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Pseudospectral Algorithms for Navier–Stokes Simulation of Turbulent Flows in Cylindrical Geometry with Coordinate Singularities

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We present a new family of algorithms for incompressible 3D Navier–Stokes equations in cylindrical geometry. A model problem of turbulent flow calculation in an infinite circular pipe $\{(r, \varphi, z)$: $0 \le r \le R, 0 \le \varphi < 2\pi, |z| < \infty\}$ is considered and used for accuracy, stability, and efficiency estimations. Algorithms are based on Galerkin trigonometric approximation for uniform variables φ, z, on pseudospectral polynomial approximation in the r-direction (with different sets of collocation nodes) and on implicit and predictor–corrector time advancement schemes. In all cases high (infinite order) spatial accuracy is retained despite the presence of coordinate singularity at $r = 0$. To achieve this we exploit the behaviour of analytic functions of variables r, φ, z in the vicinity of $r = 0$. We analyze the advantages and disadvantages of four Navier–Stokes algorithms. In method A a new splitting technique is developed which makes use of a second-order predictor–corrector scheme and nontraditional fractional step procedure. Stability and efficiency characteristics of this scheme exceed that of the usually used mixed Adams–Bashforth/Crank–Nicolson time advancement. To minimize errors due to splitting, algorithm B is suggested that has no fractional steps. In this method pressure values are eliminated from discretized Navier–Stokes equations by means of equivalent matrix operations. Although conventional Chebyshev collocation nodes $r_l = R \cos(\pi l/2Q)$, $l = 0, 1, \ldots, Q$, are used in both methods, the discrete boundary conditions at $r = 0$—consistent with analytic behaviour of solutions for small r—are fully accessible for the first time. In addition, approximations developed prevent the appearance of various pathological (with, e.g., spurious, parasitic modes, etc.) discretizations of Navier–Stokes operators. In algorithm C we propose a new set of collocation nodes $r_l = (1 - x_l)R/2$, $l = 0, 1, \ldots, Q$, where $x_l \in (-1, 1)$, $l = 1, 2, \ldots, Q - 1$, are the zeros of Jacobi polynomial $P_{Q-1}^{(2,1)}(x)$, $x_0 = -1$, $x_Q = 1$. It is demonstrated that pseudospectral polynomial approximation with this set of nodes possesses the discrete analogue to the energy conservation law of the original Navier–Stokes initial boundary value problem. The latter is of special significance for the algorithm's nonlinear stability. In method D new dependent variables are introduced that completely consider the form of the analytic pressure and velocity components at small r. We show that the discrete Navier–Stokes equations admit in this case an efficient solution procedure. Finally, we present a technique that can be used for exhaustive a priori estimates of the algorithm's accuracy and stability characteristics in the linear approach.

I. INTRODUCTION

For the past decade considerable progress has been achieved in the accurate description of transitional and turbulent wall-bounded shear flows in the simplest geometries by means of nonstationary three-dimensional Navier–Stokes solutions. See, e.g., the calculations of Orszag and Kells [1], Rozhdestvensky and Simakin [2], Kleiser and Schumann [3], Kim, Moin, and Moser [4] in a plane channel, and the results of Spalart [5], Laurien and Kleiser [6] for flat-plate boundary layer flows. Spectral and pseudospectral algorithms being used for solving these problems essentially exploit the periodic boundary conditions in two uniform directions as well as a relatively simple form of Navier–Stokes equations in Cartesian geometry. At the same time numerous attempts were undertaken to extend the class of flows under investigation. As a result, new algorithms begin to appear, being efficient enough to integrate Navier–Stokes equations under more complicated conditions:

(a) At the presence of solid boundaries leading to nonperiodic boundary conditions in two spatial directions (Le Quere and Alziary de Roquefort [7], Tuckerman [8]);

(b) When representing nontrivial geometries (more complex than parallelepipeds, cylinders, etc.). See Orszag [9], Patera [10], Macaraeg and Streett [11], Funaro, Quarteroni, and Zanolli [12];

(c) When using coordinate systems more complex than Cartesian ones—cylindrical, spherical, etc. If the integration domain contains coordinate singularities essential difficulties arise in the course of spatial discretization of the Navier–Stokes equations.

Let us consider several aspects of Navier–Stokes discretization in cylindrical geometry (including the axis $r = 0$), taking as an example the problem of the description of incompressible viscous fluid flows in an infinite circular pipe $\mathcal{A} = \{\mathbf{r} = (r, \varphi, z)$: $0 \le r \le R, 0 \le \varphi < 2\pi, |z| < \infty\}$ at supercritical Reynolds numbers. Although all the considerations are made below for

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this specific case, the results obtained have wider applicability. In addition, investigation of turbulence in a pipe represents self-dependent interest, since it relates to one of the most famous classical problems of hydrodynamics originating from Osborne Reynolds experiments [13].

Transitional flows in a circular pipe (under the condition of velocity periodicity in the streamwise direction) were simulated in an axisymmetric case by Patera and Orszag [14] and by Orszag and Patera [15] and Boberg and Brosa [16] in the nonaxisymmetric one. Although no secondary statistically stationary states (describing fully developed turbulence in long pipes) were calculated in these works, results of considerable interest concerning possible mechanisms of transition to turbulence were obtained. In each of these works the discretization of Navier–Stokes equations with respect to uniform variables φ, z is carried out by means of Galerkin trigonometric approximation. As to the r-variable the pseudospectral approximation is used in [14, 15] with the representation of Fourier coefficients of velocity in the form of Chebyshev series. Boberg and Brosa [16] exploit Galerkin approximation for the variable r with divergence-free solutions of the Stokes equations as basis functions in the representation of velocity—an approach previously checked by Salwen and Grosch [17] on the linear stability problem.

Direct Navier–Stokes simulation of *turbulent flows* in a pipe was carried out by Nikitin [18], Priymak, and Rozhdestvensky [19], Priymak [20, 21]. Calculations [18, 19] are based on low-resolution approximations of Navier–Stokes equations (only four harmonics in the uniform variables φ, z are incorporated into the Fourier series representation of the velocity field in [18], and 25 harmonics in [19]). As to [20, 21] accurate simulation of turbulent flows in a circular pipe was carried out at supercritical Reynolds number $\mathrm{Re} = U_m 2R/\nu = 4000$ (based on the mean velocity U_m) with the spatial resolution high enough to resolve the essential scales of motion. The numerical method being used by Nikitin [18] is similar to schemes developed in [16, 17]. In [19–21] one of the algorithms discussed below (see Section 4) was applied.

In addition, the algorithm suitable for Navier–Stokes simulation of turbulence in a pipe was proposed and tested on the linear stability problem for Poiseuille flow by Leonard and Wray [22]. In this work Galerkin approximation is used for all the spatial variables and a new system of divergence-free basis functions is constructed, taking advantage of the approximation properties of certain Jacobi polynomials. A new set of basis functions is an alternative to Stokes functions utilized in [16–18]. Potential interest for Navier–Stokes integration in $\mathcal{A}$ also represents the original spectral algorithm suggested by Tuckerman [8] and initially intended for simulation of Rayleigh–Benard convection in a cylindrical container.

In this paper we propose a family of pseudospectral algorithms for direct Navier–Stokes simulation of turbulent flows in a circular pipe $\mathcal{A}$. In Section 2 mathematical formulation of the problem is presented. Comparative analysis of four numerical algorithms is conducted in Sections 3–8. Their common feature is the Galerkin trigonometric approximation for variables φ, z but they differ from each other by methods of spatial discretization in the radial direction and by time integration schemes. The algorithm that was constructed first (see Section 4) is based on pseudospectral polynomial approximation with Chebyshev collocation nodes $r_l = R\cos(\pi l/2Q)$, $l = 0, 1, \ldots, Q$, and on an implicit second-order time-advancement scheme consisting of two fractional steps. On the first step the contributions of the pressure gradient and of the Navier–Stokes equations nonlinear terms, as well as viscous terms containing only derivatives with respect to uniform variables φ, z, are considered. Viscous terms containing derivatives with respect to r are taken into account on the second fractional step. The discrete nonlinear equations obtained are solved by the method of successive approximation.

Later on we succeeded in constructing three new algorithms without fractional steps where time integration is carried out by means of the Crank–Nicolson scheme for linear terms and an implicit second-order scheme for nonlinear terms. Spatial discretization of Navier–Stokes equations implies that the incompressibility condition is satisfied identically in the computational domain. Then, pressure values in the collocation points are eliminated from the resulting discrete equations. The algorithms constructed differ in the methods of spatial discretization in a radial direction. In one of them pseudospectral polynomial approximation with collocation points r_l (see above) is also used (Section 5). In the second algorithm of this type (Section 6) the preliminary mapping of segment $[0, R]$ onto the segment $[-1, 1]$ is conducted. Spatial discretization of Navier–Stokes equations is carried out by means of polynomial approximation with collocation nodes that are the roots of Jacobi polynomials $P_{Q-1}^{(2,1)}(y)$, $y \in [-1, 1]$. The points $y = \pm 1$ are also included in the set of collocation nodes. It is shown that the pseudospectral approximation used has the discrete analogue to the energy conservation law of the original boundary value problem for Navier–Stokes equations. In the third algorithm (Section 7) spatial discretization is preceded by the change of dependent variables. Written in terms of new variables properly considering the form of the pressure and velocity components at small r, the Navier-Stokes equations no longer possess singularity at $r = 0$. Special care is taken to obtain such discrete equations for that velocity components that they can be solved by the efficient influence matrix method.

The stability and accuracy of the algorithms are analyzed analytically and numerically in Section 8. Preliminary estimates can be done on the basis of comparison of the spectral characteristics of discrete equations with corresponding characteristics of linearized Navier–Stokes equations. Such analysis is reduced to the linear eigenvalue problem for the conversion matrix from time step t_j to time step t_{j+1}. Final conclusions are made according to the results of nonlinear Navier–Stokes integration.

2. GOVERNING EQUATIONS

In the present paper we develop algorithms for numerical integration of Navier–Stokes equations

$$\frac{\partial \mathbf{V}}{\partial t} = -\nabla P + \mathbf{V} \times \boldsymbol{\Omega} + \nu \nabla^2 \mathbf{V},$$
$$\nabla \cdot \mathbf{V} = 0, \tag{1}$$
$$\mathbf{V}|_{r=R} = 0, \quad \mathbf{V}|_{t=0} = \mathbf{V}_0(\mathbf{r}), \quad \nabla \cdot \mathbf{V}_0 = 0,$$

describing turbulent flows of viscous incompressible fluid in a circular pipe $\mathcal{A}$. Here $\mathbf{V}(\mathbf{r}, t)$ is the velocity; $P = p/\rho + \mathbf{V}^2/2$ is the total pressure, $p(\mathbf{r}, t)$ being the pressure; $\boldsymbol{\Omega} = \nabla \times \mathbf{V}$ is the vorticity; ν and ρ are kinematic viscosity and density of the fluid. We seek bounded nonstationary 3D solutions of (1) that satisfy the relations

$$\mathbf{V}(\mathbf{r}, t) = \mathbf{V}(r, \varphi, z + Z, t), \tag{2}$$
$$P = P_0(t)z + \overline{P}, \quad \overline{P}(\mathbf{r}, t) = \overline{P}(r, \varphi, z + Z, t), \tag{3}$$
$$U_m(t) = \langle \mathbf{V} \cdot \mathbf{e}_z \rangle_{r\varphi} = \text{const}, \tag{4}$$

where

$$\langle \cdot \rangle_{r\varphi} = (1/\pi R^2) \int_0^R r dr \int_0^{2\pi} d\varphi(\cdot), \quad \mathbf{e}_z = (0, 0, 1).$$

At arbitrary Reynolds numbers Eqs. (1)–(4) have stationary solutions

$$\mathbf{V}^0 = (0, 0, V^0), \quad V^0 = -\frac{R^2}{4\nu\rho}\frac{dp^0}{dz}(1 - r^2/R^2),$$
$$\frac{dp^0}{dz} = \text{const}, \tag{5}$$

describing laminar Poiseuille flows. It is well known [23] that at supercritical $\mathrm{Re} > (2 - 3) \times 10^3$ nonstationary (turbulent) flow regimes may also exist. Numerical algorithms under study are constructed for the description of these turbulent regimes by means of nonstationary solutions of the Navier–Stokes equations.

3. BASIC PROPERTIES OF SPATIAL DISCRETIZATION

For presentation and analysis of numerical algorithms it is convenient to introduce new dependent variables,

$$\mathbf{v} = (v, w, u) = \mathbf{V} - \mathbf{V}^0,$$
$$P = p/\rho + \mathbf{v}^2/2, \quad p = p - p^0,$$

that are the disturbances of stationary solutions (5). Navier–Stokes equations can be rewritten then as

$$\frac{\partial \mathbf{v}}{\partial t} = \Omega^0 v \mathbf{e}_z - V^0 \frac{\partial}{\partial z}\mathbf{v} + \mathbf{v} \times \boldsymbol{\omega} + \nu \nabla^2 \mathbf{v} - \nabla P,$$
$$\nabla \cdot \mathbf{v} = 0, \tag{6}$$
$$\boldsymbol{\omega} = \nabla \times \mathbf{v}, \quad \boldsymbol{\Omega}^0 = \nabla \times \mathbf{V}^0 = (0, \Omega^0, 0),$$

with the initial and boundary conditions modified correspondingly.

In all the algorithms constructed we seek Navier–Stokes solutions in the form

$$\begin{pmatrix} \mathbf{v} \\ P \end{pmatrix} = \begin{pmatrix} 0 \\ P_0(t)z \end{pmatrix} + \sum_{m=-M}^{M} \sum_{n=-N}^{N} \begin{pmatrix} \mathbf{v}_{mn}(r, t) \\ P_{mn}(r, t) \end{pmatrix} \exp(im\alpha_0 z + in\varphi),$$
$$\mathbf{v}^*_{mn} = \mathbf{v}_{-m,-n}, \quad P^*_{mn} = P_{-m,-n}, \quad \alpha_0 = 2\pi/Z, \quad i = \sqrt{-1}, \tag{7}$$

where the asterisk denotes complex conjugate values.

In the r-direction expansions based on orthogonal polynomials that are the eigenfunctions of singular Sturm–Liouville problems are utilized. In addition, these polynomial approximations have to take into account the following behaviour of the sought for solutions as $r \to 0$:

$$(v_{mn}, w_{mn}) = r^{|n|-1}(\hat{v}_{mn}, \hat{w}_{mn}) \quad (n \neq 0),$$
$$(v_{m0}, w_{m0}) = r(\hat{v}_{m0}, \hat{w}_{m0}),$$
$$g_{mn} = r^{|n-1|}\hat{g}_{mn}, \quad g_{mn} = v_{mn} - iw_{mn} \quad (n \neq 0), \tag{8}$$
$$f_{mn} = r^{|n+1|}\hat{f}_{mn}, \quad f_{mn} = v_{mn} + iw_{mn} \quad (n \neq 0),$$
$$(u_{mn}, P_{mn}) = r^{|n|}(\hat{u}_{mn}, \hat{P}_{mn}),$$

where the $\hat{}$ symbol denotes the values which may be represented as a series in terms of even powers of r.

Although these relations are known from the literature [24], they are often attributed to the local properties of Laplacian (see, e.g., [15, 25]). We want to emphasize here that formulae (8) follow solely from the analyticity of the vector $\mathbf{v}_{mn}$ and scalar P_{mn} functions of the cylindrical variables r, φ, z in the vicinity of the axis $r = 0$. It does not matter whether these functions satisfy the Navier–Stokes (Laplace) equations or not. To prove this statement one can make use of Taylor expansions in the vicinity of $r = 0$, changing over then to the cylindrical coordinates.

Discretization of Eqs. (6) is carried out by means of the Galerkin approximation with respect to the variables φ, z and by the pseudospectral method with the collocation nodes being extremums or zeros of a certain Jacobi polynomial in the radial direction.

4. THE FRACTIONAL STEP METHOD (*ALGORITHM* A)

Algorithm A represents an implicit time advancement scheme consisting of two fractional steps. At the first step

$$\tilde{\mathbf{v}} = \mathbf{v}^J + \Delta t\, L(\mathbf{v}^{J+1/2}) - \Delta t\, \nabla P^{J+1} \tag{9a}$$

$$\nabla \cdot \tilde{\mathbf{v}} = 0, \quad \tilde{v}|_{r=R} = 0, \tag{9b}$$

where

$$L(\mathbf{v}) = \Omega^0 v \mathbf{e}_z - V^0 \frac{\partial}{\partial z}\mathbf{v} + \mathbf{v} \times \boldsymbol{\omega} + \nu\left(\nabla^2 - \frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r}\right)\mathbf{v},$$

$$\mathbf{v}^J = \mathbf{v}(\mathbf{r}, t_J), \quad \mathbf{v}^{J+1/2} = \frac{1}{2}(\mathbf{v}^{J+1} + \mathbf{v}^J), \quad \Delta t = t_{J+1} - t_J,$$

the preliminary velocity $\tilde{\mathbf{v}}$ is obtained. We consider here contributions of the pressure head, nonlinear terms and viscous terms containing derivatives only with respect to uniform variables φ, z.

From the equations

$$\mathbf{v}^{J+1} = \tilde{\mathbf{v}} + \Delta t\, \nu\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right)\mathbf{v}^{J+1}, \qquad \mathbf{v}^{J+1}|_{r=R} = 0 \tag{10}$$

of the second step we find the final velocity $\mathbf{v}^{J+1}$.

The nonlinear equations (9), (10) can be solved by means of the successive approximations method. Instead of (9) we have then

$$\tilde{\mathbf{v}} = \mathbf{v}^J + \Delta t\, L(\overset{(s-1)}{\mathbf{v}}{}^{J+1/2}) - \Delta t\, \nabla \overset{(s)}{P}{}^{J+1} \tag{9'a}$$

$$\nabla \cdot \tilde{\mathbf{v}} = 0, \quad \tilde{v}|_{r=R} = 0,$$

$$\overset{(s-1)}{\mathbf{v}}{}^{J+1/2} = \frac{1}{2}(\overset{(s-1)}{\mathbf{v}}{}^{J+1} + \mathbf{v}^J) \tag{9'b}$$

and Eqs. (10) can be rewritten as

$$\overset{(s)}{\mathbf{v}}{}^{J+1} = \tilde{\mathbf{v}} + \Delta t\, \nu\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right)\overset{(s)}{\mathbf{v}}{}^{J+1}, \qquad \overset{(s)}{\mathbf{v}}{}^{J+1}|_{r=R} = 0 \tag{10'}$$

where s is the iteration counter.

For arbitrary $s \geq 1$ the iterative algorithm (9'), (10') defines the scheme of $O(\Delta t^2 + \nu\, \Delta t)$ approximation order. The initial approximation $\overset{(0)}{\mathbf{v}}{}^{J+1}$ can be calculated using the three-layer explicit scheme (9''), (10'), where Eqs. (9'') are defined as

$$\tilde{\mathbf{v}} = \mathbf{v}^J + \Delta t\,(\tfrac{3}{2}L(\mathbf{v}^J) - \tfrac{1}{2}L(\mathbf{v}^{J-1})) - \Delta t\, \nabla \overset{(s)}{P}{}^{J+1}, \qquad \nabla \cdot \tilde{\mathbf{v}} = 0, \quad \tilde{v}|_{r=R} = 0. \tag{9''}$$

It should also be noted, that if we consider the equations

$$\left(\nu\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right) - \frac{2}{\Delta t}\right)\overset{(s)}{\mathbf{v}}{}^{J+1/2} = -\frac{1}{\Delta t}(\tilde{\mathbf{v}} + \mathbf{v}^J), \tag{10''}$$

instead of Eqs. (10') we will get the time integration scheme (9'), (10'') of $O(\Delta t^2)$ approximation order.

To solve eqs. (9'), (10') we have to eliminate $\overset{(s)}{P}{}^{J+1}$ from (9'). Applying operator rot rot to (9'a) we can receive then the set of boundary value problems

$$\left(\frac{d^2}{dr^2} + a\frac{1}{r}\frac{d}{dr} - \left(\gamma + \frac{1}{r^2}b\right)\right)\tilde{v}_{mn} = c, \quad \tilde{v}_{mn}|_{r=R} = 0, \; m^2 + n^2 \neq 0, \tag{11a}$$

$$c = -\gamma \overset{(s)}{\tilde{v}}{}^{J+1}_{mn} - in\left(\frac{1}{r}\frac{d}{dr} - \frac{1}{r^2}b\right)\overset{(s)}{\tilde{w}}{}^{J+1}_{mn} - im\alpha_0\left(\frac{d}{dr} + \frac{2n^2}{\gamma r^3}\right)\overset{(s)}{\tilde{u}}{}^{J+1}_{mn},$$

$$\gamma = (m\alpha_0)^2 + n^2/r^2, \quad a = 1 + 2n^2/(r^2\gamma), \quad b = 1 - 2n^2/(r^2\gamma), \tag{11b}$$

where

$$\overset{(s)}{\tilde{\mathbf{v}}}{}^{J+1} = \mathbf{v}^J + \Delta t\, L(\overset{(s-1)}{\mathbf{v}}{}^{J+1/2}). \tag{12}$$

Discretization of Eqs. (11) with respect to r is carried out by the collocation technique with the interpolation points $r_l = R\cos(\pi l/2Q)$, $l = 0, 1, \ldots, Q$. The Fourier coefficients $\mathbf{v}_{mn}$ of the velocity are approximated by the polynomials

$$\mathbf{v}_{mn}(r, t) = \sum_{j=0}^{Q-k} \mathbf{v}_{mnj}(t) h_j^{(k)}(r), \quad \mathbf{v}_{mnj} = \mathbf{v}_{mn}|_{r=r_j}, \tag{13a}$$

$$h_j^{(k)}(r) = (2\rho_j/Q)\sum_{q=0}^{Q-k}(\rho_q + k(1-\rho_q))\cos(\pi(2q + k)j/2Q)T_{2q+k}(r/R),$$

$$\rho_0 = \rho_Q = 1/2, \quad \rho_q = 1 \quad (q = 1, 2, \ldots, Q-1), \tag{13b}$$

$$k = \begin{cases} 0 & \text{for } u_{mn}(n - \text{even}),\ v_{mn},\ w_{mn}(n - \text{odd}), \\ 1 & \text{for } u_{mn}(n - \text{odd}),\ v_{mn},\ w_{mn}(n - \text{even}). \end{cases} \tag{13c}$$

Here T_{2q+k} are Chebyshev polynomials of the first kind. Thus, the form of the interpolation polynomials (13) partly reflects the properties (8) of the sought for solution.

Consider the square matrices

$$B_{lj}^{(k)} = \left(\frac{1}{r}\frac{d}{dr}h_j^{(k)}\right)\Big|_{r=r_l}, \quad C_{lj}^{(k)} = \left(\frac{d^2}{dr^2}h_j^{(k)}\right)\Big|_{r=r_l}, \quad l, j = 0, 1, \ldots, Q-k. \tag{14}$$

Then the pseudospectral approximation of Eqs. (11) can be written in the form

$$(C^{(k)}\tilde{v}_{mn})_l + a(r_l)(B^{(k)}\tilde{v}_{mn})_l - \left(\gamma(r) + \frac{1}{r^2}b(r)\right)\Big|_{r=r_l}\tilde{v}_{mnl} = c(r_l),$$

$$l = 1, 2, ..., Q_*, \quad Q_* = Q(|n| = 1),$$

$$Q_* = Q - 1(|n| \neq 1), \tag{15a}$$

$$\tilde{v}_{mn0} = 0, \quad \tilde{v}_{mnQ} = 0 \quad (|n| \neq 1, n - \text{odd}), \tag{15b}$$

where the last equation follows from (8),

$$\tilde{v}_{mn} = (\tilde{v}_{mn0}, \tilde{v}_{mn1}, ..., \tilde{v}_{mn,Q-k})^{\mathrm{T}},$$

and $(\cdot)_l$ is the lth component of the corresponding vector. Computation of the Fourier coefficients $(\mathbf{v} \times \boldsymbol{\omega})_{mn}$ of nonlinearity is carried out by means of algorithm [26]. To avoid aliasing errors the $\frac{3}{2}$ − rule is used.

Having obtained $\tilde{v}$ one can calculate $\tilde{u}$ and $\tilde{w}$ from

$$\tilde{u}_{mnl} = \overset{(s)}{\tilde{\tilde{u}}}{}^{J+1}_{mnl} - im\alpha_0 \Delta t \overset{(s)}{P}{}^{J+1}_{mnl}, \quad \begin{cases} l = 1, 2, ..., Q & (n = 0) \\ l = 1, 2, ..., Q - 1 & (n \neq 0), \end{cases} \tag{16a}$$

$$\tilde{w}_{mnl} = \overset{(s)}{\tilde{\tilde{w}}}{}^{J+1}_{mnl} - i\frac{n}{r_l}\Delta t \overset{(s)}{P}{}^{J+1}_{mnl}, \quad l = 1, 2, ..., Q - 1,$$

$$\tilde{v}_{mnQ} + i\tilde{w}_{mnQ} = 0 \quad (|n| = 1), \tag{16b}$$

$$\Delta t \overset{(s)}{P}{}^{J+1}_{mnl} = -\frac{1}{\gamma(r_l)}\left(\frac{d}{dr}\tilde{v}_{mn}|_{r=r_l} + \frac{1}{r}\tilde{v}_{mn}|_{r=r_l} + im\alpha_0 \overset{(s)}{\tilde{\tilde{u}}}{}^{J+1}_{mnl} + \frac{in}{r_l}\overset{(s)}{\tilde{\tilde{w}}}{}^{J+1}_{mnl}\right). \tag{16c}$$

The final values of velocity $\mathbf{v}^{J+1}$ satisfy

$$\left(\nu\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}\right) - \frac{1}{\Delta t}\right)\overset{(s)}{\mathbf{v}}{}^{J+1}_{mn}|_{r=r_l} = -\frac{1}{\Delta t}\tilde{\mathbf{v}}_{mnl} \quad (m^2 + n^2 \neq 0), \tag{17a}$$

$$\overset{(s)}{\mathbf{v}}{}^{J+1}_{mn0} = 0, \quad \overset{(s)}{u}{}^{J+1}_{mnQ} = 0\,(n \neq 0), \quad \overset{(s)}{v}{}^{J+1}_{mnQ} = \overset{(s)}{w}{}^{J+1}_{mnQ} = 0\,(|n| \neq 1), \tag{17b}$$

where derivatives are approximated with the help of matrices $C^{(k)}$ and $B^{(k)}$. In the equations for $\overset{(s)}{u}{}^{J+1}_{m0}$, $\overset{(s)}{v}{}^{J+1}_{m,\pm1}$, $\overset{(s)}{w}{}^{J+1}_{m,\pm1}$, $l = 1, 2, ..., Q$; otherwise $l = 1, 2, ..., Q - 1$.

In the case $m = n = 0$ the algorithm has no fractional steps. The streamwise velocity component, for example, may be found from the equations

$$-\overset{(s)}{P}{}_0(t_{J+1}) + \left(\nu\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}\right) - \frac{1}{\Delta t}\right)\overset{(s)}{u}{}^{J+1}_{00}|_{r=r_l} = -\frac{1}{\Delta t}u^J_{001}$$

$$-(\overset{(s-1)}{\mathbf{v}}{}^{J+1/2} \times \overset{(s-1)}{\boldsymbol{\omega}}{}^{J+1/2})_{001}\mathbf{e}_z, \quad l = 1, 2, ..., Q; \tag{18a}$$

$$\overset{(s)}{u}{}^{J+1}_{000} = 0, \quad \int_0^R \overset{(s)}{u}{}^{J+1}_{00}\, r dr = 0, \tag{18b}$$

where the second equation in (18b) is the condition of flow flux constancy. Equations for the azimuth velocity component can be written in a similar way. As to the radial velocity, we have

$$\overset{(s)}{v}{}^{J+1}_{001} = 0, \quad l = 0, 1, ..., Q,$$

that follows from the incompressibility condition.

We note that the use of the implicit scheme is not a traditional practice. As a rule, mixed explicit/implicit time advancement is employed with the explicit treatment of nonlinear terms. Our motivation for considering an implicit temporal discretization is based on the well-known fact (see, e.g., [26, 27]) that stability restrictions are improved if the algorithm possesses discrete analogues to the neutrality properties of the nonlinear and pressure terms (see relations (28) in this paper). An implicit scheme (9), (10), (as well as (9′), (10′) if iterations are conducted to convergence) satisfies one of these neutrality conditions. Due to the identity

$$\mathbf{v}^{J+1/2} \cdot (\mathbf{v}^{J+1/2} \times \boldsymbol{\omega}^{J+1/2}) = 0, \quad \boldsymbol{\omega}^{J+1/2} = \nabla \times \mathbf{v}^{J+1/2},$$

it follows from (9), (10) that the nonlinearity $\mathbf{v} \times \boldsymbol{\omega}$ makes no contribution to the variation

$$\mathbf{v}^{J+1/2} \cdot \frac{(\mathbf{v}^{J+1} - \mathbf{v}^J)}{\Delta t} = \frac{1}{2}\frac{(\mathbf{v}^{J+1})^2 - (\mathbf{v}^J)^2}{\Delta t}$$

of the squared velocity over one time step. Certainly, this is correct to within the errors introduced by splitting the Navier–Stokes operators. Nevertheless, for the explicit/implicit schemes of the (9″), (10) type the parasitic contribution of the nonlinear term $\mathbf{v} \times \boldsymbol{\omega}$ to the production of the flow kinetic energy is considerably greater.

An important result was obtained in the course of our Navier–Stokes simulation [20, 21] of the turbulent pipe flow: computations demonstrated that even the small number of iterations in (9′), (10′) abruptly improves the stability characteristics of the explicit/implicit algorithm (9″), (10). In most cases we could use the simple predictor–corrector scheme: Eqs. (9″) and (10′) with $s = 0$ being the predictor; Eqs. (9′) and (10′) with the maximal $s = 1$ being the corrector. At Reynolds number Re = 4000, for example, stable and accurate predictor–corrector computations could be carried out with a time step four times greater than those in the conventional explicit/implicit

method. Thus the summary efficiency of the predictor–corrector scheme proved to be two times higher.

It should be also emphasized that there are not any spurious or parasitic modes in algorithm A. This statement is the result of algorithm's careful testing against the linear theory. Some results of this testing are presented in Section 8 (Table IV).

Another of our innovations is the decomposition of viscous terms into two parts. Derivatives with respect to the uniform variables φ, z are considered only at the first fractional step. That is why the collocation $Q \times Q$ matrix approximating Eq. (17a) of the second fractional step is the same for all wavenumbers m, n. We invert it once and then use the ready result at each time step. Storage requirements are negligible in this case.

Unfortunately this is not true for collocation matrices representing Eqs. (15); these full matrices do depend on both m and n wavenumbers. The latter requires the considerable memory of about $M \times N \times Q^2$ words. Nevertheless, scheme A is practically suitable for moderate Reynolds numbers and was used for the turbulent pipe flow simulation at Re = 4000. Computations carried out with up to $(Q + 1) \times (2N + 1) \times (2M + 1) = 33 \times 85 \times 85$ degrees of freedom in the $r-$, $\varphi-$, and z-directions demanded $\approx M \times N \times Q^2 = 1{,}806{,}336$ words to store the inverse collocation matrices. These memory requirements are admissible for the ES-1066 computer used. For the moderate (but supercritical) Reynolds number considered, the aforementioned resolution proved to be sufficient for accurate Navier–Stokes simulation of turbulence; the deminution of energies of Fourier harmonics for azimuthal and streamwise wavenumbers n and m is roughly by factors of 10^{-2} and 10^{-4}, respectively (with the computational period $Z = 2\pi R$); the minimum and maximum spacings between mesh points in the r-direction were respectively 0.18 and 7.32 wall units.

Certainly, for higher Reynolds numbers and/or larger streamwise period Z we need more efficient algorithms. In Sections 5, 6, and 7 we present several such methods with the storage requirements for collocation matrices of about $2 \times N \times Q^2$ words. Their common difference from method A is the absence of fractional steps that allows us to get rid of splitting errors. In the methods presented not only no-slip boundary conditions, but also the continuity equation, are satisfied on the t_{J+1} time level. Nonfulfillment of the incompressibility condition is one of the drawbacks of algorithm A; calculations show that it leads to the impossibility of accurate description of the near-wall behaviour of Reynolds stresses, e.g., of the $(y^+)^2$ behaviour of the normal stress, y^+ being the distance from pipe wall in wall units.

There are also several other splitting errors in method A. For example, the fine point of the algorithm is the calculation of right-hand side of Eq. $(15a)$ at $r = 0$ $(l = Q)$ when $|n| = 1$. No problems arise if the values $\tilde{\tilde{v}}^{J+1}_{mnQ}$ and $\tilde{\tilde{w}}^{J+1}_{mnQ}$, $|n| = 1$, exactly satisfy equations similar to (16b). However, some errors are introduced by the term $L(^{(s-1)}\mathbf{v}^{J+1/2})$ in (9′) and at the second fractional step. These errors are smoothed out in the course of computation.

One of our computer codes was designed for the multiprocessor vector computer IZOT ES1037-ES2706 (the hardware is manufactured in Bulgaria by IZOT and the software is developed in the Space Research Institute, Russian Academy of Science, Moscow), consisting of the central processor and 4–8 attached 38-bit array processors with a processing rate of 12 MFLOPS each. Different strategies of algorithm vectorization and parallel processing are considered by Priymak, Schevchenko, and Yulaev [28], providing the best possible utilization of the computer architecture.

So we turn to algorithms without splitting of Navier–Stokes operators. The approaches presented below differ in the methods of pressure elimination, in the conservation properties, in the iteration techniques, and in the discrete Navier–Stokes equation solvers.

5. CHEBYSHEV COLLOCATION ALGORITHM WITHOUT SPLITTING (*ALGORITHM* B)

We begin with the discretization of Navier–Stokes equations (6) with respect to the uniform variables φ, z. Afterwards we conduct the change of dependent variables: variables f_{mn}, g_{mn}, $n \neq 0$, are introduced according to (8). Finally, dropping for convenience the subscripts m, n and setting $\alpha = m\alpha_0$, we obtain for the certain Fourier mode,

$$\frac{\partial}{\partial t}\mathbf{q} = \Omega^0 \frac{1}{2}(f+g)\mathbf{e}_z - i\alpha V^0 \mathbf{q} + \mathcal{F}(\mathbf{q}) + \nu\tilde{\Delta}\mathbf{q} - \tilde{\nabla}P,$$
$$\tilde{\nabla}\cdot\mathbf{q} = 0, \quad \mathbf{q}|_{r=R} = 0, \quad \int_0^R u_{00} r dr = 0, \tag{19a}$$

where for $n \neq 0$,

$$\mathbf{q}(r,t) = (q^{(1)}, q^{(2)}, q^{(3)}) = (f, g, u)$$
$$\tilde{\nabla}P = ((D - n/r)P, (D + n/r)P, i\alpha P), \quad D = \partial/\partial r,$$
$$\tilde{\Delta}\mathbf{q} = \left(D^2 + \frac{1}{r}D - \alpha^2\right)\mathbf{q} - \frac{1}{r^2}((n+1)^2 f, (n-1)^2 g, n^2 u),$$
$$\tilde{\nabla}\cdot\mathbf{q} = (0.5D + (n+1)/2r)f + (0.5D - (n-1)/2r)g + i\alpha u,$$
$$\mathcal{F}(\mathbf{q}) = (F^{(1)}, F^{(2)}, F^{(3)}), \quad F^{(1,2)} = \mathbf{F}\cdot\mathbf{e}_r \pm i\mathbf{F}\cdot\mathbf{e}_\varphi, F^{(3)} = \mathbf{F}\cdot\mathbf{e}_z, \tag{19b}$$

$\mathbf{F}$ being the Fourier harmonic of nonlinearity $\mathbf{v} \times \boldsymbol{\omega}$.

For $n = 0$ we have, respectively,

$$\mathbf{q}(r,t) = (v, w, u),$$
$$\tilde{\nabla}P = (DP, 0, i\alpha P + P_0(t)\delta_{m0}),$$
$$\tilde{\Delta}\mathbf{q} = (D^2 + \frac{1}{r}D - \alpha^2)\mathbf{q} - \frac{1}{r^2}(v, w, 0), \tag{19c}$$
$$\tilde{\nabla}\cdot\mathbf{q} = (D + 1/r)v + i\alpha u,$$
$$\mathcal{F} = (\mathbf{v}\times\boldsymbol{\omega})_{m0},$$

δ_{m0} being the Kronecker delta. The last equation in (19a) corresponds to the flow flux constancy restriction and is utilized only in the case $m = n = 0$.

Temporal discretization of Eqs. (19) is carried out by means of the implicit second-order scheme

$$\mathbf{q}^{J+1} = \mathbf{q}^J + \Delta t\, N(\mathbf{q}^{J+1/2}) + \Delta t\, \nu \tilde{\Delta}\mathbf{q}^{J+1/2} - \Delta t\, \tilde{\nabla} P^{J+1}$$
$$\tilde{\nabla}\cdot\mathbf{q}^{J+1} = 0, \quad \mathbf{q}^{J+1}|_{r=R} = 0, \tag{20}$$

where

$$N(\mathbf{q}) = \Omega^0 \tfrac{1}{2}(f+g)\mathbf{e}_z - i\alpha V^0\mathbf{q} + \mathcal{F}(\mathbf{q}), \quad \mathbf{q}^{J+1/2} = \tfrac{1}{2}(\mathbf{q}^{J+1} + \mathbf{q}^J),$$

and the superscript index J refers to the time level, $t_J = J\,\Delta t$.

Equations (20) can be solved with the help of some successive approximations method. We make use of the algorithm

$$\overset{(s)}{\mathbf{q}}{}^{J+1} = \mathbf{q}^J + \Delta t\, N(\overset{(s-1)}{\mathbf{q}}{}^{J+1/2}) + \Delta t\, \nu \tilde{\Delta}\overset{(s)}{\mathbf{q}}{}^{J+1/2} - \Delta t\, \tilde{\nabla}\overset{(s)}{P}{}^{J+1},$$
$$\tilde{\nabla}\cdot\overset{(s)}{\mathbf{q}}{}^{J+1} = 0, \quad \overset{(s)}{\mathbf{q}}{}^{J+1}|_{r=R} = 0, \tag{21}$$

where s is the iteration counter.

For the spatial discretization of Eqs. (21) we use the pseudo-spectral method with collocation nodes $r_j = R\cos(\pi j/2Q)$, $j = 0, 1, ..., Q$, approximating the sought-for solution $\mathbf{q}$, P by the interpolation polynomial of (13a), (13b) type with a new selection rule for parameter k:

$$k = \begin{cases} 0 & \text{for } f, g\ (n - \text{odd}),\ u, P\ (n - \text{even}), \\ 1 & \text{for } f, g\ (n - \text{even}),\ u, P\ (n - \text{odd}). \end{cases} \tag{22}$$

With regard for relations (8), the fully discretized Navier–Stokes equations take then the form (we consider below only the case $n \neq 0$):

$$(L\overset{(s)}{f}{}^{J+1} - (D^{(k)} - nR^{(k)})\overset{(s)}{P}{}^{J+1})_l = \mathcal{L}_l, \quad l = 1, 2, ..., Q_n^{(1)}, \tag{23a}$$

$$(G\overset{(s)}{g}{}^{J+1} - (D^{(k)} + nR^{(k)})\overset{(s)}{P}{}^{J+1})_l = \mathcal{G}_l, \quad l = 1, 2, ..., Q_n^{(2)}, \tag{23b}$$

$$(U\overset{(s)}{u}{}^{J+1})_l - i\alpha\overset{(s)}{P}{}_l^{J+1} = \mathcal{U}_l, \qquad l = 1, 2, ..., Q-1, \tag{23c}$$

$$((D^{(k)} + (n+1)R^{(k)})\overset{(s)}{f}{}^{J+1} + (D^{(k)} - (n-1)R^{(k)})\overset{(s)}{g}{}^{J+1})_l + 2i\alpha\overset{(s)}{u}{}_l^{J+1} = 0,$$
$$l = 0, 1, ..., Q-1 \tag{23d}$$

$$\overset{(s)}{f}{}_0^{J+1} = \overset{(s)}{g}{}_0^{J+1} = \overset{(s)}{u}{}_0^{J+1} = 0, \quad \overset{(s)}{u}{}_Q^{J+1} = \overset{(s)}{P}{}_Q^{J+1} = 0\ (n - \text{even}), \tag{23e}$$

$$\overset{(s)}{f}{}_Q^{J+1} = 0\ (n - \text{odd}, n \neq -1),$$
$$\overset{(s)}{g}{}_Q^{J+1} = 0\ (n - \text{odd}, n \neq 1). \tag{23f}$$

Here

$$Q_{-1}^{(1)} = Q, \quad Q_n^{(1)} = Q - 1 \quad (n \neq -1),$$
$$Q_1^{(2)} = Q, \quad Q_n^{(2)} = Q - 1 \quad (n \neq 1),$$
$$f = (f_0, f_1, ..., f_{Q-k})^{\mathrm{T}}$$

with the similar notation for vectors g, u, and P;

$$D_{lj}^{(k)} = \frac{d}{dr}h_j^{(k)}|_{r=r_l}, \quad R_{lj}^{(k)} = \frac{1}{r}h_j^{(k)}|_{r=r_l},$$
$$l = 0, 1, ..., Q + k - 1, \quad j = 0, 1, ..., Q - k;$$
$$L_{lj} = \frac{\nu}{2}(C_{lj}^{(k)} + B_{lj}^{(k)} - \frac{1}{r_l^2}(n+1)^2\,\delta_{lj} - \alpha^2\,\delta_{lj}) - \frac{1}{\Delta t}\,\delta_{lj},$$
$$l = 1, 2, ..., Q_n^{(1)}, \quad j = 0, 1, ..., Q - k;$$
$$G_{lj} = \frac{\nu}{2}(C_{lj}^{(k)} + B_{lj}^{(k)} - \frac{1}{r_l^2}(n-1)^2\,\delta_{lj} - \alpha^2\,\delta_{lj}) - \frac{1}{\Delta t}\,\delta_{lj},$$
$$l = 1, 2, ..., Q_n^{(2)}, \quad j = 0, 1, ..., Q - k;$$
$$U_{lj} = \frac{\nu}{2}(C_{lj}^{(k)} + B_{lj}^{(k)} - \frac{1}{r_l^2}n^2\,\delta_{lj} - \alpha^2\,\delta_{lj}) - \frac{1}{\Delta t}\,\delta_{lj},$$
$$l = 1, 2, ..., Q-1, \quad j = 0, 1, ..., Q - k;$$
$$(\mathcal{L}, \mathcal{G}, \mathcal{U})_l^T = i\alpha V^0(r_l)\overset{(s-1)}{\mathbf{q}}{}_l^{J+1/2} - \frac{1}{2}\Omega^0(r_l)(0, 0, \overset{(s-1)}{f}{}_l^{J+1/2}$$
$$+ \overset{(s-1)}{g}{}_l^{J+1/2})^{\mathrm{T}} - \mathcal{F}_l(\overset{(s-1)}{\mathbf{q}}{}^{J+1/2})$$
$$- ((Lf^J)_l, (Gg^J)_l, (Uu^J)_l)^{\mathrm{T}} - \frac{2}{\Delta t}\mathbf{q}_l^J.$$

We recall here that parameter k in the above equations is the function of the azimuthal wavenumber n, according to the rule (22).

A few words about the method of solution, confining ourselves to the case $\alpha \neq 0$. Excluding with the help of (23c)–(23e), $\overset{(s)}{P}{}_l^{J+1}$, $l \neq 0$, from (23a), (23b) one can obtain the matrix equation

$$Ax = b,$$
$$x = (\overset{(s)}{f}{}_1^{J+1}, \overset{(s)}{f}{}_2^{J+1}, ..., \overset{(s)}{f}{}_{Q-1}^{J+1}, \overset{(s)}{g}{}_1^{J+1}, \overset{(s)}{g}{}_2^{J+1}, ..., \overset{(s)}{g}{}_{Q_*}^{J+1}, \overset{(s)}{P}{}_0^{J+1})^{\mathrm{T}} \quad \text{for } n > 0,$$
$$x = (\overset{(s)}{g}{}_1^{J+1}, \overset{(s)}{g}{}_2^{J+1}, ..., \overset{(s)}{g}{}_{Q-1}^{J+1}, \overset{(s)}{f}{}_1^{J+1}, \overset{(s)}{f}{}_2^{J+1}, ..., \overset{(s)}{f}{}_{Q_*}^{J+1}, \overset{(s)}{P}{}_0^{J+1})^{\mathrm{T}} \quad \text{for } n < 0,$$
$$Q_* = Q\ (n = \pm 1), \quad Q_* = Q - 1\ (n \neq \pm 1), \tag{24}$$

that is equivalent at $\alpha \neq 0$ to (23). Here b is a known vector and $A = A(\alpha, n, \mathrm{Re}, Q, \Delta t)$ is real and nonsingular in a broad range of indicated parameters. Matrices A^{-1} can be computed beforehand and then used at each time step. The required computer storage is $\cong M \times N \times (2Q)^2$ if we take into account that

$$A(-\alpha, n) = A(\alpha, -n) = A(\alpha, n) \quad (\alpha, n > 0).$$

These memory requirements exceed those of algorithm A. However, in contrast to method A algorithm (21)–(23) provides at every iteration s the simultaneous fulfilment of the incompressibility and boundary conditions. Incompressibility and boundary conditions can also be satisfied if a certain explicit/implicit algorithm without splitting is utilized. For instance, if instead of (20) we use Adams–Bashforth time advancement for the convective terms:

$$\mathbf{q}^{J+1} = \mathbf{q}^J + \Delta t \left(\frac{3}{2} N(\mathbf{q}^J) - \frac{1}{2} N(\mathbf{q}^{J-1})\right) + \Delta t\, \nu \tilde{\Delta} \mathbf{q}^{J+1/2} - \Delta t\, \nabla P^{J+1},$$

$$\tilde{\nabla} \cdot \mathbf{q}^{J+1} = 0, \quad \mathbf{q}^{J+1}|_{r=R} = 0,$$

then the discretized Navier–Stokes equations also have the form (23) (and finally (24)) with modified right-hand sides—vectors $\mathcal{L}$, $\mathcal{G}$, and $\mathcal{U}$. Storage requirements for collocation matrices therefore remain unchanged.

To improve these rather severe restrictions we suggest the following modification of the iteration technique (21):

$$\overset{(s)}{\mathbf{q}}{}^{J+1} = \mathbf{q}^J + \Delta t\, N(\overset{(s-1)}{\mathbf{q}}{}^{J+1/2}) + \Delta t\, \nu \tilde{\Delta} \overset{(s-1)}{\mathbf{q}}{}^{J+1/2} - \Delta t\, \tilde{\nabla} \overset{(s)}{P}{}^{J+1},$$

$$\tilde{\nabla} \cdot \overset{(s)}{\mathbf{q}}{}^{J+1} = 0, \quad \overset{(s)}{\mathbf{q}}{}^{J+1}|_{r=R} = 0. \tag{25}$$

Using then the same spatial discretization we finally obtain, instead of (23a)–(23d) (the case $n \neq 0$ as before),

$$(\overset{(s)}{f}{}^{J+1} + \Delta t\,(D^{(k)} - nR^{(k)})\overset{(s)}{P}{}^{J+1})_l = \tilde{\mathcal{L}}_l, \quad l = 1, 2, ..., Q_n^{(1)}, \tag{26a}$$

$$(\overset{(s)}{g}{}^{J+1} + \Delta t\,(D^{(k)} + nR^{(k)})\overset{(s)}{P}{}^{J+1})_l = \tilde{\mathcal{G}}_l, \quad l = 1, 2, ..., Q_n^{(2)}, \tag{26b}$$

$$(\overset{(s)}{u}{}^{J+1} + \Delta t\, i\alpha \overset{(s)}{P}{}^{J+1})_l = \tilde{\mathcal{U}}_l, \qquad l = 1, 2, ..., Q-1, \tag{26c}$$

$$((D^{(k)} + (n+1)R^{(k)})\overset{(s)}{f}{}^{J+1} + (D^{(k)} - (n-1)R^{(k)})\overset{(s)}{g}{}^{J+1} + 2i\alpha \overset{(s)}{u}{}^{J+1})_l = 0, \quad l = 0, 1, ..., Q-1. \tag{26d}$$

The set of Eqs. (26a)–(26d), (23e), (23f) can be solved in a more efficient way than with Eqs. (23). We eliminate $\overset{(s)}{f}{}^{J+1}$, $\overset{(s)}{g}{}^{J+1}$, and $\overset{(s)}{u}{}^{J+1}$ by taking

$$(D^{(k)} + (n+1)R^{(k)})(26a) + (D^{(k)} - (n-1)R^{(k)})(26b) + 2i\alpha(26c)$$

and setting it equal to zero (due to (26d)). The resulting equation for $\overset{(s)}{P}{}^{J+1}$ takes the form

$$(A - \alpha^2 E)x = b, \quad x = (\overset{(s)}{P}{}_0^{J+1}, \overset{(s)}{P}{}_1^{J+1}, ..., \overset{(s)}{P}{}_{Q-1}^{J+1})^{\mathrm{T}}, \tag{27}$$

where $A = A(n, \mathrm{Re}, Q, \Delta t)$ is a real nonsingular $Q \times Q$ matrix that is independent of the streamwise wavenumber α; E is the identity matrix; b is a known vector. We note that Eqs. (27) are obtained from the set (26a)–(26d), (23e), (23f) by means of the equivalent matrix operations. To solve (27) we can use the so-called collocation–diagonalization method (see, e.g., [14]) with memory requirements of about $2 \times N \times Q^2$ words. It is much better than in the previous cases considered. Vectors $\overset{(s)}{f}{}^{J+1}$, $\overset{(s)}{g}{}^{J+1}$, and $\overset{(s)}{u}{}^{J+1}$ can be obtained then from Eqs. (26a)–(26c). Direct simulation of the turbulent pipe flow shows that the iteration scheme (25)–(27) is a good choice.

In Section 7 we suggest a new method of spatial discretization admitting an efficient solution of the discretized Navier–Stokes equations for the more complicated case: when the iteration algorithm (21) is used. But first we turn to an algorithm that possesses certain conservation properties.

6. JACOBI COLLOCATION METHOD WITH DISCRETE ANALOGUES TO ENERGY CONSERVATION RELATIONS (*ALGORITHM* C)

It is well known (see, e.g., [26, 27, 29, 30]), that the stability characteristics of Navier–Stokes algorithms are closely connected with their ability to reproduce the so-called neutrality of the Navier–Stokes equations nonlinear and pressure terms. Under neutrality the zero contribution

$$\langle \mathbf{v} \cdot \nabla P \rangle_{r\varphi z} = 0, \quad \mathbf{v} \cdot (\mathbf{v} \times \boldsymbol{\omega}) = 0 \tag{28a}$$

of the total pressure and nonlinearity $\mathbf{v} \times \boldsymbol{\omega}$ to the equation for kinetic energy,

$$\frac{dE}{dt} = -\left\langle uv \frac{dV^0}{dr} \right\rangle_{r\varphi z} - \nu \langle (\nabla \times \mathbf{v})^2 \rangle_{r\varphi z}, \tag{28b}$$

where

$$E = \langle \mathbf{v}^2/2 \rangle_{r\varphi z} = \frac{1}{\pi R^2 Z} \int_{st} dr\, \mathbf{v}^2/2$$

is understood. The algorithm stated below possesses discrete analogues to the relations (28) and generalizes algorithm [30] to cylindrical geometry.

Solutions of Eqs. (19) are approximated by the polynomials

$$\begin{pmatrix}\mathbf{q}(r,t)\\ P(r,t)\end{pmatrix}=\sum_{l=0}^{Q}\begin{pmatrix}\mathbf{q}_l(t)\\ P_l(t)\end{pmatrix}\frac{h(x)}{(x-x_l)\,dh/dx(x_l)},$$
$$h(x)=(x-x_0)(x-x_Q)P_{Q-1}^{(2,1)}(x),\quad x=1-2r/R, \tag{29}$$

where $\mathbf{q}_l=\mathbf{q}(r_l,t)$, $P_l=P(r_l,t)$, $x_0=-1$, $x_Q=1$, and $x_l\in(-1,1)$, $l=1,2,\ldots,Q-1$, are the zeros of the Jacobi polynomial $P_{Q-1}^{(2,1)}(x)$.

The time integration of Eqs. (19) is carried out by means of the implicit second-order scheme (20). For spatial discretization the collocation technique with interpolation points $r_l=(1-x_l)R/2$, $l=0,1,\ldots,Q$, is used. As a result we obtain

$$(q_l^{(i),J+1}-q_l^{(i),J})/\Delta t=\Omega^0(r_l)\frac{1}{2}(f_l^{J+1/2}+g_l^{J+1/2})\delta_{i3}-i\alpha V^0(r_l)q_l^{(i),J+1/2}+F_l^{(i),J+1/2}+\nu(\tilde{\Delta}\mathbf{q}^{(i)})_l^{J+1/2}-(\tilde{\nabla}P^{(i)})_l^{J+1},\quad l=1,2,\ldots,Q_n^{(i)},\ i=1,2,3; \tag{30a}$$

$$(\tilde{\nabla}\cdot\mathbf{q})_l^{J+1}=0,\quad l=0,1,\ldots,Q-1; \tag{30b}$$

$$\mathbf{q}_0^{J+1}=0,\quad u_Q^{J+1}=P_Q^{J+1}=0\,(n\neq 0),\quad f_Q^{J+1}=0\,(n\neq -1),\quad g_Q^{J+1}=0\,(n\neq 1),\quad v_Q^{J+1}=w_Q^{J+1}=0\,(n=0). \tag{30c}$$

Here $q^{(i)}$, $\tilde{\nabla}P^{(i)}$, $\tilde{\Delta}\mathbf{q}^{(i)}$, $F^{(i)}$, $i=1,2,3$, are components of the corresponding vectors defined in (19b), (19c); $F_l^{(i),J+1/2}=F_l^{(i)}(\mathbf{q}^{J+1/2})$, $|m|\le M$, $|n|\le N$; $Q_{-1}^{(1)}=Q, Q_n^{(1)}=Q-1\ (n\neq -1)$; $Q_1^{(2)}=Q, Q_n^{(2)}=Q-1\ (n\neq 1)$; $Q_0^{(3)}=Q, Q_n^{(3)}=Q-1\ (n\neq 0)$; δ_{ij} is the Kronecker symbol.

Consider the Gauss quadrature formula

$$\frac{1}{R^2}\int_0^R rf(r)\,dr=\sum_{l=0}^{Q}c_l f(r_l),\quad r_l=R(1-x_l)/2; \tag{31}$$

it is precise for polynomials f of degree not higher than $2Q-1$.

It can be easily shown that

$$\langle\mathbf{v}^2\rangle_{\varphi z}=\mathcal{B}(\mathbf{q},\mathbf{q}),\quad \langle\mathbf{v}\cdot\nabla P\rangle_{\varphi z}=\mathcal{B}(\mathbf{q},\tilde{\nabla}P),\quad \langle\mathbf{v}\cdot(\mathbf{v}\times\boldsymbol{\omega})\rangle_{\varphi z}=\mathcal{B}(\mathbf{q},\mathcal{F})=0$$

where

$$\mathcal{B}(\mathbf{t},\mathbf{s})=\sum_{|m|\le M}\sum_{|n|\le N}(\xi_n t_{mn}^{(1)*}s_{mn}^{(1)}+\xi_n t_{mn}^{(2)*}s_{mn}^{(2)}+t_{mn}^{(3)*}s_{mn}^{(3)}),$$
$$\mathbf{t}(r,t)=(t^{(1)},t^{(2)},t^{(3)});\quad \mathbf{s}(r,t)=(s^{(1)},s^{(2)},s^{(3)}),\quad \xi_0=1,\quad \xi_n=1/2\,(n\neq 0). \tag{32}$$

From here and from relations (31) we obtain

$$2\sum_{l=0}^{Q}c_l\mathcal{B}(\mathbf{q}_l^{J+1/2},\tilde{\nabla}P_l^{J+1})\simeq\langle\mathbf{v}^{J+1/2},\nabla P^{J+1}\rangle_{r\varphi z}\simeq 0, \tag{33a}$$

$$\sum_{l=0}^{Q}c_l\mathcal{B}(\mathbf{q}_l^{J+1/2},\mathcal{F}_l^{J+1/2})=0, \tag{33b}$$

the discrete analogues of Eq. (28a). Both of the equalities in (33a) are approximate. The first one is because of the $2Q$ power of the polynomial

$$\mathcal{B}(\mathbf{q}^{J+1/2},\tilde{\nabla}P^{J+1});$$

the second one, is due to the fact that (30b) does not provide the identity fulfillment of the incompressibility condition.

Having multiplied (30a) on $2c_l(\mathbf{q}_l^{J+1/2})^*$, we take the summation over m and n in accordance with rule (32) and, afterwards, the summation over $l=0,1,\ldots,Q$. Because of (33) we obtain that the terms $(\tilde{\nabla}P^{(i)})^{J+1}$ and $F^{(i),J+1/2}$ do not contribute to the positive definite quadratic form

$$\tilde{E}^{J+1}=\sum_{l=0}^{Q}c_l\mathcal{B}(\mathbf{q}_l^{J+1},\mathbf{q}_l^{J+1})$$

that approximately equals the kinetic energy E^{J+1}.

We suggest solving Eqs. (30) by means of the successive approximations methods (21) or (25), where the resulting equations are similar to (23) or to (26), respectively.

The experience of our Navier–Stokes turbulence simulations shows that the main advantage of algorithms possessing discrete analogues to neutrality conditions (28) is their ability to carry out stable substantial time step calculations of the latest stages of the laminar-turbulent transition. Algorithm C is among these methods. On a certain stage of transition an abrupt increase of amplitudes of the disturbances initially superimposed on the laminar Poiseuille flow takes place. To calculate an explosive growth of amplitudes (Orszag and Kells [1] call it the "breakdown to turbulence") directly preceding the establishment of a statistically stationary (fully developed) turbulent flow regime is the most difficult computational problem, especially for algorithms without conservation properties. See, e.g., [31], where the author had to lower repeatedly the value of time step to pass this stage of transition. In the majority of works devoted to direct Navier–Stokes simulation of turbulence the difficulty under consideration is not mentioned at all. Apparently, flow fields that are already "close" to fully developed turbulent regimes are taken as the starting point (initial condition) for these calculations. In many other works only the early stages of transition are investigated.

Finally, we note that at the same number of collocation nodes in algorithms A, B, and C, the latter has the lowest accuracy: the viscous sublayer ($0\le y^+\le 7$, $y^+=(R-r)u_\tau/\nu$, u_τ is the shear wall velocity) of the turbulent pipe flow computed at

Re = 4000 and $Q + 1 = 33$ in [20, 21] contains seven nodes for algorithms A and B and only five nodes for algorithm C.

7. PSEUDOSPECTRAL ALGORITHM ADMITTING AN EFFICIENT SOLUTION OF THE DISCRETE NAVIER–STOKES EQUATIONS (*ALGORITHM* D)

Consider an algorithm admitting an efficient solution of the discrete Navier–Stokes equations. For this purpose we perform the change of dependent variables in Eqs. (19) introducing $\hat{\mathbf{q}}$ and $\hat{P}$ according to relations (8).

Approximating the sought-for solution by an interpolation polynomial

$$\begin{pmatrix} \hat{\mathbf{q}} \\ \hat{P} \end{pmatrix} = \sum_{j=0}^{Q} \begin{pmatrix} \hat{\mathbf{q}}_j(t) \\ \hat{P}_j(t) \end{pmatrix} h_j^{(0)}(r), \quad r_j = R\cos(\pi j/2Q), \tag{34}$$

where $h_j^{(0)}(r)$ is prescribed by (13b), and applying the pseudospectral method and time integration scheme of (21), we obtain (for the case $n > 0$)

$$(\hat{L}\overset{(s)}{\hat{f}}{}^{J+1} - B^{(0)}\overset{(s)}{\hat{P}}{}^{J+1})_l = \hat{\mathcal{L}}_l, \qquad l = 1, 2, ..., Q, \tag{35a}$$

$$(\hat{G}\overset{(s)}{\hat{g}}{}^{J+1} - (\hat{D} + 2nE)\overset{(s)}{\hat{P}}{}^{J+1})_l = \hat{\mathcal{G}}_l, \quad l = 1, 2, ..., Q, \tag{35b}$$

$$(\hat{U}\overset{(s)}{\hat{u}}{}^{J+1})_l - i\alpha\overset{(s)}{\hat{P}}{}_l^{J+1} = \hat{\mathcal{U}}_l, \qquad l = 1, 2, ..., Q, \tag{35c}$$

$$\overset{(s)}{\hat{f}}{}_0^{J+1} = \overset{(s)}{\hat{g}}{}_0^{J+1} = \overset{(s)}{\hat{u}}{}_0^{J+1} = 0, \tag{35d}$$

$$((0.5\hat{D} + (n+1)E)\overset{(s)}{\hat{f}}{}^{J+1} + 0.5B^{(0)}\overset{(s)}{\hat{g}}{}^{J+1})_l + i\alpha\overset{(s)}{\hat{u}}{}_l^{J+1} = 0, \quad l = 0, 1, ..., Q. \tag{35e}$$

Here

$\hat{f} = (\hat{f}_0, \hat{f}_1, ..., \hat{f}_Q)^{\mathrm{T}}$ with the same notation used for $\hat{g}$, $\hat{u}$, $\hat{P}$,

$$\begin{Bmatrix} \hat{L} \\ \hat{G} \\ \hat{U} \end{Bmatrix} = \frac{\nu}{2}(C^{(0)} + \begin{Bmatrix} 2n+3 \\ 2n-1 \\ 2n+1 \end{Bmatrix} B^{(0)} - \alpha^2 E) - \frac{1}{\Delta t}E,$$

where E is the identity $(Q+1) \times (Q+1)$ matrix, $C^{(0)}$ and $B^{(0)}$ are defined by (14),

$$\hat{D}_{lj} = \left(r\frac{d}{dr}h_j^{(0)}\right)\Big|_{r=r_l}, \quad l, j = 0, 1, ..., Q,$$

and $(\hat{\mathcal{L}}, \hat{\mathcal{G}}, \hat{\mathcal{U}})_l$ are values known at the iteration s.

A new procedure for solving Eqs. (35) can be suggested that is more efficient than previously used for Eqs. (23) and (30). The new solver is based on the matrix identities

$$\begin{aligned} &(\hat{D} + 2(n+1)E)\hat{L} = \hat{U}(\hat{D} + 2(n+1)E), \\ &B^{(0)}\hat{G} = \hat{U}B^{(0)}, \\ &(\hat{D} + 2(n+1)E)B^{(0)} = B^{(0)}(\hat{D} + 2nE) = C^{(0)} + (2n+1)B^{(0)}, \end{aligned} \tag{36}$$

that follows from our lemma.

LEMMA. *Let T and S be differential operators: $r(d/dr)$, $\frac{1}{r}(d/dr)$, or d^2/dr^2 defined on the interpolation polynomials* (34). *Then for the matrices T, S, H, with the elements*

$$T_{lj} = (Th_j^{(0)})|_{r=r_l}, \quad S_{lj} = (Sh_j^{(0)})|_{r=r_l}, H_{lj} = (TSh_j^{(0)})|_{r=r_l},$$

$$l, j = 0, 1, ..., Q,$$

the following matrix identity is correct:

$$H = TS.$$

Using (36), we replace (35e) by the equivalent set of Eqs. (37):

$$\begin{aligned} &((C^{(0)} + (2n+1)B^{(0)} - \alpha^2 E)\overset{(s)}{\hat{P}}{}^{J+1})_l = \hat{\mathcal{P}}_l, \quad l = 1, 2, ..., Q, \\ &((0.5\hat{D} + (n+1)E)\overset{(s)}{\hat{f}}{}^{J+1} + 0.5B^{(0)}\overset{(s)}{\hat{g}}{}^{J+1})_0 + i\alpha\overset{(s)}{\hat{u}}{}_0^{J+1} = 0, \\ &\hat{\mathcal{P}}_l = -\sum_{j=1}^{Q}(0.5\hat{D} + (n+1)E)_{lj}\hat{\mathcal{L}}_j - (0.5\hat{D} + (n+1)E)_{l0}\overset{(s)}{\hat{\tau}}{}^{(1)} \\ &\qquad - \sum_{j=1}^{Q} B_{lj}^{(0)}\hat{\mathcal{G}}_j - B_{l0}^{(0)}\overset{(s)}{\hat{\tau}}{}^{(2)} - i\alpha\hat{\mathcal{U}}_l, \\ &\overset{(s)}{\hat{\tau}}{}^{(1)} = (\hat{L}\overset{(s)}{\hat{f}}{}^{J+1} - B^{(0)}\overset{(s)}{\hat{P}}{}^{J+1})_0, \\ &\overset{(s)}{\hat{\tau}}{}^{(2)} = (\hat{G}\overset{(s)}{\hat{g}}{}^{J+1} - (\hat{D} + 2nE)\overset{(s)}{\hat{P}}{}^{J+1})_0. \end{aligned} \tag{37}$$

Equations (35a)–(35d), (37) are similar to Eqs. (3.5) in [8] and can be solved by means of an efficient method based on the Sherman–Morrison–Woodbury formula.

If we change $\overset{(s)}{\hat{\tau}}{}^{(1,2)}$ in Eqs. (37) to $\overset{(s-1)}{\hat{\tau}}{}^{(1,2)}$ values already known at iteration s, we can solve Eqs. (35a)–(35d), (37) by means of the usual influence matrix technique. In the course of the solution one should use the possibility of diagonalization of the matrix operators $A + \varphi(n)B - \alpha^2 E$ by means of transferring them to the matrix $A + \varphi(n)B$ eigenvector space.

TABLE I

Convergence of the Least Stable Eigenvalues at $\mathrm{Re}_0 = 9600$, $\alpha = n = 1$

	$\overline{\lambda}_1$	
	Salwen, Cotton, & Grosch [33]	
	−.02317	−.95048 i
	Leonard & Wray [22]	
$N + 2 = 22$	−.02312	−.95050 i
27	−.02317074	−.95048142 i
32	−.023170795769	−.950481396659 i
37	−.023170795764	−.950481396668 i
	Algorithm B	
$Q + 1 = 22$	−.02318	−.95049 i
27	−.02317072	−.9504811 i
32	−.023170797	−.950481399 i
37	−.023170795759	−.950481396659 i
42	−.02317079576503	−.95048139666992 i
47	−.02317079576500417	−.950481396669903170 i
52	−.02317079576500421524	−.950481396669903170 i
57	−.023170795765004215205	−.950481396699031794844 i
62	−.023170795765004215205	−.950481396699031794843 i
	Algorithm C	
$Q + 1 = 22$	−.02308	−.95043 i
27	−.02316	−.9504808 i
32	−.0231705	−.9504817 i
37	−.023170799	−.95048141 i
42	−.0231707961	−.950481396696 i
47	−.0231707957653	−.950481396663 i
52	−.0231707957649	−.95048139666988 i
57	−.0231707957650045	−.9504813966699037 i
62	−.0231707957650042	−.950481396669903178 i
	Algorithm D	
$Q + 1 = 22$	−.02318	−.950497 i
27	−.0231710	−.9504815 i
32	−.023170795	−.9504813961 i
37	−.023170795770	−.950481396671 i
42	−.02317079576499	−.950481396669905 i
47	−.02317079576500423	−.950481396669903171 i
52	−.023170795765004215199	−.950481396669903170 i
57	−.023170795765004215205	−.950481396699031794843 i
62	−.023170795765004215205	−.950481396699031794843 i

We emphasize here that Eqs. (23) and (30) cannot be written in the form similar to (35a)–(35d), (37).

8. ACCURACY AND STABILITY CHARACTERISTICS A PRIORI ESTIMATES

Navier–Stokes simulation of turbulence makes high demands of the algorithm's accuracy and stability. Due to nonlinearity of the discrete Navier–Stokes equations complete a priori investigation of their characteristics is a very complicated problem. Some preliminary estimates can be obtained by means of a spectral technique [32] based on the requirement of closeness of spectral characteristics of the linear problem of hydrodynamic stability and of the discrete linearized Navier–Stokes equations. In other words the numerical method must properly reproduce time evolution of small disturbances of Navier–Stokes laminar stationary solutions $\mathbf{V}^0$, P^0.

Time evolution of these disturbances is determined by the solutions (the case $\alpha^2 + n^2 \neq 0$)

$$\begin{pmatrix} \mathbf{v}(\mathbf{r}, t) \\ P(r, t) \end{pmatrix} = \exp(i\alpha z + in\varphi) \sum_{k=1}^{\infty} a_k \begin{pmatrix} \mathbf{v}_k(r) \\ P_k(r) \end{pmatrix} \exp(\lambda_k t),$$

$$\alpha = 2\pi/Z, n = 0, \pm 1, \pm 2, ..., \tag{38}$$

of Navier–Stokes equations linearized on $\mathbf{V}^0$, P^0. Here $\lambda_k = \lambda_k(\alpha, n, \mathrm{Re}_0)$, $re\lambda_k \geq re\lambda_{k+1}$, $k = 1, 2, ...$, eigenvalues, and $\mathbf{v}_k$, P_k, eigenfunctions, of the problem

TABLE II

Nine First Eigenvalues at $\mathrm{Re}_0 = 9600$, $\alpha = n = 1$

k	λ_k	
1	−.023170795765004215	−.950481396669903179 i
2	−.047586081470067203	−.276842738665522835 i
3	−.049457844142055134	−.976681656624860195 i
4	−.049939191128628251	−.918858226047491525 i
5	−.077299966311528997	−.888174706374086770 i
6	−.080880040967004304	−.949767712360271294 i
7	−.082053066334950830	−.148388982676809416 i
8	−.104964149781276119	−.857937705687900834 i
9	−.111346833528618748	−.922252896844621581 i

Note. True digits that can be obtained with $Q + 1 = 32$ collocation nodes are underlined.

$$\lambda \mathbf{v} = -\nabla P + \mathbf{v} \times \boldsymbol{\Omega}^0 + \mathbf{V}^0 \times \boldsymbol{\omega} + \frac{1}{\mathrm{Re}_0} \nabla^2 \mathbf{v}, \quad \nabla \cdot \mathbf{v} = 0, \mathbf{v}|_{r=R} = 0, \quad (39)$$

where $\mathrm{Re}_0 = u^0_{CL} R/\nu$, $u^0_{CL} = V^0|_{r=0}$. Approximate solutions of Eqs. (39) can be obtained by means of spatial discretizations used in algorithms B, C, or D. Instead of $\{\lambda_k(\alpha, n, \mathrm{Re}_0)\}_{k=1}^{\infty}$ we receive then the finite number of approximate eigenvalues $\{\bar{\lambda}_k(\alpha, n, \mathrm{Re}_0, Q)\}_{k=1}^{K}$.

In Table I for $\alpha = n = 1$, $\mathrm{Re}_0 = 9600$, we compare the values of $\bar{\lambda}_1$ with the corresponding results from Leonard and Wray [22] and Salwen *et al.* [33]. Here $N + 2$ and $Q + 1$ equal the total number of degrees of freedom in [22] and in our work, respectively. One can see that the convergence rates of algorithms B and D are comparable [22], while that of algorithm C is relatively lower. Nevertheless, in all cases almost the "exponential" (in Q) convergence is demonstrated, which allows us to state that algorithms B, C, and D (as well as [22]) are all methods "without satiation." The latter is typical for spectral methods, the corresponding concept was introduced by Babenko in [34].

TABLE III

Convergence of Eigenvalues at $\mathrm{Re}_0 = 9600$ and $\alpha = n = 20$

$Q + 1$	k	$\bar{\lambda}_k$	
32	1	−.357184	−13.1939 i
	2	−.359880	−12.2153 i
	3	−.361510	−14.1407 i
	4	−.369130	−11.2147 i
62	1	−.713982	−1.10611 i
	2	−.813027	−1.84159 i
	3	−.857136	−15.8335 i
	4	−.858351	−15.4049 i
82	1	−.713982	−1.10611 i
	2	−.813027	−1.84159 i
	3	−1.18296	−1.92255 i
	4	−1.31254	−16.7317 i
102	1	−.713982	−1.10611 i
	2	−.813027	−1.84159 i
	3	−1.18296	−1.92255 i
	4	−1.33409	−18.5810 i
122	1	−.713982	−1.10611 i
	2	−.813027	−1.84159 i
	3	−1.18296	−1.92255 i
	4	−1.33409	−18.5810 i

Tables II and III permit us to estimate the number of collocation points necessary for adequate polynomial approximation of the spectral problem (39) when $\mathrm{Re}_0 = 9600$, $\alpha = n = 1$, and $\alpha = n = 20$. As it is often stated (see, e.g., Fig. 1 in [22]) spectral (pseudospectral) methods approximate a considerable number ($K \gg 1$) of eigenvalues $\{\bar{\lambda}_k\}_{k=1}^{K}$ for a relatively small number of expansion functions (collocation nodes). This is also true for spatial approximations B, C, and D. In Table II (the case of algorithm B) we show nine first eigenvalues $\{\bar{\lambda}_k\}_{k=1}^{9}$ when $\alpha = n = 1$. Digits that coincided for computations with a number of different collocation points $Q + 1 = 102$, 129 were assumed to be truly significant. We then underline the digits which coincide also for the calculation with $Q + 1 = 32$ nodes. Thus, a large number of eigenvalues can be accurately calculated with only 32 collocation points in the r-direction.

The situation changes for large values of wavenumbers $\alpha = n = 20$. Table II shows us that no one true eigenvalue can be obtained in this case with $Q + 1 = 32$ nodes. And what is more, only two eigenvalues can be correctly computed with much finer resolution when $Q + 1 = 62$. Besides, this is quite an ordinary situation for spectral problems of (39) type. We demonstrate it here once more in order to stress the necessity of investigating the spectral characteristics of Eqs. (39) for the full range of wavenumbers that we intend to take into account during the nonlinear Navier–Stokes calculations. However, the common practice at present is to test the time evolution of the first (least stable) eigenvalue $\bar{\lambda}_1$ only. The above-mentioned (and some other) inaccuracies in the description of Eqs. (39) spectrum can be, in addition, amplified by the time advancement scheme. To investigate the latter influence on the stability and accuracy characteristics of algorithms, without direct time-consuming Navier–Stokes integration in time, we suggest the following technique.

Consider for definiteness Eqs. (15)–(17) of algorithm A and assume that nonlinearity $\mathbf{v} \times \boldsymbol{\omega}$ equals zero. The resulting equations appear to be the discrete analogue of the linearized Navier–Stokes equations and possess solutions that, similarly to (38), are defined by eigenvectors and eigenvalues of conversion matrix from time step t_j to time step t_{j+1}. Using these eigenvalues the spectra $\{\lambda_k(\alpha, n, \mathrm{Re}_0, Q, \Delta t, s)\}$ of a discrete problem can be computed and compared with the spectra $\bar{\lambda}_k(\alpha, n, \mathrm{Re}_0, Q)\}$ of the corresponding differential problem.

TABLE IV

The Least Stable Eigenvalues of the Discrete and Differential Problems

α, n	Δt	$\tilde{\lambda}_1(\alpha, n, \mathrm{Re}_0, Q, \Delta t, s)$ $\langle \mathrm{Re}_0 = 4000, Q = 32, s = 1\rangle$	$\bar{\lambda}_1(\alpha, n, \mathrm{Re}_0, Q)$ $\langle \mathrm{Re}_0 = 4000\rangle$
1, 1	.00625	$-.357 \times 10^{-1} - i\ .923$	$-.358 \times 10^{-1} - i\ .923$ $\langle Q = 32\rangle$
			$-.358 \times 10^{-1} - i\ .923$ $\langle Q = 64\rangle$
4, 4	.2	$-.293 - i\ .493$	$-.189 - i\ .372 \times 10^{+1}$ $\langle Q = 32\rangle$
	.1	$-.224 - i\ .369 \times 10^{+1}$	$-.189 - i\ .372 \times 10^{+1}$ $\langle Q = 64\rangle$
	.00625	$-.189 - i\ .372 \times 10^{+1}$	
10, 10	.1	$-.529 - i\ .453 \times 10^{+1}$	$-.529 - i\ .800 \times 10^{+1}$ $\langle Q = 32\rangle$
	.05	$-.371 - i\ .657 \times 10^{+1}$	$-.574 - i\ .928$ $\langle Q = 64\rangle$
	.00625	$-.284 - i\ .714 \times 10^{+1}$	$-.574 - i\ .928$ $\langle Q = 128\rangle$
	.0001	$-.275 - i\ .715 \times 10^{+1}$	
	.00001	$-.275 - i\ .715 \times 10^{+1}$	
20, 20	.05	$+.172 \times 10^{+2} + i\ .240 \times 10^{+2}$	$-.881 - i\ .135 \times 10^{+2}$ $\langle Q = 32\rangle$
	.025	$-.536 - i\ .104 \times 10^{+2}$	$-.104 \times 10^{+1} - i\ .148 \times 10^{+1}$ $\langle Q = 64\rangle$
	.00625	$-.410 - i\ .115 \times 10^{+2}$	$-.104 \times 10^{+1} - i\ .148 \times 10^{+1}$ $\langle Q = 128\rangle$
	.0001	$-.369 - i\ .115 \times 10^{+2}$	
	.00001	$-.369 - i\ .115 \times 10^{+2}$	
42, 42	.0125	$+.669 \times 10^{+2} + i\ .514 \times 10^{+2}$	$-.198 \times 10^{+1} - i\ .206 \times 10^{+2}$ $\langle Q = 32\rangle$
	.00625	$-.125 \times 10^{+1} - i\ .182 \times 10^{+2}$	$-.227 \times 10^{+1} - i\ .242 \times 10^{+1}$ $\langle Q = 64\rangle$
	.0001	$-.103 \times 10^{+1} - i\ .202 \times 10^{+2}$	$-.227 \times 10^{+1} - i\ .242 \times 10^{+1}$ $\langle Q = 128\rangle$
	.00001	$-.102 \times 10^{+1} - i\ .202 \times 10^{+2}$	

Without loss of generality we shall explain the technology of spectral analysis in the case $\alpha = m\alpha_0 \neq 0$, $n \neq 0$. It follows from Eqs. (11b), (15), and (16) that

$$\mathbf{V} = A\overset{(s)}{\tilde{\mathbf{V}}}{}^{J+1},$$

where

$$\mathbf{V} = (u_{mn1}, \ldots, u_{mn,Q-1}, v_{mn1}, \ldots, v_{mnQ_*}, w_{mn1}, \ldots, w_{mnQ_*})^{\mathrm{T}},$$

$$Q_* = Q\ (|n| = 1), \qquad Q_* = Q - 1\ (|n| \neq 1)$$

and A is a complex square matrix. From here and Eqs. (17) we obtain

$$\overset{(s)}{\mathbf{V}}{}^{J+1} = -\frac{1}{\Delta t} B^{-1} A \overset{(s)}{\tilde{\mathbf{V}}}{}^{J+1} \quad (s \geq 0), \tag{40}$$

where B is a real nonsingular matrix approximating the differential operator at the left-hand side of Eq. (17a) with boundary conditions (17b).

In the case $s = 0$, instead of Eq. (12), we have

$$\overset{(0)}{\tilde{\mathbf{v}}}{}^{J+1}_{mn} = \mathbf{v}^J_{mn} + \Delta t\, \Omega^0 \left(\tfrac{3}{2} v^J_{mn} - \tfrac{1}{2} v^{J-1}_{mn}\right)\mathbf{e}_z - i\alpha\, \Delta t\, V^0 \left(\tfrac{3}{2}\mathbf{v}^J_{mn} - \tfrac{1}{2}\mathbf{v}^{J-1}_{mn}\right)$$

$$+ \Delta t\, \nu \left(\nabla^2 - \frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr}\right)\left(\frac{3}{2}\mathbf{v}^J_{mn} - \frac{1}{2}\mathbf{v}^{J-1}_{mn}\right).$$

From here with regard to (40) we receive

$$\overset{(0)}{\tilde{\mathbf{V}}}{}^{J+1} = T_1 \tilde{\mathbf{V}}^J - T_2 \tilde{\mathbf{V}}^{J-1}, \tag{41a}$$

where complex $(Q - 1 + 2Q_*) \times (Q - 1 + 2Q_*)$ matrices T_1, T_2 are functions of α, n, Re_0, Q and Δt. For $s \geq 1$ we have, instead of (41a),

$$\overset{(s)}{\tilde{\mathbf{V}}}{}^{J+1} = T_2 \overset{(s-1)}{\tilde{\mathbf{V}}}{}^{J+1} + T_3 \tilde{\mathbf{V}}^J, \tag{41b}$$

where T_3 is also square complex matrix of the $(Q - 1 + 2Q_*)$th order.

Using the recurrence relations (41) one can finally obtain

$$\overset{(s)}{\tilde{\mathbf{V}}}{}^{J+1} = T_4 \tilde{\mathbf{V}}^J + (-T_2)^s \tilde{\mathbf{V}}^{J-1} \quad (s \geq 1),$$

where

$$T_4 = (T_2^s T_1 + (T_2^{s-1} + T_2^{s-2} + \cdots + T_2 + E)T_3).$$

Since the matrices T_4 and $(-T_2)^s$ do not depend on the index J,

$$\overset{(s)}{\tilde{\mathbf{V}}}{}^{J+1} = \overset{(s)}{\rho}{}^{J+1}\tilde{\mathbf{V}},$$

where $\overset{(s)}{\rho}$ and $\tilde{\tilde{v}}$ are among the eigenvalues and eigenvectors of the spectral problem

$$\overset{(s)}{\rho}\mathbf{x} = \begin{pmatrix} T_4 & (-T_2)^s \\ E & 0 \end{pmatrix}\mathbf{x}, \quad \mathbf{x} = (\overset{(s)}{\rho}\tilde{\mathbf{V}}, \tilde{\mathbf{V}})^{\mathrm{T}},$$

that can be solved by means of the QR algorithm.

Eigenvalues $\tilde{\lambda}_k$ are calculated then according to the following formula:

$$\tilde{\lambda}_k(\alpha, n, \mathrm{Re}_0, Q, \Delta t, s) = \frac{1}{\Delta t}\ln \overset{(s)}{\rho}_k, \quad k = 1, \ldots, 2(Q - 1 + 2Q_*).$$

Comparison of the sets $\{\bar{\lambda}_k\}$ and $\{\tilde{\lambda}_k\}$, $re\lambda_k \geq re\lambda_{k+1}$, $k = 1, 2, \ldots$, permits us to obtain important information about the stability and accuracy characteristics of the numerical scheme at different values $\alpha, n, \mathrm{Re}_0, Q, \Delta t, s$ of the problem parameters.

Periodic with respect to z with period $Z = \pi 2R$ nonstationary Navier–Stokes solutions describing the turbulent flow regimes in a circular pipe at Re = 4000 were obtained in [20, 21]. The calculations were performed with $(Q + 1) \times (2N + 1) \times (2M + 1) = 33 \times 9 \times 9$, $33 \times 21 \times 21$, and $33 \times 41 \times 41$ basis functions in r, φ, z. Nowadays more precise computations with $33 \times 85 \times 85$ functions are also carried out. In all the cases algorithm A was used with $Q = 32$, $s = 1$, and, depending on the number of basis functions, with time steps $\Delta t = 0.1$, 0.05, 0.025, and 0.00625, respectively. Here the radius R is chosen as a unit of length and the centre-line velocity u^0_{CL} at $\mathrm{Re}_0 = \mathrm{Re} = 4000$ as a unit of velocity. For $33 \times 9 \times 9$, $33 \times 21 \times 21$, $33 \times 41 \times 41$, and $33 \times 85 \times 85$ computer runs instability was observed at $\Delta t = 0.2$, $\Delta t = 0.1$, $\Delta t = 0.05$, and $\Delta t = 0.0125$, respectively.

In Table IV we compare the least stable eigenvalues $\bar{\lambda}_1$ and $\tilde{\lambda}_1$ of the differential and discrete spectral problems. For $M, N \geq 20$ in the linear approach algorithm A loses stability approximately at the same values of Δt as it does in the nonlinear case. In fact (cf. Table IV), the stationary solution (5) is stable in the linear approach at $\Delta t = 0.00625$ and unstable at $\Delta t = 0.0125$ with respect to the Fourier harmonic with $\alpha = 42$, $n = 42$ ($Z = 2\pi$ and $M = N = 42$ in representation (7)); similarly, it is stable at $\Delta t = 0.025$ and unstable at $\Delta t = 0.05$ with respect to the harmonic with $\alpha = 20$, $n = 20$ ($M = N = 20$). In the case $M = N = 4$, although the stability survives, while Δt increases from 0.1 to 0.2, the spectra undergo undesirable qualitative changes.

Data of Table IV allow us also to estimate the rate of convergene of eigenvalues $\tilde{\lambda}_1$ and the number $Q + 1$ of collocation points necessary for the adequate description of Fourier harmonics with different wavenumbers α, n when $\mathrm{Re}_0 = 4000$.

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