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Divergence-free Velocity Fields in Nonperiodic Geometries

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The influence matrix method of enforcing incompressibility in pseudospectral simulations of fluid dynamics, as described by Kleiser and Schumann for channel flow, is generalized to other geometries, A formalism of projection and matrix operators is introduced, in which the influence matrix method is shown to be an application of the classic Sherman–Morrison–Woodbury formula of numerical linear algebra. Special attention is paid to the tau correction. Applications to Cartesian geometries illustrate the concepts and highlight the role of symmetry. A coded implementation in a cylindrical geometry, requiring special treatment of coordinate singularities, is used to investigate properties of the influence matrix and to provide estimates of timings. © 1989 Academic Press, Inc.

1. INTRODUCTION

In incompressible flow, the pressure serves as the degree of freedom necessary to ensure that the velocity field is divergence-free. It is therefore necessary to derive equations and boundary conditions for the pressure which correctly express this constraint on the velocity. There has been a great deal of interest in this problem for pseudospectral simulations of three-dimensional flows with one or more nonperiodic directions.

Most methods solve a Poisson equation for the pressure; the difficulty then centers on deriving appropriate boundary conditions. Among the approaches which have been used are: (1) the influence, or capacitance, matrix method which is the subject of this article (Kleiser and Schumann [1]; Marcus [2]; Patera [3]; Sulem, Sulem, and Thual [4]; Alziary de Roquefort and Le Quéré [5]), (2) iterative solution of the pressure (Haldenwang [6], Maday and Patera [7]), and (3) time-splitting methods in which boundary conditions on the pressure approximately enforce incompressibility (Orszag and Kells [8]; Patera and Orszag [9]; Orszag, Deville, and Israeli [10]; Zang and Hussaini [11], and Streett and Hussaini [12]).

Other techniques bypass the Poisson equation, either: (4) solving the coupled momentum and incompressibility equations for the pressure and velocity together (Moin and Kim [13], Malik, Zang, and Hussaini [14]), (5) using an inherently divergence-free basis set for the velocity (Leonard [15]; Leonard and Wray [16];

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Moser, Moin, and Leonard [17]; Spalart [18]), or (6) using vector potentials (Marcus [19], Glatzmaier [20], and Murdock [21]).

Gresho and Sani [22] have given an excellent and comprehensive treatment of the pressure boundary conditions necessary for enforcing incompressibility. The purpose of this article is not to compare the different numerical methods of treating the pressure (for such a comparison, see Orszag, Israeli, and Deville [10]; Deville, Kleiser, and Montigny-Rannou [23]; Ku, Taylor, and Hirsh [24]), but rather to discuss in detail the influence matrix method.

It is well known that pseudospectral methods are best suited to periodic geometries; there, the pressure is easy to treat. Indeed one of the main directions of recent effort has been to extend the use of the pseudospectral method to arbitrary geometries (Patera [3], Maday and Patera [7]). Most of the approaches listed above grow increasingly difficult, if not impossible, as the geometry becomes more complicated. Restricting ourselves to regular geometries, the complexities can be of two kinds, both of which will be encountered in this article:

(1) The coordinate system itself can be complicated. A Cartesian system is simplest, followed by cylindrical, then by spherical. Cylindrical and spherical domains which contain coordinate singularities such as poles, origins, or axes are more difficult to treat than those which do not, requiring either special basis functions (e.g., spherical harmonics) or special treatment of the coordinate singularities.

(2) Solid boundaries may be present, leading to nonperiodic directions, i.e. directions in which there are nonperiodic boundary conditions. Computations involving one nonperiodic direction have by now become fairly commonplace. Applying the same methods to two or three nonperiodic directions will, however, cause nontrivial coupling between the directions. Even a nonperiodic Cartesian cube poses formidable problems which have long been resolved for a periodic box.

TABLE I

Representative Pseudospectral Calculations in Nonperiodic Geometries

Nonperiodic directions	Cartesian	Cylindrical	Spherical
One	*Kleiser & Schumann* [1] *Sulem, Sulem & Thual* [4] Orszag & Kells [8] Zang & Hussaini [11] Moin & Kim [13]	*Marcus* [2] Patera & Orszag [9]* Leonard & Wray [16]*	Marcus [19] Glatzmaier [20]
	Moser, Moin, & Leonard [17]		
	Spalart [18]		
Two	*Le Quéré & Alziary de Roquefort* [5]	Streett & Hussaini [12]	
Three	Haldenwang [6]		

Some of the references have treated relatively complex geometries. We classify them according to this scheme in Table I, italicizing those which use the influence matrix method. (Asterisks denote cylindrical geometries like ours, which include the axis.)

Green's functions are a classic tool in the solution of elliptic partial differential equations (see, for example, Morse and Feshbach [25]), in particular for imposing boundary conditions. Numerical discretization leads to influence, or capacitance, matrices. Hockney [26] was among the first to implement this technique numerically in order to solve the Poisson equation via finite differences in an irregular domain. Buzbee, Dorr, George, and Golub [27] gave a precise exposition of the method and of its interpretation in terms of the Sherman–Morrison–Woodbury [28–32] formula for matrix inversion. Proskurowski and Widlund [33] and O'Leary and Widlund [34] returned to the original elliptic differential equations to analyze the numerical Green's functions as kernels of Fredholm integral equations. They were then able to exploit known analytic results about the well- or ill-posedness of such integral equations to formulate numerical methods yielding well-conditioned influence matrices.

The use of Green's functions or influence matrices as a means of imposing incompressibility in the Stokes or Navier–Stokes equations is, however, a fairly recent idea. Canuto and Sacchi-Landriani [35] have proved the mathematical convergence of the influence matrix algorithm developed by Kleiser and Schumann [1]. Quartapelle and Napolitano [36] have analyzed the method in terms of integral boundary conditions; an analogy can be drawn between their work and [33, 34]. In this article, we will show that the Kleiser–Schumann influence matrix method of enforcing incompressibility can, like [26, 27], also be recast as an application of the Sherman–Morrison–Woodbury formula.

Kleiser and Schumann presented their algorithm as algebraic equations relating coefficients, in a geometry with one nonperiodic direction. Our formulation using matrix operators facilitates the generalization of their method to other geometries. We have applied the method to Rayleigh–Benard convection in a cylindrical container with radial and vertical boundaries (i.e., two nonperiodic directions), and we present results specific to this geometry.

We have organized the article in the following way. In the remainder of this section, we transform the time-dependent Navier–Stokes equations to the Stokes-like problem we will study throughout the paper. In Section 2 we review the pseudospectral method for space-discretization and the tau method for imposing boundary conditions, with a view towards introducing our notation.

Sections 3 and 4 form the heart of the paper. Section 3.1 derives the discrete Poisson equation for the pressure. Section 3.2 discusses the tau correction, which has been overlooked in most other articles. Section 3.3 expresses the fluid-dynamical problem in matrix form and discusses the Sherman–Morrison–Woodbury formula [28–32], which gives the inverse of a matrix in terms of the inverse of a related matrix. Section 3.4 sets up the correspondance between the various terms of the Sherman–Morrison–Woodbury formula and the fluid-dynamical problem.

Section 4 applies the formalism of Section 3 to two Cartesian geometries. The first, a rectangle with two nonperiodic directions, has been treated by Le Quéré and Alziary de Roquefort [5]. The second, a channel with two periodic and one nonperiodic direction, is the geometry studied by Kleiser and Schumann [1]. With these examples we explain how symmetry can be used to reduce the size of influence matrices.

Section 5, an application to cylindrical coordinates, should be of interest to those using curvilinear coordinates. It explains the difficulties posed by the coupling of the cylindrical coordinates and the coordinate singularity at the axis and shows how they can be dealt with, both in elliptic solvers and in the influence matrix. Section 6 discusses the singularity of the influence matrix and an easy empirical algorithm for rendering it invertible. Timings, condition numbers, and error bounds are also presented here. While these results are obtained for the cylindrical case, they should be generally applicable. After the conclusion is a glossary listing our notation.

1.1. *Time-Discretization*

We begin by discretizing the Navier–Stokes equations in time. We assume the use of any implicit time discretization (here, Crank–Nicolson) for the viscous term, and of any explicit time-discretization (here, Adams–Bashforth) for nonlinear terms and external forces $\mathbf{f}$ (e.g., buoyancy). The following system of equations is obtained for proceeding from the velocity field $\mathbf{u}^i$ to $\mathbf{u}^{i+1}$:

$$\left(\mathbf{I}-\frac{\nu\Delta t}{2}\nabla^2\right)\mathbf{u}^{i+1}+\Delta t\,\nabla p^{i+1}=\left(\mathbf{I}+\frac{\nu\Delta t}{2}\nabla^2\right)\mathbf{u}^i$$

$$+\frac{\Delta t}{2}\left[3(\mathbf{u}^i\times(\nabla\times\mathbf{u}^i)+\mathbf{f}^i)-(\mathbf{u}^{i-1}\times(\nabla\times\mathbf{u}^{i-1})+\mathbf{f}^{i-1})\right] \tag{1.1a}$$

$$\mathbf{B}\mathbf{u}^{i+1}=0 \tag{1.1b}$$

$$\nabla\cdot\mathbf{u}^{i+1}=0, \tag{1.1c}$$

where ν, Δt, and p are the viscosity, time step, and pressure head, respectively. The notation $\mathbf{Bu}$ means $\mathbf{u}$ evaluated at the boundary of the domain, and ∇^2 is the vector Laplacian. Defining $\varepsilon\equiv\nu\Delta t/2$, let $\mathbf{E}\equiv\mathbf{I}-\varepsilon\nabla^2$ be the elliptic operator appearing on the left-hand side of (1.1a), and let $\mathbf{s}$ be the entire right-hand side of (1.1a). Dropping the now-superfluous superscripts and setting $\phi\equiv p\Delta t$, we obtain this system of equations to be solved for $\mathbf{u}$ and ϕ:

$$\mathbf{E}\mathbf{u}+\nabla\phi=\mathbf{s} \tag{1.2a}$$

$$\mathbf{B}\mathbf{u}=\mathbf{0} \tag{1.2b}$$

$$\nabla\cdot\mathbf{u}=0. \tag{1.2c}$$

If $\mathbf{E}$ is replaced by ∇^2, this becomes the Stokes problem. Most of this article

(except for Sections 6.2–6.3) will pertain to the Stokes problem as well. We assume that we have a procedure for inverting **E** with given boundary conditions. The difficulty in solving (1.2) lies in the coupling of **u** and ϕ in (1.2a) and between the different scalar components of the vector field **u** in (1.2c). The remainder of the article is addressed to the modification and solution of the system (1.2). We will first need to be more precise about our means of discretizing operators in space and of imposing boundary conditions.

2. Boundary Conditions—Pseudospectral Method

In this section, we describe the collocation and tau methods of imposing boundary conditions in the pseudospectral method. Although these methods are already well known and documented (Gottlieb and Orszag [37]; Voigt, Gottlieb, and Hussaini [38]; Canuto, Hussaini, Quateroni, and Zang [39]), we include this treatment to make the article relatively self-contained. However, our primary purpose here is to introduce our notation of projection operators and matrix decompositions in familiar surroundings. This notation is rather elaborate, but we hope it will serve to clarify points which have remained vague in the literature, sometimes leading to errors in algorithms. It is summarized in a glossary at the end of the article. The reader who, with the help of the glossary, understands equations (2.1) and (2.2) at the end of Section 2 may wish to skip to Section 3.

2.1. *Grid and Coefficients*

Using the ideas of the pseudospectral method, we can go freely back and forth between gridpoints and basis functions. For illustrative purposes we discuss the case of a rectangle with a Chebyshev grid and polynomials. We begin by defining the Chebyshev polynomials:

$$\mathscr{C}_j(x) \equiv \cos(j \arccos(x))$$

and the Chebyshev grid $\hat{G} \equiv \{(x_j, y_k): 0 \leqslant j \leqslant J, 0 \leqslant k \leqslant K\}$, where

$$x_j \equiv X \cos \frac{\pi j}{J}$$

$$y_k \equiv Y \cos \frac{\pi k}{K}$$

(Hats, $\hat{}$, will always be used to refer to physical space quantities.) Each $\mathscr{C}_j$ is either an even or an odd polynomial of degree j. A function on the rectangle $\{(x, y): -X \leqslant x \leqslant X, \ -Y \leqslant y \leqslant Y\}$ can be specified by either its physical space representation, i.e., its values on the grid $\hat{f}(x_j, y_k)$, or by its spectral space represen-

tation, i.e., its Chebyshev coefficients $f(j,k)$, where $(j,k)\in G\equiv\{0\leqslant j\leqslant J, 0\leqslant k\leqslant K\}$. A transformation $\hat{f}=Uf$ relates the two:

$$\hat{f}(x_{j'},y_{k'})=\sum_{\substack{0\leqslant j\leqslant J\\0\leqslant k\leqslant K}}\mathscr{C}_j\left(\frac{x_{j'}}{X}\right)\mathscr{C}_k\left(\frac{y_{k'}}{Y}\right)f(j,k).$$

We define $\mathscr{G}$ and $\hat{\mathscr{G}}$ to be the vector space of all (real-valued) functions defined on the grid sets G or $\hat{G}$, respectively, so that $f\in\mathscr{G}$ and $\hat{f}\in\hat{\mathscr{G}}$ and $U:\mathscr{G}\to\hat{\mathscr{G}}$. The dimensionality of $\mathscr{G}$ and of $\hat{\mathscr{G}}$ is equal to the cardinality of G and of $\hat{G}$, which we will denote by $|G|$ or $|\hat{G}|$. (Vertical bars around a set or vector space will always denote its cardinality or dimensionality.)

By calculating its effect on the $\mathscr{C}_j(x)$, a differential operator can be expressed in spectral space as a matrix $E:\mathscr{G}\to\mathscr{G}$ acting on f. Alternatively, it can be expressed in physical space as $\hat{E}:\hat{\mathscr{G}}\to\hat{\mathscr{G}}$ acting on $\hat{f}$. The two matrices are related by the transformation $\hat{E}=UEU^{-1}$. In the remainder of the article, all operators, such as those used in Eqs. (1.2), will be replaced by spectral space matrices (except when coordinate singularities are treated in Section 5.2).

We now wish to solve an elliptic equation,

$$Ef=g,$$

imposing homogeneous boundary conditions on the perimeter of the rectangle.

2.2. *Collocation Method*

The two representations, so far equivalent, lead to different methods of imposing boundary conditions. In the collocation method the differential equation is not imposed at the boundary, but is instead replaced by the boundary conditions. Let $\hat{T}_x$, $\hat{T}_y$, and $\hat{T}_{xy}$ be the x- and y-boundaries and the corners of the rectangle, i.e.,

$$\hat{T}_x\equiv\{(x_j,y_k): j=0 \text{ or } j=J,\ 1\leqslant k\leqslant K-1\},$$
$$\hat{T}_y\equiv\{(x_j,y_k): 1\leqslant j\leqslant J-1, k=0 \text{ or } k=K\},$$
$$\hat{T}_{xy}\equiv\{(x_j,y_k): j=0 \text{ or } j=J, k=0 \text{ or } k=K\}.$$

Then the perimeter of the rectangle is $\hat{T}=\hat{T}_x\cup\hat{T}_y\cup\hat{T}_{xy}$. Let $\hat{\mathscr{T}}$, $\hat{\mathscr{T}}_x$, and $\hat{\mathscr{T}}_y$ be subspaces of $\hat{\mathscr{G}}$ consisting of all functions which are nonzero only on $\hat{T}$, $\hat{T}_x$, and $\hat{T}_y$, respectively. Let Q_{bdy} and $Q_{\text{int}}\equiv I-Q_{\text{bdy}}$ be projection operators onto the boundary and interior subspaces $\hat{\mathscr{T}}$ and $\hat{\mathscr{G}}-\hat{\mathscr{T}}$, respectively. (The notation $\hat{\mathscr{G}}-\hat{\mathscr{T}}$ here means the *orthogonal complement* of $\hat{\mathscr{T}}$ in $\hat{\mathscr{G}}$. It does not mean "all elements of $\hat{\mathscr{G}}$ which are not elements of $\hat{\mathscr{T}}$," but instead "all elements of $\hat{\mathscr{G}}$ which contain no component of $\hat{\mathscr{T}}$," i.e., the vector space of functions on $\hat{G}$ which are zero on $\hat{T}$. Thus $\hat{\mathscr{G}}\neq\hat{\mathscr{T}}\cup(\hat{\mathscr{G}}-\hat{\mathscr{T}})$, but rather $\hat{\mathscr{G}}=\hat{\mathscr{T}}\oplus(\hat{\mathscr{G}}-\hat{\mathscr{T}})$.)

The collocation method consists of replacing the equation

$$\hat{E}\hat{f}=\hat{g}$$

by the pair of equations

$$Q_{\text{int}}\,\hat{E}\hat{f} = Q_{\text{int}}\,\hat{g}$$
$$Q_{\text{bdy}}\hat{f} = 0$$

so that the differential equation is no longer satisfied on the boundary. An equivalent formulation is to introduce an additional variable $\hat{\tau} \in \hat{\mathcal{T}}$, serving as a kind of "placeholder" (its value is not significant),

$$Q_{\text{int}}\,\hat{E}\hat{f} = Q_{\text{int}}\,\hat{g}$$
$$Q_{\text{bdy}}\,\hat{E}\hat{f} = \hat{\tau}$$
$$Q_{\text{bdy}}\hat{f} = 0$$

or

$$\hat{E}\hat{f} = Q_{\text{int}}\hat{g} + \hat{\tau}$$
$$Q_{\text{bdy}}\hat{f} = 0.$$

If we reorder the points so that all boundary points are located at the end of the vectors, we can partition the square matrix $\hat{E}$ as

$$\hat{E} = \begin{pmatrix} Q_{\text{int}}\hat{E} \\ Q_{\text{bdy}}\hat{E} \end{pmatrix}.$$

In matrix form we have

$$\begin{matrix} |\hat{G}-\hat{T}| \\ |\hat{T}| \\ |\hat{T}| \end{matrix} \begin{pmatrix} Q_{\text{int}}\hat{E} & 0 \\ Q_{\text{bdy}}\hat{E} & -I \\ Q_{\text{bdy}} & 0 \end{pmatrix} \begin{pmatrix} \hat{f} \\ \hat{\tau} \end{pmatrix} = \begin{pmatrix} Q_{\text{int}}\,\hat{g} \\ 0 \\ 0 \end{pmatrix}.$$
$$\qquad\qquad |\hat{G}| \qquad |\hat{T}|$$

Despite containing six blocks, the matrix above is square, as can be seen from the dimensions of these blocks, specified to the left and below the matrix. Similarly, it can be seen that the vectors on the left-and right-hand sides are both of length $|\hat{G}| + |\hat{T}|$. A vector or matrix of all zeroes is denoted by 0, and I is the identity matrix of appropriate dimension. Note that unlike $\hat{g}$, $\hat{f}$ is not projected: $Q_{\text{int}}\hat{f}$ and $Q_{\text{bdy}}\hat{f}$ are treated on an equal footing.

2.3. *Tau Method*

In the tau method, rather than eliminating the rows evaluating the differential equation at the boundary, we eliminate the rows expressing the highest frequency modes of the differential equation. Define the sets T_x, T_y, and T_{xy} by

$$T_x = \{(j,k): j \geqslant J-1, k \leqslant K-2\},$$
$$T_y \equiv \{(j,k): j \leqslant J-2, k \geqslant K-1\},$$
$$T_{xy} \equiv \{(j,k): j \geqslant J-1, k \geqslant K-1\}.$$

Then the *tau set* is $T = T_x \cup T_y \cup T_{xy}$. Note that the boundary and tau sets are of the same size: $|T_x| = |\hat{T}_x| = 2(K-1)$, $|T_y| = |\hat{T}_y| = 2(J-1)$, $|T_{xy}| = |\hat{T}_{xy}| = 4$, and $|T| = |\hat{T}| = 2(J+K)$. As before we will denote by $\mathcal{T}_x$, $\mathcal{T}_y$, $\mathcal{T}_{xy}$, and $\mathcal{T}$ the vector spaces of functions which are nonzero only on sets T_x, T_y, T_{xy}, and T, and we define projection operators Q_{hi} and $Q_{\text{lo}} = I - Q_{\text{hi}}$ onto the spaces $\mathcal{T}$ and $\mathcal{G} - \mathcal{T}$ of high- and low-frequency functions, respectively. The differential equation with the boundary conditions imposed by the tau method is

$$Q_{\text{lo}} Ef = Q_{\text{lo}} g$$
$$Q_{\text{hi}} Ef = \tau$$
$$Bf = 0.$$

Equivalent forms are

$$EF = Q_{\text{lo}}\, g + \tau$$
$$Bf = 0$$

and

$$\begin{matrix} |G-T| \\ |T| \\ |T| \end{matrix} \begin{pmatrix} Q_{\text{lo}} E & 0 \\ Q_{\text{hi}} E & -I \\ B & 0 \end{pmatrix} \begin{pmatrix} f \\ \\ \tau \end{pmatrix} = \begin{pmatrix} Q_{\text{lo}} g \\ 0 \\ 0 \end{pmatrix}. \tag{2.1}$$
$$\begin{matrix} & |G| & |T| \end{matrix}$$

The boundary operator B may compute either function values ($B \equiv Q_{\text{bdy}}\, U$) or Chebyshev coefficients along the boundary. We use the latter, for reasons to be explained in Section 4. This yields boundary values that are defined on a mixed physical-spectral grid, such as

$$(Bf)(x_0, k) \equiv \sum_j \mathcal{C}_j(x_0) f(j,k),$$

which we will write (without a hat) as $b(x_0, k)$.

We have deliberately emphasized the analogy between the collocation and tau methods, but they are not equivalent, as can easily be seen from the fact that $\hat{f}$ depends only on $Q_{\text{int}}\, g$, while f is determined by $Q_{\text{lo}} g$. Nor does the nomenclature τ and $\hat{\tau}$ imply that $\hat{\tau} = U\tau$. We have introduced the collocation method first because it is more intuitive, but since differential operators such as ∇^2 and $\nabla \cdot$ are local in spectral space, it will be far more economical to use the tau method, both in solving the elliptic equations and in reducing the set $\mathcal{T}$, as we shall see in Sections 3 and 4.

If the functions are *vector-valued*, they and the spaces to which they belong will be denoted by bold letters, and called *bi-* or *tri-directional*, so as to avoid confusion with the dimensionality of vector spaces. For example, if $\mathbf{f}=\mathbf{e}_x f_x+\mathbf{e}_y f_y$, we will say that $d=2$, and that $\mathbf{f}$ is bi-directional. Then $\mathbf{f}$, $\mathbf{g}\in\mathscr{G}\oplus\mathscr{G}$ and $\boldsymbol{\tau}\in\mathscr{T}\oplus\mathscr{T}$. We then require vector operators

$$\mathbf{E}:\mathscr{G}\oplus\mathscr{G}\to\mathscr{G}\oplus\mathscr{G},$$
$$\mathbf{Q}_{\mathrm{hi}}:\mathscr{G}\oplus\mathscr{G}\to\mathscr{T}\oplus\mathscr{T},$$
$$\mathbf{Q}_{\mathrm{lo}}:\mathscr{G}\oplus\mathscr{G}\to(\mathscr{G}-\mathscr{T})\oplus(\mathscr{G}-\mathscr{T}).$$

Generally, for $d=1$, 2, or 3, we have $\mathbf{f},\mathbf{g}\in\mathscr{G}\equiv\oplus_{i=1}^{d}\mathscr{G}$ and $\boldsymbol{\tau}\in\mathscr{T}\equiv\oplus_{i=1}^{d}\mathscr{T}$, or $\mathbf{f},\mathbf{g}: G\to\mathfrak{R}^d$ and $\tau: T\to\mathfrak{R}^d$, and the corresponding vector operators. Note that the grid G and tau set T, pertaining to the *domain* (which for the rectangular case we also call bi-directional), remain unchanged. The d-directional equation with boundary conditions becomes

$$\begin{matrix} d|G-T| \\ d|T| \\ d|T| \end{matrix}\begin{pmatrix} \mathbf{Q}_{\mathrm{lo}}\mathbf{E} & \mathbf{0} \\ \mathbf{Q}_{\mathrm{hi}}\mathbf{E} & -\mathbf{I} \\ \mathbf{B} & \mathbf{0} \end{pmatrix}\begin{pmatrix} \mathbf{f} \\ \boldsymbol{\tau} \end{pmatrix}=\begin{pmatrix} \mathbf{Q}_{\mathrm{lo}}\mathbf{g} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \tag{2.2}$$
$$\begin{matrix} d|G| & d|T| \end{matrix}$$

3. The Influence Matrix Method

3.1. *The Poisson Equation*

We now return to the fluid dynamical problem at hand. Using the tau method to impose the boundary conditions, and the notation defined in the previous section, we express equations (1.2) as

$$\mathbf{E}\mathbf{u}+\nabla\phi=\mathbf{Q}_{\mathrm{lo}}\mathbf{s}+\boldsymbol{\tau} \tag{3.1a}$$
$$\mathbf{B}\mathbf{u}=\mathbf{0} \tag{3.1b}$$
$$\nabla\cdot\mathbf{u}=0. \tag{3.1c}$$

Recall that the symbols $\mathbf{E}$, ∇, and $\nabla\cdot$ no longer refer to differential operators, but to the corresponding spectrally discretized matrices, as explained in Section 2.1.

This is a well-posed problem, but all of the unknowns $\mathbf{u}$, $\boldsymbol{\tau}$, and ϕ are coupled. Worse yet, Eq. (3.1c) and the presence of $\nabla\phi$ as an unknown in (3.1a) couple the different scalar components of the vector $\mathbf{u}$. We assume that we have a rapid numerical algorithm for solving (3.1a)–(3.1b) if ϕ were known. Our goal is to reduce (3.1) to a form in which we can solve for ϕ independently of $\mathbf{u}$.

The usual starting point is to derive a Poisson equation for the pressure. We operate with $Q_{\mathrm{lo}}\nabla\cdot$ on (3.1a), obtaining

$$Q_{\mathrm{lo}}(\nabla\cdot\mathbf{E}\mathbf{u}+\nabla^2\phi)=Q_{\mathrm{lo}}\nabla\cdot(\mathbf{Q}_{\mathrm{lo}}\mathbf{s}+\boldsymbol{\tau}). \tag{3.2}$$

In order to eliminate the term involving $\mathbf{u}$ in (3.2), we use the fact that an elliptic equation with homogeneous right-hand side and boundary conditions has only the null solution; this is true for the discretized equation as well. Defining the *scalar* elliptic operator $E \equiv I - \varepsilon\nabla^2$, (3.1c) is equivalent to

$$Q_{\text{lo}}\, E(\nabla \cdot \mathbf{u}) = 0 \tag{3.3a}$$

$$B(\nabla \cdot \mathbf{u}) = 0. \tag{3.3b}$$

Using $\nabla^2(\nabla \cdot \mathbf{u}) = \nabla \cdot \mathbf{V}^2\mathbf{u}$, we obtain the commutation relation

$$\begin{aligned} E(\nabla \cdot \mathbf{u}) &= (I - \varepsilon\nabla^2)(\nabla \cdot \mathbf{u}) \\ &= \nabla \cdot (\mathbf{I} - \varepsilon\nabla^2)\,\mathbf{u} \\ &= \nabla \cdot \mathbf{E}\mathbf{u}, \end{aligned}$$

allowing us to replace (3.3a) by

$$Q_{\text{lo}} \nabla \cdot \mathbf{E}\mathbf{u} = 0.$$

Equation (3.2) becomes

$$Q_{\text{lo}} \nabla^2 \phi = Q_{\text{lo}} \nabla \cdot (\mathbf{Q}_{\text{lo}}\mathbf{s} + \tau). \tag{3.4}$$

Projecting Eq. (3.1a) into the low- and high-subspaces, and reordering equations (3.1b), (3.4), and (3.3b), the full problem now reads

$$\mathbf{Q}_{\text{lo}}(\mathbf{E}\mathbf{u} + \nabla\phi) = \mathbf{Q}_{\text{lo}}\mathbf{s} \tag{3.5a}$$

$$\mathbf{B}\mathbf{u} = \mathbf{0} \tag{3.5b}$$

$$Q_{\text{lo}} \nabla^2 \phi = Q_{\text{lo}} \nabla \cdot (\mathbf{Q}_{\text{lo}}\mathbf{s} + \tau) \tag{3.5c}$$

$$B(\nabla \cdot \mathbf{u}) = 0 \tag{3.5d}$$

$$\mathbf{Q}_{\text{hi}}(\mathbf{E}\mathbf{u} + \nabla\phi) = \tau. \tag{3.5e}$$

The desired decoupling has not yet been accomplished, for two reasons: first, (3.5d) continues to couple the different components of $\mathbf{u}$, and second, the unknown τ still appears in (3.5c). Both types of coupling can be reduced, though not completely eliminated, as we shall see in Section 3.2.

3.2. *The Tau Correction*

Before continuing, we briefly discuss a point which has often been overlooked. Note that τ appears in the Poisson equation (3.5c), causing additional coupling with (3.5e): it is for this reason that we explicitly introduced τ in Section 2. It might be thought that this could be avoided by taking the divergence of the projected equation (3.5a) instead of the full equation (3.1a). However, $\nabla\cdot$ and the projected operator $\mathbf{Q}_{\text{lo}}\mathbf{E}$ do not obey a commutation relation, that is,

$$\nabla \cdot \mathbf{Q}_{\text{lo}}\mathbf{E}\mathbf{u} \neq Q_{\text{lo}}\, E \nabla \cdot \mathbf{u},$$

preventing the elimination of $\mathbf{Q}_{\text{lo}}\mathbf{Eu}$ via (3.3a). This noncommutation has long been the bane of incompressible computational fluid dynamics and has often been ignored in the interests of expediency. Another possibility might seem to be to take the divergence of the original equation (1.2a) *before discretization* and imposition of boundary conditions (1.2b), leading to

$$Q_{\text{lo}}\nabla^2\phi = Q_{\text{lo}}\nabla\cdot\mathbf{s} \tag{3.5c'}$$

instead of (3.5c). The error here is that (1.2a) is not satisfied numerically: the discrete Poisson equation should be derived from the discrete momentum equation (3.1a).

Our derivation of (3.5c) is very similar to that of Haldenwang [6]; both are multi-directional versions of Kleiser and Schumann's [1] treatment. Kleiser and Schumann propose a remedy, called the *tau correction*, for this coupling; we will generalize their tau correction and make it an integral part of our influence matrix formalism in Section 3.4. The description by Kleiser and Schumann is very specific to their case and has proven to be far more difficult to generalize than the rest of their algorithm. It is therefore perhaps not surprising that all of the other articles we cite [2–5] as implementing the influence matrix method have solved (3.5c') instead of (3.5c).

Without the tau correction, a small error (discussed further in Section 6.2) occurs in satisfying $\nabla\cdot\mathbf{u}=0$ at interior points although $B\nabla\cdot\mathbf{u}=0$ is enforced. We emphasize that this error is not inherent in Kleiser and Schumann's method, but a consequence of its incomplete implementation. A number of authors have successfully used the influence matrix method without tau correction; however, Kleiser has found the stability boundary in channel flow calculations to change if the tau correction is neglected (see Canuto, Hussaini, Quateroni, and Zang [39]).

Returning to our transformation of system (3.5), we note that τ appears in (3.5c) only as $Q_{\text{lo}}\nabla\cdot\tau$, so that the coupling between (3.5c) and (3.5e) occurs only via elements of τ (high-frequency modes) whose divergence contains low-frequency modes. The coupling can then be reduced by further partitioning of $\mathscr{T} = \oplus_{i=1}^{d}\mathscr{T}$. Define $\mathscr{T}_*$, of dimension $|\mathscr{T}_*|$, to be the orthogonal complement (in $\mathscr{T}$) of the null space of $Q_{\text{lo}}\nabla\cdot$, so that $\tau\in\mathscr{T}-\mathscr{T}_*$ implies that $Q_{\text{lo}}\nabla\cdot\tau=0$. Just as we can partition the space $\mathscr{T}$, we can decompose $\mathbf{Q}_{\text{hi}}$ by defining the projection operators $\mathbf{Q}_*:\mathscr{G}\to\mathscr{T}_*$ and $(\mathbf{Q}_{\text{hi}}-\mathbf{Q}_*):\mathscr{G}\to\mathscr{T}-\mathscr{T}_*$. Then the coupling occurs only via $\mathbf{Q}_*\tau$, since by definition,

$$Q_{\text{lo}}\nabla\cdot\tau = Q_{\text{lo}}\nabla\cdot\mathbf{Q}_*\tau.$$

We can now decompose (3.5e) into

$$\mathbf{Q}_*(\mathbf{Eu}+\nabla\phi) = \mathbf{Q}_*\tau \tag{3.6a}$$

$$(\mathbf{Q}_{\text{hi}}-\mathbf{Q}_*)(\mathbf{Eu}+\nabla\phi) = (\mathbf{Q}_{\text{hi}}-\mathbf{Q}_*)\,\tau \tag{3.6b}$$

Equation (3.6b) serves only to determine $(\mathbf{Q}_{\text{hi}}-\mathbf{Q}_*)\,\tau$ and can be dropped.

Finally, we reduce the coupling by (3.5d) of different components of $\mathbf{u}$ by noting that the equations

$$\mathbf{Bu} = \mathbf{0}$$

$$B\nabla \cdot \mathbf{u} = \mathbf{0}$$

are not independent. $\mathbf{Bu} = \mathbf{0}$ implies the vanishing at the boundary, not only of $\mathbf{u}$, but also of its derivatives *tangent* to the boundary. The only contribution to $B\nabla \cdot \mathbf{u}$ comes from the *normal* derivatives, which we denote by $\nabla_n \cdot$. We can then replace (3.5d) by

$$B\nabla_n \cdot \mathbf{u} = \mathbf{0}. \tag{3.7}$$

Assembling Eqs. (3.5a)–(3.5c), (3.7), and (3.6a), we arrive at

$$\mathbf{Q}_{\text{lo}}(\mathbf{Eu} + \nabla\phi) = \mathbf{Q}_{\text{lo}}\mathbf{s} \tag{3.8a}$$

$$\mathbf{Bu} = \mathbf{0} \tag{3.8b}$$

$$Q_{\text{lo}}(\nabla^2\phi - \nabla \cdot \mathbf{Q}_*\tau) = Q_{\text{lo}}\nabla \cdot \mathbf{Q}_{\text{lo}}\mathbf{s} \tag{3.8c}$$

$$B(\nabla_n \cdot \mathbf{u}) = 0 \tag{3.8d}$$

$$\mathbf{Q}_*(\mathbf{Eu} + \nabla\phi) - \mathbf{Q}_*\tau = \mathbf{0}. \tag{3.8e}$$

At this point, no further decoupling seems possible, although the terms $\nabla_n \cdot \mathbf{u}$ and $\mathbf{Q}_*\tau$ still remain in (3.8d)–(3.8e). The influence matrix method calls for *arbitrarily* replacing these last two equations, obtaining

$$\mathbf{Q}_{\text{lo}}(\mathbf{Eu} + \nabla\phi) = \mathbf{Q}_{\text{lo}}\mathbf{s} \tag{3.9a}$$

$$\mathbf{Bu} = \mathbf{0} \tag{3.9b}$$

$$Q_{\text{lo}}(\nabla^2\phi - \nabla \cdot \mathbf{Q}_*\tau) = Q_{\text{lo}}\nabla \cdot \mathbf{Q}_{\text{lo}}\mathbf{s} \tag{3.9c}$$

$$B\phi = b \tag{3.9d}$$

$$-\mathbf{Q}_*\tau = -\boldsymbol{\sigma}. \tag{3.9e}$$

This new system of equations is no longer equivalent to (3.8) and contains two additional quantities on the right-hand side, b and $\boldsymbol{\sigma}$. However, it is now possible to solve for ϕ and $\mathbf{Q}_*\tau$ (which no longer has any relation to the tau error) before knowing $\mathbf{u}$. There exist values of b and $-\boldsymbol{\sigma}$ for which the solutions to (3.8) and (3.9) are the same: the task now becomes to determine those values.

3.3. *The Sherman-Morrison-Woodbury Formula*

We can derive some insight about the systems of Eqs. (3.8) and (3.9) by writing them in matrix notation. Now that we have derived precise equations, we will shed

some of the notation in the interest of increased readability. We will drop Q_{lo} and $\mathbf{Q}_{lo}$, assuming that they precede $\mathbf{E}$, $\nabla\cdot$, $\mathbf{s}$, ∇^2, and $\nabla\cdot$, and we will abbreviate $\mathbf{Q}_*$ by $\mathbf{Q}$, and $\mathbf{Q}_*\boldsymbol{\tau}$ by $\boldsymbol{\tau}_*$. We rewrite the true system (3.8) we have derived above in block matrix form:

$$\begin{array}{r|c|ccc|c|c|l}
d|G-T| & \mathbf{E} & \nabla & 0 & & \mathbf{u} & & \mathbf{s} & (3.8a)\\
d|T| & \mathbf{B} & \mathbf{0} & \mathbf{0} & & & & \mathbf{0} & (3.8b)\\
\hline
|G-T| & 0 & \nabla^2 & -\nabla\cdot & & \phi & = & \nabla\cdot\mathbf{s} & (3.8c)\\
|T| & B\nabla_n\cdot & 0 & 0 & & & & 0 & (3.8d)\\
|\mathscr{T}_*| & \mathbf{QE} & \mathbf{Q}\nabla & -\mathbf{I} & & \boldsymbol{\tau}_* & & \mathbf{0} & (3.8e)\\
\multicolumn{1}{c}{} & d|G| & |G| & |\mathscr{T}_*| & & & & &
\end{array}$$

The lines are drawn to partition the matrix into separate systems for $\mathbf{u}$ and $(\phi, \boldsymbol{\tau}_*)$, but we can see that the system is still fully coupled due to the fact that both offdiagonal blocks are nonzero. The altered system (3.9) is written

$$\begin{array}{r|c|ccc|c|c|l}
d|G-T| & \mathbf{E} & \nabla & 0 & & \mathbf{u} & & \mathbf{s} & (3.9a)\\
d|T| & \mathbf{B} & \mathbf{0} & \mathbf{0} & & & & \mathbf{0} & (3.9b)\\
\hline
|G-T| & 0 & \nabla^2 & -\nabla\cdot & & \phi & = & \nabla\cdot\mathbf{s} & (3.9c)\\
|T| & 0 & B & 0 & & & & b & (3.9d)\\
|\mathscr{T}_*| & \mathbf{0} & \mathbf{0} & -\mathbf{I} & & \boldsymbol{\tau}_* & & -\boldsymbol{\sigma} & (3.9e)\\
\multicolumn{1}{c}{} & d|G| & |G| & |\mathscr{T}_*| & & & & &
\end{array}$$

Here we see clearly the decoupling of the two systems, manifested by the zero offdiagonal block on the bottom left. Thus by the criterion and assumptions stated previously, (3.9) is numerically soluble.

We wish to solve (3.8) using only a procedure for solving (3.9). A classic formula, first stated by Sherman and Morrison [28, 29] and generalized by Woodbury [30] (see also [31, 32]), will accomplish this purpose;

$$(H+VW^\dagger)^{-1} = H^{-1} - H^{-1}\,V\,C^{-1}\,W^\dagger\,H^{-1}, \tag{3.10a}$$

where

$$C \equiv I + W^\dagger H^{-1} V. \tag{3.10b}$$

Here $(H+VW^\dagger)$ is the matrix we wish to invert, and H^{-1} is a matrix we know (or rather, whose action we can compute on a vector, as will be discussed later). Any method which directly (rather than iteratively) solves a linear system by modification of a related linear system implicitly makes use of the Sherman–Morrison–Woodbury formula. For example, the decomposition into homogeneous and particular solutions is an application of this formula. Green's function methods, also called influence or capacitance matrix methods, fall into this category and the matrix C in (3.10) is in fact what is called the influence or capacitance matrix.

The matrices in (3.10) are of different sizes. H and C are square matrices: H is $\mathcal{N}\times\mathcal{N}$ and C is $n\times n$. V is $\mathcal{N}\times n$ and $W^\dagger$ is $n\times\mathcal{N}$ (here † means transpose). The Sherman–Morrison–Woodbury formula is only advantageous insofar as n, which measures the extent to which H is modified, is less than $\mathcal{N}$, the size of the original problem. (The limiting case in which $n=1$, so that C is a scalar and V and $W^\dagger$ are column and row vectors, is the original Sherman–Morrison formula.) Note that (3.10) can easily be derived via Gaussian elimination on the expanded system:

$$\begin{pmatrix} H & V \\ W^\dagger & -I \end{pmatrix}\begin{pmatrix} u \\ \ell \end{pmatrix}=\begin{pmatrix} \delta \\ c \end{pmatrix}.$$

While Eqs. (3.10) represent a convenient form of the Sherman–Morrison–Woodbury procedure, it can also be stated as follows. Given a vector δ, if ℓ is a solution to

$$C\ell \equiv (I+W^\dagger H^{-1}V)\,\ell = W^\dagger H^{-1}\delta \tag{3.11a}$$

and we define

$$u \equiv H^{-1}(\delta - V\ell), \tag{3.11b}$$

then

$$(H+VW^\dagger)\,u=\delta. \tag{3.11c}$$

In this formulation neither of the inverses C^{-1} nor $(H+VW^\dagger)^{-1}$ appear. Thus we stress that this procedure can be used to generate solutions to the problem (3.11c) even when the matrices C or $(H+VW^\dagger)$ are noninvertible. By construction it can be seen that if (3.11a) has a solution for a given δ, then (3.11c) has a solution for that δ. The converse is easily shown by replacing definition (3.11b) with

$$\ell \equiv W^\dagger u. \tag{3.11b'}$$

O'Leary and Widlund [34] have in fact proven that C is invertible if and only if $(H+VW^\dagger)$ is invertible by observing that if ℓ is a nontrivial null vector of C, then $H^{-1}V\ell$ is a nontrivial null vector of $(H+VW^\dagger)$.

3.4. *Applying the Sherman–Morrison–Woodbury Formula*

Applying the Sherman–Morrison–Woodbury formula to our problem (3.8)–(3.9), we set

$$H+VW^\dagger=\left|\begin{array}{ccc} \mathbf{E} & \nabla & 0 \\ \mathbf{B} & \mathbf{0} & \mathbf{0} \\ 0 & \nabla^2 & -\nabla\cdot \\ \hline B\nabla_n\cdot & 0 & 0 \\ \mathbf{QE} & \mathbf{Q}\nabla & -\mathbf{I} \end{array}\right| \qquad H=\left|\begin{array}{ccc} \mathbf{E} & \nabla & 0 \\ \mathbf{B} & \mathbf{0} & \mathbf{0} \\ 0 & \nabla^2 & -\nabla\cdot \\ \hline 0 & B & 0 \\ \mathbf{0} & \mathbf{0} & -\mathbf{I} \end{array}\right|.$$

Here the horizontal lines are drawn to emphasize the part of the matrix that changes. We obtain the matrices V and $W^\dagger$ by

$$VW^\dagger = (H + VW^\dagger) - H = \quad V \qquad\qquad W^\dagger$$

$$\left(\begin{array}{ccc} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ 0 & 0 & 0 \\ B\nabla_n\cdot & -B & 0 \\ \mathbf{QE} & \mathbf{Q}\nabla & \mathbf{0} \end{array}\right) = \left(\begin{array}{cc} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ 0 & 0 \\ I & 0 \\ \mathbf{0} & \mathbf{I} \end{array}\right) \left(\begin{array}{ccc} B\nabla_n\cdot & -B & 0 \\ \mathbf{QE} & \mathbf{Q}\nabla & \mathbf{0} \end{array}\right)$$

We see that $W^\dagger$ evaluates the term $\nabla_n \cdot \mathbf{u} - \phi$ at the boundary, and the components of $\mathbf{Eu} + \nabla\phi$ which are in $\mathcal{T}_*$. V takes b and $-\boldsymbol{\sigma}$, the boundary values of ϕ and the values imposed on $-\boldsymbol{\tau}_*$, and inserts them into the otherwise homogeneous problem ($\mathbf{s} = \mathbf{0}$). The dimension $n = |T| + |\mathcal{T}_*|$ is considerably less than $\mathcal{N} = (d+1)|G| + |\mathcal{T}_*|$ as desired ($|T|/|G|$ is on the order of the ratio of surface to volume of the domain). The vectors u, ℓ, and ϑ of (3.11) are, for this case,

$$u \equiv \begin{pmatrix} \mathbf{u} \\ \phi \\ \boldsymbol{\tau}_* \end{pmatrix}, \qquad \ell \equiv \begin{pmatrix} b \\ -\boldsymbol{\sigma} \end{pmatrix}, \qquad \vartheta \equiv \begin{pmatrix} \mathbf{s} \\ \mathbf{0} \\ \nabla\cdot\mathbf{s} \\ 0 \\ \mathbf{0} \end{pmatrix}.$$

The role of the influence matrix C can be seen as follows. If $(\mathbf{u}^h, \phi^h, \boldsymbol{\tau}_*^h)$ is the solution to the homogeneous problem for a given b and $-\boldsymbol{\sigma}$, i.e., the solution to (3.9) with

$$\mathbf{s} = \mathbf{0}$$

$$B\phi^h = b$$

$$-\boldsymbol{\tau}_*^h = -\boldsymbol{\sigma}$$

then

$$C\ell = (W^\dagger H^{-1} V + I)\begin{pmatrix} b \\ -\boldsymbol{\sigma} \end{pmatrix} = \begin{pmatrix} B(\nabla_n\cdot\mathbf{u}^h - \phi^h) + b \\ \mathbf{Q}(\mathbf{Eu}^h + \nabla\phi^h) - \boldsymbol{\sigma} \end{pmatrix} = \begin{pmatrix} B\nabla_n\cdot\mathbf{u}^h \\ \mathbf{Q}(\mathbf{Eu}^h + \nabla\phi^h) - \boldsymbol{\tau}_*^h \end{pmatrix}. \quad (3.12)$$

This vector would be zero if all of the conditions which we seek to impose on the solution were satisfied, that is, if we had been able to guess the correct b and $-\boldsymbol{\sigma}$ in Eqs. (3.9d)–(3.9e) so as to satisfy Eqs. (3.8d)–(3.8e). As it is, C provides us with the error ("influence") in (3.8d)–(3.8e) arising from any given b and $-\boldsymbol{\sigma}$ in the homogeneous problem. C is generated in a preprocessing step by setting b and $-\boldsymbol{\sigma}$ equal to each basis vector in turn, finding the corresponding homogeneous solution, and performing the calculation (3.12), which corresponds to Eq. (3.10b).

In contrast, the operations symbolized by (3.10a) are to be carried out at each time step, with a different **s**. One first calculates a particular solution, i.e., a solution to (3.9) with $b=0$, $-\boldsymbol{\sigma}=\mathbf{0}$. This corresponds to the first term on the right-hand side of (3.10a). The sequence of vectors produced by the second term on the right-hand side is shown below, reading right to left. Below each step ($\Leftarrow$) is the matrix which transforms the vector on the right to the vector on the left:

$$\begin{pmatrix} \mathbf{u}^h \\ \phi^h \\ \boldsymbol{\tau}_*^h \end{pmatrix} \Leftarrow \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ 0 \\ b \\ -\boldsymbol{\sigma} \end{pmatrix} \Leftarrow \begin{pmatrix} b \\ -\boldsymbol{\sigma} \end{pmatrix} \Leftarrow \left\{ \begin{pmatrix} B(\nabla_n \cdot \mathbf{u}^p - \phi^p) \\ \mathbf{Q}(\mathbf{E}\mathbf{u}^p + \nabla\phi^p) \end{pmatrix} = \begin{pmatrix} B(\nabla_n \cdot \mathbf{u}^p) \\ \mathbf{Q}(\mathbf{E}\mathbf{u}^p + \nabla\phi^p) - \boldsymbol{\tau}_*^p \end{pmatrix} \right\} \Leftarrow \begin{pmatrix} \mathbf{u}^p \\ \phi^p \\ \boldsymbol{\tau}_*^p \end{pmatrix} \Leftarrow \begin{pmatrix} \mathbf{s} \\ \mathbf{0} \\ \nabla \cdot \mathbf{s} \\ 0 \\ \mathbf{0} \end{pmatrix}.$$

$$H^{-1} \qquad V \qquad C^{-1} \qquad\qquad W^{\dagger} \qquad H^{-1} \qquad (3.13)$$

That is, $H^{-1}VC^{-1}W^{\dagger}H^{-1}$ generates the homogeneous solution which has the same error in satisfying (3.8d)–(3.8e) as does the particular solution. By subtracting the homogeneous from the particular solution, the last step of (3.10a), we arrive at the true solution, which has no error. Note that the same operations are used to evaluate $W^{\dagger}$ on particular solutions in (3.13), as to generate the matrix C from homogeneous solutions in (3.12).

The matrix operations in (3.13) should be interpreted as a symbolic shorthand, rather than as explicit matrix multiplication. Indeed, as stated in Section 3.3, the matrix C need not even be invertible: the multiplication by C^{-1} in (3.13) should be treated as notation for finding a solution to (3.11a) and will be discussed further in Section 6. Although H is invertible, multiplication by H^{-1} would require $O(\mathcal{N}^2)$ operations and storage of the full H^{-1} would require $\mathcal{N}^2$ words. This would be prohibitively expensive, since $\mathcal{N}$ is assumed to be large. However, H, like $\mathbf{E}$ and ∇^2, has a relatively sparse and highly regular structure which is destroyed by ordinary matrix inversion, so we assume that we have instead some procedure (which we call a *solve*) for solving Eq. (3.9). The multiplications by V and $W^{\dagger}$ are also carried out by procedures more economical than matrix multiplication.

By writing

$$H^{-1} - H^{-1}VC^{-1}W^{\dagger}H^{-1} = H^{-1}(I - VC^{-1}W^{\dagger}H^{-1}) \qquad (3.14a)$$

$$= (I - H^{-1}VC^{-1}W^{\dagger})H^{-1}, \qquad (3.14b)$$

we see that only two solves are actually required per time step. In fact the $\mathcal{N}$ by n matrix $H^{-1}VC^{-1}$ may be calculated and stored in the preprocessing stage, thereby reducing the number of solves in (3.14b) to only one. Economical in time, but costly in storage, this last reduction is possible only if n is sufficiently small; in practice, if the domain is unidirectional. $H^{-1}VC^{-1}$ contains the Green functions, i.e., the set of homogeneous solutions for all possible values of $(b, -\boldsymbol{\sigma})$. (Since

neither the values of ϕ nor of τ_* are required, the effective $H^{-1}VC^{-1}$ is actually smaller: of size $d|G|$ by n.)

A different shortcut is possible when the Green's functions are not stored and Eq. (3.14a) is used. Note that $W^\dagger$ does not use all of the information in $\mathbf{u}$: specifically $\mathbf{u}$ can be replaced by the normal velocity in the term $\nabla_n \cdot \mathbf{u} - \phi$. This means that to evaluate $\nabla_n \cdot \mathbf{u} - \phi$, we need not calculate the velocity components which are tangent to *all* boundaries. In most cases these velocity components are also not used in the term $\mathbf{QEu}$ (but not always, as we shall see in Section 5). We define $\bar{\mathbf{u}}$ to be that part of $\mathbf{u}$ that is relevant to $W^\dagger$; i.e., $\bar{\mathbf{u}}$ is the projection of $\mathbf{u}$ that is orthogonal to the kernels both of $B\nabla_n \cdot$ and of $\mathbf{QE}$. In calculating particular velocities in (3.14a), we need only find $\bar{\mathbf{u}}$ and not the full $\mathbf{u}$.

Since some of the operations and storage required in the algorithm are $O(n^2)$, it is highly advantageous to reduce n as much as possible. This is one of the reasons for having introduced the projection operator $\mathbf{Q}$ and the subspace $\mathscr{T}_*$ before replacing (3.8e) by (3.9e); we will work further on reducing n by symmetry in Section 4.

4. Cartesian Applications

4.1. *The Rectangle Revisited*

We return to our rectangular example of Section 2 in order to determine the composition of the space $\mathscr{T}_*$ for a concrete case. Recall that $\mathscr{T} - \mathscr{T}_*$ is the set of all $\tau \in \mathscr{T}$ such that $Q_{1o}\nabla \cdot \tau = 0$. We will find the elements of $\mathscr{T}$ which have this property by listing and examining its basis vectors. Define basis vectors g^{jk} by $g^{jk}(j', k') = \delta(j, j')\,\delta(k, k')$. We then have for the vector space $\mathscr{G}$ the usual basis set $\{g^{jk}: (j, k) \in G\}$, and for $\mathscr{T}$ the basis set $\{g^{jk}: (j, k) \in T\}$. $T \equiv T_x \cup T_y \cup T_{xy}$, where the definitions of T_x, T_y, and T_{xy} are recalled in Table II.

We first consider the case $d = 2$ (the case $d = 1$ has only the trivial solution), so that we have for $\mathscr{T}$ the basis set $\{\mathbf{e}_x g^{jk}, \mathbf{e}_y g^{jk}: (j, k) \in T\}$. In Cartesian coordinates,

$$\nabla \cdot \tau = \partial_x \tau_x + \partial_y \tau_y.$$

TABLE II

Tau Sets for the Rectangle

k \ j	0 ⋯ $J-2$	$J-1$ J
0 ⋮ $K-2$		T_x
$K-1$ K	T_y	T_{xy}

The operation ∂_x on the Chebyshev polynomial $\mathscr{C}_j(x)$ generates lower j indices,

$$\partial_x \mathscr{C}_j(x) = j \sum_{\substack{j' \le j-1 \\ j+j' \text{ odd}}} \mathscr{C}_{j'}(x)(2-\delta(j',0)),$$

but leaves the k index unchanged. We now examine the effect of ∂_x on basis elements of $\mathscr{T}$:

(1) $\partial_x g^{jK}$ has components of $g^{j'K}$ for *all* $j'=j-1, j-3$, etc. Because the k index has not been changed from its original value of K, these are all in the "high-frequency" set $\mathscr{T}$, so $Q_{\text{lo}}\nabla\cdot\mathbf{e}_x g^{jK}=0$, and $\mathbf{e}_x g^{jK}\in\mathscr{T}-\mathscr{T}_*$.

(2) Similarly, $\mathbf{e}_x g^{j(K-1)}\in\mathscr{T}-\mathscr{T}_*$.

(3) $\partial_x g^{Jk}$ has components of g^{jk} for $j=J-1$, $J-3$, etc. So, unless $k\ge K-1$, components in the "low-frequency" set $\mathscr{G}-\mathscr{T}$ are generated, $Q_{\text{lo}}\nabla\cdot\mathbf{e}_x g^{Jk}\neq 0$, and $\mathbf{e}_x g^{Jk}\in\mathscr{T}_*$.

(4) Similarly, $\mathbf{e}_x g^{(J-1)k}\in\mathscr{T}_*$ unless $k\ge K-1$.

We can combine (1)–(4) into the statements:

(5) $\mathbf{e}_x g^{jk}\in\mathscr{T}-\mathscr{T}_*$ iff $(j,k)\in T-T_x$, iff $g^{jk}\in\mathscr{T}-\mathscr{T}_x$

(6) $\mathbf{e}_x g^{jk}\in\mathscr{T}_*$ iff $(j,k)\in T_x$, i.e., iff $g^{jk}\in\mathscr{T}_x$.

By reversing the roles of x and y, j and k, we see that

(7) $\mathbf{e}_y g^{jk}\in\mathscr{T}_*$, i.e., iff $(j,k)\in T_y$, i.e., iff $g^{jk}\in\mathscr{T}_y$.

We combine (6) and (7) to get the final result,

(8) $\mathscr{T}_*=\mathscr{T}_x\oplus\mathscr{T}_y$, which is of dimension $2(J+K-2)$.

For $d=3$, the set $\mathscr{T}$ contains additional components $\mathbf{e}_z\tau_z(j,k)$, or in the physical space representation, $\mathbf{e}_z\hat{\tau}_z(x,y)$. However, the additional term $\partial_z\tau_z$ in the divergence is always zero, since all functions are independent of z. Therefore, $\mathbf{e}_z\tau_z\in\mathscr{T}-\mathscr{T}_*$ for any τ_z, and so $\mathscr{T}_*=\mathscr{T}_x\oplus\mathscr{T}_y\oplus 0$, meaning that $\boldsymbol{\tau}\in\mathscr{T}_*$ has components $\tau_x\in\mathscr{T}_x$, $\tau_y\in\mathscr{T}_y$, and $\tau_z=0$. $\mathscr{T}_*$ is still of dimension $|T_x\cup T_y|=2(J+K-2)$. (This can be compared with $\mathscr{T}=\mathscr{T}\oplus\mathscr{T}\oplus\mathscr{T}$, which is of dimension $d|T|=6(J+K)$.) The influence matrix, including boundary values b as well as tau values $\boldsymbol{\tau}_*$, is independent of d and is of dimension

$$n=|T|+|\mathscr{T}_*|=2(J+K)+2(J+K-2)=4(J+K-1).$$

The Green's function matrix is probably too large to be stored in this case. Can any advantage be gained from calculating only those components of the particular velocity $\bar{\mathbf{u}}$ needed by $W^{\dagger}$? It can be verified that

$$\bar{\mathbf{u}}=\mathbf{e}_x u_x+\mathbf{e}_y u_y.$$

That is, there is no need to calculate the z-component of the particular solution. Thus $\bar{\mathbf{u}}$ differs from $\mathbf{u}$ only if $d=3$. We defer a more detailed discussion of $\bar{\mathbf{u}}$ to Section 4.2.

4.2. *The Channel—Periodicity*

We need to extend these considerations to periodic domains. In the case considered by Kleiser and Schumann [1], the domain is tri-directional, with periodic x- and y-directions, and a nonperiodic z-direction. Functions are represented by

$$\hat{f}(x, y, z) = \sum_{\ell=-L/2}^{L/2} \sum_{m=-M/2}^{M/2} \sum_{k=0}^{K} f(\ell, m, k)\, e^{i\ell x}\, e^{imy}\, \mathscr{C}_k(z) \left\{ \begin{array}{c} 0 \leqslant x < 2\pi \\ 0 \leqslant y < 2\pi \\ -1 \leqslant z \leqslant +1 \end{array} \right\}.$$

In order for $\hat{f}$ to be real, $f(-\ell, -m, k)$ must be the complex conjugate of $f(\ell, m, k)$. The periodicity of the domain is inherent in these basis functions, and thus no boundary conditions are required on $\mathbf{u}$ or ϕ in either the x- or the y- directions of the domain.

The operators ∇^2, $\mathbf{\nabla}^2$, ∇, $\nabla\cdot$, E, and $\mathbf{E}$, which contain the operators ∂_x and ∂_y, act differently on modes with different values of ℓ and m, but without coupling them. If we define the boundary operator B so that it calculates boundary values for the pressure and for the divergence as Fourier coefficients, then it, too, does not couple the different (ℓ, m) modes. Then the matrices H, V, $W^\dagger$, and C are decoupled, since they are comprised of decoupled operators. The net result is that, although the *velocity* remains tri-directional ($d=3$), the *domain* can be considered to be effectively uni-directional: the z direction is the only direction in which boundary conditions are imposed and for which tau coefficients exist. We may apply all of the nomenclature and operations of the preceding sections to each of the modes independently. We define the uni-directional grid $G^{\ell m} = \{k: 0 \leqslant k \leqslant K\}$ and tau sets $T^{\ell m} = \{K-1, K\}$. We then define operators and functions particular to each (ℓ, m) mode. For example, $E^{\ell m}$ acts on $f^{\ell m}$ by

$$\begin{aligned}
(Ef)(\ell, m, k) &= \sum_{\ell'} \sum_{m'} \sum_{k'} E(\ell, m, k; \ell', m', k') f(\ell', m', k') \\
&= \sum_{\ell'} \sum_{m'} \sum_{k'} E(\ell, m, k; \ell, m, k')\, \delta(\ell, \ell')\, \delta(m, m') f(\ell', m', k') \\
&= \sum_{k'} E(\ell, m, k; \ell, m, k') f(\ell, m, k') \\
&\equiv \sum_{k'} E^{\ell m}(k, k') f^{\ell m}(k') \\
&= (E^{\ell m} f^{\ell m})(k).
\end{aligned}$$

(Note that the superscripts here do not signify basis vectors as they did in Section 4.1.)

To determine the set $\mathcal{T}_*^{\ell m}$, we need to consider the action of $Q_{\text{lo}}\nabla\cdot$ on $\tau \in \mathcal{T} = \bigoplus_{i=1}^{3} \mathcal{T}^{\ell m}$. The operations ∂_x on u_x and ∂_y on u_y leave the k index unchanged, but by operating with ∂_z on u_z we can lower the k-index and exit the tau set. We therefore have

$$\mathcal{T}_*^{\ell m} = 0 \oplus 0 \oplus \mathcal{T}^{\ell m}.$$

The dimensionality of $C^{\ell m}$ is thus

$$n^{\ell m} = |T^{\ell m}| + |\mathcal{T}_*^{\ell m}| = 2|T^{\ell m}| = 4.$$

Storing the Green's function matrices $(H^{\ell m})^{-1} V^{\ell m} C^{\ell m}$ is still possible for this case, since each requires $d|T^{\ell m}|\,|G^{\ell m}| = 3 \times 4 \times (K+1)$ words, giving a total storage count of $12 \times (L+1)(M+1)(K+1)$.

If (as in Kleiser and Schumann [1]) the Green's function matrices are not stored, it becomes of interest to calculate only reduced particular solutions $\bar{\mathbf{u}}$. Recall that $\bar{\mathbf{u}}$ is the projection of $\mathbf{u}$ which is used by $W^\dagger$ (it is orthogonal to the kernels of $B\nabla_n\cdot$ and of $\mathbf{Q}_*\mathbf{E}$). Clearly, the projection of $\mathbf{u}$ used by the operator $B\nabla_n\cdot$ is the velocity normal to the boundaries, i.e., the z-velocity: $\mathbf{u}_n = \mathbf{e}_z u_z$. On the other hand, the operator $\mathbf{Q}_*\mathbf{E}$ cannot use any component other than the z-velocity. This is because (4.1) shows that $\mathbf{Q}_*$ projects onto the (high-frequency) z-component of the velocity, and $\mathbf{E}$ does not mix z- with x- or y-velocities:

$$\begin{aligned}\mathbf{Q}_*\mathbf{E}\mathbf{u} &= \mathbf{e}_z(\mathbf{e}_z \cdot \mathbf{Q}_{hi}\,\mathbf{E}\mathbf{u}) \\ &= \mathbf{e}_z(Q_{hi}\,E u_z).\end{aligned}$$

Therefore $\bar{\mathbf{u}} = \mathbf{e}_z u_z$ is the only component of the particular velocity that need be calculated.

4.3. *Reflection Symmetry*

The problem can be further reduced, since the domain is reflection-symmetric in z. This symmetry is manifested in the spectral representation by the fact that odd and even Chebyshev polynomials are decoupled. Operators which are $(K+1)$ by $(K+1)$ matrices, such as $E^{\ell m}$, can be replaced by two matrices $E^{\ell m p}$, for symmetric $(p=s)$ and antisymmetric $(p=a)$ functions, each $(K+1)/2$ by $(K+1)/2$. (Here and throughout the rest of the article, the order of the highest Chebyshev polynomial—here K—will be odd, so that the total number of polynomials or gridpoints—here $K+1$—is even. This simplifies the discussion since the number of even and odd polynomials is the same.) Presumably the inversion procedures chosen for H, i.e., for $\mathbf{E}$ and ∇^2, already take advantage of reflection symmetry. This is accomplished merely by decoupling the even polynomials from the odd, and so requires little additional throught. Here we consider how reflection-symmetry is manifested in the full three-directional problem.

TABLE III

Parity and Symmetry of Vectors and Operators

Solution	V	$W^\dagger$		$p=s$	$p=a$
ϕ	b	$B(\nabla_n \cdot \mathbf{u} - \phi)$		Even	Odd
$\mathbf{u}, \tau$	$-\sigma$	$\mathbf{Q}_*(\mathbf{E}\mathbf{u} + \nabla\phi)$	$\mathbf{e}_x \cdot$	Even	Odd
			$\mathbf{e}_y \cdot$	Even	Odd
			$\mathbf{e}_z \cdot$	Odd	Even

The intricacy comes from the fact that ∂_x and ∂_y are parity preserving operators, but that ∂_z reverses parity, changing even Chebyshev polynomials to odd and vice versa. The requirement that $\nabla \cdot \mathbf{u} = 0$ means that the even (odd) Chebyshev polynomials in u_x and u_y are coupled to the odd (even) Chebyshev polynomials in u_z, as shown in Table III. The role of $\nabla\phi$ in the equations tells us that ϕ has the same parity as u_x, u_y (opposite to that of u_z). The boundary conditions b behave like ϕ; τ and σ behave like $\mathbf{u}$. The same conclusions can be drawn by considering that the z reflection operator, defined by,

$$(\hat{u}_x, \hat{u}_y, \hat{u}_z)(x, y, z) \to (\hat{u}_x, \hat{u}_y, -\hat{u}_z)(x, y, -z)$$
$$\hat{\phi}(x, y, z) \to \hat{\phi}(x, y, -z)$$

commutes with all the operators in the problem. Therefore the full space of solutions $(\mathbf{u}, \phi)$ can be decomposed into symmetric and antisymmetric invariant subspaces.

Decoupled influence matrices $C^{\ell mp}$ require that the procedures represented by V and $W^\dagger$ take parity into account as shown by Table III. In addition, to classify boundary conditions as symmetric or antisymmetric, the boundary operator B must not couple odd and even Chebyshev polynomials. That is, instead of the natural boundary conditions,

$$\phi^{\ell m}(z = +1) = \beta^{\ell m +}$$
$$\phi^{\ell m}(z = -1) = \beta^{\ell m -},$$

we should specify that

$$\phi^{\ell m}(z = +1) + \phi^{\ell m}(z = -1) = b^{\ell m, p=s} \tag{4.1a}$$
$$\phi^{\ell m}(z = +1) - \phi^{\ell m}(z = -1) = b^{\ell m, p=a}. \tag{4.1b}$$

This requirement is analogous to—but less obvious than—the requirement in the periodic case that B calculate Fourier coefficients.

Note that classification of a tau set as symmetric or antisymmetric will depend on the variable (u_x, u_y, u_z, or ϕ) with which it is associated. To avoid ambiguity, we must unfortunately introduce yet another superscript on the tau sets T and $\mathcal{T}$ in order to indicate the variable. For instance, $T_z^{\phi\ell ms}$ is the tau set along the z boundary for $\phi^{\ell ms}$ (the subscript refers to a part of the domain, and the first super-

script to a component or function). But in the interest of legibility, *all* superscripts (including those referring to symmetry) will be implied rather than written out wherever possible. We introduce two conventions:

(1) T without superscripts will refer to the tau sets for ϕ (here $\phi^{\ell mp}$; other symmetry superscripts will be implied later). For example, $T \equiv T^{\phi \ell mp}$ and $T_z \equiv T_z^{\phi \ell mp}$.

(2) $\mathscr{T}_z$ without superscripts will denote $\mathscr{T}_z^z$—the space of functions defined on T_z^z, the z-directional tau set of u_z. The same convention applies to x- and y-, or r- and θ-directions, and again the symmetry superscripts such as (ℓ, m, p) are implied.

The rectangle is also reflection-symmetric, in both x and y. Just as the physical grid $\hat{G}$ can be divided into four identical quarters, the spectral grid G can be partitioned into four pieces: (s, s) functions symmetric both in x and in y, (s, a) functions symmetric in x but antisymmetric in y, and (a, s) and (a, a) functions defined analogously. The original problem of size $|G| = (J+1)(K+1)$ is decomposed into four entirely decoupled problems, each defined on a domain of size $(J+1)(K+1)/4$. Table IV is similar to Table III: for example, the set $(p = s, p' = s)$ contains functions u_x which are odd polynomials in x (j odd) and even polynomials in y (k even).

The dimensionality of the influence matrices $C^{pp'}$ is

$$n = |T| + |\mathscr{T}_*| = |T^{\phi pp'}| + |\mathscr{T}_*^{pp'}| = \frac{(J+K)}{2} + \frac{(J+K-2)}{2} = J+K-1.$$

Periodicity is a manifestation of the absence of boundaries—all locations are equivalent, indistinguishable by their distance from a boundary—whereas reflection symmetry occurs in the presence of boundaries whose geometry is such as to make certain set of points equivalent. Tables III and IV, and especially boundary conditions (4.1) show that reflection symmetry is more elusive than periodicity. As a result, *none* of the articles we have cited that implemented the influence matrix method used reflection symmetry to reduce the size n of their influence matrices. Recall that reduction of n is particularly desirable because C is multiplied and

TABLE IV

Parity and Symmetry for the Rectangle

	j		k	
	$p = s$	$p = a$	$p' = s$	$p' = a$
ϕ	Even	Odd	Even	Odd
u_x	Odd	Even	Even	Odd
u_y	Even	Odd	Odd	Even

stored as a full matrix, taking time and space proportional to n^2. The savings due to symmetry are not significant in channel flow simulations (one nonperiodic direction, e.g., Kleiser and Schumann [1]): there, multiplication by C takes a very small portion of the calculation time whether or not n is reduced from 4 to 2. However, sacrificing symmetry becomes more wasteful as we increase the number of nonperiodic directions (because multiplication by and storage of C represents a larger proportion of the total calculation), or symmetric directions (because n can be reduced by a larger factor). Rectangular symmetry leads to a 16-fold reduction in n^2. For Le Quéré and Alziary de Roquefort [5], whose finest grids used $J = K = 64$, the reduction would be substantial, reducing n from ≈ 512 to ≈ 128. (They have $n \approx 256$, but this is because they did not include the tau correction.)

5. Cylindrical Coordinates

The cylindrical coordinates for which we developed this formalism involve aspects from both of the cases discussed in Section 4. The velocity is tri-directional. Scalar functions, as well as u_z, are represented by

$$\hat{f}(r, \theta, z) = \sum_{m=-M}^{M} \sum_{\substack{j=0 \\ j+m \text{ even}}}^{2J+1} \sum_{k=0}^{K} f(j, m, k)\, \mathscr{C}_j\left(\frac{r}{R}\right) e^{im\theta} \mathscr{C}_k(z) \begin{Bmatrix} 0 \leqslant r \leqslant R \\ 0 \leqslant \theta < 2\pi \\ -1 \leqslant z \leqslant +1 \end{Bmatrix}.$$

Since $f(j, -m, k)$ is the complex conjugate of $f(j, m, k)$, only $m \geqslant 0$ are required. For the functions u_r and u_θ, the representation is the same except that $j+m$ *odd* is required. Corresponding to these parity restrictions is the fact that r/R ranges over the half interval $[0, 1]$ rather than $[-1, 1]$.

The r direction has peculiar properties: sometimes it has one boundary point at $r = R$, and sometimes a second "boundary point" at the axis $r = 0$. Because the θ direction is periodic, the different m-modes are decoupled, as in Section 4.2. The z direction is effectively Cartesian, with two boundary points at $z = \pm 1$, and the symmetric and antisymmetric modes are decoupled. Thus the domain is made effectively bi-directional, and we have operators $\mathbf{E}^{mp}$, C^{mp}, and so on. Determination of the sets T^{mp} and $\mathscr{T}_*^{mp}$ is complicated but can be done systematically, by accounting carefully for each boundary condition imposed. This is what we will do in this section.

5.1. *Axisymmetric Case*

The axisymmetric case $m = 0$ is relatively simple and analogous to our rectangle example. One boundary condition is applied in the r direction at $r = R$, and the tau set for ϕ^{0p} is

$$T = T_r \cup T_z \cup T_{rz},$$

where

$$T_r = \{(j, m, k): j = 2J, m = 0, 0 \leqslant k \leqslant K-2, k+p \text{ even}\} \text{ is of size } (K-1)/2,$$

$$T_z = \{(j, m, k): 0 \leqslant j \leqslant 2J-2, j \text{ even}, m = 0, k = K-1 \text{ or } K, k+p \text{ even}\} \text{ is of size } J,$$

and

$$T_{rz} = \{(j, m, k): j = 2J, m = 0, k = K-1 \text{ or } K, k+p \text{ even}\} \text{ is of size } 1.$$

Since ∂_θ multiplies axisymmetric functions by zero, the set $\mathscr{T}_*$ is

$$\mathscr{T}_* = \mathscr{T}_r \oplus 0 \oplus \mathscr{T}_z,$$

where $\mathscr{T}_r \equiv \mathscr{T}_r^{r0p}$ is the set of vectors defined on

$$T_r^{r0p} = \{(j, m, k): j = 2J+1, m = 0, 0 \leqslant k \leqslant K-2, k+p \text{ even}\}, \text{ of size } (K-1)/2$$

and $\mathscr{T}_z \equiv \mathscr{T}_z^{z0p}$ is the set of vectors defined on

$$T_z^{z0p} = \{(j, m, k): 0 \leqslant j \leqslant 2J-2, j \text{ even}, m = 0, k = K-1 \text{ or } K, k+p \text{ odd}\}, \text{ of size } J$$

(where $k+p$ is odd because of parity reversal of τ_z by reflection in z). Adding the sizes of all these sets, we see that the dimensionality of the influence matrix for each z-parity is

$$n = K + 2J.$$

5.2. *Nonaxisymmetric Case*

Before embarking on this section, we should point out that the complications to be encountered are not due to the influence matrix method, but to the cylindrical coordinate system. These difficulties—axis conditions, decoupling of the Laplacian—reflect those which arise in developing an algorithm for inverting the elliptic operators $\mathbf{E}$ and ∇^2. This section will show that the inversion algorithm and the influence matrix must be formulated together.

It might seem that, with no boundary condition in θ (and thus no set T_θ), $\mathscr{T}_*$ should contain no element of the form $\mathbf{e}_\theta \tau_\theta$. But in fact, since

$$\nabla \cdot \mathbf{u} = \frac{1}{r} \partial_r (r u_r) + \frac{1}{r} \partial_\theta u_\theta + \partial_z u_z,$$

the operation $\nabla_\theta \equiv (1/r)\, \partial_\theta$ lowers the order of r-polynomials. Thus if $\tau_\theta \in \mathscr{T}_r$ and $m \geqslant 1$, then $\mathbf{e}_\theta \tau_\theta \in \mathscr{T}_*$. In order to say more about the nonaxisymmetric case we

must recall the form of the Laplacian (and the operator $\mathbf{E} \equiv \mathbf{I} - \varepsilon \nabla^2$) in cylindrical coordinates. It is not diagonal in that $\mathbf{e}_r \cdot \nabla^2$ and $\mathbf{e}_\theta \cdot \nabla^2$ both depend on u_r and u_θ:

$$\begin{aligned}\nabla^2 \mathbf{u} = \mathbf{e}_r &\left(\left(\nabla^2 - \frac{1}{r^2}\right) u_r - \frac{2}{r^2}\,\partial_\theta u_\theta\right) \\ &+ \mathbf{e}_\theta \left(\left(\nabla^2 - \frac{1}{r^2}\right) u_\theta + \frac{2}{r^2}\,\partial_\theta u_r\right) \\ &+ \mathbf{e}_z \nabla^2 u_z.\end{aligned}$$

(Note that u_r and u_θ are uncoupled in the axisymmetric case.) The Laplacian can be diagonalized (Patera and Orszag [9]) by the transformation

$$\begin{aligned}u_+ &= u_r + i u_\theta \\ u_- &= u_r - i u_\theta,\end{aligned}$$

so that

$$\begin{aligned}\nabla^2 \mathbf{u} = \mathbf{e}_+ &\left(\left(\nabla^2 - \frac{1}{r^2}\right) + \frac{2i}{r^2}\,\partial_\theta\right) u_+ \\ &+ \mathbf{e}_- \left(\left(\nabla^2 - \frac{1}{r^2}\right) - \frac{2i}{r^2}\,\partial_\theta\right) u_- \\ &+ \mathbf{e}_z \nabla^2 u_z.\end{aligned}$$

The *independent* variables are not affected by this transformation: $\hat{u}_+$ and $\hat{u}_-$ are still functions of r and θ.

The functions u_+ and u_- are also the appropriate ones on which to impose regularity conditions at the axis, necessitated by the coordinate singularity at $r = 0$. To explain what is meant by regularity conditions, we introduce another (equivalent) basis set, consisting of monomials in r and z instead of Chebyshev polynomials, i.e., $r^j e^{im\theta} z^k$ instead of $\mathscr{C}_j(r/R)\, e^{im\theta} \mathscr{C}_k(z)$. Coefficients in the monomial basis are denoted by $\tilde{u}(j, m, k)$.

$$u \begin{Bmatrix} + \\ z \\ - \end{Bmatrix} = \sum_{j,m,k} \tilde{u} \begin{Bmatrix} + \\ z \\ - \end{Bmatrix} (j, m, k)\, r^j e^{im\theta} z^k \tag{5.1}$$

with the same parity rules as before. (The notation of (5.1) allows us to compress expansions for each of u_+, u_-, and u_z into one formula.)

Consider the form of the vector Laplacian in this basis:

$$\mathbf{e}\begin{Bmatrix}+\\ z\\ -\end{Bmatrix}\cdot\nabla^2\mathbf{u}=\sum_{j,m,k}\tilde{u}\begin{Bmatrix}+\\ z\\ -\end{Bmatrix}(j,m,k)$$

$$\left[\left(j^2-\begin{Bmatrix}m+1\\ m\\ m-1\end{Bmatrix}^2\right)r^{j-2}e^{im\theta}z^k+k(k-1)\,r^j e^{im\theta}z^{k-2}\right]. \tag{5.2}$$

Equation (5.2) shows that the operator ∇^2 can produce negative powers of r, whereas negative powers of z are all preceded by a coefficient of zero. The representation (5.1) cannot, of course, include singular functions; however, it can include functions whose derivatives have singularities which are projected out by the numerical differentiation operators. In Cartesian coordinates, any function of the form $x^j y^m z^k$ $(j, m, k \geq 0)$ is analytic, i.e., infinitely differentiable, and can serve as a scalar component of a vector field. But in cylindrical coordinates, a velocity field $\mathbf{u}$, in order to be analytic, must have components with series expansions of the forms

$$\hat{u}_+(r,\theta,z)=\sum_{\substack{j\geq m+1\\ j+m\text{ odd}}}\tilde{u}_+(j,m,k)\,r^j e^{im\theta}z^k$$

$$\hat{u}_z(r,\theta,z)=\sum_{\substack{j\geq m\\ j+m\text{ even}}}\tilde{u}_z(j,m,k)\,r^j e^{im\theta}z^k$$

$$\hat{u}_-(r,\theta,z)=\sum_{\substack{j\geq |m-1|\\ j+m\text{ odd}}}\tilde{u}_-(j,m,k)\,r^j e^{im\theta}z^k$$

or, generally,

$$\hat{u}\begin{Bmatrix}+\\ z\\ -\end{Bmatrix}(r,\theta,z)=\sum_{j-\begin{Bmatrix}m+1\\ m\\ |m-1|\end{Bmatrix}\text{even}}{}'\tilde{u}\begin{Bmatrix}+\\ z\\ -\end{Bmatrix}(j,m,k)\,r^j e^{im\theta}z^k. \tag{5.3}$$

The prime means that, in addition to the parity rule, the sum is to be restricted to

$$j\geq\begin{Bmatrix}m+1\\ m\\ |m-1|\end{Bmatrix}, \tag{5.4}$$

where the three possibilities in brackets refer to $\tilde{u}\left\{\begin{smallmatrix}+\\ z\\ -\end{smallmatrix}\right\}$. Following Orszag [39] we require only the weaker and more easily implemented condition that $\nabla^2\mathbf{u}$ (the

TABLE V

Axis Conditions Imposed On **u**

m	0	1	2	3	4	5
$+$	$j \geq 1$	$j \geq 2$	$j \geq 3$	$j \geq 2$	$j \geq 3$	$j \geq 2$
z	$j \geq 0$	$j \geq 1$	$j \geq 2$	$j \geq 3$	$j \geq 2$	$j \geq 3$
$-$	$j \geq 1$	$j \geq 0$	$j \geq 1$	$j \geq 2$	$j \geq 3$	$j \geq 2$

highest derivative of **u** appearing in the equations) be nonsingular, i.e., contain no negative powers of r. We make the sum in (5.3) less restrictive, replacing (5.4) by

$$j \geq \min \left(\left\{ \begin{matrix} m+1 \\ m \\ |m-1| \end{matrix} \right\}, 2 \right). \tag{5.5}$$

Inequality (5.5), shown in Table V, can be considered to specify boundary conditions at the axis. In the table, a line delimits the functions and m-values which require a condition at the axis. We see that for $m=0$ there are no axis conditions, for $m=1$ there is a condition on u_+ only, for $m=2$ there are conditions on both u_+ and u_z, and for $m \geq 3$ there are axis conditions on all three, u_+, u_z, and u_-. Scalar functions such as ϕ are treated like u_z.

For computation, the axis conditions are expressed as conditions on the Chebyshev coefficients of ϕ and $u \left\{ \begin{matrix} + \\ z \\ - \end{matrix} \right\}$ for $j=0$ or 1, using the fact that the coefficient of r^0 in $\mathscr{C}_{2j}(r)$ is $(-1)^j$, and the coefficient of r^1 in $\mathscr{C}_{2j+1}(r)$ is $j(-1)^j$. For the scalar function ϕ, we can define the axis operator A and express the axis condition as:

$$(A\phi)(m,k) \equiv \left\{ \begin{matrix} \sum_j (-1)^j \phi(j,m,k) & \text{for } m \text{ even} \\ \\ \sum_j j(-1)^j \phi(j,m,k) & \text{for } m \text{ odd} \end{matrix} \right\} = 0.$$

We can express the axis conditions on **u** in a similar way. We use the tau method to impose an axis condition by replacing the equation corresponding to the $j=2J-2$ or $2J-1$ Chebyshev component (depending on whether j is required to be even or odd), since we have already dropped the $2J$ or $2J+1$ equation in favor of the boundary condition at $r=R$. We define tau sets $T_r^{\pm} = T_r^{\pm mp}$ for u_+ and u_-, enlarged by the inclusion of the axis conditions:

$$T_r^{\pm} \equiv \{(j,m,k): j \geq 2J \text{ if } m \pm 1 < 2, j \geq 2J-2 \text{ if } m \pm 1 \geq 2,$$
$$j+m \text{ odd}, k \leq K-2, k+p \text{ even}\}.$$

For $m \geq 1$, the tau terms τ_+ and τ_- will belong to $\mathcal{T}_r^+$ and $\mathcal{T}_r^-$, leading to

$$\mathcal{T}_* = \mathcal{T}_r^+ \oplus \mathcal{T}_r^- \oplus \mathcal{T}_z. \tag{5.6}$$

The definition implied by (5.6) for the projection operator $\mathbf{Q}_*$ onto $\mathcal{T}_*$ shows that $\mathbf{Q}_*\mathbf{E}$, and thus $\mathbf{W}^+$, acts on *all* components of $\mathbf{u}$ (although u_θ is tangent to all boundaries). Therefore the particular solution requires the full velocity $\mathbf{u}$.

How do the axis conditions affect the boundary conditions on ϕ? Replacing Eq. (3.8d), we now have the two equations,

$$B\nabla \cdot \mathbf{u} = 0 \tag{5.7a}$$

$$A\phi = 0. \tag{5.7b}$$

Equation (5.7b) does not involve any coupling of ϕ or of different $\mathbf{u}$ components; it can be imposed as it stands. Equation (5.7a) is replaced, as before, by

$$B\phi = b.$$

There is one component of b for each of the boundary conditions, but not the axis conditions. We say that b is $|B|$-, rather than $|T|$-, dimensional. The total size and composition of the influence matrices for all values of m is given in Table VI.

Use of (5.5) rather than (5.4) leads to a subtle difficulty, which can be traced back to the derivation of Eqs. (3.5) from Eqs. (3.1). When the numerical operator $\mathbf{E}$ projects out singularities, Eqs. (3.3) are no longer sufficient to insure that $\nabla \cdot \mathbf{u} = 0$; we must also impose

$$\begin{aligned}(\nabla \cdot \tilde{\mathbf{u}})(j=1, m, k) &= (3+m)\,\tilde{u}_+(2, m, k) + (3-m)\,\tilde{u}_-(2, m, k) \\ &= 0 \qquad \text{for} \quad m \geq 3 \text{ and odd.}\end{aligned} \tag{5.8}$$

TABLE VI

Size of Influence Matrices for Cylindrical Coordinates

m	$\lvert\mathcal{T}_r^+\rvert$	$\lvert\mathcal{T}_r^-\rvert$	$\lvert\mathcal{T}_z\rvert$	$\lvert B\rvert$	Total
0	$\frac{K-1}{2}$		J	$\frac{K-1}{2}+J+1$	$K+2J$
m	$\lvert\mathcal{T}_r^+\rvert$	$\lvert\mathcal{T}_r^-\rvert$	$\lvert\mathcal{T}_z\rvert$	$\lvert B\rvert$	Total
1, 2	$K-1$	$\frac{K-1}{2}$	J	$\frac{K-1}{2}+J+1$	$2K+2J-1$
≥ 3	$K-1$	$J-1$	J	$\frac{K-1}{2}+J+1$	$5\frac{K-1}{2}+2J+1$

Another point of view is that all of the terms of Eq. (3.1a) must be sufficiently differentiable to allow their divergence to be taken. When ϕ satisfies the conditions of Table V, $\nabla\phi$ poses no problem. But **Eu**, **s**, and τ may have singular divergences. For example, the monomial representation

$$\nabla\cdot\mathbf{s}=\sum\left[((j+1)\,\tilde{s}_r(j,m,k)+im\tilde{s}_\theta(j,m,k))\,r^{j-1}\,e^{im\theta}\,z^k + k\,\tilde{s}_z(j,m,k)\,r^j\,e^{im\theta}z^{k-1}\right]$$

shows that $\nabla\cdot(\mathbf{s}+\tau)$ may have an r^{-1} singularity unless

$$(1+m)(\tilde{s}_+ + \tilde{\tau}_+)(j=0,m,k)+(1-m)(\tilde{s}_- + \tilde{\tau}_-)(j=0,m,k)=0 \qquad \text{for } m \text{ odd.} \tag{5.9}$$

(Although τ contains only high order Chebyshev polynomials, these contain terms in r^0.)

To enforce (5.9), we change the $j=0$ component of $(s+\tau)_+$ (for m odd, $m\geqslant 3$). This alters the $j=0$ component of $(\tilde{s}+\tilde{\tau})_+$ while preserving all other components, and leads to no additional coupling since $\nabla\cdot(\mathbf{s}+\tau)$ is not affected. After solving (3.8), we find that (5.8) is satisfied. Lest changing the $j=0$ component seem like a drastic alteration of the differential equation, note that both (5.8) and (5.9) are themselves axis conditions. Thus if **s** and **u** were analytic vector fields, the conditions would be satisfied automatically. In fact, in the time-dependent iterations of Eqs. (1.1), the $j=0$ terms in $\tilde{s}_+$ may be considered to arise from the insufficient constraints of analyticity on previous iterations of **u**.

6. Properties of the Influence Matrix

6.1. *Null Vectors and Invertibility*

The influence matrix C, as defined in Sections 3 through 5, is singular. We recall from Section 3.3 that C is singular if and only if the full matrix $(H+VW^\dagger)$ is singular [34]. The singularity of $(H+VW^\dagger)$ can be anticipated from the structure of the original problem. (Haldenwang [6] gives a thorough discussion of this.) For example, since ϕ appears only as $\nabla\phi$, it is determined only up to a constant; this shows the existence of a nontrivial null vector for $(H+VW^\dagger)$. Another source of noninvertibility is the operator $B\nabla_n\cdot\mathbf{u}$ appearing in the matrix $(H+VW^\dagger)$ (see Eq. (3.8d)). As defined in Section 3.2, $\nabla_n\cdot$ is the derivative normal to the boundary (of the velocity normal to the boundary). At a *corner*, there is no direction normal to the boundary, a criterion which coincides with the definition introduced in Section 2.2. Therefore $B\nabla_n\cdot\mathbf{u}$ is always zero at a corner: this shows that the range of $(H+VW^\dagger)$ is deficient. The problem (3.8) remains soluble because the right-hand side of Eq. (3.8d) is also always zero. In the cylindrical geometry, the "corners" lie on the two circles $\hat{T}_{rz}=\{(r,\theta,z): r=R,\ 0\leqslant\theta\leqslant 2\pi,\ z=\pm 1\}$.

We shall analyze a few of the null vectors of C in order to provide insight into

the Poisson equation and boundary conditions, as well as to demonstrate the concepts and notation we have introduced. For $m=0$ and $p=s$, there are two null vectors, both with $\boldsymbol{\sigma}=\mathbf{0}$. Recalling that $p=s$ means symmetric in z and that boundary values are given on a mixed physical-spectral grid, the first null vector is

$$b(r=R, n)=\delta(k, 0)$$
$$b(j, z=\pm 1)=\delta(j, 0),$$

which signifies the pressure boundary conditions

$$\hat{\phi}(r=R, z)=\mathscr{C}_0(z)=1$$
$$\hat{\phi}(r, z=1)+\hat{\phi}(r, z=-1)=\mathscr{C}_0(r/R)=1$$
$$\hat{\phi}(r, z=1)-\hat{\phi}(r, z=-1)=0.$$

The solution to the homogeneous problem with these boundary conditions is the zero velocity, constant pressure solution

$$\hat{\mathbf{u}}^h=\mathbf{0}$$
$$\hat{\phi}^h(r, z)=\mathscr{C}_0(r/R)\,\mathscr{C}_0(z)=1.$$

This solution has, of course, neither divergence nor tau error, and therefore definition (3.12) shows that C acting on this $(b, -\boldsymbol{\sigma})$ is zero. A cure for this singularity is to specify the arbitrary value of $\phi(j=0, k=0)$.

The second null vector has the pressure boundary conditions

$$\hat{\phi}(r=R, z)=0$$
$$\hat{\phi}(r, z=1)+\hat{\phi}(r, z=-1)=\mathscr{C}_{2J}(r/R)$$
$$\hat{\phi}(r, z=1)-\hat{\phi}(r, z=-1)=0.$$

These boundary conditions generate the solution

$$\hat{\mathbf{u}}^h=\mathbf{0}$$
$$\hat{\phi}^h(r, z)=\mathscr{C}_{2J}(r/R)\,\mathscr{C}_{K-1}(z).$$

Although here $\nabla\phi^h$ is non-zero, it contains only high-frequency modes, so that $\mathbf{Q}_{\text{lo}}\nabla\phi^h=0$, allowing $\mathbf{u}^h$ to be zero.

For $m=0$, there are also two antisymmetric $(p=a)$ null vectors,

$$\hat{\phi}(r=R, z)=0$$
$$\hat{\phi}(r, z=1)+\hat{\phi}(r, z=-1)=0$$
$$\hat{\phi}(r, z=1)-\hat{\phi}(r, z=-1)=\mathscr{C}_{2J}(r/R)$$
$$\boldsymbol{\sigma}=\mathbf{0}$$

and

$$\hat{\phi}(r=R, z) = K\mathscr{C}_{K-2}(z)$$

$$\hat{\phi}(r, z=1) + \hat{\phi}(r, z=-1) = 0$$

$$\hat{\phi}(r, z=1) - \hat{\phi}(r, z=-1) = 2\mathscr{C}_0(r/R)$$

$$\boldsymbol{\sigma}(j, k) = \mathbf{e}_z\, 4K(K-2)\,\delta(j, 0)\,\delta(k, K-1).$$

The noninvertibility of C does not pose a fundamental problem, since, as stated in Section 3.3, we need only find one solution to Eq. (3.11a), which is possible whenever the original problem (3.11c) has a solution. However, we still need a method of solving (3.11a), which cannot be accomplished by straightforward multiplication of both sides of (3.11a) by C^{-1}.

In their implementations of the influence matrix method for solving scalar elliptic equations in an irregular region, Proskurowski, Widlund, and others [33, 34, 40, 41] used the iterative conjugate gradient method to solve their version of Eq. (3.11a). In addition to being feasible when the influence matrix is large and direct solution impossible, this procedure also yields a solution when the matrix is singular.

Our implementation of the Kleiser–Schumann method for enforcing incompressibility generates influence matrices whose size n is small enough that direct inversion is the most economical method of solving (3.11a). This still leaves unresolved the problem of the noninvertibility of C. This difficulty has previously been circumvented on a case-by-case basis, by identifying the null vectors and then modifying the fluid-dynamical equations or boundary conditions. For example, Le Quéré and Alziary de Roquefort [5] believed that the "corner deficiency" of the range of $(H + VW^{\dagger})$ implied the *mathematical* necessity of additional constraints on the problem. They derived such conditions from the Poisson equation for ϕ, effectively evaluating the unprojected version of Eq. (3.3a) at the corners instead of Eq. (3.3b). This procedure is unnecessary, although in no way incorrect. In our nonaxisymmetric cylindrical case, analysis of the null vectors for all m grows increasingly complex, if not impossible, as axis conditions come into play. Some null vectors still have an obvious meaning but others are complicated combinations of all of the various taus and boundary values.

Armed with the formulation (3.11a)–(3.11c), we know that *any* solution to (3.11a) will suffice. The procedure we have chosen is to form a closely related, but invertible, matrix C' in the following way: because C is singular, a certain number of its eigenvalues are zero. We first diagonalize C (its eigenvectors and eigenvalues are complex) by a similarity transformation, then replace the zero eigenvalues by any nonzero value (we use the value one), and transform back. The resulting invertible matrix C' acts like C except on its null space, on which it acts like the identity. We have verified that use of $(C')^{-1}$ in Eq. (3.13) yields the desired result: a solution to (3.8). Understanding the relationship between our regularization procedure and

the filtering of spurious pressure modes discussed in Bernardi, Maday, and Métivet [42] would be of interest.

6.2. *Eigenvalues and Condition Number*

Since the numerical results we will discuss depend upon the details of our program and parameters, we will briefly describe them here. We have implemented the influence matrix method as part of a computer program for solving the time-dependent Boussinesq equations (the Navier–Stokes equations supplemented by an equation for the temperature). We have run the program on a Cray X-MP/24 to study departures from axisymmetry in convection in a cylindrical container of large aspect ratio $R/2$. The geometry has influenced our choice of algorithm: J, the number of radial points or modes, is assumed large, while M and K, the number of modes in θ and z, are assumed small. All parts of the program have been written to scale linearly with J, the number of radial points—except the unavoidable multiplication by $(C')^{-1}$—and to vectorize over J wherever possible. We have used resolutions of up to $J+1=200$, $2M+2=20$, and $K+1=48$, and we shall shortly list timings obtained. In the Boussinesq equations, the Prandtl number Pr is substituted for ν, while in the Navier–Stokes equations, ν should be considered to represent $1/Re$. We have investigated various Prandtl numbers ranging from 1 to 500, and generally used $\Delta t/2 \approx 10^{-3}$.

We return to the implementation of the regularization procedure of Section 6.1 for forming C'. Finite precision will cause some eigenvalues which should be zero (for analytic reasons like those in Section 6.1) to actually have small nonzero values. When C' is generated automatically, we must therefore apply a threshold for the absolute value of the eigenvalues, below which an eigenvalue is considered to be zero and is replaced by an arbitrary finite value. If the threshold is too large, eigenvectors which are necessary to the proper performance of the method are eliminated, and if the threshold is too small, small eigenvalues are retained which greatly magnify error; in either case, the divergence will be nonzero and large. By numberical experimentation we have found that, in our case, an appropriate threshold is $|\lambda| > 10^{-7}$.

There is no truncation error in this method: $|\nabla \cdot \mathbf{u}|$ is not proportional to Δt, $1/J$, or $1/K$. The only error is due to round-off: the finite precision of numerical matrix inversion and multiplication causes the magnitude of the divergence to be proportional to the magnitude of the right-hand side $|\mathbf{s}|$ (not to $|\nabla \cdot \mathbf{s}|$). On the Cray X-MP/24, with 14 decimal digits of accuracy, we have found that

$$|\nabla \cdot \mathbf{u}| \sim 10^{-10} |\mathbf{s}|.$$

If the tau correction is not included (see Section 3.2), $\mathscr{R}$ will be reduced by about a factor of two. However, for an $\mathbf{s}$ with an arbitrary functional form (as, for example, in debugging a program) $|\nabla \cdot \mathbf{u}|$ may then be very large. The authors who have made this approximation have implicitly relied on the fact that $\mathbf{s}$ is *not* arbitrary. The error made depends on $|Q_{1_0} \nabla \cdot \tau|$, as stated by Haldenwang [6], and should

decrease as the resolution increases. Kleiser and Schumann [1] calculate the error in the (l, m) mode to be proportional to $\max_{k=K-1,K}(k/\varepsilon)\,u(\ell, m, k)$ in their one-directional geometry.

The relevant measure for accuracy of matrix inversion is the condition number, the ratio of the largest eigenvalue $|\lambda|_{\max}$ to the smallest $|\lambda|_{\min}$ (here the smallest eigenvalue *retained*). The eigenvalues depend on m and p (Fourier mode in θ and symmetry in z), on J and K (resolution in r and z), and on $\varepsilon = v\Delta t/2$. We find that $|\lambda|_{\max}$ depends mainly on ε, with $0.6/\varepsilon \lesssim |\lambda|_{\max} \lesssim 1/\varepsilon$. $|\lambda|_{\min}$ is nearly independent of ε, but varies a great deal with m and p, ranging from 10^{-4} to 0.6, with the lowest values for $p = a$. The condition number then varies between $10^4/\varepsilon$ and $1/\varepsilon$, so that in our case, the influence matrix can be reliably inverted (i.e., without suffering severe loss of accuracy) for $\varepsilon > 10^{-4}$. Using $v \geqslant 1$ and $\Delta t/2 \approx 10^{-3}$, the accuracy is quite sufficient. Further analysis shows that the eigenvalues of C fall into two sets. The first set is associated with the boundary values of ϕ and the replacement of Eq. (3.8d) by (3.9d), and these eigenvalues fall between 1 and $1/\varepsilon$. The second set is associated with the tau correction, i.e., with $|\mathscr{T}_*|$ and Eqs. (3.8e)–(3.9e). These eigenvalues do not depend on ε and range from 1 to 10^{-4}. (The condition number of C is improved when the tau correction is not included). The two classes merge as ε increases.

6.3. *Timing*

We now discuss the time required to execute the program on the Cray X-MP/24. Table VII shows the time taken by various steps in the program for different resolutions. Except for the last column, all times are given in units of 6.5×10^{-2} s, which is the time required for the linear step for the smallest resolution (first line) in the table.

The resolution for each case is given in terms of $J+1$, $2M+2$, and $K+1$, the number of gridpoints or modes in each direction (their product is the total number of gridpoints or modes). The next column gives the maximum size n of the influence matrices for the resolution. Recall from Section 5 that the problem decouples: it is most efficient to treat C (and $(C')^{-1}$) not as a single matrix, but as a collection of $2M+2$ decoupled influence matrices C^{mp}. Their sizes n are functions of J and K which depend on m according to Table VI, with the maximum given by $n = 5((K-1)/2) + 2J + 1$. The next column gives the time required for computing C and $(C')^{-1}$. These computations are extremely time-consuming, taking as long as 130 s for the largest resolution shown. However, since this is a preprocessing step, this time becomes negligible as a percentage of the total in a typical run with many thousands of timesteps; $(C')^{-1}$ can also be stored for use in later runs with the same parameters. The time for computing C and $(C')^{-1}$ should scale asymptotically like $JMKn$ and Mn^3, respectively, but the dependence of the timings on the resolution is less than that predicted by the operation count, due to the economy of scale of vectorization.

The next three columns give the time required for multiplications by $(C')^{-1}$ and H^{-1} and for the entire linear step. Multiplication by $(C')^{-1}$ is actually very fast,

TABLE VII

Timings

$J+1$	$2M+2$	$K+1$	max(n)	Multiplication by			Total Linear	Nonlinear	s/mode
				Preprocessing	$(C')^{-1}$	H^{-1}			
50	20	12	124	171.	0.09	0.38	1.00	1.75	5.3×10^{-6}
100	20	24	254	1222.	0.38	1.80	4.40	6.50	5.9×10^{-6}
100	4	24	243	232.	0.07	0.38	0.97	1.66	6.5×10^{-6}
200	4	48	491	2017.	0.28	2.18	5.18	6.24	8.7×10^{-6}

and always requires less than 9% of the total linear step. While the time obeys the predicted quadratic dependence on n (and linear dependence on $2M+2$), it has a small prefactor (for which the optimized Cray assembly language routine for matrix multiplication is partly responsible). We see that the linear step therefore consists primarily of two solves, each of which requires approximately 40% of the time of the total linear step; operating with $\nabla\cdot$ and multiplying by $W^\dagger$ are responsible for most of the remainder. The first solve is, of course, a necessary step for any method, and the second is necessitated by the influence matrix method when the Green's functions cannot be stored.

The next column gives the time required to calculate the nonlinear terms, i.e., the right-hand side **s** of Eq. (3.9a). (These computations include Fourier and Chebyshev transforms and have not been discussed in this article.) The nonlinear portion of the iteration requires between 1.2 and 1.8 of the time required for the linear step. The additional calculations necessitated by the influence matrix method (i.e., one multiplication by each of $(C')^{-1}$, $W^\dagger$, and H^{-1}), while taking 58–62% of the *linear* step time, actually take only 22–26% of the *total* iteration time: while certainly not negligible, they do not dominate the calculation. We also see that, as expected, the time for both the linear and nonlinear steps scale approximately like the number of gridpoints or modes. Finally, the last column gives the linear step time in actual CPU seconds divided by the number of modes. The values, ranging from 5×10^{-6} to 9×10^{-6} s per mode, are typical for a program of this kind.

7. Conclusion

We have developed a formalism for describing the influence matrix method in a general (but regular) geometry. The Sherman–Morrison–Woodbury [28–32] formula offers an elegant notation for generalizing the one-directional treatment of Kleiser and Schumann [1]. This formalism has permitted us to apply the method to cylindrical coordinates, complicated by boundaries in two directions and by the coordinate singularity at the axis. It also provides a framework for discussing questions that remain open, such as the compatibility of different pressure boundary conditions and initial conditions [6, 22], the necessity for the tau correction [1, 35, 39], and the filtering of spurious pressure modes [6, 42].

A very crucial question that remains is that of applicability to geometries with three nonperiodic dimensions. One promising approach is a hybrid method, using conjugate gradient or other iteration procedures [6, 7, 43]. We hope that descriptions of other methods of enforcing boundary conditions and incompressibility can be facilitated by the concepts introduced in this article.

Our timings using a realistic resolution confirm the feasibility of the influence matrix method for calculating tri-directional flows in a geometry with two nonperiodic directions. The results pertaining to Rayleigh–Bénard convection which we have obtained with our program will be described in future publications.

APPENDIX: GLOSSARY

A	axis operator
a	antisymmetric parity
b	vector of imposed boundary values (in mixed physical-spectral space)
ℓ	extended vector $\ell \equiv (b, -\sigma)^\dagger$ of length n
B, $\mathbf{B}$	boundary operator for scalar or vector-valued functions
$\mathscr{C}_j$	jth Chebyshev polynomial
C	influence, or capacitance, matrix
C'	"regularized" (invertible) influence matrix
d	"directionality": velocity field $\mathbf{u}$ values in $\Re^d$; d can equal 1, 2, or 3; used to avoid confusion with dimensionality of vectors or vector spaces; bold face used to denote multi-directional functions, operators, and vector spaces
$\delta(k, k')$	Kronecker delta function
Δt	size of time step
ε	$\nu\Delta t/2$
E, $\mathbf{E}$	scalar and vector elliptic operators $I-\varepsilon\nabla^2$ and $\mathbf{I}-\varepsilon\mathbf{V}^2$
$E^{\ell m}$, $E^{\ell mp}$, $E^{pp'}$, etc.	decoupled operator E acting on (ℓ, m), (ℓ, m, p), or (p, p') modes
$\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$, $\mathbf{e}_r$, $\mathbf{e}_\theta$	unit vectors for Cartesian and cylindrical geometries
$\mathbf{e}_+$, $\mathbf{e}_-$	unit vectors in cylindrical geometry which diagonalize the vector Laplacian: $\mathbf{e}_+ = \frac{1}{2}(\mathbf{e}_r - i\mathbf{e}_\theta)$, $\mathbf{e}_- = \frac{1}{2}(\mathbf{e}_r + i\mathbf{e}_\theta)$
f, g	functions on spectral grid
$\hat{f}, \hat{g}$	functions on physical grid
G	spectral grid: set of Chebyshev coefficients
$\hat{G}$	physical grid: grid of Chebyshev points on the domain
$\mathscr{G}, \hat{\mathscr{G}}$	vector space of real-valued functions on G, and on $\hat{G}$
$\|G\|$	cardinality (size) of G and of $\hat{G}$, also equal to the dimensionality of $\mathscr{G}$ and of $\hat{\mathscr{G}}$
$\mathscr{G}$	vector space of vector-valued functions on G; $\mathscr{G} \equiv \oplus_{i=1}^{d} \mathscr{G}$
g^{jk}	basis vector for $\mathscr{G}$ (rectangular case), defined by $g^{jk}(j', k') \equiv \delta(j, j')\,\delta(k, k')$
h	superscript used for homogeneous solution
H	soluble (decoupled) fluid-mechanical problem or matrix
i	(1) time step, (2) $\sqrt{-1}$
j, J	index of x-mode in rectangular geometry, or of r mode in cylindrical geometry, and highest such mode
k, K	index of y-mode in rectangular geometry, or of z-mode in channel or cylindrical geometry, and highest such mode
ℓ, L	periodic index of x-mode in channel geometry, and highest such mode
m, M	periodic index of y-mode in channel geometry, or of θ-mode in cylindrical geometry, and highest such mode
n	dimensionality of influence matrix C
$\mathcal{N}$	dimensionality of full fluid-mechanical problem, e.g., of matrix H
p	(1) pressure head, (2) superscript for particular solution, (3) parity (symmetric, s, or antisymmetric, a)
ϕ	pressure head multiplied by time interval: $\phi \equiv p\Delta t$
$\phi^{\ell m}$, $\phi^{\ell mp}$, $\phi^{pp'}$, etc.	decoupled (ℓ, m), (ℓ, m, p), or (p, p') modes of ϕ
Q_{bdy}, Q_{int}	projection operators onto boundary, or interior of physical grid
Q_{lo}, $\mathbf{Q}_{\text{lo}}$	projection operator onto low-frequency modes of spectral grid, for scalar or vector-valued functions
Q_{hi}, $\mathbf{Q}_{\text{hi}}$	projection operator onto high-frequency (tau) modes, for scalar or vector-valued functions
$\mathbf{Q}_*$, $\mathbf{Q}$	projection operator onto those high-frequency modes whose divergence contains low-frequency modes

r, R	radial coordinate, and radius of cylindrical container
$\mathbf{s}$	right-hand side (explicit part) in semi-implicit scheme for solving Stokes or Navier–Stokes equations
$\mathscr{s}$	extended vector $\mathscr{s} \equiv (\mathbf{s}, \mathbf{0}, \nabla \cdot \mathbf{s}, 0, \mathbf{0})^\dagger$ of length $\mathscr{N}$
s	symmetric parity
$\boldsymbol{\sigma}$	vector of imposed tau values
θ	angular coordinate in cylindrical geometry
T	tau set: in the tau method, set of indices of high-frequency components of differential equation discarded in favor of boundary conditions. Superscripts, if any, refer to functions (ϕ, u_r, etc.) and to symmetry (ℓ, m, p, etc.). Subscripts refer to parts of the domain.
$\hat{T}$	boundary set, e.g., perimeter of rectangular grid: in the collocation method, differential equation evaluated on these points are discarded in favor of boundary conditions
$\mathscr{T}, \hat{\mathscr{T}}$	vector space of real-valued functions on T, and on $\hat{T}$
$\lvert T \rvert$	cardinality (size) of T (and of $\hat{T}$), also equal to the dimensionality of $\mathscr{T}$ (and of $\hat{\mathscr{T}}$)
$\boldsymbol{\mathscr{T}}$	vector space of vector-valued functions on T; $\boldsymbol{\mathscr{T}} \equiv \oplus_{i=1}^{d} \mathscr{T}$
$\mathscr{T}_*$	orthogonal complement in $\mathscr{T}$ of null space of $Q_{1_0} \nabla \cdot$
$\lvert \mathscr{T}_* \rvert$	dimensionality of $\mathscr{T}_*$
$\tau, \hat{\tau}, \boldsymbol{\tau}$	elements of $\mathscr{T}$, $\hat{\mathscr{T}}$, and $\boldsymbol{\mathscr{T}}$
$\tau_x, \tau_y, \tau_z, \tau_r, \tau_\theta$	components of $\boldsymbol{\tau}$ in Cartesian and cylindrical coordinates
τ_+, τ_-	components of $\boldsymbol{\tau}$ in cylindrical geometry in $\mathbf{e}_+, \mathbf{e}_-$ basis
$\boldsymbol{\tau}_*$	element of $\boldsymbol{\mathscr{T}}_*$; $\boldsymbol{\tau}_* \equiv \mathbf{Q}_* \boldsymbol{\tau}$
$\hat{T}_x, \hat{T}_y, \hat{T}_z, \hat{T}_r$	x-, y-, z-, and r- boundaries: points which are on the boundary by virtue of their x, y, z, or r coordinates only
T_x, T_y, T_z, T_r	x-, y-, z-, and r- tau sets: points which are in the tau set by virtue of their x, y, z, or r coefficients only
$\mathscr{T}_x, \mathscr{T}_y, \mathscr{T}_z, \mathscr{T}_r$	vector spaces of real-valued functions on T_x, T_y, T_z, and T_r, respectively
$\hat{T}_{xy}, \hat{T}_{rz}$	set of corners in physical grid, for rectangular and cylindrical geometry
T_{xy}, T_{rz}	set of "corners" in spectral grid, for rectangular and cylindrical geometry: points *both* of whose coordinates are high-frequency (tau) components
$\mathbf{u}$	velocity field on spectral (Chebyshev polynomial) grid
$u_x, u_y, u_z, u_r, u_\theta$	velocity components in Cartesian and cylindrical geometries
u_+, u_-	velocity components in cylindrical geometry which diagonalize the vector Laplacian: $u_+ = u_r + iu_\theta$, $u_- = u_r - iu_\theta$
$\hat{\mathbf{u}}$	velocity field on physical grid
$\tilde{\mathbf{u}}$	velocity field on spectral (monomial) grid
$\bar{\mathbf{u}}$	projection of velocity operated on by $\mathbf{W}^\dagger$
$\mathscr{u}$	extended vector $\mathscr{u} = (\mathbf{u}, \phi, \boldsymbol{\tau}_*)^\dagger$ of length $\mathscr{N}$
U	operator relating physical and spectral representation
ν	viscosity
V	matrix in Sherman-Morrison-Woodbury formula. In the influence matrix method, V inserts values of $(b, -\boldsymbol{\sigma})$ into a homogeneous right-hand-side.
$W^\dagger$	matrix in Sherman-Morrison-Woodbury formula. In the influence matrix method, $W^\dagger$ acts on $(\mathbf{u}, \phi, \boldsymbol{\tau}_*)$.
x, y	coordinates in Cartesian geometry
X, Y	half-length and half-width of rectangle
(x_j, y_k)	points in physical grid in rectangular geometry
z	coordinate in Cartesian or cylindrical geometry

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