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Numerical Methods for the Simulation of Turbulence

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Two schemes for the numerical solution of the Navier–Stokes equations at moderate Reynolds number are discussed. The essential ingredient of the present methods is the use of the fast Fourier transform. In one scheme, discrete Fourier transformation is used to compute the convolution sums appearing in the formally Fourier-transformed Navier–Stokes equations. This results in an aliasing-free, energetically conservative (when $\nu = 0$) scheme that can be used convincingly as a model on which to test turbulence theories. The second scheme calculates in real space. Fast Fourier transform is used to solve Poisson's equation for the pressure. The latter scheme offers the advantages of speed and flexibility. The schemes are critically compared and a survey of applications is made.

I. INTRODUCTION

In this paper we introduce and analyze two schemes for the numerical solution of the Navier–Stokes equations at moderate Reynolds number. These schemes are being used in an extensive series of numerical experiments which will be reported in detail elsewhere.

The present considerations originated in an attempt to assess the feasibility of testing turbulence theories (particularly those of Refs. 1–3) by comparison with the results of three-dimensional numerical calculations. In contrast to the lack of control of initial conditions in comparing turbulence theory with the results of laboratory experiment, numerical experiments offer the advantage that initial conditions may be matched to those used by the turbulence theory. Specifically, it is possible to construct an initial random velocity field having a multivariate Gaussian distribution and arbitrary energy spectrum (see Appendix).

It appears that available computer facilities (meaning an IBM Model 360–95 computer with 5×10^5 double-precision word memory and typical multiplication time of order 1 μsec) limit direct numerical calculation of turbulent flows to $R_\lambda \sim 20$ (where R_λ is the Reynolds number based on the Taylor microscale[4]). The estimate $R_\lambda \sim 20$ is discussed in Sec. V. These Reynolds numbers are characteristic of some classic wind-tunnel experiments.[5] In this range of R_λ, we shall see that direct solution of the Navier–Stokes equations is competitive in terms of computation time with solution of the equations of the turbulence theories.

In view of these estimates, one may question what advantages there are to formulating and solving a turbulence theory rather than performing direct simulation of turbulent flows on computers. In the author's opinion, there are at least three evident benefits of pursuing turbulence theory at this time. First, it is apparent that a satisfactory turbulence theory implies a much deeper understanding of turbulent flow than do stacks of computer output. Second, the statistically averaged quantities of turbulence theory exhibit symmetries and invariances, such as isotropy and homogeneity, not evident in individual realizations.

Third, the statistically averaged quantities of turbulence theories are *smooth* functions of their arguments. Accurate integration of the equations of motion of a single realization of homogeneous turbulence requires retaining as dynamical variables all Fourier modes up to a cutoff wavenumber K lying within the dissipation range (see Secs. II and IV). Turbulence theory suggests that it is necessary to choose K proportional to $R_\lambda^{3/2}$, so that the number of dynamical variables is proportional to $K^3 \propto R_\lambda^{9/2}$. In contrast, since spectra typically have power-law behavior outside the dissipation range, accurate integration of the equations of turbulence theory requires only a fixed number of dynamical variables per octave of wavenumber. It follows that the number of dynamical variables is proportional to a low power of $\log K \propto \log R_\lambda$. Consequently, calculation of a turbulence theory at, say, $R_\lambda \sim 100$ requires few more mesh points than calculation at $R_\lambda \sim 20$. For these three reasons, we choose to justify our studies as tests of turbulence theories, rather than as simulations for their own sake. Direct simulation of very high Reynolds number turbulence appears to be beyond at least the next few genera-

[1] R. H. Kraichnan, J. Fluid Mech. **5**, 497 (1959); Phys. Fluids **7**, 1030 (1964).
[2] R. H. Kraichnan, Phys. Fluids **8**, 575 (1965); **9**, 1728 (1966).
[3] R. H. Kraichnan, J. Math. Phys. **2**, 124 (1961); Phys. Rev. **174**, 240 (1968).
[4] G. K. Batchelor, *Theory of Homogeneous Turbulence* (Cambridge University Press, Cambridge, England, 1953), p. 47.
[5] R. W. Stewart and A. A. Townsend, Phil. Trans. Roy. Soc. (London) **A243**, 359 (1951).

tions of computers. However, it is not beyond turbulence theory.[2]

In Sec. II, we describe a Fourier mode calculation of homogeneous turbulence. In Sec. III, we describe a real-space numerical scheme for homogeneous turbulence having the advantage of speed and flexibility over the Fourier mode method. In Sec. IV, we compare the methods of Secs. II and III, and in Sec. V we describe some applications that have been and are being made.

II. DISCRETE FOURIER MODES

The Navier–Stokes equations for incompressible fluid flow may be written

$$\frac{\partial \mathbf{v}(\mathbf{x}, t)}{\partial t} + \mathbf{v}(\mathbf{x}, t)\cdot\nabla\mathbf{v}(\mathbf{x}, t) = -\nabla p(\mathbf{x}, t) + \nu\nabla^2\mathbf{v}(\mathbf{x}, t), \quad (1)$$

$$\nabla\cdot\mathbf{v}(\mathbf{x}, t) = 0, \quad (2)$$

where $\mathbf{v}(\mathbf{x}, t)$ is the velocity field, $p(\mathbf{x}, t)$ the pressure, and ν the kinematic viscosity. Approximately homogeneous turbulence may be most conveniently realized numerically by imposing periodic boundary conditions,

$$\mathbf{v}(\mathbf{x} + \mathbf{n}, t) = \mathbf{v}(\mathbf{x}, t),$$

where $\mathbf{n} = (n_1, n_2, n_3)$, $n_i = 0, \pm1, \pm2, \cdots$.

With this assumption of periodicity, the velocity field may be written

$$\mathbf{v}(\mathbf{x}, t) = \sum_{\mathbf{k}} \mathbf{u}(\mathbf{k}, t) \exp(i\mathbf{k}\cdot\mathbf{x}), \quad (3)$$

where $\mathbf{k} = 2\pi\mathbf{n}$. It may be shown[6] that Eqs. (1) and (2) become

$$\left(\frac{\partial}{\partial t} + \nu k^2\right)u_\alpha(\mathbf{k}, t) = -\frac{i}{2}P_{\alpha\beta\gamma}(\mathbf{k}) \sum_{\mathbf{p}} u_\beta(\mathbf{p})u_\gamma(\mathbf{k} - \mathbf{p}), \quad (4)$$

$$k_\alpha u_\alpha(\mathbf{k}, 0) = 0, \quad (5)$$

$$P_{\alpha\beta\gamma}(\mathbf{k}) = k_\beta P_{\alpha\gamma}(\mathbf{k}) + k_\gamma P_{\alpha\beta}(\mathbf{k}), \qquad P_{\alpha\beta}(k) = \delta_{\alpha\beta} - k_\alpha k_\beta/k^2, \quad (6)$$

where the summation convention is implied. Equation (4) is not yet suitable for numerical integration because of the infinity of coupled $\mathbf{k}$ (owing to the continuum of points in the unit box).

A natural truncation of the system (4) is to cut off artificially all wavevector sums in Eqs. (3) and (4). Such a cutoff would result if the viscosity acting on modes above the cutoff were allowed to become infinite. An asymptotic ordering argument indicates that modes subject to such a viscosity are indeed cut off—in effect, they can never be excited. The most convenient cutoff for the work to follow is $-2\pi K \leq k_i < 2\pi K (i = 1, 2, 3)$, where $2\pi K$ is the cutoff, although the most convenient cutoff for isotropic turbulence theory is $|\mathbf{k}| \leq 2\pi K$.

In this way we obtain

$$\left(\frac{\partial}{\partial t} + \nu k^2\right)u_\alpha(\mathbf{k}, t) = -\frac{i}{2}P_{\alpha\beta\gamma}(\mathbf{k}) \sum{}' u_\beta(\mathbf{p}, t)u_\gamma(\mathbf{k} - \mathbf{p}, t) \quad (-2\pi K \leq k_i < 2\pi K), \quad (7)$$

where $\sum'$ extends over all wavevectors $\mathbf{p}$ satisfying $-2\pi K \leq p_i < 2\pi K$ *and* $-2\pi K \leq k_i - p_i < 2\pi K (i = 1, 2, 3)$. It may be shown that when $\nu = 0$, Eq. (7) conserves energy:

$$\frac{\partial}{\partial t} \sum u_\alpha(\mathbf{k}, t)u_\alpha(-\mathbf{k}, t) = 0, \quad (8)$$

where it is assumed that we *identify* $u_\alpha(\mathbf{k} + 2\pi K\mathbf{n}, t)$ with $u_\alpha(\mathbf{k}, t)$.

Equation (7) is to be solved numerically. In applications, we typically treat problems in which $K = 16$ so that there are $32 \times 32 \times 32 = 2^{15}$ independent Fourier modes [counting real and imaginary parts separately and noting that $\mathbf{v}(\mathbf{x}, t)$ given by Eq. (5) is real]. In this case, computation of the convolution sums in Eq. (7) would appear to require approximately 2^{15} multiplications for each of the 2^{15} possible Fourier modes and each of the six independent β, γ subscript choices. Actually with $K = 16$, the total number of multiplications involved in the right-hand side of Eq. (7) is close to 3×10^9. Even with a multiplication time of 1 μsec, this gives a step time of about 1 h, and this is neglecting additions, indexing, etc.! Clearly, this is unreasonable. In the past, such difficulty in computing large convolution sums has deterred use of Fourier mode methods. Note that computation of the right-hand side of Eq. (7) requires approximately $6 \times (27/64) \times (2K)^6$ multiplications and additions, where the factor $27/64 = (\frac{3}{4})^3$ is due to the restrictions implied by $\sum'$. The methods described below reduce the number of multiplications to about $36(2K)^3 \log_2 (2K)^3$ and the number of additions to approximately $72(2K)^3 \log_2 (2K)^3$. With $K = 16$, the efficiency gain is several orders of magnitude.

To simplify discussion, we shall treat a one-dimensional analog of the sums appearing in Eq. (7), namely,

[6] S. A. Orszag and M. D. Kruskal, Phys. Fluids 11, 43 (1968).

$$S(k) = \sum_{\substack{-K\le p<K \\ -K\le k-p<K}} a(p)b(k-p) \tag{9}$$

with k, p now quantized to take on only integer values. The necessary generalization to calculate Eq. (7) is straightforward but complicated. As before, an *a priori* estimate of the number of arithmetical operations gives $\frac{3}{4}(2K)^2$. The method to be described reduces this to a number of order $6[(2K/2)\log_2 2K]$.

The crucial observation is that the difficulty in computing Eq. (9) is the "nonlocal" character of the sums $S(k)$. Roughly speaking, if $\mathfrak{F}$ denotes discrete Fourier transform [Eq. (11) below], then the convolution theorem states

$$\tilde{S}(k) = \tilde{a}(k)\tilde{b}(k),$$

where $\tilde{S} = \mathfrak{F}S$, $\tilde{a} = \mathfrak{F}a$, $\tilde{b} = \mathfrak{F}b$. This symbolic result indicates the advantage gained by a "local" (or diagonalized) computation.

Define

$$r(n) = a(n-K),$$

$$s(n) = b(n-K),$$

where $0 \le n < N = 2K$. It is straightforward to express $S(k)$ in terms of $r(n)$, $s(n)$ as

$$S(k) = \sum_{n=0}^{N+k} r(n)s(N+k-n), \qquad (-K \le k < 0),$$
$$S(k) = \sum_{n=k+1}^{N-1} r(n)s(N+k-n), \qquad (0 \le k < K). \tag{10}$$

We introduce $\tilde{r}_1 = \mathfrak{F}r$, $\tilde{s}_1 = \mathfrak{F}s$ defined by

$$\tilde{r}_1(n) = \sum_{m=0}^{N-1} r(m)\exp\left(\frac{i2\pi nm}{N}\right), \quad (0 \le n < N-1),$$
$$\tilde{s}_1(n) = \sum_{m=0}^{N-1} s(m)\exp\left(\frac{i2\pi nm}{N}\right), \quad (0 \le n < N-1), \tag{11}$$

and define

$$\tilde{r}_2(n) = \sum_{m=0}^{N-1} r(m)\exp\left(\frac{i2\pi m(n+\frac{1}{2})}{N}\right), \qquad (0 \le n < N-1),$$
$$\tilde{s}_2(n) = \sum_{m=0}^{N-1} s(m)\exp\left(\frac{i2\pi m(n+\frac{1}{2})}{N}\right), \qquad (0 \le n < N-1). \tag{12}$$

Finally, we set

$$S_1(m) = \frac{1}{N}\sum_{n=0}^{N-1} \tilde{r}_1(n)\tilde{s}_1(n)\exp\left(-\frac{i2\pi nm}{N}\right), \qquad (0 \le m < N-1), \tag{13}$$

$$S_2(m) = \frac{1}{N}\sum_{n=0}^{N-1} r_2(n)s_2(n)\exp\left(-\frac{i2\pi nm}{N}\right), \qquad (0 \le m < N-1). \tag{14}$$

It follows easily from Eqs. (11)–(14) that

$$S_1(m) = \sum_{n=0}^{m} r(n)s(m-n) + \sum_{n=m+1}^{N-1} r(n)s(N+m-n), \qquad (0 \le m < N-1),$$
$$S_2(m) = \exp\frac{i\pi m}{N}\sum_{n=0}^{m} r(n)s(m-n) - \exp\frac{i\pi m}{N}\sum_{n=m+1}^{N-1} r(n)s(N+m-n), \qquad (0 \le m < N-1). \tag{15, 16}$$

Therefore, we find

$$S(k) = \tfrac{1}{2}[S_1(k+N) - \exp(-i\pi k/N)S_2(k+N)], \qquad -K \le k < 0,$$
$$S(k) = \tfrac{1}{2}[S_1(k) - \exp(-i\pi k/N)S_2(k)], \qquad 0 \le k < K. \tag{17}$$

Equation (17) is the essential algebraic result.

Some comments on Eqs. (11)–(17) are necessary. Equation (11) is a discrete Fourier transform on N points. The complication of Eqs. (12)–(17) is due to the fact that $S(k)$ is not the inverse discrete Fourier transform of $\tilde{r}_1$ times $\tilde{s}_1$, as might be suggested by the continuous version of the convolution theorem. When $-K \le k < 0$ ($K \le m = k+N < N$), the second term on the right-hand side of Eq. (15) is due to "aliasing," or in the language of solid-state physics, "umklapp" processes. Similarly, when $0 \le k < K$ ($0 \le m = k < K$), the first term is aliasing. These aliasing interactions arise because, when r, s have harmonic components up to N, then rs has harmonic components up to $2N$ and discrete Fourier transform on N points cannot distinguish between wavenumbers modulo N. The most straightforward way to eliminate aliasing is to perform the discrete Fourier transform on a mesh of $2N$ points rather than N. In three dimensions elimination of aliasing interactions requires Fourier transforms using eight times the number of retained modes. Since the computations we perform usually have the computer bursting at its seams without this extra factor of 8, this straightforward method of eliminating aliasing is not satisfactory. On the other

hand, Eqs. (11) –(17) offer the advantage of eliminating aliasing while remaining on the mesh of N points. This is done at the cost of computing twice as many Fourier transforms on N points. In three dimensions, the algorithm corresponding to Eq. (17) requires 8 times as many Fourier transforms on N^3 points as Fourier transforms on $(2N)^3$ points to eliminate exactly the aliasing interactions. With $N^3 = 32\,768$ the practical advantage of the present method should be clear.

It appears that Eqs. (11) and (12) each require order N^2 multiplications to compute $\tilde{r}_1$, etc., at all N points. Fortunately, Eqs. (11)–(14) may be calculated using fast Fourier transforms[7] so that when $N = 2^a$, the calculation of $\tilde{r}_1(n)$ from $r(m)$ requires only $\frac{1}{2}N \log_2 N - (N-1)$ complex multiplications and $N \log_2 N$ complex additions. The idea behind the fast Fourier transform may be illustrated when $N = 8$. *A priori* it seems that calculation of Eq. (11) requires 64 multiplications and 56 additions. However, if we set $w(n) = \exp[i(n\pi/4)]$, $c(n) = r(n) + r(n+4)$, $d(n) = w(n)[r(n) - r(n+4)]$ for $n = 0, 1, 2, 3$ and define $e(n) = c(n) + c(n+2)$, $f(n) = d(n) + d(n+2)$, $g(n) = w(2n)[c(n) - c(n+2)]$, $h(n) = w(2n) \cdot [d(n) - d(n+2)]$ for $n = 0, 1$, then

$$\tilde{r}_1(0) = e(0) + e(1), \qquad \tilde{r}_1(4) = e(0) - e(1),$$
$$\tilde{r}_1(1) = f(0) + f(1), \qquad \tilde{r}_1(5) = f(0) - f(1),$$
$$\tilde{r}_1(2) = g(0) + g(1), \qquad \tilde{r}_1(6) = g(0) - g(1),$$
$$\tilde{r}_1(3) = h(0) + h(1), \qquad \tilde{r}_1(7) = h(0) - h(1).$$

In this way, Eq. (11) with $N = 8$ may be calculated with only 5 multiplications and 24 additions.

In summary, the method of calculating the right-hand side of Eq. (7) involves use of the convolution theorem (in its aliasing-free form) and fast Fourier transform. Elimination of repeated Fourier transform of the same quantity reduces the total number of Fourier transforms per step to 72 (three dimensions) or 20 (two dimensions).

In numerical calculations of Eq. (7) using this method, we have used second-order Adams–Bashforth time discretization[8] and have treated vsicous dissipation to first-order implicitly. That is, suppose that Eq. (7) has the form

$$\left(\frac{\partial}{\partial t} + \nu k^2\right) u_\alpha(\mathbf{k}, t) = f_\alpha(\mathbf{k}, t)$$

and that time is discretized so that $t = n\delta$, $n = 0, +1, \cdots$. Then, we set

$$u_\alpha(\mathbf{k}, (n+1)\,\delta) = [u_\alpha(\mathbf{k}, n\,\delta) + \delta(\tfrac{3}{2} f_\alpha(\mathbf{k}, n\,\delta) - \tfrac{1}{2} f_\alpha(\mathbf{k}, (n-1)\,\delta)]/(1 + \nu k^2\,\delta).$$

III. REAL-SPACE DISCRETIZATION

After some experimentation, we found the most convenient way to solve Eqs. (1) and (2) in primitive variables to be the use of the Harlow–Welch staggered-mesh space-differencing scheme,[9] fast Fourier transform to solve exactly the discretized form of the Poisson equation for the pressure field, and Adams–Bashforth time differencing (viscous dissipation treated explicitly). The only essential new feature here is the use of the fast Fourier transform to insure exact incompressibility.

In the staggered mesh, velocities are defined at cell boundaries and pressures at cell centers. Thus, if we let $\mathbf{v} = (u, v, w)$ and label space points by subscripts so that $v_{i,j+1/2,k} = v(i\delta x, (j + \frac{1}{2})\,\delta y, k\delta z)$, etc., where δx, δy, δz specifies the cell size, then if $\delta x = 1/N_1$, $\delta y = 1/N_2$, $\delta z = 1/N_3$, the $4N_1N_2N_3$ dynamical variables are chosen to be

$$u_{i+\frac{1}{2},j,k},\ v_{i,j+\frac{1}{2},k},\ w_{i,j,k+\frac{1}{2}},\ p_{i,j,k}$$

with

$$0 \le i < N_1, \qquad 0 \le j < N_2, \qquad 0 \le k \le N_3.$$

The staggered-mesh approximation to

$$-\mathbf{v}\cdot\nabla u - \frac{\partial p}{\partial x} + \nu\nabla^2 u = -\nabla\cdot(\mathbf{v}u) - \frac{\partial p}{\partial x} + \nu\nabla^2 u$$

at the point $(i + \frac{1}{2}, j, k)$ is

$$\begin{aligned}
&\frac{1}{\delta x}\left[(u_{i,j,k})^2 - (u_{i+1,j,k})^2\right] + \frac{1}{\delta y}\left[(u_{i+1/2,j-1/2,k})(v_{i+1/2,j-1/2,k}) - (u_{i+1/2,j+1/2,k})(v_{i+1/2,j+1/2,k})\right] \\
&+ \frac{1}{\delta z}\left[(u_{i+\frac{1}{2},j,k-\frac{1}{2}})(w_{i+\frac{1}{2},j,k-\frac{1}{2}}) - (u_{i+\frac{1}{2},j,k+\frac{1}{2}})(w_{i+\frac{1}{2},j,k+\frac{1}{2}})\right] \\
&+ \frac{1}{\delta x}(p_{i,j,k} - p_{i+1,j,k}) + \nu\Bigg[\frac{1}{(\delta x)^2}(u_{i+3/2,j,k} + u_{i-1/2,j,k} - 2u_{i+1/2,j,k}) \\
&+ \frac{1}{(\delta y)^2}(u_{i+1/2,j+1,k} + u_{i+1/2,j-1,k} - 2u_{i+1/2,j,k}) + \frac{1}{(\delta z)^2}(u_{i+1/2,j,k+1} + u_{i+1/2,j,k-1} - 2u_{i+1/2,j,k})\Bigg]. \qquad (18)
\end{aligned}$$

[7] J. W. Cooley and J. W. Tukey, Math. Comput. 19, 90 (1965); N. M. Brenner, Lincoln Laboratory Massachusetts Institute of Technology Tech. Note No. 2 (1967).

[8] D. K. Lilly, Monthly Weather Rev. 93, 11 (1965).

[9] F. H. Harlow and J. E. Welch, Phys. Fluids 8, 2182 (1965).

Whenever a velocity value appears in (18) that is not centered at the proper point, an average of adjacent points is implied. Representative examples are

$$u_{i+1/2,j+1/2,k} = \tfrac{1}{2}(u_{i+1/2,j+1,k} + u_{i+1/2,j,k}),$$
$$v_{i+1/2,j+1/2,k} = \tfrac{1}{2}(v_{i+1,j+1/2,k} + v_{i,j+1/2,k}),$$
$$u_{i,j,k} = \tfrac{1}{2}(u_{i-1/2,j,k} + u_{i+1/2,j,k}).$$

The finite-difference approximation to Eq. (2) is taken to be

$$D_{i,j,k} \equiv \left[\frac{1}{\delta x}(u_{i+1/2,j,k} - u_{i-1/2,j,k}) + \frac{1}{\delta y}(v_{i,j+1/2,k} - v_{i,j-1/2,k}) + \frac{1}{\delta z}(w_{i,j,k+1/2} - w_{i,j,k-1/2})\right] = 0. \quad (19)$$

Applying the differencing operator in Eq. (19) to the discretized form of Eq. (1) gives a discretized form of a Poisson equation to determine the pressure field. It follows that

$$\left[\frac{1}{(\delta x)^2}(p_{i+1,j,k} + p_{i-1,j,k} - 2p_{i,j,k}) + \frac{1}{(\delta y)^2}(p_{i,j+1,k} + p_{i,j-1,k} - 2p_{i,j,k}) + \frac{1}{(\delta z)^2}(p_{i,j,k+1} + p_{i,j,k-1} - 2p_{i,j,k})\right] = -Q_{i,j,k}, \quad (20)$$

where $Q_{i,j,k}$ is a nonlinear combination of the velocity variables at mesh points near i, j, k. If we write

$$p_{i,j,k} = \sum_{l=0}^{N_1-1}\sum_{m=0}^{N_2-1}\sum_{n=0}^{N_3-1} \tilde{p}(l, n, m) \cdot \exp\left[i2\pi\left(\frac{li}{N_1} + \frac{mj}{N_2} + \frac{nk}{N_3}\right)\right] \quad (21)$$

and similarly express $Q_{i,j,k}$ in terms of $\tilde{Q}(l, m, n)$, it follows from Eq. (20) that

$$\tilde{p}(l, m, n) = \tilde{Q}(l, m, n)\left[4\left(\frac{1}{(\delta x)^2}\sin^2\frac{\pi l}{N_1} + \frac{1}{(\delta y)^2}\sin^2\frac{\pi m}{N_2} + \frac{1}{(\delta z)^2}\sin^2\frac{\pi n}{N_3}\right)\right]^{-1}. \quad (22)$$

Equations (20)–(22) are implemented by the fast Fourier transform.[7]

Incompressibility is maintained exactly with two Fourier transformations for each time step requiring about $\frac{1}{2}N_1N_2N_3 \log_2 (N_1N_2N_3)$ multiplications and $N_1N_2N_3 \log_2 (N_1N_2N_3)$ additions when N_1, N_2, N_3 are of the form 2^a.

It may be shown by lengthy but straightforward algebra that when $\nu = 0$, the staggered mesh conserves momentum

$$\frac{\partial}{\partial t}\sum_{i,j,k}(u_{i+1/2,j,k}, v_{i,j+1/2,k}, w_{i,j,k+1/2}) = 0,$$

and energy

$$\frac{\partial}{\partial t}\sum_{i,j,k}\tfrac{1}{2}[(u_{i+1/2,j,k})^2 + (v_{i,j+1/2,k})^2 + (w_{i,j,k+1/2})^2] = 0, \quad (23)$$

except for time differencing errors. (Such loss of nonlinear conservation properties by time differencing can apparently only be avoided by implicit schemes such as the modified Euler method.[8])

Finally, we mention that the method of this section can easily be extended to flows which have periodic boundary conditions in all but one space dimension. Examples of such problems are three-dimensional plane-parallel Bénard convection, plane-parallel Poiseuille flow and plane-parallel Couette flow. The procedure is to solve the discretized version of the Poisson equation for the pressure field by Fourier transforming in the directions where the boundary conditions are periodic to obtain a discretized version of the equation

$$\frac{\partial^2}{\partial z^2}\tilde{p}(\mathbf{k}, z) - k^2\tilde{p}(\mathbf{k}, z) = -\tilde{Q}(\mathbf{k}, z)$$

[see Eq. (20)] which may then be solved using well-known methods for tridiagonal systems of linear equations. In fact, this procedure gives a slight increase in speed over the Fourier-transform method employed above to solve Poisson's equation with fully periodic boundary conditions, but programming convenience and the fact that solving Poisson's equation already involves less than 50% of the computing time per step makes further economies unnecessary.

The scheme described here was tested by comparison with an exactly soluble two-dimensional test problem proposed by Taylor.[10] The initial data are

$$u = -\cos x \sin y, \quad v = \sin x \cos y, \quad w = 0.$$

The exact solution of the problem is

[10] G. I. Taylor, Scientific Papers **2**, 190 (1960). See also C. E. Pearson, Sperry-Rand Research Center Report No. SRRC-RR-64-17 (1964).

TABLE I. Results of two-dimensional test problem (Ref. 10). Scheme I is the method of Sec. III, while scheme II is due to Chorin (Ref. 11). With scheme I, $\delta x = \delta y = \pi/16$, while with scheme II, $\delta x = \delta y = \pi/39$. For both schemes, the time step $\Delta t = 0.0648$ and $\nu = 0.05$. In the table, n is the number of integration steps, $e(u)$ is the maximum error in the velocity field, and $e(p)$ is the maximum error in the pressure field. l_{II} is the number of iterations for scheme II to obtain convergence to within $(\delta x)^2 \approx 0.0065$.

n	$e(u)_I$	$e(u)_{II}$	$e(p)_I$	$e(p)_{II}$	l_{II}
1	2.1×10^{-5}	1.2×10^{-3}	1.6×10^{-7}	2.2×10^{-2}	15
3	6.1×10^{-5}	2.1×10^{-3}	4.0×10^{-5}	2.3×10^{-2}	9
5	1.0×10^{-4}	2.8×10^{-3}	7.8×10^{-5}	2.4×10^{-2}	9
7	1.4×10^{-4}	3.3×10^{-3}	1.1×10^{-4}	2.5×10^{-2}	9
9	1.7×10^{-4}	4.0×10^{-3}	1.5×10^{-4}	2.5×10^{-2}	8
20	3.7×10^{-4}	5.8×10^{-3}	3.1×10^{-4}	2.6×10^{-2}	8

$$u = -\cos x \sin y \exp(-2\nu t),$$

$$v = \sin x \cos y \exp(-2\nu t),$$

$$w = 0,$$

$$p = -\tfrac{1}{4}(\cos 2x + \cos 2y) \exp(-4\nu t).$$

The results are given in Table I. For comparison we present results of a similar computation using a new scheme of a relaxation type developed by Chorin.[11] It is apparent that the accuracy of the present method compares quite favorably with relaxation methods. The method of Sec. II was not applied to this test problem because the very nature of the Fourier mode method insures that the numerical solution follows the exact solution except for time differencing errors.

IV. COMPARISON OF METHODS

In this section, we list and critically compare seven properties of the Fourier mode and real-space methods outlined above.

(a) Incompressibility of the flow field is maintained exactly by both schemes. In the case of the Fourier mode method, this means that $k_\alpha u_\alpha(\mathbf{k}, t) = 0$ for all t. In the real-space method of Sec. III, this means that $D_{i,j,k} = 0$.

(b) Both schemes are conservative when $\nu = 0$. In the Fourier method, energy conservation is given by Eq. (8) while in real space it is given by Eq. (23). In the presence of viscosity, each of these energy integrals is decreasing with time. Consequently, except for possible instabilities induced by time differencing, both schemes are stable in the sense that the quadratic integrals (8) or (23) put bounds on the magnitude of the velocity at each mesh point.

(c) The errors associated with the truncation of Fourier space and the discretization of real space take different forms. In the Fourier-mode method, all interactions among harmonic components up to cutoff are treated exactly. In Eq. (7), the coupling constant between retained modes is exact, i.e., $P_{\alpha\beta\gamma}(\mathbf{k})$. In this way, we see that there are none of the usual aliasing errors associated with numerical schemes. Instead, the errors arise from a "damming-up" of the nonlinear transfer of energy in Fourier space. We base the following argument on the Kolmogoroff theory of the inertial range.[2,4,6] At high Reynolds numbers, dissipation occurs principally around the wavenumber

$$k_d \sim \tfrac{1}{10}(\epsilon/\nu^3)^{1/4} \sim \tfrac{1}{10}(\tfrac{1}{10}R_\lambda^2)^{3/4} k_0,$$

where ϵ is the rate of nonlinear energy transfer and k_0 is a wavenumber characteristic of the energy-containing eddies. Damming-up is insignificant when $k_d \ll K$ and, in this case, we may expect that solutions of Eq. (7) approximate those of Eq. (4). However, when $k_d \gg K$, the transfer mechanism is strongly inhibited by the cutoff. In this latter asymptotic limit, it may be argued that solutions of Eq. (7) do not at all approximate solutions of Eq. (4), but rather exhibit approach to an equipartition, equilibrium state (slightly damped by the small viscosity).

In terms of interaction among harmonic components, the errors associated with the real-space discretization method of Sec. III take the form of errors in coupling constants and aliasing errors.[8] The coupling constant errors already appear in Eq. (22) where the denominator should be $[(2\pi l)^2 + (2\pi m)^2 + (2\pi n)^2]$ if the equation determining p were really the Poisson equation $\nabla^2 p = -Q$. It is seen that there is serious distortion of interactions involving wavevectors any of whose components are larger than $\frac{1}{4}N_1$, $\frac{1}{4}N_2$, or $\frac{1}{4}N_3$. Aliasing errors involve a whole set of spurious interaction coefficients among harmonic components due to the finiteness of the grid. Phillips[12] has shown that aliasing inter-

[11] A. J. Chorin, Math. Comput. 22, 745 (1968).

[12] N. A. Phillips, in *The Atmosphere and the Sea in Motion* (Rockefeller Institute Press, New York, 1959), p. 501.

actions, i.e., couplings which should be zero but are not because of discretization, can sometimes lead to instability. In any case, it is unlikely that the real-space discretization can provide a valid description of wavevectors with components larger than $\frac{1}{4}N_1$, $\frac{1}{4}N_2$, $\frac{1}{4}N_3$.

(d) The Fourier mode method offers the advantage that in time differencing it is an easy matter to treat viscosity implicitly. At the high Reynolds numbers considered here, this is not much of an advantage since the size of time steps is not usually dictated by diffusive-stability considerations but rather by the condition that eddies not execute much circulation per step. At this point, one may question why we do not consider some fancier form of time differencing than Adams–Bashforth. The reason is that in effect we are using rather sophisticated space-differencing techniques on which implicit methods are inconvenient. In three-dimensional calculations it is much cheaper in terms of computation time to halve a time step than it is to halve a space step.

(e) The real-space method offers the advantage of speed over the Fourier-mode method. Using Fourier modes, it is necessary to do 72 fast Fourier transforms per time step in three dimensions, compared with only two to solve Poisson's equation. Allowing for the time to compute Eq. (18), etc., the real-space method is about a factor 20 times faster than the method of Sec. II when the same numbers of grid points are used. However, aliasing and derivative errors indicate that the accuracy of a real-space calculation with $8N^3$ points is about the same as that of a Fourier-mode calculation with N^3 modes, which negates most of the advantage in speed. In two dimensions, the Fourier-mode method requires only 20 fast Fourier transforms per step so that the speeds of both methods are comparable.

We find execution times per step on the IBM Model 360-95 to be about 1 min for a Fourier mode calculation with $32 \times 32 \times 32$ modes and 3 sec for a real-space calculation with $32 \times 32 \times 32$ points. A typical calculation involves about 100 time steps. It seems possible to extend the real-space mesh to $64 \times 64 \times 64$ with a more refined use of disk and tape facilities.

(f) An important advantage of the Fourier-mode method as a tool in testing turbulence theories is that they may be formulated on the truncated system (7) rather than the Navier–Stokes system (4). For example, the random-coupling model (Ref. 3) may be formulated directly on Eq. (7) without the intermediate step of deriving the theory first for Eq. (4) and then imposing the cutoff K on the equations of the theory. This feature of the Fourier method is very attractive since it means that except for possible time-differencing errors, the comparison between theory and numerical experiment is exact. There is no possibility of arguing that any observed discrepancy could be due to poor space differencing.

(g) As mentioned in Sec. III, the real-space method can be applied to plane-parallel shear flows, etc. Apparently, the only type of shear flow to which the Fourier-mode method may be applied is the rather artificial one where one (or a few) Fourier mode(s) is (are) constrained to have a fixed nonzero value. Such flows would not exhibit boundary layers, but they could test effects of interactions between mean and fluctuating fields.

V. APPLICATIONS

The results of the application of our methods to a variety of turbulent flows will be reported in detail in forthcoming publications. Some of these applications are:

(a) The solution of the Taylor–Green model[13] for turbulence decay. This problem involves the study of the decay of a special class of vortices. Because of special symmetries which may be exploited in real space but not with Fourier modes, the real-space method offers considerable advantages for this problem. An interesting result of this study concerns the apparent independence of the rate of energy dissipation on Reynolds number at large Reynolds number.

(b) A study of the statistical properties of solutions to Burgers' equation[14] at large Reynolds number using the Fourier-mode method.

(c) An investigation of the decay of three-dimensional homogeneous, isotropic turbulence at $R_\lambda \sim 20$. With a $32 \times 32 \times 32$ grid and $R_\lambda \sim 20$, simple estimates show that there about 4 or 5 grid thicknesses in a typical shear layer that develops. Both the Fourier-mode and real-space method have been and are being used in this study.

(d) A contemplated study similar to that of (c) for two-dimensional turbulence using the Fourier-mode method. This work should be complementary to the real-space calculation reported by Lilly.[15]

(e) The study of a variety of shear and thermal flows using the real-space method. This work belongs to the future.

[13] G. I. Taylor and A. E. Green, Proc. Roy. Soc. (London) **A158**, 499 (1937).

[14] J. M. Burgers, in *Advances in Applied Mechanics*, R. V. Mises and Th. V. Kármán, Eds. (Academic Press Inc., New York, 1948), Vol. 1, p. 171.

[15] D. K. Lilly, Phys. Fluids Suppl. II, **12**, II-240 (1969).

In conclusion, it seems that the numerical study of interesting three-dimensional turbulent flows is not beyond the capabilities of existing computer hardware. However, the results so obtained appear useful only as tests of turbulence theories at moderate Reynolds number. It does not appear likely that three-dimensional solutions with inertial ranges extending over several decades of wavenumber will be obtained numerically in the near future.

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APPENDIX

In this Appendix we describe a method of generating an initial random velocity profile which is multivariate Gaussian statistically homogeneous, statistically isotropic, incompressible and whose energy spectrum is $E(k)$.

We first choose $\mathbf{r}(\mathbf{k})$ and $\mathbf{s}(\mathbf{k})$ to be zero-mean Gaussian, independent, real, random vector fields satisfying

$$\langle r_\alpha(\mathbf{k}) r_\beta(\mathbf{k}')\rangle = \langle s_\alpha(\mathbf{k}) s_\beta(\mathbf{k}')\rangle = 0 \qquad (\mathbf{k} \neq \mathbf{k}'),$$

$$\langle r_\alpha(\mathbf{k}) r_\beta(\mathbf{k})\rangle = \langle s_\alpha(\mathbf{k}) s_\beta(\mathbf{k})\rangle = \delta_{\alpha\beta}[\pi^2 E(k)/2k^2],$$

$$\langle r_\alpha(\mathbf{k}) s_\beta(\mathbf{k}')\rangle = 0,$$

where $\langle\ \rangle$ means ensemble average, and $\mathbf{k}$ is quantized as in Eq. (3), i.e., $\mathbf{k} = 2\pi\mathbf{n}$. A realization of $\mathbf{r}(\mathbf{k})$ and $\mathbf{s}(\mathbf{k})$ may be obtained using a Gaussian random number generator. We set

$$u_\alpha(\mathbf{k}) = P_{\alpha\beta}(\mathbf{k})[r_\beta(\mathbf{k}) + r_\beta(-\mathbf{k}) + is_\beta(\mathbf{k}) - is_\beta(-\mathbf{k})],$$

where

$$P_{\alpha\beta}(\mathbf{k}) = \delta_{\alpha\beta} - k_\alpha k_\beta / k^2.$$

It follows that $u_\alpha(\mathbf{k})$ is Gaussian with zero mean and satisfies

$$\langle u_\alpha(\mathbf{k}) u_\beta(\mathbf{k}')\rangle = 0 \qquad \mathbf{k} \neq -\mathbf{k}',$$

$$\langle u_\alpha(\mathbf{k}) u_\beta(-\mathbf{k})\rangle = 2\pi^2[E(k)/k^2]P_{\alpha\beta}(\mathbf{k}),$$

$$k_\alpha u_\alpha(\mathbf{k}) = 0,$$

$$u_\alpha(\mathbf{k}) = [u_\alpha(-\mathbf{k})]^*,$$

where the asterisk denotes complex conjugate. Finally, $\mathbf{v}(\mathbf{x})$ is constructed by fast Fourier transform,

$$\mathbf{v}(\mathbf{x}) = \sum_{\mathbf{k}} \mathbf{u}(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{x}).$$

It can easily be verified that $\mathbf{v}(\mathbf{x})$ is Gaussian, real, incompressible, statistically homogeneous and isotropic and

$$\tfrac{1}{2}\langle v_\alpha(\mathbf{x}) v_\alpha(\mathbf{x} + \mathbf{y})\rangle = \int_0^\infty E(k) \frac{\sin ky}{ky}\, dk.$$

To obtain the latter equation a wave vector sum has been replaced by an integral as if the periodicity interval of $\mathbf{v}(\mathbf{x})$ were infinite.