NUMERICAL CHALLENGES FOR TURBULENCE COMPUTATION: STATISTICAL EQUIPARTITION AND THE METHOD OF SPECTRAL REDUCTION

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Abstract. Numerical issues in the implementation of spectral reduction, a new method for the computation of statistical moments of homogeneous turbulence, are examined. The method implements a coarse graining in Fourier space and exploits the fact that statistical moments are much smoother functions of wave number than the underlying fluctuating velocities. A notable feature of this turbulence model is the existence of a control parameter (bin size) that can be varied to increase the accuracy of the approximation. The inviscid version of spectral reduction satisfies a Liouville theorem and yields statistical equipartition solutions. However, if the wavenumber bins are of nonuniform size (as is desirable for efficiency), an additional bin-dependent rescaling of time by the relative bin area must be introduced to obtain the correct equipartition. This rescaling of the time derivative term drastically increases the stiffness of the spectrally reduced equations. The prospect of developing an implicit nonlinear integrator for this highly stiffened convection problem is examined.

Key words. homogeneous turbulence, statistical closures, spectral reduction, stiff differential equations

AMS subject classifications. 76F05, 34A65

1. Introduction.

Over the past forty years, much effort has been devoted to the development of a satisfactory statistical theory of turbulence. For example, statistical closures were developed in an attempt to find closed expressions for the unknown triplet correlation function that arises upon averaging the Navier–Stokes equation. Familiar examples include Kraichnan's direct-interaction approximation [10, 11] and Lagrangian-history direct-interaction approximation [12]. Unfortunately, there is considerable arbitrariness in the formulation of statistical closures. Moreover, it is generally believed that low-order statistical theories are not capable of capturing the effects of coherent structures [9, 15]. But probably the greatest weakness of these methods is that there exists neither an error estimate nor a control parameter that can be varied to increase the accuracy of the approximation.

Recently, a method called spectral reduction [5] has been proposed for calculating statistical moments of turbulent quantities by implementing a coarse-graining in Fourier space. The bin size serves as a control parameter that can be varied to increase the accuracy of the approximation. The method exploits the fact that statistical moments are much smoother functions of wave number than are the underlying stochastic amplitudes. Collections of Fourier amplitudes are represented by nonuniformly spaced sample modes that interact via enhanced coupling coefficients. By assigning most of these sample modes to the scales of greatest physical interest, the technique makes optimal use of limited computational resources. The approximation reduces to the exact Navier–Stokes equation as the number of fundamental wave numbers associated with each sample mode tends to one. Even at large values of this parameter, the

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statistics of the full dynamics may be accurately recovered from the time-averaged predictions of the theory.

2. Spectral Reduction. Let us restrict our attention to homogeneous and isotropic incompressible turbulence in two dimensions, for which the Fourier-transformed Navier–Stokes vorticity equation takes the form

$$\frac{\partial \omega_{\boldsymbol{k}}}{\partial t} + \nu_{\boldsymbol{k}} \omega_{\boldsymbol{k}} = \int_{\mathcal{D}} d\boldsymbol{p} \int_{\mathcal{D}} d\boldsymbol{q}\, \frac{\epsilon_{\boldsymbol{kpq}}}{q^2} \omega^*_{\boldsymbol{p}} \omega^*_{\boldsymbol{q}}, \tag{2.1}$$

where * denotes complex conjugation. Here $\nu_{\boldsymbol{k}}$ models time-independent linear dissipation and the interaction coefficient $\epsilon_{\boldsymbol{kpq}} \doteq (\hat{\boldsymbol{z}} \cdot \boldsymbol{p} \times \boldsymbol{q})\, \delta(\boldsymbol{k} + \boldsymbol{p} + \boldsymbol{q})$ is antisymmetric under permutation of any two indices, where $\hat{\boldsymbol{z}}$ is the unit normal to the plane of motion ($\doteq$ denotes a definition). We restrict the integration to a bounded wave-number domain $\mathcal{D}$ that excludes a neighborhood of $\boldsymbol{k} = \boldsymbol{0}$. As a consequence of the antisymmetry of $\epsilon_{\boldsymbol{kpq}}$, (2.1) conserves in the inviscid limit $\nu_{\boldsymbol{k}} = 0$ both the energy $\frac{1}{2} \int_{\mathcal{D}} d\boldsymbol{k}\, |\omega_{\boldsymbol{k}}|^2 / k^2$ and the enstrophy $\frac{1}{2} \int_{\mathcal{D}} d\boldsymbol{k}\, |\omega_{\boldsymbol{k}}|^2$.

We introduce an arbitrary coarse-grained grid on $\mathcal{D}$, to which we associate new variables $\Omega_{\boldsymbol{K}} \doteq \Delta_{\boldsymbol{K}}^{-1} \int_{\boldsymbol{K}} \omega_{\boldsymbol{k}}\, d\boldsymbol{k}$, where $\Delta_{\boldsymbol{K}}$ is the area of bin $\boldsymbol{K}$. The exact evolution of $\Omega_{\boldsymbol{K}}$ is given by

$$\frac{\partial \Omega_{\boldsymbol{K}}}{\partial t} + \langle \nu_{\boldsymbol{k}} \omega_{\boldsymbol{k}} \rangle_{\boldsymbol{K}} = \sum_{\boldsymbol{P},\boldsymbol{Q}} \Delta_{\boldsymbol{P}} \Delta_{\boldsymbol{Q}} \left\langle \frac{\epsilon_{\boldsymbol{kpq}}}{q^2} \omega^*_{\boldsymbol{p}} \omega^*_{\boldsymbol{q}} \right\rangle_{\boldsymbol{KPQ}}, \tag{2.2}$$

where $\langle \cdot \rangle_{\boldsymbol{K}}$ denotes a bin average and the operator

$$\langle f \rangle_{\boldsymbol{KPQ}} \doteq \frac{1}{\Delta_{\boldsymbol{K}} \Delta_{\boldsymbol{P}} \Delta_{\boldsymbol{Q}}} \int_{\boldsymbol{K}} d\boldsymbol{k} \int_{\boldsymbol{P}} d\boldsymbol{p} \int_{\boldsymbol{Q}} d\boldsymbol{q}\, f, \tag{2.3}$$

depends only on the bin geometry. The geometric factors $\langle f \rangle_{\boldsymbol{KPQ}}$ can be efficiently computed using a combination of analytical and numerical methods [1, 2, 3]; being independent of both time and initial conditions, they need only be computed once for each new wave-number partition. The *reality condition*[1] $\Omega_{\boldsymbol{K}} = \Omega^*_{-\boldsymbol{K}}$, where $-\boldsymbol{K}$ denotes the inversion of bin $\boldsymbol{K}$ through the origin, will be respected for partitions that possess inversion symmetry.

Equation (2.2) is unfortunately not closed. If $\omega_{\boldsymbol{k}}$ were naively approximated by its bin-averaged value $\Omega_{\boldsymbol{K}}$, one would obtain

$$\frac{\partial \Omega_{\boldsymbol{K}}}{\partial t} + \langle \nu_{\boldsymbol{k}} \rangle_{\boldsymbol{K}}\, \Omega_{\boldsymbol{K}} = \sum_{\boldsymbol{P},\boldsymbol{Q}} \Delta_{\boldsymbol{P}} \Delta_{\boldsymbol{Q}} \left\langle \frac{\epsilon_{\boldsymbol{kpq}}}{q^2} \right\rangle_{\boldsymbol{KPQ}} \Omega^*_{\boldsymbol{P}} \Omega^*_{\boldsymbol{Q}}. \tag{2.4}$$

In the inviscid limit, (2.4) conserves the coarse-grained enstrophy $\frac{1}{2} \sum_{\boldsymbol{K}} |\Omega_{\boldsymbol{K}}|^2 \Delta_{\boldsymbol{K}}$ since $\left\langle \epsilon_{\boldsymbol{kpq}} / q^2 \right\rangle_{\boldsymbol{KPQ}}$ is antisymmetric in $\boldsymbol{K} \leftrightarrow \boldsymbol{P}$. However, the coarse-grained energy $\frac{1}{2} \sum_{\boldsymbol{K}} |\Omega_{\boldsymbol{K}}|^2 \Delta_{\boldsymbol{K}} / K^2$ is not conserved since $\left\langle \epsilon_{\boldsymbol{kpq}} / q^2 \right\rangle_{\boldsymbol{KPQ}} / K^2$ is not antisymmetric in $\boldsymbol{K} \leftrightarrow \boldsymbol{Q}$ (here K denotes the magnitude of some characteristic wave number in bin $\boldsymbol{K}$). However, both of these desired symmetries can be reinstated by replacing the factor $\left\langle \epsilon_{\boldsymbol{kpq}} / q^2 \right\rangle_{\boldsymbol{KPQ}}$ in (2.4) with the slightly modified coefficient $\langle \epsilon_{\boldsymbol{kpq}} \rangle_{\boldsymbol{KPQ}} / Q^2$. The relative error introduced by this modification is negligible in the limit of small bin

[1] The reality condition $\omega_{\boldsymbol{k}} = \omega^*_{-\boldsymbol{k}}$ guarantees that the inverse Fourier transform of $\omega_{\boldsymbol{k}}$ be real.

size, being on the order of the squared relative variation in the wavenumber magnitude over a bin. The result,

$$\frac{\partial \Omega_{\boldsymbol{K}}}{\partial t} + \langle \nu_{\boldsymbol{k}} \rangle_{\boldsymbol{K}} \, \Omega_{\boldsymbol{K}} = \sum_{\boldsymbol{P},\boldsymbol{Q}} \Delta_{\boldsymbol{P}} \Delta_{\boldsymbol{Q}} \frac{\langle \epsilon_{\boldsymbol{kpq}} \rangle_{\boldsymbol{KPQ}}}{Q^2} \Omega^*_{\boldsymbol{P}} \Omega^*_{\boldsymbol{Q}}, \tag{2.5}$$

is a more acceptable alternative as an approximation of (2.2) since it conserves both energy and enstrophy. Moreover, the time-averaged (or ensemble-averaged) moments of (2.5) satisfy equations that closely approximate the equations governing the exact bin-averaged statistics, even when each bin contains many statistically independent modes. That is, spectral reduction can provide an accurate statistical description of turbulence, *even if the assumptions leading to (2.5) are themselves violated*.

Let us justify the above claim. A time average (denoted by an over-bar) of the bin-averaged enstrophy equation derived from (2.1) leads to

$$\frac{1}{2} \overline{\frac{\partial \left\langle |\omega_{\boldsymbol{k}}|^2 \right\rangle_{\boldsymbol{K}}}{\partial t}} + \mathrm{Re} \left\langle \nu_{\boldsymbol{k}} \overline{|\omega_{\boldsymbol{k}}|^2} \right\rangle_{\boldsymbol{K}} = \mathrm{Re} \sum_{\boldsymbol{P},\boldsymbol{Q}} \Delta_{\boldsymbol{P}} \Delta_{\boldsymbol{Q}} \left\langle \frac{\epsilon_{\boldsymbol{kpq}}}{q^2} \overline{\omega^*_{\boldsymbol{k}} \omega^*_{\boldsymbol{p}} \omega^*_{\boldsymbol{q}}} \right\rangle_{\boldsymbol{KPQ}}. \tag{2.6}$$

If the true vorticity is a continuous function of wave number, there will exist a wave number $\boldsymbol{\kappa}$ in bin $\boldsymbol{K}$ such that $\omega_{\boldsymbol{\kappa}} = \Omega_{\boldsymbol{K}}$. Furthermore, time-averaged quantities such as $\overline{|\omega_{\boldsymbol{k}}|^2}$ are generally smooth functions of the wave number $\boldsymbol{k}$. We thus deduce that $\overline{|\Omega_{\boldsymbol{K}}|^2} = \overline{|\omega_{\boldsymbol{\kappa}}|^2} \approx \overline{|\omega_{\boldsymbol{k}}|^2}$ for all $\boldsymbol{k}$ in bin $\boldsymbol{K}$. Similarly, the triplet correlation $\overline{\omega^*_{\boldsymbol{k}} \omega^*_{\boldsymbol{p}} \omega^*_{\boldsymbol{q}}}$ is a smooth function of $\boldsymbol{k}$, $\boldsymbol{p}$, $\boldsymbol{q}$ when restricted to the surface defined by the triad condition $\boldsymbol{k} + \boldsymbol{p} + \boldsymbol{q} = \boldsymbol{0}$.

To good accuracy the statistical averages in (2.6) may therefore be evaluated at the characteristic wave numbers $\boldsymbol{K}$, $\boldsymbol{P}$, $\boldsymbol{Q}$ of each bin. Hence, to the extent that the wave-number magnitudes vary slowly over a bin, (2.6) may be reduced to the (nonlinearly conservative) approximation

$$\frac{1}{2} \frac{\partial \overline{|\Omega_{\boldsymbol{K}}|^2}}{\partial t} + \mathrm{Re} \, \langle \nu_{\boldsymbol{k}} \rangle_{\boldsymbol{K}} \, \overline{|\Omega_{\boldsymbol{K}}|^2} = \mathrm{Re} \sum_{\boldsymbol{P},\boldsymbol{Q}} \Delta_{\boldsymbol{P}} \Delta_{\boldsymbol{Q}} \frac{\langle \epsilon_{\boldsymbol{kpq}} \rangle_{\boldsymbol{KPQ}}}{Q^2} \overline{\Omega^*_{\boldsymbol{K}} \Omega^*_{\boldsymbol{P}} \Omega^*_{\boldsymbol{Q}}}, \tag{2.7}$$

which is precisely the evolution equation for the time-averaged enstrophy obtained from (2.5). Similar arguments for the higher-order statistical moments can also be made, suggesting that spectral reduction can indeed provide an accurate statistical description of turbulence, even when each bin contains many statistically independent modes. As the partition is refined, one expects the solutions of (2.7) to converge to the those of (2.6). Note that spectral reduction does not make a closure assumption on the triplet correlation $\overline{\Omega^*_{\boldsymbol{K}} \Omega^*_{\boldsymbol{P}} \Omega^*_{\boldsymbol{Q}}}$ appearing in (2.7); it circumvents the closure problem entirely by reducing the number of triplet correlations to a tractable number, instead of eliminating them in favor of lower-order statistical variables. Unlike statistical closures, spectral reduction thus does not destroy the phase information embodied in the triplet correlation.

In Fig. 2.1, we demonstrate the excellent agreement obtained in comparison with a forced-dissipative pseudospectral simulation for a two-dimensional fluid containing coherent structures. We also compare to the predictions of the realizable test-field model [3]. In Fig. 2.2 we illustrate the scaling with distance r of the angular average $S_{10}(r)$ of the tenth moment of velocity increments $\overline{|\boldsymbol{v}(\boldsymbol{r}) - \boldsymbol{v}(\boldsymbol{0})|^{10}}$. Slight variations in the predicted large-scale velocities are evident as overall vertical offsets.

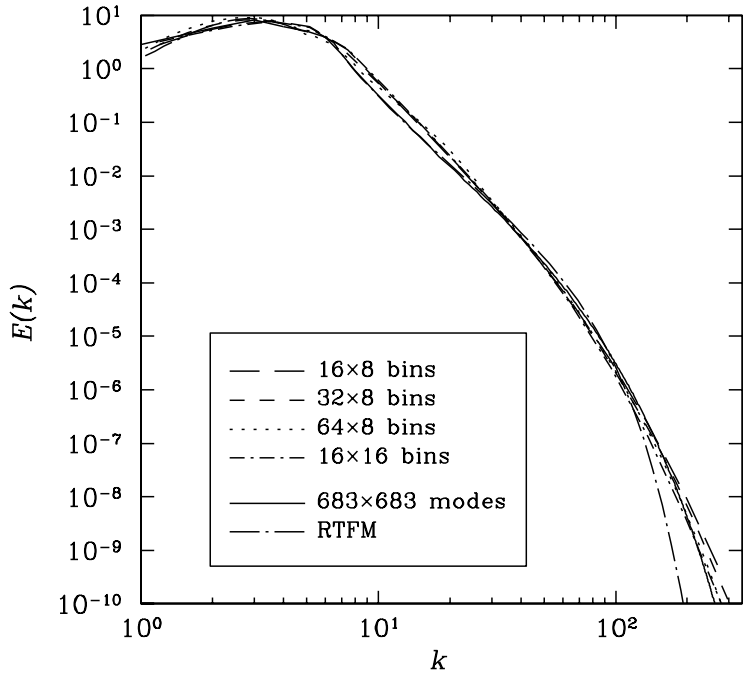

FIG. 2.1. *Comparison of the energy spectra obtained with several (radial × angular) wavenumber partitions, the realizable test-field model, and a* 683×683 *dealiased pseudospectral simulation.*

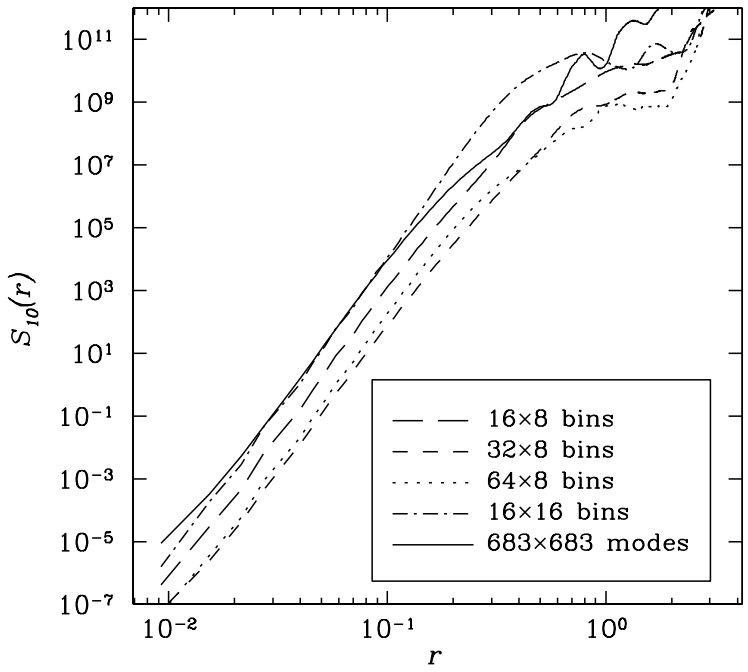

FIG. 2.2. *Angle-averaged structure function* $S_{10}(r)$.

3. Statistical Equipartition. In the inviscid limit, spectral reduction has been shown to satisfy a Liouville theorem [5]. If the dynamics is *mixing*, the inviscid system will then evolve toward a state of equipartition [6, 8, 14, 16]. Unlike in three dimensions, where there is an equipartition of the modal energies, one obtains in two dimensions an equipartition of a linear combination of the modal energies and enstrophies [13], as shown in Fig. 3.1.

When applying the method of spectral reduction with nonuniform bins it is necessary to account for additional internal statistical degrees of freedom by rescaling the time derivative $\partial/\partial t$ in (2.5) to $(\Delta_0/\Delta_{\boldsymbol{K}})\partial/\partial t$, where Δ_0 is the minimum bin area:

$$\frac{\Delta_0}{\Delta_{\boldsymbol{K}}}\frac{\partial \Omega_{\boldsymbol{K}}}{\partial t} + \langle \nu_{\boldsymbol{k}} \rangle_{\boldsymbol{K}}\, \Omega_{\boldsymbol{K}} = \sum_{\boldsymbol{P},\boldsymbol{Q}} \Delta_{\boldsymbol{P}} \Delta_{\boldsymbol{Q}} \frac{\langle \epsilon_{\boldsymbol{kpq}} \rangle_{\boldsymbol{KPQ}}}{Q^2} \Omega^*_{\boldsymbol{P}} \Omega^*_{\boldsymbol{Q}}. \tag{3.1}$$

Equation (3.1) correctly leads to an equipartition of a linear combination of the modal (instead of bin) invariants, as illustrated in Fig. 3.1 numerically, using a specially designed fifth-order conservative Runge–Kutta integration algorithm that conserves quadratic invariants to all orders in the time step [4, 18].

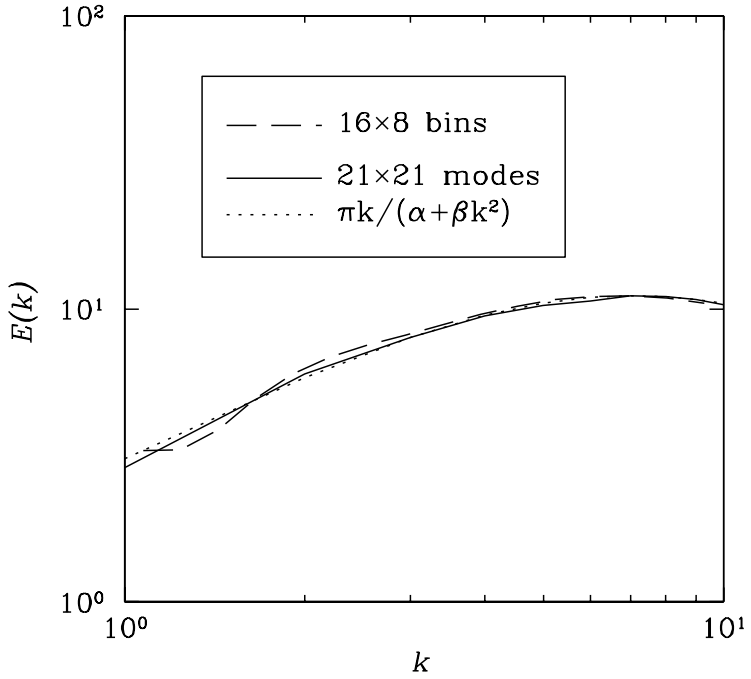

FIG. 3.1. *Statistical equipartition by spectral reduction with* 16×8 *(radial × angular) nonuniform polar bins. The dotted curve is the equipartition solution.*

While this rescaling of time by the relative bin area does not change the steady-state moment equations, it does affect the statistical trajectory of the nonlinear system of equations and consequently can affect the resulting statistical solution, even in the presence of forcing and dissipation. In particular, the use of the rescaled formulation (3.1) appears to be necessary to obtain the theoretically expected $k^{-5/3}$ scaling of the two-dimensional energy inverse cascade illustrated in Fig. 3.2.

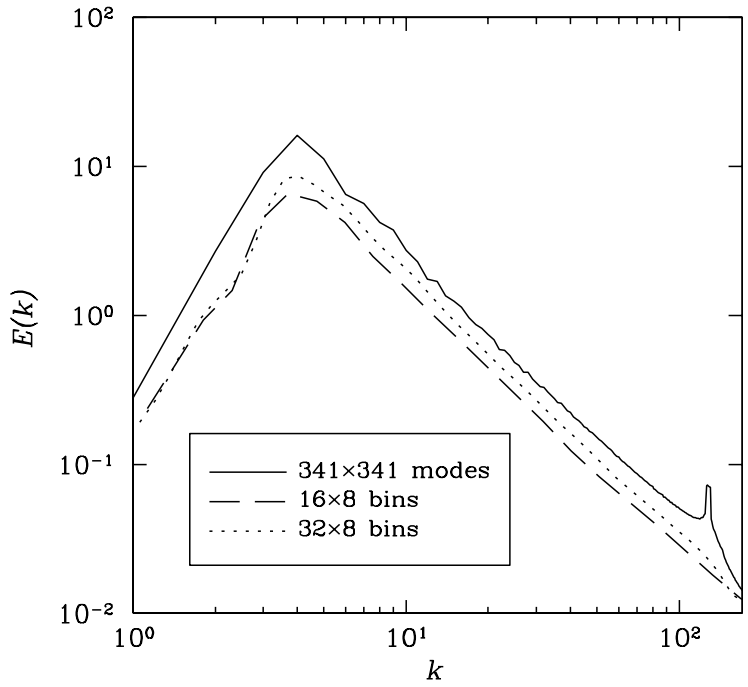

FIG. 3.2. *The inverse energy cascade obtained using rectangular wave-number partitions and a* 341×341 *dealiased pseudospectral simulation.*

4. Implicit Integration Algorithm. Unfortunately, the introduction of the factor $\Delta_0/\Delta_{\boldsymbol{K}}$ in (3.1) greatly increases the stiffness of the spectrally reduced equations. Let us rewrite (2.5) in the form

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{F}(\boldsymbol{y}), \tag{4.1}$$

where $\boldsymbol{F}$ represents both the linear and nonlinear terms in (2.5). We are faced with the following problem: although there are many efficient explicit (*e.g.* Runge–Kutta) schemes for evolving (4.1), these methods do not necessarily provide efficient algorithms for the rescaled system

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{\Lambda}\boldsymbol{F}(\boldsymbol{y}) \doteq \boldsymbol{S}, \tag{4.2}$$

where $\boldsymbol{\Lambda}$ is a constant real diagonal matrix. The diagonal elements of $\boldsymbol{\Lambda}$ are the relative areas of the wavenumber bins. In a practical application of spectral reduction, it is desirable to use wavenumber bins that become larger as the length scale (and hence time scale) decreases. Consequently, the effect of introducing the $\boldsymbol{\Lambda}$ factor is to increase the stiffness of the problem drastically.

In this work, we examined the prospect of developing an implicit nonlinear integrator for this highly stiffened convection problem. We tried to solve (4.2) with the implicit midpoint rule (implicit second-order Runge–Kutta algorithm)

$$\boldsymbol{y}(t+\tau) = \boldsymbol{y}(t) + \tau\boldsymbol{S}\left(\frac{\boldsymbol{y}(t)+\boldsymbol{y}(t+\tau)}{2}\right). \tag{4.3}$$

This algorithm can be easily be shown to conserve all invariants that are quadratic in $\boldsymbol{y}$ (which, for simulating a turbulent cascade, is a desirable property). However, it is difficult to find solutions to the nonlinear system of equations (4.3) when τ is large. One might try the Newton iteration

$$\left(1 - \frac{1}{2}\tau \boldsymbol{\nabla} \boldsymbol{S}\Big|_{\widetilde{\boldsymbol{y}}_i}\right) \boldsymbol{y}_{i+1} = \boldsymbol{y}(t) + \tau \boldsymbol{S}(\widetilde{\boldsymbol{y}}_i) - \frac{1}{2}\tau \boldsymbol{\nabla} \boldsymbol{S}\Big|_{\widetilde{\boldsymbol{y}}_i} \boldsymbol{y}_i, \tag{4.4}$$

where $\widetilde{\boldsymbol{y}}_i \doteq [\boldsymbol{y}_i + \boldsymbol{y}(t)]/2$, for $i = 1, 2, \ldots$. Line-searching (backtracking) does not appear to be effective for this problem since the local search direction specified by the gradient of the squared error is not adequate for finding an initial guess $\boldsymbol{y}_1$ inside the basin of attraction. We found that one solution to this problem was to start with a small value of τ and increase it geometrically each iteration, re-evaluating the Jacobian at every iteration. Convergence was then obtained with time steps approximately 10 times larger than that possible with conventional Newton iteration.

However, a more elegant solution to the problem of divergence of the Newton iteration is to use an adaptive time-step. If the Newton iterator does not converge after a specified number of iterations, the time step is automatically reduced. Otherwise the time step can be adjusted using an error estimate based on the effect of a single implicit fourth-order Runge–Kutta iteration on the converged solution of (4.4). With this scheme, we found that it was then no longer necessary to increase the time step geometrically from a small starting value, as described above. The adaptive scheme effectively accomplished the same behavior automatically. In the end we were able to use a time step that was about 500 times larger than the stability limit of an explicit second-order Runge–Kutta method. However, with such a large time step we observed that the implicit method introduced significant error in the high-wavenumber energy spectrum. Given the higher cost per time step of an implicit method, the explicit Runge–Kutta methods still seem to be the most suitable integrators that we have found for (3.1). We therefore used these explicit methods for all of the results presented in this paper. The prospect of developing a better implicit integrator for (3.1) remains a difficult, unsolved problem. Perhaps it is possible to develop an alternative algorithm that exploits the fact that we seek only moments to (3.1) and not the instantaneous values of the solution.

Although a practical numerical method has not yet been developed to solve the rescaled spectrally reduced equations, the rescaling can be shown to be unnecessary to obtain the correct small-scale statistical relaxation in the two-dimensional enstrophy inertial range. The unscaled formulation (2.5), which is numerically tractable, may thus be sufficient for describing (*e.g.* as a subgrid model) the small-scale dynamics of two-dimensional fluid and plasma turbulence.

5. Discussion. Spectral reduction appears to be a promising candidate as a statistical description of turbulence, although for some applications, a better numerical scheme to solve (3.1) has yet to be devised. The method affords a dramatic reduction in the number of degrees of freedom that must be explicitly evolved in turbulence simulations. It has been successfully applied to confirm the existence of logarithmic corrections to the velocity structure functions in the enstrophy cascade and to lend numerical support to recent theoretical and experimental claims [7, 17] that there are no intermittency corrections in the 2D enstrophy cascade in the absence of an energy cascade. We propose that spectral reduction could be used to assess the effect of various dissipation mechanisms in large-eddy simulations, as a subgrid model, or even as a substitute for full simulation of high-Reynolds number turbulence.

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