathbf{S} + \mathbf{B}^{n+1}, \qquad (18)$$

where $\mathbf{B}$ is the residue in the discretized momentum equations and is zero at the interior collocation points but non-zero on the boundaries. The non-zero value of $\mathbf{B}$ on the boundary is not known a priori. The corresponding Poisson equation for pressure is

$$\nabla^2 p^{n+1} = -\nabla\cdot\mathbf{S} - \nabla\cdot\mathbf{B}^{n+1}. \qquad (19)$$

The non-zero value of $\mathbf{B}$ on the boundary directly influences only the pressure equation and not the momentum equations. It is now desired to include the effect of $\mathbf{B}$ in determining the pressure field such that both the interior and the boundary divergences are zero.

The crux of this correction procedure is to generate another complementary solution that will account for the non-zero boundary residual in the momentum equations. The second complementary solution is again represented as a sum of a series of complementary functions. Thus, the pressure and velocity are given by

$$\begin{aligned} p^{n+1} &= p_p + \sum \alpha_i \bar{p}_i + \sum \beta_i \bar{\bar{p}}_i, \\ \mathbf{u}^{n+1} &= \mathbf{u}_p + \sum \alpha_i \bar{\mathbf{u}}_i + \sum \beta_i \bar{\bar{\mathbf{u}}}_i. \end{aligned} \qquad (20)$$

The summation is once again over all the boundary points excluding the corners. The particular solutions and the first set of complementary functions are obtained as before. The second set of complementary functions are to account for the boundary residual in the momentum equations. Each of these complementary functions $(\bar{\bar{p}}_i, \bar{\bar{\mathbf{u}}}_i)$ is a solution to the governing equations with zero source terms (i.e., $\mathbf{S} = \mathbf{0}$) and homogeneous boundary conditions. The pressure field is solved with a unit momentum residual at one of the boundary nodes. The momentum equations are then solved using this pressure field. These complementary functions are thus solutions to the equations

$$\begin{aligned} \nabla^2 \bar{\bar{p}}_i &= \nabla\cdot\mathbf{b}_i,\ \mathbf{b}_i = \mathbf{0} && \text{in } \Omega \text{ with} \\ (\bar{\bar{p}}_i)_j &= 0,\ (\mathbf{b}_i\cdot\boldsymbol{n})_j = \delta_{ij} && \text{on } \partial\Omega \end{aligned} \qquad (21)$$

$$\begin{aligned} (\nabla^2 - 2\mathrm{Re}/\Delta t)\,\bar{\bar{\mathbf{u}}}_i - \nabla\bar{\bar{p}}_i &= \mathbf{0} && \text{in } \Omega \text{ with} \\ \bar{\bar{\mathbf{u}}}_i &= \mathbf{0} && \text{on } \partial\Omega, \end{aligned} \qquad (22)$$

where $\mathbf{b}_i$ is the vector field of momentum residuals and $\boldsymbol{n}$ is the normal to the boundary. It should be noted that in a spectral collocation procedure, only the normal component of the momentum residual $(\mathbf{B}\cdot\boldsymbol{n})$ at the boundary contributes to $\nabla\cdot\mathbf{B}$ at the interior points. The residuals in the tangential momentum equations on the boundary are inconsequential and, therefore, only the normal momentum residuals are used in the construction of the second set of the complementary functions.

The unknown coefficients α_i's and β_i's in Eq. (20) are to be determined such that the velocity field has zero interior as well as boundary divergences. Physically, the α_i's represent the boundary pressure distribution and it will be shown later that the β_i's represent the residuals in the normal momentum equation at the boundary. An extended influence matrix is therefore constructed to evaluate these $2N_b$ unknowns. The incompressibility condition and the normal momentum equation at the boundary provide the necessary relations. The divergence-free condition on the boundary requires that

$$\nabla \cdot \mathbf{u}_p + \sum \alpha_i \nabla \cdot \bar{\mathbf{u}}_i + \sum \beta_i \nabla \cdot \bar{\bar{\mathbf{u}}}_i = 0 \quad \text{on } \partial\Omega. \tag{23}$$

The discretized normal momentum equation at the boundary is written as

$$\Big[(\nabla^2 - 2\mathrm{Re}/\Delta t) \Big[\mathbf{u}_p + \sum \alpha_i \bar{\mathbf{u}}_i + \sum \beta_i \bar{\bar{\mathbf{u}}}_i \Big] - \nabla \Big(p_p + \sum \alpha_i \bar{p}_i + \sum \beta_i \bar{\bar{p}}_i \Big) = \mathbf{S} + \mathbf{B} \Big]_j \cdot \boldsymbol{n}, \tag{24}$$

where $j = 1$ to N_b denotes the boundary points. Substituting the governing equations for the particular and complementary solutions, we obtain

$$(B_p \cdot \boldsymbol{n})_j + \sum \alpha_i (\bar{B}_i \cdot \boldsymbol{n})_j + \sum \beta_i (\bar{\bar{B}}_i \cdot \boldsymbol{n})_j = (\mathbf{B} \cdot \boldsymbol{n})_j, \tag{25}$$

where

$$\begin{aligned} B_p &= (\nabla^2 - 2\mathrm{Re}/\Delta t)\, \mathbf{u}_p - \nabla p_p - \mathbf{S} \\ \bar{B}_i &= (\nabla^2 - 2\mathrm{Re}/\Delta t)\, \bar{\mathbf{u}}_i - \nabla \bar{p}_i \\ \bar{\bar{B}}_i &= (\nabla^2 - 2\mathrm{Re}/\Delta t)\, \bar{\bar{\mathbf{u}}}_i - \nabla \bar{\bar{p}}_i \end{aligned} \tag{26}$$

are the residuals in the momentum equations of the particular and the two sets of complementary functions. Using the Poisson equations for the particular and the two sets of complementary solutions of pressure (Eqs. (11), (14), (21)) along with Eq. (19), it can be shown that the total residual in the normal momentum equation at the boundary, $(\mathbf{B} \cdot \boldsymbol{n})_j$, is given by

$$(\mathbf{B} \cdot \boldsymbol{n})_j = -\sum \beta_i (\mathbf{b}_i \cdot \boldsymbol{n})_j = -\beta_j. \tag{27}$$

Upon substituting Eq. (27) in Eq. (25) and combining Eq. (23) and (25), we obtain for the unknowns α_i's and β_i's:

$$\begin{bmatrix} (\nabla \cdot \bar{\mathbf{u}}_i)_j & (\nabla \cdot \bar{\bar{\mathbf{u}}}_i)_j \\ (\bar{B}_i \cdot \boldsymbol{n})_j & (\bar{\bar{B}}_i \cdot \boldsymbol{n})_j + \delta_{ij} \end{bmatrix} \begin{bmatrix} \alpha_i \\ \beta_i \end{bmatrix} = - \begin{bmatrix} (\nabla \cdot \mathbf{u}_p)_j \\ (B_p \cdot \boldsymbol{n})_j \end{bmatrix}. \tag{28}$$

The matrix on the left-hand side of the above equation is the total influence matrix when the "collocation correction" is included and accounts for both the boundary divergences and the boundary momentum residuals. Denoting this matrix by **C**, we have

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = -[\mathbf{C}]^{-1} \begin{bmatrix} (\nabla \cdot \mathbf{u}_p)_b \\ (B_p \cdot \boldsymbol{n})_b \end{bmatrix}. \tag{29}$$

The influence matrix **C** is computed for each wavenumber in z and its inverse is stored at the beginning of the solution procedure. This inverse is then used to compute the weights α_i's and β_i's of the complementary functions at all other time steps. As before, after obtaining the α_i's and β_i's, the pressure and momentum equations are solved for the second time. Since the second set of pressure complementary functions are solved with homogeneous boundary conditions, the final pressure equation is solved with the boundary condition $p_i = \alpha_i$ on $\partial\Omega$ and the right-hand side given by $-\nabla \cdot \mathbf{S} + \sum \nabla \cdot \beta_i \mathbf{b}_i$. This pressure field is then used to solve the momentum equations in the non-periodic directions for the second time. Since the momentum equation in the periodic direction does not affect the computation of α_i's and β_i's, it is solved only after obtaining the final pressure field. The resulting velocity field is then divergence-free everywhere in the domain at the end of the time advancement. The solution cycle can be summarized as follows:

(i) Generate the influence matrix (**C**) for each wavenumber in the periodic direction and store its inverse at the beginning of the solution procedure. Then at any time step;

(ii) First solve for the particular solution of the pressure;

(iii) Solve the momentum equations in the non-periodic directions to obtain the particular solutions of the velocities in the non-periodic directions;

(iv) Compute the boundary divergence and the boundary residual in the normal momentum equation corresponding to the particular solution;

(v) Determine the boundary pressures (α_i's) and the boundary residuals of the normal momentum equation (β_i's) using the influence matrix;

(vi) Recompute the pressure field using the new boundary pressures and a modified right-hand side, i.e., solve $\nabla^2 p^{n+1} = -\nabla \cdot \mathbf{S} + \sum \nabla \cdot \beta_i \mathbf{b}_i$ with $p_i = \alpha_i$ on $\partial\Omega$;

(vii) Solve the momentum equations in the non-periodic directions once again using the new pressure field;

(viii) Finally, solve the momentum equation corresponding to the periodic direction.

An important issue relating to the influence matrix is its invertibility for incompressible flows. The influence matrix is singular for the zeroth wave number ($k = 0$). One reason for this is the arbitrariness of the level of pressure field in incompressible flows. In addition, the "collocation correction" procedure introduces more singularities. The influence matrix without the "collocation correction" has one zero eigenvalue while that with the "collocation correction" has four zero eigenvalues. Tuckerman [19] discussed in detail the implication of these zero eigenvalues of the singular matrix and the associated null vectors. She suggested a procedure to obtain a related non-singular matrix which would behave the same way as the original matrix for the purpose of obtaining a solution. In this procedure, first the eigenvalues and the eigenvectors of the singular influence matrix are determined. The zero eigenvalues are then replaced with any non-zero value (say, one) and a modified influence matrix with the new eigenvalues and the original eigenvectors is constructed. This influence matrix is then inverted and used in the computation of α_i's and β_i's. In the present computations, the threshold value below which the magnitude of an eigenvalue on the CRAY Y-MP is considered to be "zero" has been set to 1.0×10^{-10}. The selection of this threshold value depends on the grid size, Reynolds number and Δt.

Another important consideration in the present procedure is the storing of the influence matrix. Without the "collocation correction," the size of the influence matrix is $2(N_x + N_y - 2) \times 2(N_x + N_y - 2)$ per wavenumber, where $N_x + 1$ (0 to N_x) and $N_y + 1$ (0 to N_y) are the number of collocation points in the x and y directions, respectively. When the "collocation correction" is included, the size of the matrix increases to $4(N_x + N_y - 2) \times 4(N_x + N_y - 2)$. For $N_x \approx N_y$, this matrix requires for each wavenumber a storage of approximate size $64N_x^2$. While the CPU overhead for the generation of the influence matrix is amortized over the total integration time of the problem, the memory requirement of these arrays for all streamwise wavenumbers is large and practically unaffordable for large grid sizes. To tackle this problem, we have used the BUFFER IN/BUFFER OUT option available on CRAY computers. This option reduces the active memory requirement by retaining in memory only the inverse of the influence matrix for two wavenumbers at any time. While computations are being carried out for the first of these two wavenumbers, the influence matrix corresponding to the second wavenumber will be read in an asynchronous manner. For the examples considered here, this asynchronous data read neither increases the CPU time nor the wall clock turn-around time in any significant manner when implemented on CRAY computers. Also, significant reduction in the size of the influence matrix can be achieved by utilizing the quadrant or octant symmetry present in rectangular geometries.

To summarize, the collocation correction is an additional correction to the pressure field such that the interior and boundary divergences are identically zero to machine accuracy. This correction is necessary because the boundary residuals in the momentum equations are non-zero due to the discrete representation of the spatial operators and their effect should be included in determining the pressure distribution.

4. APPLICATIONS AND RESULTS

The above described numerical procedure (including the "collocation correction") has been applied to two test problems: (a) 2D flow in a driven square cavity and (b) the decay of a 3D perturbation in a fully developed laminar flow through a square duct. The test problems are intended to verify that the time-evolving flow field remains divergence-free in the interior as well as on the boundary of the domain. The test problems have also been solved using the influence matrix method without the "collocation correction" and the fractional step method [15]. In the fractional step method, zero Neumann boundary conditions were used for the scalar potential (ϕ^{n+1}). The normal component of the intermediate velocity was set to zero on the boundary and the tangential velocity was calculated using the following expression: $\tilde{\mathbf{u}} \cdot \tau = \Delta t(2\nabla\phi^n - \nabla\phi^{n-1}) \cdot \tau$ on $\partial\Omega$. Results from all three methods have been compared to assess the relative magnitudes of the velocity divergences as well as their effect on the flow field. For the ease of comparison, the three methods are numbered as follows: Method 1 represents the influence matrix method with the "collocation correction"; Method 2 corresponds to the influence matrix method without the "collocation correction"; and Method 3 represents the fractional step method.

4.1. *2D Flow in a Driven-Square Cavity*

The 2D flow in a driven-square cavity is simulated at a Reynolds number of 200, based on the half-width of the cavity and the velocity of the top wall using a grid of 16×16 in the x and y directions, respectively. The Gauss–Lobatto distribution is used to generate the grid. To avoid singularity at the top corners, the velocity distribution along the top wall is ramped using an exponential function ($u_{\text{top}} = 1 - \exp[-100\{1 - x^2\}^2]$). The calculation is started with fluid at rest and the top wall is suddenly moved at $t = 0^+$. Table I gives the CPU time per time step (on the CRAY Y-MP), the boundary slip velocities, and the maximum interior and boundary divergences for the three methods after 60 time units. It can be seen that with the collocation correction, the velocity divergence in the interior as well as on the boundary is machine-zero while

TABLE I

Comparison of CPU Time, Maximum Boundary Slip Velocity, and Maximum Interior and Boundary Divergences in a Driven Square-Cavity Flow Computed Using the Three Methods

	Method 1	Method 2	Method 3
CPU time (s)/ time step	0.008	0.007	0.0056
Max. interior divergence	3.74×10^{-11}	0.543	7.73×10^{-12}
Max. boundary divergence	5.0×10^{-11}	7.68×10^{-6}	3.32
Max. boundary slip velocity	0.0	0.0	3.8×10^{-11}

TABLE II

u-Velocity at Selected Points along the Vertical Centerline in a Driven Cavity Flow Computed Using the Three Methods

y	Method 1	Method 2	Method 3
−1	0	0	1.77678×10^{-12}
−0.980785	−0.0153093	−0.0151103	−0.0148264
−0.92388	−0.0576761	−0.0576926	−0.0582984
−0.707107	−0.206494	−0.20079	−0.206106
−0.382683	−0.323367	−0.320364	−0.327129
0.382683	0.113123	0.110917	0.109836
0.707107	0.292598	0.293723	0.297072
0.92388	0.627434	0.630469	0.633536
0.980785	0.902351	0.902287	0.901518
1	1	1	1

TABLE IV

Comparison of CPU Time, Maximum Boundary Slip Velocity, and Maximum Interior and Boundary Divergences Computed Using the Three Methods in a Fully Developed Laminar Flow through a Square Duct Subject to a 3D Perturbation

	Method 1	Method 2	Method 3
CPU time (s)/ time step	0.268	0.245	0.18
Max. interior divergence	1.4×10^{-11}	7.99×10^{-4}	2.34×10^{-11}
Max. boundary divergence	4.0×10^{-11}	1.28×10^{-11}	2.98×10^{-3}
Max. boundary slip velocity	0.0	0.0	4.06×10^{-6}

the maximum divergences in the other two methods are appreciable. Tables II and III show the values of u and v velocities at selected points along the vertical centerline. The differences in the velocity field are a result of not satisfying the divergence conditions everywhere in the domain. The differences are largest near the boundaries. Accordingly the velocity gradients implied by the three solutions could differ significantly near the boundaries.

4.2. *Decay of a 3D Perturbation in a Laminar Flow*

To test the scheme for a 3D problem with two non-periodic directions and one periodic direction, the decay of a 3D perturbation in a fully developed laminar flow through a square duct has been simulated. For this problem, z represents the streamwise (periodic) direction, and x and y represent the transverse directions. A divergence-free 3D perturbation is superimposed on the fully developed laminar flow and the temporal evolution of the solution is computed using the three methods. The induced perturbation is similar to that used by Moin and Kim [11] and is given by

$$\begin{aligned} u'(x, y, z) &= -\varepsilon[1+\cos(\pi x)]\sin(\pi y)\sin(z) \\ v'(x, y, z) &= -\varepsilon \sin(\pi x)[1+\cos(\pi y)]\sin(z) \\ w'(x, y, z) &= 2\pi\varepsilon \sin(\pi x)\sin(\pi y)\cos(z), \end{aligned} \tag{30}$$

where ε is the amplitude of the perturbation. The normalized domain of computation is $2 \times 2 \times 2\pi$. The grid used was $32 \times 32 \times 16$ and the time increment was 5×10^{-3}. The Reynolds number based on the friction velocity and the duct half-width was 30 and a fairly large value (0.3) was chosen for ε. Table IV shows the CPU time, the boundary slip velocities, and the maximum interior and boundary divergences for the three methods after one time unit. Once again, the velocity field obtained by Method 1 is divergence-free while the velocity fields obtained by Methods 2 and 3 have small divergences. However, the differences in the velocity fields are negligibly small. The CPU time for Method 1 is 44% more than that for Method 3.

Finally, the CPU time, memory requirements, and

TABLE III

v-Velocity at Selected Points along the Vertical Centerline in a Driven Cavity Flow Computed Using the Three Methods

y	Method 1	Method 2	Method 3
−1	0	0	0
−0.980785	5.6308×10^{-5}	0.00121361	−0.0030767
−0.92388	−0.0004967	0.00255354	-2.808×10^{-5}
−0.707107	−0.0030082	−0.0005287	−0.0012029
−0.382683	0.02485599	0.02650375	0.02688145
0.382683	0.07176275	0.06782609	0.06725114
0.707107	0.0707148	0.07537123	0.07703139
0.92388	0.0068781	0.00929236	0.00721779
0.980785	−0.0002314	0.00059931	−0.0002377
1	0	0	0

TABLE V

Run Time Statistics for Method 1 on Different Grids

Grid size	CPU time (s) for generation of influence matrix	CPU time (s)/ time step	Memory (MW)	MFLOPS
$16 \times 16 \times 16$	1.12	0.061	0.4	145
$32 \times 32 \times 16$	9.0	0.268	1.0	236
$32 \times 32 \times 32$	14.15	0.50	1.45	238
$64 \times 64 \times 16$	86.4	1.7	2.9	266
$64 \times 64 \times 32$	152.0	3.4	4.72	267
$100 \times 100 \times 16$	438.0	6.15	6.53	290

computational performance (MFLOPS) for six grid sizes [$16 \times 16 \times 16$, $32 \times 32 \times 16$, $32 \times 32 \times 32$, $64 \times 64 \times 16$, $64 \times 64 \times 32$, and $100 \times 100 \times 16$] are given in Table V for Method 1. Also given in this table are the CPU times for the generation of influence matrix.

5. CONCLUSIONS

A Chebyshev collocation procedure that satisfies the divergence-free condition on the boundary as well as in the interior of an incompressible flow with two non-periodic directions has been presented. An influence matrix technique combined with a correction methodology [16, 19] is used to satisfy the continuity equation everywhere in the domain. Details of implementing this procedure in a collocation method are presented. This "collocation correction" accounts for the effect of non-zero residuals in the boundary momentum equations arising due to the discrete representation of the spatial operators. The procedure has been demonstrated to yield machine-zero divergences in two test problems. An efficient solution procedure based on matrix diagonalization has been used to solve the discretized equations. Results are also presented for the fractional step method and the influence matrix method without the collocation correction. It is seen that the CPU time and the memory requirements for the present procedure are not significantly greater than those for the fractional step method and the influence matrix method without the collocation correction.

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