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Simulation of Taylor–Couette flow. Part 1. Numerical methods and comparison with experiment

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We present a numerical method that allows us to solve the Navier–Stokes equation with boundary conditions for the viscous flow between two concentrically rotating cylinders as an initial-value problem. We use a pseudospectral code in which all of the time-splitting errors are removed by using a set of Green functions (capacitance matrix) that allows us to satisfy the inviscid boundary conditions exactly. For this geometry we find that a small time-splitting error can produce large errors in the computed velocity field. We test the code by comparing our numerically determined growth rates and wave speeds with linear theory and by comparing our computed torques with experimentally measured values and with the values that appear in other published numerical simulations. We find good agreement in all of our tests of the numerical calculation of wavy vortex flows. A test that is more sensitive than the comparison of torques is the comparison of the numerically computed wave speed with the experimentally observed wave speed. The agreements between the simulated and measured wave speeds are within the experimental uncertainties; the best-measured speeds have fractional uncertainties of less than 0.2%.

1. Introduction

We have developed a numerical method for calculating the equilibrium states and the transitions of a viscous flow between two differentially rotating concentric cylinders (Taylor–Couette flow). In this paper we shall generally limit our study to the case where the outer cylinder is not rotating, so that the fluid is driven solely by the angular velocity Ω_{in} of the inner cylinder. By further limiting ourselves to the case of a very large aspect ratio Γ (i.e. the height in the axial, or z, direction of the cylinder is much greater than the radial gap between the two cylinders), we can assume that the motion is periodic in z with fundamental wavenumber α. Taylor (1923) showed that equations of motion of this axially periodic system depend on three dimensionless numbers: the radius ratio $\eta = a/b$ (where $a \equiv$ inner-cylinder radius, $b \equiv$ outer-cylinder radius), the dimensionless axial wavelength $\lambda = 2\pi/\alpha d$ (where $d = b-a$) and the Reynolds number $R \equiv a\Omega_{\text{in}} d/\nu$ (where ν is the kinematic viscosity). Throughout this paper, unless otherwise specified, we use d as the unit of length, $a\Omega_{\text{in}}$ as the unit of velocity and ρd^3 as the unit of mass, where ρ is the fluid density.

Description of the numerical problem

We remind the reader that there are several qualitatively different, stable equilibria of the Navier–Stokes equation when the inner cylinder is rotating and the outer

cylinder is held stationary. For a good description of some of these equilibria see the review article by DiPrima & Swinney (1981). There is only one closed-form analytic solution for a Taylor–Couette flow, and that is the circular Couette flow $\tilde{v}$:

$$\tilde{v}_\phi = \frac{\eta}{1-\eta^2}\left[\frac{1}{r}\left(\frac{\eta}{1-\eta}\right) - r(1-\eta)\right], \tag{1.1}$$

$$\tilde{v}_r = \tilde{v}_z = 0. \tag{1.2}$$

Circular Couette flow is stable only for low Reynolds numbers. Another well-known solution to the Navier–Stokes equation is axisymmetric Taylor-vortex flow. Two of the best documented non-axisymmetric stable equilibrium solutions that have been studied experimentally are (1) wavy-vortex flow, which has one non-axisymmetric travelling wave with fundamental azimuthal wavenumber m_1 and azimuthal speed s_1 (for the earliest systematic study of wavy vortices cf. Coles 1965) and (2) modulated wavy-vortex flow, which has two non-axisymmetric travelling waves. The waves both travel in the ϕ-direction. The fundamental wavenumbers of the travelling waves are m_1 and m_2, and their angular velocities are s_1 and s_2. A quantitative description of the two-travelling-wave flow appears in Gorman & Swinney (1982).

The earliest analytic studies of Taylor–Couette flow (for a review see Chandrasekhar 1961) were primarily concerned with the determination of the critical Reynolds number R_c where circular Couette flow becomes unstable to axisymmetric Taylor vortices. Finite-amplitude calculations of the torque exerted by the Taylor-vortex flow on the stationary outer cylinder were pioneered by Stuart (1958) and improved upon by Davey (1962). DiPrima (1967) re-examined the flow with an Eckhaus expansion. These expansions are, of course, valid only for $(R-R_c)/R_c \ll 1$. Davey, DiPrima & Stuart (1968) extended the finite-amplitude study to three-dimensional non-axisymmetric flows and determined the critical Reynolds number for the onset of wavy vortices and their torques. Their calculation was verified and extended by Eagles (1971), who used a fifth-order expansion. In a subsequent paper, Eagles (1974) computed the torques of the non-axisymmetric one-travelling-wave flows and compared them with the experimentally measured values. The comparison is only qualitative because the experiments were made without any flow visualization. (The outer cylinder of the Couette apparatus was opaque.) Therefore the exact states of the flow (i.e. the values of λ and m_1) in the experiment are unknown and must be assumed.

One of the earliest axisymmetric numerical simulations of Taylor-vortex flow was carried out by Meyer (1966), who later (1969*a*, *b*) extended the calculations to three dimensions for Reynolds numbers just greater than the critical value for the onset of wavy vortices. More recently, Meyer-Spasche & Keller (1980) simulated axisymmetric Taylor vortices numerically using a continuation method that forces the solution to relax to a steady state. Jones (1981) also computed the Taylor-vortex flow, and used his solutions to determine the linearized eigenfunctions corresponding to the non-axisymmetric waves. In a series of papers Yahata (1983 and references cited therein) used a truncated modal expansion of the Navier–Stokes equations to represent Taylor–Couette flow. His truncations are very severe (at most four modes in the axial direction). Yahata's model equations exhibit a frequency locking that is not observed in the laboratory experiments. The fact that the modal and laboratory results do not agree qualitatively is not surprising since Marcus (1981) and Loncaric (1981) showed that erroneous temporal behaviour can occur whenever truncations are so severe that they disallow effective viscous dissipation at the small scales. In

addition to having a small number of modes, Yahata's choice of modes (e.g. Chandrasekhar–Reid functions) is not well-suited for numerical approximation. The poor convergence properties of these modes are well-documented (Gottlieb & Orszag 1977). Recently, an extremely well-resolved numerical study of three-dimensional wavy-vortex flow with a set of modes that exhibit exponential (spectral) convergence was carried out by Moser, Moin & Leonard (1983).

Purpose of paper

The purpose of this paper is first to present a numerical initial-value method that will allow us to compute non-axisymmetric time-dependent Taylor–Couette flows. The method is sufficiently robust, fast and memory-efficient to allow us to calculate solutions for Reynolds numbers as large as ~ 1500. Typical runs for $R \approx 1000$ require (for physical, not numerical, reasons) on the order of 15 rotation periods of the inner cylinder for the fluid to come to equilibrium. Computing the flow for 15 rotation periods requires approximately 2400 timesteps with approximately 10^6 operations per timestep or roughly 20 min on a CRAY-1. The storage requirement to resolve a typical flow fully at $R \approx 1000$ is approximately 700000 words.

The second purpose of this paper is to show that the computer can serve as a useful tool in understanding and predicting the results of Taylor–Couette flow. Despite the fact that this classical flow was first observed almost 100 years ago (Mallock 1888) and that the conditions for linear stability with respect to axisymmetric disturbances were found over 50 years ago (Taylor 1923), much less progress has been made in understanding the physical mechanisms that produce non-axisymmetric disturbances. Several mechanisms have been proposed (cf. Coles 1965; Meyer 1966; Davey *et al.* 1968), but no single scenario explains why the waves form easily in narrow-gap geometries but are inhibited in wide gaps, why the waves are themselves unstable to modulations, and why the waves disappear at very large Reynolds numbers while the Taylor cells persist. In this paper we demonstrate that we can quantitatively simulate Taylor–Couette flow. The simulations not only agree with past experiments, but also have predicted experimental results (King *et al.* 1984). Although experimentalists find it easier and cheaper than numericists to measure torques and wave speeds for several different values of the parameters η, Γ, R, λ and m, *for any particular flow* numericists can determine the entire velocity field *everywhere*. Numericists can also compute the torque, wave speed, enstrophy, angular momentum and energy spectrum of a flow. Experimentalists can generally only measure the velocity at a few points, and cannot obtain a global picture of the flow. Therefore numerical simulation is a useful way of examining Taylor–Couette flow and is complementary to laboratory measurements.

In Part 2 (Marcus 1984) we use the numerical code described in this paper to produce a family of simulations. From these we propose a scenario for the physical instability that drives the wavy vortices, and marginal-stability/mixing-length theory. Our scenario predicts the speed of the travelling waves at onset and at high Reynolds number in the narrow-gap limit. We also show that the observed spatial symmetries and computed energy spectra are consistent with our scenario.

In §2 of this paper we outline the fundamental numerical methods that we use in a pseudospectral initial-value calculation. We emphasize the fact that a small time-splitting error can cause a large error in the travelling-wave speeds s_1 and s_2. The splitting error is removed by the use of Green functions. In §3 we present evidence of the code's accuracy by comparing our results to analytic calculations and independently obtained numerical results. We also show that the Navier–Stokes

equation is solved in a self-consistent manner. In §4 we test the validity of our numerical simulations by direct comparison with the experimentally measured stability boundaries, torques and wave speeds. Our discussion appears in §5.

2. Numerical methods

General equations

The fluid velocity $\boldsymbol{v}'(c, r, \phi, z, t)$, as measured by an observer in a frame rotating with angular velocity c about the z-axis of the cylindrical Couette apparatus is related to the velocity $\boldsymbol{v}'(r, \phi, z, t)$ as viewed by an inertial observer by

$$\boldsymbol{v}'(c, r, \phi, z, t) = \boldsymbol{v}'(r, \phi + ct, z, t) - cr\hat{\boldsymbol{e}}_\phi. \tag{2.1}$$

The computational variable that we use in all of our numerical calculations is

$$\boldsymbol{v}(c, r, \phi, z, t) \equiv \boldsymbol{v}'(c, r, \phi, z, t) + cr\hat{\boldsymbol{e}}_\phi - \tilde{\boldsymbol{v}}(r) \tag{2.2}$$

$$= \boldsymbol{v}'(r, \phi + ct, z, t) - \tilde{\boldsymbol{v}}(r), \tag{2.3}$$

where $\tilde{\boldsymbol{v}}(r)$ is the primary Couette-flow velocity (1.1), (1.2). The advantage of $\boldsymbol{v}$ as the computational variable is that, unlike $\boldsymbol{v}'$, $\boldsymbol{v}$ obeys homogeneous radial boundary conditions

$$\boldsymbol{v}(c, r = a, \phi, z, t) = \boldsymbol{v}(c, r = b, \phi, z, t) = 0. \tag{2.4}$$

In dimensionless units, $a = \eta/(1-\eta)$ and $b = 1/(1-\eta)$. The advantage of using the velocity calculated in a rotating frame over the velocity in the inertial frame is that, with the proper choice of c, the one-travelling-wave flows are steady-state and the two-travelling-wave flows are periodic in time. Our code has been designed to search for the proper rotating frame and then to shift automatically into that frame.

As seen in a frame rotating with speed c, the Navier–Stokes equation written in terms of $\boldsymbol{v}(c, r, \phi, z, t)$ is

$$\frac{\partial \boldsymbol{v}}{\partial t} = (\boldsymbol{v} + \tilde{\boldsymbol{v}} - cr\hat{\boldsymbol{e}}_\phi) \times (\boldsymbol{\omega} + \tilde{\boldsymbol{\omega}}) - \boldsymbol{\nabla} \Pi + R^{-1} \nabla^2 \boldsymbol{v}, \tag{2.5}$$

where $\boldsymbol{\omega}$ is the vorticity in the rotating frame:

$$\boldsymbol{\omega}(c, r, \phi, z, t) = \boldsymbol{\nabla} \times \boldsymbol{v}(c, r, \phi, z, t), \tag{2.6}$$

$$\tilde{\boldsymbol{\omega}}(r) \equiv \boldsymbol{\nabla} \times \tilde{\boldsymbol{v}}(r) = \frac{-2\eta}{1+\eta} \hat{\boldsymbol{e}}_z, \tag{2.7}$$

and Π is the pressure head in the rotating frame. The Navier–Stokes equation is solved subject to the kinematic condition

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} = 0, \tag{2.8}$$

the radial boundary conditions (2.4) and an imposed periodicity in the axial direction of length λ.

Equations (2.4)–(2.8) are solved pseudospectrally, and we adopt the notation that each variable $Q(c, r, \phi, z, t)$ is written as a spectral sum

$$Q(c, r, \phi, z, t) = \mathrm{Re} \left\{ \sum_{n=0}^{N} \sum_{k=-K+1}^{K} \sum_{m=0}^{M} \hat{Q}(c, n, m, k, t)\, T_n(r)\, \mathrm{e}^{\mathrm{i}(2\pi kz/\lambda + m\phi)} \right\}, \tag{2.9}$$

where $\hat{Q}$ is complex and $T_n(x)$ are Chebyshev polynomials. Note that (2.8) requires that $v_r(c, n, m = 0, k = 0, t)$ is always identically equal to zero for all n. All derivatives are evaluated spectrally. The nonlinear cross-product of the velocity and the vorticity is computed by transforming the velocity and vorticity into physical space, multiplying the values at the collocation points, and then inverse-transforming. We do not remove aliasing errors. A discussion of the magnitude of these errors appears at the end of §3. A description of these pseudospectral operations is given by Gottlieb & Orszag (1977). Often, we shall need the quantity Q in a mixed physical–spectral space, and we adopt the notation

$$Q(c, r, m, k, t) \equiv \sum_{n=0}^{N} \hat{Q}(c, n, m, k, t)\, T_n(r). \tag{2.10}$$

A time-splitting method

The velocity can be advanced from timestep N to timestep $N+1$ by using three fractional steps. The first fractional step accounts for the nonlinear terms, and is made second-order accurate in time Δt by using an Adams–Bashforth method. We denote the velocity at the end of this third of the full timestep as $\boldsymbol{v}^{N+\frac{1}{3}}$:

$$\boldsymbol{v}^{N+\frac{1}{3}} = \boldsymbol{v}^N + \Delta t[\tfrac{3}{2}(\boldsymbol{v}^N + \tilde{\boldsymbol{v}} - cr\hat{\boldsymbol{e}}_\phi) \times (\boldsymbol{\omega}^N + \tilde{\boldsymbol{\omega}})] - \Delta t[\tfrac{1}{2}(\boldsymbol{v}^{N-1} + \tilde{\boldsymbol{v}} - cr\hat{\boldsymbol{e}}_\phi) \times (\boldsymbol{\omega}^{N-1} + \tilde{\boldsymbol{\omega}})]. \tag{2.11}$$

The stability of the explicit nonlinear step in (2.11) is governed by a Courant condition. We can modify (2.11) to allow bigger timesteps by observing that, even in a rotating frame, the largest velocity component is the z-independent axisymmetric ($m = 0$, $k = 0$) component of the azimuthal velocity. In Taylor–Couette flow the mean azimuthal velocity is analogous to the mean temperature gradient in thermal convection; it drives the primary instability and has a profile that is modified by order unity owing to the nonlinear interactions. Like the mean temperature gradient, the mean velocity becomes modified so that in the interior of the flow the mean profile is almost neutrally stable. Typically, for Reynolds numbers less than $15R_c$ and $\eta \approx 0.875$, $v_\phi(c, n, m = 0, k = 0, t)$ is $O(1)$; whereas the rest of the velocity, $[\boldsymbol{v}(c, n, \phi, z, t) - v_\phi(c, n, m = 0, k = 0, t)\,\hat{\boldsymbol{e}}_\phi]$, is much smaller, approximately 0.1. We can therefore break the nonlinear term in (2.11) into two pieces: a term that does not depend on $v_\phi(c, n, m = 0, k = 0, t)$ (and/or the vorticity produced by this piece of the mean velocity), which we compute explicitly, and a term that contains $v_\phi(c, n, m = 0, k = 0, t)$, which we treat implicitly to first order in Δt. By using a Richardson extrapolation at the end of all three fractional steps, we can recover second-order accuracy in Δt. The implicit method is practical only when we are computing a final equilibrium state that is very far from the initial condition. Generally, we use (2.11) as it stands and avoid a Richardson extrapolation.

The second fractional step is due to the pressure contribution

$$\boldsymbol{v}^{N+\frac{2}{3}} = \boldsymbol{v}^{N+\frac{1}{3}} - \Delta t\, \boldsymbol{\nabla} \Pi^{N+1}. \tag{2.12}$$

With the time-splitting method, the pressure head Π^{N+1} is computed by requiring that $\boldsymbol{v}^{N+\frac{2}{3}}$ be divergence-free:

$$\Delta t\, \nabla^2 \Pi^{N+1} = \boldsymbol{\nabla} \cdot \boldsymbol{v}^{N+\frac{1}{3}}, \tag{2.13}$$

with the boundary condition

$$\hat{\boldsymbol{e}}_r \cdot \boldsymbol{v}^{N+\frac{2}{3}} = 0 \quad \text{at} \quad r = a \quad \text{and} \quad r = b, \tag{2.14}$$

or equivalently

$$\Delta t \frac{\partial \Pi^{N+1}}{\partial r} = \hat{\boldsymbol{e}}_r \cdot \boldsymbol{v}^{N+\frac{1}{3}} \quad \text{at} \quad r = a \quad \text{and} \quad r = b. \tag{2.15}$$

Equation (2.15) is exact for the pressure head in the inviscid limit $R \to \infty$. We shall show that (2.15) causes a large time-splitting error near the radial boundaries.

The third fractional step, which completes the integration from timestep N to timestep $N+1$, is the viscous step

$$\boldsymbol{v}^{N+1} = \boldsymbol{v}^{N+\frac{2}{3}} + \Delta t \, R^{-1} \nabla^2 \boldsymbol{v}^{N+1}, \tag{2.16}$$

where ∇^2 is inverted subject to the no-slip boundary condition (2.4). We have chosen the backwards Euler method rather than the second-order-accurate Crank–Nicholson method to avoid a numerical neutrally stable oscillation that can occur at large wavenumbers. By using the backwards Euler method, our final accuracy will be reduced from $O(\Delta t^2)$ to $O(\Delta t^2, \Delta t/R)$. We can formally recover second-order accuracy by using a Richardson extrapolation, but we have found experimentally that an extrapolation does not improve our results. Since $R > 100$ for all of our calculations, the $O(\Delta t/R)$ error is always smaller than the $O(\Delta t^2)$ error; a plot of the error in the velocity as a function of Δt reveals that the error is proportional to Δt^2, not Δt.

We note that the most expensive numerical operation in stepping $\boldsymbol{v}$ forward in time is inverting the ∇^2 operator. The inversion must be done four times per timestep: once for evaluating the pressure head (2.13) and once for each component of the velocity in the viscous fractional step (2.16). We use the Haidvogel–Zang (1979) factorization in the inversion (for efficient implementation in cylindrical geometries see Patera & Orszag 1981), which requires $O(4N^2MK)$ multiplications per inversion, where N is the number of radial Chebyshev points, $2K$ is the number of axial modes and M is the number of azimuthal modes. Since ∇^2 is inverted in the pressure fractional step with Neumann boundary conditions and is inverted in the viscous step with Dirichlet boundary conditions, we are required to store two different eigenvector decompositions of ∇^2 for a total of $4N^2M$ words of storage. This is a significant fraction of the total storage requirements of the code, and we show presently that the storage can be reduced.

In solving the Navier–Stokes equation, we could have used the two vector potentials Ψ and Φ as the computational variables rather than the three components of the velocity. The velocity is defined in terms of the vector potentials by

$$\boldsymbol{v} = \nabla \times (\Psi \hat{\boldsymbol{e}}) + \nabla \times \nabla \times (\Phi \hat{\boldsymbol{e}}), \tag{2.17}$$

where $\hat{\boldsymbol{e}}$ is an arbitrary unit vector. In spherical and Cartesian geometries (see e.g. Marcus 1979), use of the two vector potentials requires only three and not four inversions of the ∇^2 operator (one inversion for the pressure and one inversion each for $\nabla^2\Psi$ and $\nabla^2\Phi$ in the viscous fractional step). In these two geometries, use of the vector potential reduces the total computational cost by a factor of approximately $\frac{3}{4}$. In cylindrical coordinates, depending on the choice of $\hat{\boldsymbol{e}}$, either the two equations for the boundary conditions for Ψ and ϕ do not separate (and thereby make the numerics intractable) or the viscous fractional step cannot be put into a form where the Laplacian operators on Φ and Ψ can be implicitly (stably) inverted in a numerically efficient manner. We have therefore opted to use the velocity and not the vector potential as our computational variable throughout the calculations.

Occasionally, we have used a computational shortcut when we have had a poor guess for the initial velocity field and when we were interested only in finding a

steady-state equilibrium (or in finding a new equilibrium state that could serve as a 'good' initial guess for the velocity field). This shortcut uses the fact that the mean angular momentum profile $\bar{L}(r,t) \equiv r v_\phi(c,r,m=0,k=0,t)$, which drives the Taylor-vortex flow, changes to its final equilibrium value near the radial boundary only in a viscous timescale and not in the faster dynamic timescale. In our shortcut, we replace the dynamic equation that governs the growth of $v_\phi(c,r,m=0,k=0,t)$,

$$\frac{\partial v_\phi(c,r,m=0,k=0,t)}{\partial t} = \hat{\boldsymbol{e}}_\phi \cdot [\boldsymbol{v} \times (\boldsymbol{\omega}+\tilde{\boldsymbol{\omega}})]_{m=0,\,k=0} + R^{-1}\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{1}{r^2}\right] v_\phi(c,r,m=0,k=0,t), \quad (2.18)$$

with the kinematic equation

$$v_\phi(c,r,m=0,k=0,t) = -R\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{1}{r^2}\right]^{-1} \hat{\boldsymbol{e}}_\phi \cdot [\boldsymbol{v} \times (\boldsymbol{\omega}+\tilde{\boldsymbol{\omega}})]_{m=0,\,k=0}, \quad (2.19)$$

where $\partial^2/\partial r^2 + (1/r)\,\partial/\partial r - 1/r^2$ is inverted using homogeneous Dirichlet boundary conditions. All of the other dynamic equations for $v(c,r,m,k,t)$ remain unchanged. When the time derivative of $v_\phi(c,r,m=0,t)$ is small, (2.19) is a good approximation to (2.18) (cf. the amplitude expansions of Stuart 1958), and in a steady state it reduces exactly to (2.18). However, even for large time derivatives, we have found that the shortcut equations are stable and converge much faster to a steady-state (and therefore exact) equilibrium than the Navier–Stokes equations. We emphasize that, whenever we have found a steady equilibrium solution by using the shortcut, we have tested its stability by using the equilibrium solution (plus small perturbations) as the initial value of the full Navier–Stokes equations. We have also experimentally determined that any solution produced by the shortcut method is physically realizable; by starting with a physically realizable initial condition (i.e. circular Couette flow or some other observed equilibrium plus perturbations) and integrating it forward in time with the full Navier–Stokes equation, the same solution is obtained. In summary, we have used our shortcut method not to produce 'real' solutions but merely to explore a large area of parameter space for interesting features in a short amount of computational time.

Analysis of the time-splitting error

We have found that the time-splitting error due to solving (2.13) for the pressure-head with the inviscid boundary condition (2.15) can cause large errors in many of the diagnostic tests that we use to test our code's accuracy. In particular, we have found that, as the ratio η of inner- to outer-cylinder radii approaches unity, the travelling-wave speeds predicted by the initial-value solver differ markedly from the speeds predicted by a numerical calculation of the linear eigenvalues. (See §3 for a full discussion.)

Orszag & Deville (1984) studied the numerical errors produced by solving the incompressible Stokes equation with the method of fractional steps in a simplified geometry. Using the globally first-order-accurate backwards Euler method in the viscous fractional step, they found that in the interior of the domain, far from the boundary, the time-splitting causes an error of $O(\Delta t)$ in the velocity and $O(\Delta t^{\frac{1}{2}})$ in the pressure. The time-splitting errors in the interior can be reduced by Richardson extrapolation. A local Richardson extrapolation reduces the time-splitting error in the velocity to $O(\Delta t^{\frac{3}{2}})$ and in the pressure to $O(\Delta t)$. A disadvantage of Richardson

extrapolation is that it nearly doubles the required computer time and storage. Higher-order extrapolations can further reduce the error in the velocity to $O(\Delta t^2)$.

Orszag & Deville found that the method of fractional steps causes much larger errors near the boundary in a layer with thickness of order $(\Delta t/R)^{\frac{1}{2}}$. In the boundary layer the time-stepping errors in the pressure, $\partial v_r/\partial r$, $\partial^2 v_\phi/\partial r^2$, $\partial^2 v_z/\partial r^2$ and $\boldsymbol{\nabla}\cdot\boldsymbol{v}$, are $O(\Delta t^{\frac{1}{2}})$ and the errors in the radial derivative of the pressure and $\partial^2 v_r/\partial r^2$ are $O(1)$. The errors that are in the boundary layer cannot be reduced by Richardson extrapolation.

The Δt-dependence of the time-splitting errors in the radial derivatives of the velocity in Orszag & Deville's model problem is consistent with the results of our numerical experiments in Taylor–Couette flow. Note that the inviscid boundary condition (2.14) used in solving for the pressure head along with (2.4) and (2.16) impose the condition

$$\hat{\boldsymbol{e}}_r\cdot\boldsymbol{\nabla}^2\boldsymbol{v} = 0 \quad \text{at} \quad r = a \quad \text{and} \quad r = b. \tag{2.20}$$

Equation (2.20) is incorrect since the correct boundary condition is

$$\hat{\boldsymbol{e}}_r\cdot\boldsymbol{\nabla}^2\boldsymbol{v} = R\frac{\partial \Pi}{\partial r} - R(\tilde{v}_\phi - cr)\frac{1}{r}\frac{\partial}{\partial r}[r(\tilde{v}_\phi + v_\phi)] \quad \text{at} \quad r = a \quad \text{and} \quad r = b. \tag{2.21}$$

The discrepancy between (2.20) and (2.21) is consistent with Orszag & Deville's time-splitting error $O(1)$ in $\partial^2 v_r/\partial^2 r$ (or $\hat{\boldsymbol{e}}_r\cdot\boldsymbol{\nabla}^2\boldsymbol{v}$) at the radial boundaries. Since the imposed boundary condition in (2.20) is not modified by using a Richardson extrapolation, it is not surprising that an extrapolation does not reduce the time-splitting error at the boundary.

In cylindrical pipe flow (Orszag & Patera 1983) the time-splitting error does not appear to cause inaccuracies; in cylindrical Couette flow it does. The linear momentum and energy that drive the flow in cylindrical pipe flow enter and leave the cylinder primarily at the axial boundaries (not at the radial boundaries), and the rates of energy and momentum transfer between the cylinder and the outside world are independent of viscosity. In cylindrical Couette flow the energy and angular momentum that drive the flow enter only at the radial boundaries. Furthermore, the rates at which angular momentum and energy leave or enter the cylinder are proportional to the viscosity (or R^{-1}) and are also proportional to the derivative of the velocity at the radial boundaries. It is therefore not surprising that time-splitting errors that are $O(1)$ in $\partial^2\boldsymbol{v}/\partial r^2$ and $O(\Delta t^{\frac{1}{2}})$ in $\partial\boldsymbol{v}/\partial r$ at the radial boundaries cause large errors in cylindrical Couette flow. In particular our numerical experiments show that Richardson extrapolation (which reduces the error at the interior but not at the radial boundaries) does not reduce the error in the speed s_1 of the travelling wave. Our experiments indicate that s_1 depends strongly on the physics at the radial boundaries, and as $n \to 1$ the error in s_1 becomes very large.

Reducing the time-splitting error

The most straightforward way of removing the time-splitting error is to solve for the pressure head with the correct boundary condition. In inverting (2.13), the correct boundary condition is

$$\hat{\boldsymbol{e}}_r\cdot\boldsymbol{v}^{N+1} = 0 \tag{2.22}$$

or

$$\Delta t\frac{\partial \Pi^{N+1}}{\partial r} = \hat{\boldsymbol{e}}_r\cdot(\boldsymbol{v}^{N+\frac{1}{3}} + R^{-1}\boldsymbol{\nabla}^2\boldsymbol{v}^{N+1}). \tag{2.23}$$

Equation (2.23) cannot be solved directly since $\boldsymbol{v}^{N+1}$ is still an unknown quantity during the pressure fractional step. We can, however, approximate (2.23) by

$$\Delta t \frac{\partial \Pi^{N+1}}{\partial r} = \hat{\boldsymbol{e}}_r \cdot (\boldsymbol{v}^{N+\frac{1}{3}} + R^{-1} \nabla^2 \boldsymbol{v}^N). \tag{2.24}$$

This approximation reduces the splitting error in $\partial^2 \boldsymbol{v}/\partial r^2$ by a factor of Δt. Results obtained using (2.24) in our initial-value code for short times have given excellent agreement (one part in 10^6) with the wave speeds and growth rates produced by our linear eigenvalue code (which does not use fractional steps). Unfortunately, (2.24) makes the initial-value code algebraically unstable, and after several revolutions of the inner cylinder the numerical results are meaningless.

A method with no time-splitting error

We have removed the time-splitting error entirely by using a new Green-function or capacitance-matrix method. We solve for the pressure head Π^{N+1} by using (2.13) with the correct viscous boundary condition (2.22). We define

$$\Pi^{N+1} \equiv \overline{\Pi}^{N+1} + \Pi_{\mathrm{c}}^{N+1} \tag{2.25}$$

and

$$\boldsymbol{v}^{N+\frac{2}{3}} \equiv \bar{\boldsymbol{v}}^{N+\frac{2}{3}} + \boldsymbol{v}_{\mathrm{c}}^{N+\frac{2}{3}}, \tag{2.26}$$

where $\overline{\Pi}^{N+1}$ is defined to be the partial pressure head

$$\Delta t \nabla^2 \overline{\Pi}^{N+1} \equiv \nabla \cdot \boldsymbol{v}^{N+\frac{1}{3}} \tag{2.27}$$

determined by the (arbitrary) Dirichlet boundary condition

$$\overline{\Pi}^{N+1} = 0 \quad \text{at} \quad r = a \quad \text{and} \quad r = b, \tag{2.28}$$

and where

$$\bar{\boldsymbol{v}}^{N+\frac{2}{3}} \equiv \boldsymbol{v}^{N+\frac{1}{3}} - \Delta t \nabla \overline{\Pi}^{N+1}, \tag{2.29}$$

$$\boldsymbol{v}_{\mathrm{c}}^{N+\frac{2}{3}} = -\Delta t \nabla \Pi_{\mathrm{c}}^{N+1}. \tag{2.30}$$

(We could have chosen to define $\overline{\Pi}^{N+1}$ and the correction Π_{c}^{N+1} by imposing the Neumann boundary condition (2.15) instead of (2.28). The Neumann boundary condition gives a correction that is smaller than the Dirichlet condition, but both methods give the same final answer for $\boldsymbol{v}^{N+1}$. We show at the end of this section that the Dirichlet method is much more memory-efficient than the Neumann method.) The correction Π_{c}^{N+1} that must be added to the partial pressure head obeys the homogeneous equation

$$\nabla^2 \Pi_{\mathrm{c}}^{N+1} = 0, \tag{2.31}$$

with the inhomogeneous boundary condition (from (2.21))

$$\Delta t \frac{\partial \Pi_{\mathrm{c}}^{N+1}}{\partial r} = \boldsymbol{e}_r \cdot [\boldsymbol{v}^{N+\frac{1}{3}} + R^{-1} \nabla^2 \boldsymbol{v}^{N+1}] - \Delta t \frac{\partial \overline{\Pi}^{N+1}}{\partial r} \quad \text{at} \quad r = a \quad \text{and} \quad r = b. \tag{2.32}$$

The equations (2.27) and (2.28) for the partial pressure head can be solved immediately since $\boldsymbol{v}^{N+\frac{1}{3}}$ is known; the equations for Π_{c}^{N+1} cannot yet be solved because $\boldsymbol{v}^{N+1}$ is still unknown. The viscous fractional timestep (2.16) becomes

$$\boldsymbol{v}^{N+1} = \bar{\boldsymbol{v}}^{N+1} + [1 - \Delta t R^{-1} \nabla^2]^{-1} \boldsymbol{v}_{\mathrm{c}}^{N+\frac{2}{3}}, \tag{2.33}$$

where $\bar{\boldsymbol{v}}^{N+1}$ is defined by

$$\bar{\boldsymbol{v}}^{N+1} \equiv [1 - \Delta t R^{-1} \nabla^2]^{-1} \bar{\boldsymbol{v}}^{N+\frac{2}{3}}, \tag{2.34}$$

and where $1-R^{-1}\Delta t\nabla^2$ is inverted subject to the boundary condition

$$\bar{v}^{N+1}=0 \quad \text{at} \quad r=a \quad \text{and} \quad r=b. \tag{2.35}$$

The equations for $\bar{v}^{N+1}$ can be solved immediately. Knowing $\bar{v}^{N+1}$, we could in principle solve (2.31) and (2.32) directly for Π_c. However, the numerical solution of (2.31) is numerically expensive – it involves solving Poisson's equation. We now show how we solve directly for v^{N+1} without any additional Poisson solves.

It can be shown that the boundary conditions (2.32) for the pressure correction Π_c are satisfied if and only if

$$\nabla\cdot v^{N+1}=0 \quad \text{at} \quad r=a \quad \text{and} \quad r=b, \tag{2.36}$$

or, using (2.30) and (2.33),

$$\Delta t\,\nabla\cdot[1-\Delta t R^{-1}\nabla^2]^{-1}\nabla\Pi_c^{N+1}=\nabla\cdot\bar{v}^{N+1} \quad \text{at} \quad r=a \quad \text{and} \quad r=b. \tag{2.37}$$

Expressing Π_c^{N+1} as a spectral sum of Fourier modes m and k in the azimuthal and axial directions, we see that $\Pi_c^{N+1}(r,m,k)$ can be written at each timestep as a linear combination of $\chi_1(r,m,k)$ and $\chi_2(r,m,k)$:

$$\Pi_c^{N+1}(r,m,k)=a_1^{N+1}(m,k)\,\chi_1(r,m,k)+a_2^{N+1}(m,k)\,\chi_2(r,m,k), \tag{2.38}$$

where χ_1 and χ_2 are two linearly independent solutions of Laplace's equation (2.31):

$$\nabla^2[\chi_1(r,m,k)\,e^{i(m\phi+2\pi kz/\lambda)}]=\nabla^2[\chi_2(r,m,k)\,e^{i(m\phi+2\pi kz/\lambda)}]=0, \tag{2.39}$$

and at the boundaries

$$\chi_1=1, \quad \chi_2=0 \quad \text{at} \quad r=a, \tag{2.40}$$

$$\chi_1=0, \quad \chi_2=1 \quad \text{at} \quad r=b. \tag{2.41}$$

The boundary conditions (2.40) and (2.41) are arbitrary except that they ensure linear independence of χ_1 and χ_2. Dirichlet rather than Neumann conditions are chosen for computational convenience in evaluating χ_1 and χ_2 (see below).

To implement this method efficiently, we evaluate *once* in a preprocessing stage the functions χ_1 and χ_2 for all Fourier modes. We don't store χ_1 and χ_2; instead we store the two Green functions, $G_1(r,m,k)$ and $G_2(r,m,k)$:

$$G_i(r,m,k)\equiv-\Delta t[1-\Delta t R^{-1}\nabla^2]^{-1}\nabla\chi_i, \tag{2.42}$$

where $i=1,2$ and where $[1-\Delta t R^{-1}\nabla^2]^{-1}$ is inverted with homogeneous Dirichlet boundary conditions. The Green functions depend only on the cylindrical geometry η and not on the fluid velocity. We also calculate and store the four constants $b_{11}(m,k)$, $b_{12}(m,k)$, $b_{21}(m,k)$ and $b_{22}(m,k)$:

$$b_{1i}(m,k)\equiv\Delta t\,\nabla\cdot\{[1-R^{-1}\Delta t\nabla^2]^{-1}\nabla\chi_i\}|_{r=a}, \tag{2.43}$$

$$b_{2i}(m,k)\equiv\Delta t\,\nabla\cdot\{[1-R^{-1}\Delta t\nabla^2]^{-1}\nabla\chi_i\}|_{r=b}, \tag{2.44}$$

where $i=1,2$. From (2.33) and the definitions of G_i and χ_i we see that the final velocity is

$$v^{N+1}(r,m,k)=\bar{v}^{N+1}(r,m,k)+a_1^{N+1}(m,k)\,G_1(r,m,k)+a_2^{N+1}(m,k)\,G_2(r,m,k). \tag{2.45}$$

G_1 and G_2 are not functions of timestep; therefore at each step we need only evaluate $a_1^{N+1}(m,k)$ and $a_2^{N+1}(m,k)$ for each Fourier mode (i.e. we do not have to solve Poisson's

equation at each timestep to get $\boldsymbol{v}^{N+1}$ from $\bar{\boldsymbol{v}}^{N+1}$). The constants $a_1^N(m,k)$ and $a_2^N(m,k)$ are determined from (2.37) and are seen to obey

$$\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \begin{pmatrix} a_1^{N+1} \\ a_2^{N+1} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\nabla}\cdot\bar{\boldsymbol{v}}^{N+1} & \text{at } r=a \\ \boldsymbol{\nabla}\cdot\bar{\boldsymbol{v}}^{N+1} & \text{at } r=b \end{pmatrix} \tag{2.46}$$

Equation (2.46) is a trivial algebraic equation that is solved for each mode, (m,k). There is no coupling in (2.46) between modes. In practice we need only tabulate and store half of the Green functions, since they always have the symmetries

$$\hat{\boldsymbol{e}}_z\cdot\boldsymbol{G}_i(r,m,k) = \hat{\boldsymbol{e}}_z\cdot\boldsymbol{G}_i(r,-m,k), \tag{2.47}$$

$$\hat{\boldsymbol{e}}_r\cdot\boldsymbol{G}_i(r,m,k) = \hat{\boldsymbol{e}}_r\cdot\boldsymbol{G}_i(r,-m,k), \tag{2.48}$$

$$\hat{\boldsymbol{e}}_\phi\cdot\boldsymbol{G}_i(r,m,k) = -\hat{\boldsymbol{e}}_\phi\cdot\boldsymbol{G}_i(r,-m,k), \tag{2.49}$$

where $i = 1, 2$. Note that $\hat{\boldsymbol{e}}_r\cdot\boldsymbol{G}_i(r,m,k)$ is a real function and that $\hat{\boldsymbol{e}}_\phi\cdot\boldsymbol{G}_i(r,m,k)$ and $\hat{\boldsymbol{e}}_z\cdot\boldsymbol{G}_i(r,m,k)$ are purely imaginary.

We conclude this section by noting that the additional numerical calculations needed to remove the time-splitting error by this Green-function method are negligible. On the other hand, the amount of memory needed to store the Green functions appears to be significant since it is $O(NMK)$. However, with the method of fractional steps outlined previously ((2.11)–(2.16)) it is necessary to invert ∇^2 once with Neumann boundary conditions (for the pressure step) and once with Dirichlet boundary conditions (for the viscous step). The two types of inversions require storing Haidvogel–Zang factorizations of ∇^2 for both types of boundary conditions. By using the Green functions we only invert ∇^2 with Dirichlet boundary conditions and thereby save the $O(2N^2M)$ words of memory needed to store the Haidvogel–Zang factorization with Neumann boundary conditions. (We would not have this saving if we used Neumann boundary conditions in defining $\overline{\Pi}$ (see (2.28)) or in the definition of χ_i (see (2.40) and (2.41)).) Therefore no net increase in storage is needed to use the Green-function method. We note that this Green-function procedure is similar to one that was used by Marcus (1979) for a simulation of thermal convection in spheres. It is also similar to a capacitance-matrix method used by Kleiser & Schumann (1980) for simulation of channel flow. We note, however, that Kleiser & Schumann's method does not use the Haidvogel–Zang factorization for inverting ∇^2, and therefore it is not efficient to store the Green function. Kleiser & Schumann must recalculate their set of Green functions at every timestep, which makes their method twice as time consuming as our method.

3. Tests of the numerical code

Linear eigenvalues

To determine how well our initial-value code for solving the Navier–Stokes equation works, we have written a second, independent, code that computes the linear eigenvalues and eigenfunctions of the general circular Couette flow where the angular velocity Ω_{out} of the outer cylinder is non-zero. The eigenvalue code uses a fourth-order solver and has no time-splitting errors. In table 1 we list for several values of radius ratio, Reynolds number and $\Omega_{\text{in}}/\Omega_{\text{out}}$ the published eigenvalues σ of eigenmodes of the form $\boldsymbol{v} = \boldsymbol{f}(r)\exp(\mathrm{i}m_1\phi + \mathrm{i}\alpha z - \mathrm{i}\sigma t)$ that have been calculated by other authors using a variety of analytic and numerical methods. Also listed in the table are the eigenvalues produced by our fourth-order solver and the eigenvalues (that is, the growth rates for Im (σ) and wave speeds for Re (σ)) produced by our initial-value code

η	R	$\frac{\Omega_{out}}{\Omega_{in}}$	α	m_1	Published eigenvalue		Linear eigenvalue from fourth-order solver		Eigenvalue from initial-value code	
					Imaginary	Real	Imaginary	Real	Imaginary	Real
0.5000	63.134	0.11765	3.100	0	0	0†	1.59×10^{-2}	$< 10^{-20}$	1.57×10^{-2}	0.0
0.5000	66.397	0.16667	3.000	0	0	0†	-1.60×10^{-2}	$< 10^{-20}$	-1.65×10^{-2}	0.0
0.5000	74.924	0	3.161	0	—	—	0.035637	$< 10^{-20}$	0.035636	0.0
0.8770	238.20	0	2.662	1	—	—	0.025330	0.43044	0.025325	0.43040
0.8770	238.20	0	2.662	4	—	—	0.067245	0.28432	0.067241	0.28430
0.8770	1191.0	0	2.662	6	—	—	0.073329	0.50111	0.073225	0.50109
0.9500	184.99	0	3.128	0	0	0‡	4.58×10^{-4}	$< 10^{-20}$	5.16×10^{-4}	0.0
0.9500	490.72	−0.80000	3.561	3	0	0.030783‡	4.00×10^{-4}	0.030781	4.35×10^{-4}	0.030773
0.9500	625.42	−1.00000	3.680	4	0	0.037348‡	7.64×10^{-4}	0.037351	8.30×10^{-4}	0.037348
0.9500	1050.6	−1.5000	4.002	6	0	0.041517‡	6.14×10^{-4}	0.041513	6.26×10^{-4}	0.041516
0.9500	1633.7	−2.0000	4.483	7	0	0.039265‡	-3.97×10^{-4}	0.039269	-4.16×10^{-4}	0.039264

† Chandrasekhar (1961).
‡ Krueger, Gross & DiPrima (1966).

TABLE 1. Comparison of previously published eigenvalues, values from our fourth-order solver, and from the initial-value code

where we have used the eigenmodes (produced by the fourth-order solver) as the initial value for the velocity field.

Note that the published eigenvalues correspond to calculations with the Reynolds number equal to the critical value for the onset of the perturbation. Therefore the imaginary parts of the published eigenvalues are all zero. The comparison between our eigenvalues and the published eigenvalues tests our numerical computation of the critical Reynolds numbers and (for $m \neq 0$) the numerical calculation of the wave speed. From table 1 it is clear that the real part of the eigenvalues computed by Krueger, Gross & DiPrima (1966) and those produced by our fourth-order solver agree to within one part in 10^4. At the Reynolds numbers corresponding to the critical values determined by Krueger *et al.* the imaginary parts of our eigenvalues (growth rates) are negligible. It is also apparent from table 1 that the eigenvalues from the fourth-order solver and those implied by the growth rates and wave speeds from our initial-value code also agree to within one part in 10^4.

Numerical consistency of computed solutions

One useful measure of the accuracy of our code is the calculation of $\nabla \cdot \boldsymbol{v}$ in units of the characteristic Taylor-vortex velocity v_{char} divided by the characteristic length d of the Taylor vortices. This normalized divergence is less than 10^{-6} everywhere in the fluid at all times. (Without using the Green functions to remove the time-splitting errors, this normalized divergence is of order unity at the boundaries for typical timesteps.)

When a solution converges to a steady state, either to the axisymmetric Taylor-vortex flow or to the non-axisymmetric one-travelling-wave state (viewed in the correct rotating frame), we can compute a second test of the solution's accuracy. We define Y by

$$Y \equiv |\nabla \times [-(\boldsymbol{v}' \cdot \nabla)\, \boldsymbol{v}' + R^{-1} \nabla^2 \boldsymbol{v}']|. \tag{3.1}$$

If the flow appears as a steady state to an observer in some rotating frame, then Y will be identically equal to zero in that frame. When Y is measured in units of $(v_{\text{char}}/d)^2$ we find it to be less than 10^{-6} at every point in the fluid for both the axisymmetric Taylor-vortex flows and for the one-travelling-wave states. The fact that we have independently numerically determined that the velocity is divergence-free and that Y is zero (and that the no-slip boundary conditions on the velocity are satisfied) verifies that our initial-value code produces correct steady-state solutions.

Temporal accuracy

The temporal accuracy of our code has been checked in several ways. The code was designed to have temporal errors of $O(R^{-1}\,\Delta t, \Delta t^2)$ (see §2). By varying the timestep Δt at large Reynolds numbers ($R > 100$) we have confirmed experimentally that the errors in the velocity's growth rate and wave speed are proportional to Δt^2. Furthermore, we have computed the one-travelling-wave state in the inertial frame (which is periodic in time) and followed this flow for several revolutions of the inner cylinder. We have compared this time-dependent calculation of the flow with the steady-state calculation of the same flow (computed in the proper rotating frame). We find that after 10 inner-cylinder revolutions the amplitudes of the two calculations agree to one part in 10^6 and the phases agree to one part in 10^5. The timestep used in this comparison was $\Delta t =$ the inner-cylinder rotation period/48.

Two other tests of the temporal accuracy of the code are the measurements of the

energy and angular momentum. The total rate of change of the angular momentum of the fluid is the difference in the torques applied at the inner and outer cylinders. The angular momentum of the fluid per unit length of the cylinder is

$$\mathscr{L} = 2\pi \int_a^b \mathrm{d}r\, v'_\phi(r, m = 0, k = 0, t)\, r^2, \tag{3.2}$$

where the inner radius a and outer radius b are respectively $\eta/(1-\eta)$ and $1/(1-\eta)$ in dimensionless units. The torques (per unit axial length) exerted on the fluid by the inner and the outer cylinders are respectively

$$G_{\mathrm{in}} = -2\pi a^3 R^{-1} \frac{\partial}{\partial r}\left[\frac{v'_\phi(r, m = 0, k = 0, t)}{r}\right]\Bigg|_{r=a} \tag{3.3}$$

and

$$G_{\mathrm{out}} = -2\pi b^3 R^{-1} \frac{\partial}{\partial r}\left[\frac{v'_\phi(r, m = 0, k = 0, t)}{r}\right]\Bigg|_{r=b} \tag{3.4}$$

A good test of the temporal accuracy of the code is to determine the numerical accuracy of the angular-momentum-balance equation

$$\mathscr{L}(t_2) - \mathscr{L}(t_1) = \int_{t_1}^{t_2} \mathrm{d}t\, (G_{\mathrm{in}} - G_{\mathrm{out}}), \tag{3.5}$$

where the flow at time t_1 is in a different state (for example, the axisymmetric Taylor-vortex state) than the flow is in at time t_2 (such as the one-travelling-wave state) and where $t_2 - t_1$ is several inner-cylinder rotation periods. We have found that (3.5) is typically satisfied to 1 part in 10^5 for $t_2 - t_1 = 10$ inner-cylinder rotation periods.

The rate at which energy enters the fluid (per unit length) at the inner cylinder is

$$\dot{E}_{\mathrm{in}} = G_{\mathrm{in}}\, \Omega_{\mathrm{in}}. \tag{3.6}$$

We remind the reader that Ω_{in} in dimensionless units is $(1-\eta)/\eta$. If the outer cylinder is held stationary there is no energy exchange at the outer cylinder. The rate of loss due to viscosity (per unit axial length) of the fluid is

$$\dot{E}_{\mathrm{dis}} = 2R^{-1}(2\pi + \mathscr{E}), \tag{3.7}$$

where $\mathscr{E}$ is the enstrophy per unit axial length:

$$\mathscr{E} = \frac{\frac{1}{2}\int \mathrm{d}r\, r(\nabla \times \boldsymbol{v})^2\, \mathrm{d}\phi\, \mathrm{d}z}{\int \mathrm{d}z}. \tag{3.8}$$

For a steady-state solution $\dot{E}_{\mathrm{dis}}$ should of course be equal to $\dot{E}_{\mathrm{in}}$, but a much more stringent test of the numerical temporal accuracy is to see how well the integrated energy-balance equation is satisfied:

$$E(t_2) - E(t_1) = \int_{t_1}^{t_2} \mathrm{d}t\, (\dot{E}_{\mathrm{in}} - \dot{E}_{\mathrm{dis}}), \tag{3.9}$$

where E is the kinetic energy per unit axial length of the flow. Typically, we find that (3.9) is accurate to one part in 10^4 for $t_2 - t_1 = 10$ inner-cylinder rotation periods. The energy-balance equation is more prone to numerical round-off error than the angular-momentum-balance equation because the angular momentum and torques involve only the large-scale ($m = 0, k = 0$) Fourier mode, whereas the kinetic energy and the viscous dissipation rate $\dot{E}_{\mathrm{dis}}$ depend on all of the Fourier modes.

Since angular momentum is conserved, we can define an angular-momentum flux $\boldsymbol{F}_{\bar{L}}$

$$\frac{\partial \bar{L}}{\partial t} = -\boldsymbol{\nabla}\cdot\boldsymbol{F}_{\bar{L}}, \tag{3.10}$$

where $\bar{L}$ is the angular momentum density (i.e. $\rho r v_\phi(r, m = 0, k = 0, z)$ in dimensional units). The outward radial component of the mean (averaged over ϕ and z) angular-momentum flux per unit axial length in dimensionless units is

$$\bar{F}_{\bar{L}}(r,t) = -R^{-1}r^2\frac{\partial}{\partial r}\left[\frac{v'_\phi(r, m=0, k=0, t)}{r}\right] + \frac{r}{2\pi}\frac{\int \mathrm{d}\phi\,\mathrm{d}z\, v'_r v'_\phi}{\int \mathrm{d}z}. \tag{3.11}$$

At the cylinders' boundaries $2\pi r\bar{F}_{\bar{L}}(r)$ is, of course, equal to G_{in} and G_{out}. If a flow appears as a steady state in any rotating frame, then $2\pi r\bar{F}_{\bar{L}}(r)$ should be independent of radius. For the Taylor-vortex flow and for the one-travelling-wave flow we find that the fractional variation in $2\pi r\bar{F}_{\bar{L}}(r)$ over the entire radius is about one part in 10^6.

Finally, we note that our results have been checked for adequate spatial resolution. Truncation and aliasing errors are both due to miscalculation of the nonlinear term $\boldsymbol{v}\times\boldsymbol{\omega}$. We now estimate upper bounds for both errors and show that they have the same order of magnitude. Let us restrict ourselves to errors due to insufficient truncation and aliasing in the axial direction. We denote by $\boldsymbol{v}_k$ and $(\boldsymbol{v}\times\boldsymbol{\omega})_k$, the kth axial Fourier components of $\boldsymbol{v}$ and $\boldsymbol{v}\times\boldsymbol{\omega}$, where $-K \leqslant k < K$. By numerical experimentation with $R_{\mathrm{c}} \leqslant R \leqslant 15R_{\mathrm{c}}$ and $\eta \approx 0.875$ we have found that $\boldsymbol{v}_k \approx \boldsymbol{\omega}_k \approx O(\mathrm{e}^{-\alpha|k|})$ (see figure 5 of Part 2). The product $(\boldsymbol{v}\times\boldsymbol{\omega})_k$ is the convolution sum

$$(\boldsymbol{v}\times\boldsymbol{\omega})_k = \sum_{\substack{p\\ p+q=k}}\sum_{q} \boldsymbol{v}_p\times\boldsymbol{\omega}_q. \tag{3.12}$$

Owing to the exponential nature of the spectrum, the k largest terms in the sum are $O(\mathrm{e}^{-\alpha|k|})$. The truncation error in the sum is dominated by the neglected terms that contain either $\boldsymbol{\omega}_{\pm(K+1)}$ or $\boldsymbol{v}_{\pm(K+1)}$. The neglected terms are $O(\mathrm{e}^{-\alpha(2K+2-k)})$. Therefore an upper bound on the *fractional* error in $(\boldsymbol{v}\times\boldsymbol{\omega})_k$ due to truncation is $O(\mathrm{e}^{-2\alpha(K+1-k)})$.

Typically, α is approximately 1.5 (see Part 2). Therefore, with $K = 16$ the upper-bound fractional truncation error in $(\boldsymbol{v}\times\boldsymbol{\omega})_k$ is less than the machine precision of 10^{-15} for $|k| < 6$. In the worst case, when $|k| = K$, the upper-bound fractional error is e^{-3}. However, a fractional error in $(\boldsymbol{v}\times\boldsymbol{\omega})_k$ of e^{-3} does not mean that there is a fractional error of e^{-3} in $\boldsymbol{v}_k$ (see below).

The aliasing error in $(\boldsymbol{v}\times\boldsymbol{\omega})_k$ is due to our collocation method, which contaminates $(\boldsymbol{v}\times\boldsymbol{\omega})_k$ with terms that really belong to $(\boldsymbol{v}\times\boldsymbol{\omega})_{2K-k}$. Since the characteristic term in $(\boldsymbol{v}\times\boldsymbol{\omega})_{2K-k}$ is $O(\mathrm{e}^{-\alpha(2K-k)})$, the *upper bound* to the fractional aliasing error in $(\boldsymbol{v}\times\boldsymbol{\omega})_k$ is $O(\mathrm{e}^{-2\alpha(K-k)})$, or $\mathrm{e}^{2\alpha}$ times the upper bound to the fractional truncation error. Therefore it is apparent that aliasing errors have the same k- and K-dependences as, and are not much greater than, the truncation errors. Although the aliasing error can be found directly by comparing the values of $(\boldsymbol{v}\times\boldsymbol{\omega})_k$ computed with $2K$ collocation points with the value computed with 3K collocation points (which is alias-free), it is more useful to find the combined effects of truncation and aliasing on $\boldsymbol{v}$ by doubling the number of spectral modes. For an axisymmetric Taylor-vortex flow with $n = 0.95$, $\alpha = 2\pi/1.988$ and $R = 1.3R_{\mathrm{c}}$ and $K = 16$ and 32 we have found that the greatest fractional change in value of $\boldsymbol{v}_k$ occurs for the largest $|k|$ and is $O(10^{-6})$. The reason that the fractional error of $\boldsymbol{v}_K$ is much smaller than the fractional error in $(\boldsymbol{v}\times\boldsymbol{\omega})_K$ is that the modal equation for $\boldsymbol{v}_K$ is dominated by the linear viscous term, not the

nonlinear term. We also note that errors due to aliasing and truncation can usually be easily detected by plotting the energy spectrum of $\boldsymbol{v}_k$. An upward curl in the spectrum at large harmonic numbers usually indicates lack of spatial resolution (see figure 24 of Part 2).

4. Comparison of simulations with laboratory measurements

Torques

We have compared our numerically calculated torques with those measured experimentally by Donnelly & Simon (1960) for axisymmetric Taylor-vortex flow with a radius ratio of $\eta = 0.5$ and for Reynolds numbers up to four times the critical Reynolds number for transition to Taylor-vortex flow. One difficulty in comparing the calculated torques with the experiments is that the torque depends on the axial wavelength. The torque measurements of Donnelly & Simon (and almost all other experimentalists) are done with opaque outer cylinders so that the axial wavenumber is not known and must be assumed *a priori*. (It is also not known how constant the axial wavelength is among the different Taylor cells nor is it known how the finite length of the cylinder affects the torque – see Alziary de Roquefort & Grillaud (1978).) For these reasons we do not present a detailed comparison between our numerical torques and the experimental values. We are content with noting that for $R_c < R < 4R_c$ the torque of Taylor-vortex flow varies by a factor of three, and over this entire range our numerical values agree with the experimental values to within 2%. We believe that a more detailed comparison (i.e. more detailed than the experimental uncertainties warrant) is highly misleading.

We have not attempted to compare our calculated torques with the experimentally measured values for non-axisymmetric travelling-wave flows. For laboratory data acquired without simultaneous flow visualization, the comparison would require assuming not only the axial wavelengths and the effects of finite-length cylinders, but also the azimuthal wavenumbers of the experimentally measured flow (cf. Eagles 1974).

For Taylor-vortex flow with $\eta = 0.5$ and $\alpha = 2\pi/1.988$, we have compared the torques computed by our initial-value code with those computed by Meyer-Spasche & Keller (1980, figure 3), who used a steady-state solver. For $R < 2.0R_c$ our torques agree within 1%. For $R = 3.0R_c$ the agreement is within 2.5%. For computations at this Reynolds number Meyer-Spasche & Keller used a Galerkin spectral sum with 9 cosine modes in the axial direction. By plotting the energy spectra as a function of axial wavenumber and observing an upward curl at high axial harmonic numbers, we found that 9 axial modes are insufficient for complete spatial resolution at $R = 3.0R_c$. To determine whether the truncated spatial resolution could be a source of error, we calculated the torques with our initial-value code using both a 9- and a 32-term cosine series. The two torques differed by 2%. Another possible source of disagreement between our code and the code of Meyer-Spasche & Keller is that we have a stricter convergence criterion; a necessary condition for our terminating a calculation (for steady-state equilibrium) is that the fractional variation of the angular momentum flux (or torque) over the entire radius of the fluid be less than 10^{-6} (see (3.11)). Meyer-Spasche & Keller report fractional variations of up to 3%.

Wave speeds

We believe that a comparison of the numerically computed and experimentally measured speeds of the waves in wavy-vortex flow is the best test of a numerical

$\frac{R}{R_c}$	$\frac{2\pi}{\alpha}$	s_1	
		Computed	Measured
3.98	2.4	0.3443 ± 0.0001	0.3440 ± 0.0008
3.98	3.0	0.3344 ± 0.0001	0.3347 ± 0.0007
5.97	2.2	0.3370 ± 0.0001	0.3370 ± 0.0002

TABLE 2. Comparison of computed and measured wave speeds ($\eta = 0.868$, $m_1 = 6$)

simulation. Not only can the wave speed be measured much more precisely than the torque, but also the numerical experiments show that the wave speeds are a sensitive indicator of a code's accuracy. We have found that any compromise in numerical resolution changes the wave speed by several percent. In particular, improper treatment of boundary conditions markedly changes the wave speeds, especially in the limit as $\eta \to 1$ (see §2).

To determine the degree of accuracy which we expect our numerical code to reproduce the laboratory values of the wave speed, we note that there are strong physical constraints on s_1. As shown in Part 2, the wave speed is determined by the azimuthal velocity of a fluid surface located far from both boundary layers. For large R (i.e. $R > 4R_c$) and large η (i.e. $\eta > 0.8$) the azimuthal velocity of the fluid far from the boundary layers has only about a 25% variation; therefore we believe that even a poorly resolved code *with the correct boundary conditions* should be able to reproduce wave speeds within 25% of their measured values for $R > 4R_c$ and $\eta > 0.8$. A code that produces wave speeds with errors of 5 or 10% is not necessarily quantitatively accurate. A quantitatively correct code should produce wave-speed errors on the order of the experimental accuracy, which is less than 1%.

Our numerically calculated wave speeds correspond to an infinite aspect ratio Γ, so to compare our numerical speeds with laboratory experiments (made at finite Γ), it is necessary that the speeds be measured in the laboratory as a function of Γ and then extrapolated to $\Gamma = \infty$. For $\eta = 0.876$ and $R \approx 4R_c$ the difference between the extrapolated value of s_1 at $\Gamma = \infty$ and the s_1 observed at the largest aspect ratio measured ($\Gamma \approx 80$) is approximately 2%. The experimental uncertainty in the extrapolated value of s_1 at $\Gamma = \infty$ is approximately 0.2%.

In table 2 we summarize the results of King *et al.* (1984), which compares the experimental and numerical value of the speeds of $m_1 = 6$ one-travelling-wave flows at $\eta = 0.868$ for different values of λ and R/R_c. The important feature of the table is that the numerical and laboratory speeds agree to within the laboratory uncertainties. Details of the laboratory measurements appear in King *et al.* The numerical wave speeds in table 2 were computed with 33 radial Chebyshev modes, 32 axial Fourier modes, and 32 azimuthal Fourier modes where the modes were chosen so that all symmetries of the one-travelling-wave flow were fully exploited.

The errors in the numerical calculations are due to both the finite timestepping and the finite spatial resolution (which includes the aliasing error). The error due to spatial resolution was estimated by computing the flow three more times, each recalculation corresponding to reducing the spatial by half in each of the three dimensions. The fractional change in s_1 is $O(5 \times 10^{-4})$, which is less than the timestepping error.

The timestepping errors in the flow velocity (see §2), are of $O(\Delta t/R, \Delta t^2)$. By plotting the change in the velocity field as a function of Δt, we have found that the error in the velocity scales as $(\Delta t)^2$. Presumably the Δt^2 error dominates the $\Delta t/R$ error

because R is large (greater than 100) for wavy-vortex flows, with $\eta \approx 0.875$. Typical calculations were made with Δt in the range $\tau/160 \leqslant \Delta t \leqslant \tau/2000$, where τ is the period of the inner cylinder.

The uncertainty shown in table 2, $\Delta s_1/s_1 \approx 3 \times 10^{-4}$, is due to the uncertainty in extrapolating the value of s_1 to $\Delta t = 0$. Note that this fractional uncertainty is three times the fractional error in the wave speeds that we found when we compared the speeds from our initial-value solver with the speeds from our fourth-order eigenvalue solver (see table 1).

5. Discussion

In this paper we have presented the details of a numerical method that computes Taylor–Couette flow by solving the Navier–Stokes equation as an initial-value problem. Furthermore, we have demonstrated that the method works, by showing that the numerical results are self-consistent, that they agree with other published numerical work, that they agree with analytic results, and most importantly that they agree with laboratory measurements.

The most difficult numerical task solved in this paper is the removal of the time-splitting error that occurs if the viscous fractional step and calculation of the pressure head are not done simultaneously. It is interesting that, although both cylindrical pipe flow (Patera & Orszag 1981) and Taylor–Couette flow require solving the Navier–Stokes equation for a divergence-free velocity field in a cylindrical geometry with periodic boundary conditions in the axial direction, the time-splitting does not cause an appreciable error in pipe flow, but does cause a large error in Taylor–Couette flow. The reason why the rotating flow is sensitive to the splitting error is that the forcing terms for Taylor–Couette flow are at the radial boundaries, while in the pipe flow the radial boundaries are rather unimportant. This difference in sensitivity to the time-splitting error illustrates the fact that numerical codes that solve the Navier–Stokes equation in some particular geometry are not equally good for all problems. The subtleties of the physics of a flow should be considered before blindly applying a numerical method. All numerical codes produce small errors that contaminate the velocity. If the flow is not sensitive to these errors it is pointless to remove them, but if the flow is sensitive then some additional care must be taken.

There are several extensions of the use of Green functions to remove time-splitting errors that would be useful. Green functions can be used efficiently in our calculation because in two spatial dimensions (ϕ and z) our flow is periodic. We would like to modify the Green-function method so that it is efficient for flows where only one spatial dimension is periodic (for example Rayleigh–Bénard convection in a cylinder) or for flows with no spatial periodicity.

Another planned extension of this work is to use the method of artificial time, outlined in §2, to compute unstable equilibria. A disadvantage of initial-value codes is that often they cannot converge to an unstable equilibrium, while steady-state solvers usually can. It may be possible to compute these unstable equilibria using an initial-value code with artificial time. We have already found examples of flows that are unstable with respect to real-time perturbations, but are stable to perturbations in artificial time. An initial-value code that uses artificial time converges to these unstable equilibria. The advantage of using an initial-value code over a conventional steady-state solver that uses a Newton–Raphson method is that the matrix inversion required with the latter method frequently prohibits detailed spatial resolution.

We believe that the best test of a code that simulates Taylor–Couette flow numerically is the comparison between the numerically simulated wave speeds and the experimentally measured speeds. At the present time torques have not been measured sufficiently accurately (i.e. with fractional errors less than 2%) to allow measurements to be a definitive comparison between experiments and numerics. For all comparisons it is necessary that the laboratory flow be measured in a way that allows the axial wavelength and azimuthal wavenumber to be unambiguously determined. It is also necessary that either the numerically simulated flows include the same finite-axial-length end effects as the experiments or that the experiments be done for a sequence of large aspect ratios, so that the experimental results can be extrapolated to infinite aspect ratio. In this paper we have compared the numerical simulations to experimental results that were extrapolated to infinite aspect ratio. The fractional errors in our numerically computed wave speeds are within the experimental uncertainties. For $\eta = 8.75$ and $R \lesssim 4R_c$, the experimental uncertainty is less than 0.2%.

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