Pseudospectral Reduction of Incompressible Two-Dimensional Turbulence

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Abstract

Spectral reduction was originally formulated entirely in the wavenumber domain as a coarse-grained wavenumber convolution in which bins of modes interact with enhanced coupling coefficients. A Liouville theorem leads to inviscid equipartition solutions when each bin contains the same number of modes. A pseudospectral implementation of spectral reduction which enjoys the efficiency of the fast Fourier transform is described. The model compares well with full pseudospectral simulations of the two-dimensional forced-dissipative energy and enstrophy cascades.

Key words: spectral reduction, decimation, pseudospectral, collocation, two-dimensional turbulence, incompressible turbulence, equipartition, coarse graining
2010 MSC: 65M70,65T50,76D06,76M22

1. Introduction

Turbulence researchers have long sought to reduce the number of degrees of freedom that must be retained in simulations of turbulent phenomena [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]. About ten years ago a novel decimation method called spectral reduction [11], which accounts for the deleted modes by coarse-graining the nonlinearity, was developed in collaboration with Prof. Philip Morrison, to whom we dedicate this paper, on the occasion of his 60th birthday.

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Spectral reduction is formulated as a coarse-grained wavenumber convolution over bins of modes that interact with enhanced coupling coefficients. The approximation possesses many desirable properties: coarse-grained analogues of primitive conservation laws, a Liouville theorem, plausible moment balance equations that resemble the exact moment balances, and a control parameter (bin size) that can be varied to increase accuracy incrementally, until the exact dynamics is recovered. In the case where each bin contains an identical number of modes, spectral reduction recovers (for mixing dynamics) the well known inviscid equipartition solutions of spectrally truncated turbulence [12, 13, 14, 15, 16]. In particular, in two dimensions, one obtains an equipartition of a linear combination of the modal energies and enstrophies [17], as shown in Fig. 1.

Two serious limitations have prevented spectral reduction from being adopted for general use. First, if the bins contain different numbers of modes (a case of practical significance, e.g. for subgrid modelling), the Liouville theorem, together with the coarse-grained conservation laws, incorrectly leads to equipartitions of bin, rather than modal, energies and enstrophies [16]. Second, because spectral reduction coarse grains the convolution arising from the advective nonlinearity, it was originally formulated entirely in the wavenumber domain. This limited its use to situations where the wavenumber reduction factor is large enough to offset the inefficiency of spectral methods relative to their pseudospectral counterparts.

In this work, we report on a recent pseudospectral implementation of spectral reduction that exploits the efficiency of the fast Fourier transform (FFT). The resulting implementation of *pseudospectral reduction* agrees well with full pseudospectral simulations of the energy and enstrophy cascades of two-dimensional (2D) forced-dissipative turbulence.

Let us begin by writing in Fourier space the 2D vorticity equation

$$\frac{\partial \omega_{\boldsymbol{k}}}{\partial t} + \nu_{\boldsymbol{k}} \omega_{\boldsymbol{k}} = \sum_{\boldsymbol{p},\boldsymbol{q}} \frac{\epsilon_{\boldsymbol{kpq}}}{q^2} \omega^*_{\boldsymbol{p}} \omega^*_{\boldsymbol{q}} + f_{\boldsymbol{k}}\, \xi(t), \tag{1}$$

where $\nu_{\boldsymbol{k}} \doteq \nu k^2$ models molecular viscosity, $\epsilon_{\boldsymbol{kpq}} \doteq (\hat{\boldsymbol{z}} \cdot \boldsymbol{p} \times \boldsymbol{q})\, \delta_{\boldsymbol{k}+\boldsymbol{p}+\boldsymbol{q},0}$ is antisymmetric under permutation of any two indices, $f_{\boldsymbol{k}}$ is an external stirring amplitude, and $\xi(t)$ represents a unit Gaussian stochastic white-noise process ($\doteq$ is used to emphasize a definition). According to a result by Novikov, the steady-state enstrophy injection rate is given by $\epsilon_Z = \frac{1}{2} \sum_{\boldsymbol{k}} |f_{\boldsymbol{k}}|^2$ [18].

We introduce a uniform coarse-grained grid that partitions the two-dimensional wavenumber domain into bins, each containing the same number r^2 of

Fourier wave vectors (assuming for simplicity that the binning reductions r in each direction are identical). The bins are labeled by capital letters to distinguish them from the underlying Fourier wave vectors, which we represent by lower-case letters. To each bin $\boldsymbol{K}$ on this grid, we associate the coarse-grained vorticity $\Omega_{\boldsymbol{K}} \doteq \frac{1}{r^2}\sum_{\boldsymbol{k}\in\boldsymbol{K}} \omega_{\boldsymbol{k}}$ and assign a characteristic Fourier wave vector $\boldsymbol{K}$ (whether $\boldsymbol{K}$ refers to a bin or its characteristic wave vector should always be clear from context).

On introducing the bin averaging operations

$$\langle f\rangle_{\boldsymbol{K}} \doteq \frac{1}{r^2}\sum_{\boldsymbol{k}\in\boldsymbol{K}} f_{\boldsymbol{k}} \quad \text{and} \quad \langle f\rangle_{\boldsymbol{K},\boldsymbol{P},\boldsymbol{Q}} \doteq \frac{1}{r^6}\sum_{\boldsymbol{k}\in\boldsymbol{K}}\sum_{\boldsymbol{p}\in\boldsymbol{P}}\sum_{\boldsymbol{q}\in\boldsymbol{Q}} f, \tag{2}$$

we may write the exact evolution equation for $\Omega_{\boldsymbol{K}}$ as

$$\frac{\partial\Omega_{\boldsymbol{K}}}{\partial t} + \langle\nu_{\boldsymbol{k}}\omega_{\boldsymbol{k}}\rangle_{\boldsymbol{K}} = r^4\sum_{\boldsymbol{P},\boldsymbol{Q}}\left\langle \frac{\epsilon_{\boldsymbol{kpq}}}{q^2}\omega^*_{\boldsymbol{p}}\omega^*_{\boldsymbol{q}}\right\rangle_{\boldsymbol{K},\boldsymbol{P},\boldsymbol{Q}} + \langle f_{\boldsymbol{k}}\rangle_{\boldsymbol{K}}\,\xi(t), \tag{3}$$

Spectral reduction [11] approximates the evolution of $\Omega_{\boldsymbol{K}}$ solely in terms of coarse-grained variables:

$$\frac{\partial\Omega_{\boldsymbol{K}}}{\partial t} + \langle\nu_{\boldsymbol{k}}\rangle_{\boldsymbol{K}}\,\Omega_{\boldsymbol{K}} = r^4\sum_{\boldsymbol{P},\boldsymbol{Q}}\frac{1}{Q^2}\,\langle\epsilon_{\boldsymbol{kpq}}\rangle_{\boldsymbol{K},\boldsymbol{P},\boldsymbol{Q}}\,\Omega^*_{\boldsymbol{P}}\Omega^*_{\boldsymbol{Q}} + F_{\boldsymbol{K}}\xi(t), \tag{4}$$

where $F_{\boldsymbol{K}}$ represents a coarse-grained stirring force. In this work we choose $F_{\boldsymbol{K}} = 2\epsilon_Z f_K/\sqrt{\sum_{\boldsymbol{K}}|f_K|^2}$ to inject exactly ϵ_Z units of enstrophy in a steady state. In the absence of forcing and dissipation, Eq. (4) is readily seen to conserve the coarse-grained energy $\frac{1}{2}\sum_{\boldsymbol{K}} K^{-2}\,|\Omega_{\boldsymbol{K}}|^2\,\Delta_{\boldsymbol{K}}$ and enstrophy $\frac{1}{2}\sum_{\boldsymbol{K}}|\Omega_{\boldsymbol{K}}|^2\,\Delta_{\boldsymbol{K}}$. However, since the $\delta_{\boldsymbol{k}+\boldsymbol{p}+\boldsymbol{q},0}$ factor appearing in the nonlinear coefficient $\epsilon_{\boldsymbol{kpq}}$ is averaged in Eq. (4) over $\boldsymbol{k}$, $\boldsymbol{p}$, and $\boldsymbol{q}$, the resulting equation is no longer a convolution. This means that Eq. (4) cannot be solved directly by the usual pseudospectral method. Nevertheless, in the case of uniform binning a generalization of the pseudospectral method can be developed to efficiently implement Eq. (4). To illustrate this, we first develop in the following section an efficient method for computing coarse-grained convolutions.

2. One-dimensional coarse-grained convolution

On defining the Nth primitive root of unity, $\zeta_N \doteq \exp(2\pi i/N)$, the one-dimensional *backwards discrete Fourier transform* of a complex vector $\{F_k :$

$k = 0, \ldots, N-1\}$ may be written as

$$\hat{F}_j \doteq \sum_{k=0}^{N-1} \zeta_N^{jk} F_k, \qquad j = 0, \ldots, N-1.$$

We recall that the FFT exploits the properties $\zeta_N^r = \zeta_{N/r}$ and $\zeta_N^N = 1$.

Pseudospectral reduction relies on the following construction. On taking $N = rM$ and $f_{rK+\ell} = F_K$ for $\ell = 0, 1, \ldots r-1$ and $K = 0, 1, \ldots, M-1$, then for $J = 0, \ldots, M-1$ and $s = 0, \ldots, r-1$ the *backwards Fourier transform of the coarse-grained data* F_K is given by

$$\hat{f}_{sM+J} = \sum_{K=0}^{M-1} \sum_{\ell=0}^{r-1} \zeta_N^{(sM+J)(rK+\ell)} F_K = S_{J,s} \hat{F}_J,$$

where

$$S_{J,s} \doteq \sum_{\ell=0}^{r-1} \zeta_N^{J\ell} \zeta_r^{s\ell} \quad \text{and} \quad \hat{F}_J \doteq \sum_{K=0}^{M-1} \zeta_M^{JK} F_K.$$

The *coarse-grained forwards Fourier transform* is given by

$$\begin{aligned} F_K &\doteq \frac{1}{Nr} \sum_{\ell=0}^{r-1} f_{rK+\ell} = \frac{1}{r^2 M} \sum_{\ell=0}^{r-1} \sum_{J=0}^{M-1} \sum_{s=0}^{r-1} \zeta_N^{-(rK+\ell)(sM+J)} \hat{f}_{sM+J} \\ &= \frac{1}{r^2 M} \sum_{J=0}^{M-1} \zeta_M^{-KJ} \sum_{s=0}^{r-1} \bar{S}_{J,s} \hat{f}_{sM+J}. \end{aligned}$$

The *coarse-grained convolution* $\langle f * g \rangle_K$ of f and g can then be computed as

$$\begin{aligned} \langle f * g \rangle_K &\doteq \frac{1}{r} \sum_{\ell=0}^{r-1} (f * g)_{rK+\ell} = \frac{1}{r^2 M} \sum_{J=0}^{M-1} \zeta_M^{-KJ} \sum_{s=0}^{r-1} \bar{S}_{J,s} \hat{f}_{sM+J} \hat{g}_{sM+J} \\ &= \frac{1}{r^2 M} \sum_{J=0}^{M-1} \zeta_M^{-KJ} W_J \hat{F}_J \hat{G}_J, \end{aligned}$$

where $W_J \doteq \sum_{s=0}^{r-1} |S_{J,s}|^2 S_{J,s}$.

Similarly, the bin-averaged Fourier transform of F_K weighted by ℓ is given by

$$\hat{f}_{sM+J} = \sum_{K=0}^{M-1} \sum_{\ell=0}^{r-1} \zeta_N^{(sM+J)(rK+\ell)} \ell F_K = T_{J,s} \hat{F}_J,$$

where

$$T_{J,s} \doteq \sum_{\ell=0}^{r-1} \ell \zeta_N^{J\ell} \zeta_r^{s\ell}.$$

For the formulation of pseudospectral reduction in the next section, it will be convenient to define

$$W'_J \doteq \sum_{s=0}^{r-1} |S_{J,s}|^2 T_{J,s}.$$

3. Pseudospectral reduction

Let us now rewrite Eq. (4), on substituting $-\boldsymbol{p}$ for $\boldsymbol{p}$ and $-\boldsymbol{q}$ for $\boldsymbol{q}$, as

$$\frac{\partial \Omega_{\boldsymbol{K}}}{\partial t} + \langle \nu_{\boldsymbol{k}} \omega_{\boldsymbol{k}} \rangle_{\boldsymbol{K}} = r^4 \sum_{\boldsymbol{P},\boldsymbol{Q}} \frac{1}{Q^2} \langle \delta_{\boldsymbol{p}+\boldsymbol{q},\boldsymbol{k}} (p_x q_y - p_y q_x) \rangle_{\boldsymbol{K},\boldsymbol{P},\boldsymbol{Q}} \, \Omega_{\boldsymbol{P}} \Omega_{\boldsymbol{Q}}.$$

Denoting $F^0 \doteq K_x \Omega_{\boldsymbol{K}}$, $F^1 \doteq K_y \Omega_{\boldsymbol{K}}$, $F^2 \doteq \Omega_{\boldsymbol{K}}$, $G^0 \doteq K_x K^{-2} \Omega_{\boldsymbol{K}}$, $G^1 \doteq K_y K^{-2} \Omega_{\boldsymbol{K}}$, and $G^2 \doteq K^{-2} \Omega_{\boldsymbol{K}}$, the nonlinear coupling may then be efficiently evaluated using 2D bin-averaged FFTs:

$$\begin{aligned}
&\sum_{\boldsymbol{P},\boldsymbol{Q}} \frac{1}{Q^2} \langle \delta_{\boldsymbol{p}+\boldsymbol{q},\boldsymbol{k}} (p_x q_y - p_y q_x) \rangle_{\boldsymbol{K},\boldsymbol{P},\boldsymbol{Q}} \, \Omega_{\boldsymbol{P}} \Omega_{\boldsymbol{Q}} \\
&= \frac{1}{r^2} \sum_{\boldsymbol{\ell}} \left([(rK_x + \ell_x) \Omega_{\boldsymbol{K}}] * \left[(rK_y + \ell_y) K^{-2} \Omega_{\boldsymbol{K}} \right] \right)_{r\boldsymbol{K}+\boldsymbol{\ell}} \\
&\qquad - \frac{1}{r^2} \sum_{\boldsymbol{\ell}} \left([(rK_y + \ell_y) \Omega_{\boldsymbol{K}}] * \left[(rK_x + \ell_x) K^{-2} \Omega_{\boldsymbol{K}} \right] \right)_{r\boldsymbol{K}+\boldsymbol{\ell}} \\
&= \frac{1}{r^4 M^2} \sum_{\boldsymbol{J}} \zeta_M^{-\boldsymbol{K}\cdot\boldsymbol{J}} \Big[r^2 W_{J_x} W_{J_y} (\hat{F}^0_{\boldsymbol{J}} \hat{G}^1_{\boldsymbol{J}} - \hat{F}^1_{\boldsymbol{J}} \hat{G}^0_{\boldsymbol{J}}) \\
&\qquad + r W'_{J_x} W_{J_y} (\hat{F}^2_{\boldsymbol{J}} \hat{G}^1_{\boldsymbol{J}} - \hat{F}^1_{\boldsymbol{J}} \hat{G}^2_{\boldsymbol{J}}) + r W_{J_x} W'_{J_y} (\hat{F}^0_{\boldsymbol{J}} \hat{G}^2_{\boldsymbol{J}} - \hat{F}^2_{\boldsymbol{J}} \hat{G}^0_{\boldsymbol{J}}) \Big],
\end{aligned} \tag{5}$$

noting that the two terms involving $\ell_x \ell_y$ cancel. The term proportional to r^2 represents the usual 2D pseudospectral contribution to the convolution, which would normally require five 2D Fourier transforms. The two terms proportional to r require two additional Fourier transforms (to compute $\hat{F}^2_{\boldsymbol{J}}$ and $\hat{G}^2_{\boldsymbol{J}}$), as well as a few extra multiplications and additions. Asymptotically, the computation time for pseudospectral reduction is thus seen to be $\mathcal{O}(N \log N)$, but with a coefficient $7/5 = 1.4$ times greater than the scaling for a conventional pseudospectral method.

4. Hermitian case

In view of the reality condition $\omega_{-\boldsymbol{k}} = \omega^*_{\boldsymbol{k}}$, only the independent modes (say those in the upper half wavenumber plane) are evolved in an efficient pseudospectral simulation. For this reason, one would typically restrict the decimation radix r to be odd, taking the the coarse-grained index $\boldsymbol{K}$ to correspond to the central wave vector in each bin of a uniform $r \times r$ lattice. In each direction, the fine scale wave vector components can then expressed as $k = rK + \ell$, where ℓ takes on one of the r integral values in $[-(r-1)/2, (r-1)/2]$. In this case one chooses the Hermitian fields $F^0 \doteq iK_x \Omega_{\boldsymbol{K}}$, $F^1 \doteq iK_y \Omega_{\boldsymbol{K}}$, $F^2 \doteq \Omega_{\boldsymbol{K}}$, $G^0 \doteq -iK_x K^{-2} \Omega_{\boldsymbol{K}}$, $G^1 \doteq -iK_y K^{-2} \Omega_{\boldsymbol{K}}$, and $G^2 \doteq -K^{-2} \Omega_{\boldsymbol{K}}$. The corresponding spatial weight factors are then real:

$$S_{J,s} \doteq \sum_{\ell=-(r-1)/2}^{(r-1)/2} \zeta_N^{J\ell} \zeta_r^{s\ell} = 1 + 2\,\mathrm{Re} \sum_{\ell=1}^{(r-1)/2} \zeta_N^{J\ell} \zeta_r^{s\ell},$$

$$T_{J,s} \doteq \sum_{\ell=-(r-1)/2}^{(r-1)/2} i\ell \zeta_N^{J\ell} \zeta_r^{s\ell} = -2\,\mathrm{Im} \sum_{\ell=1}^{(r-1)/2} \ell \zeta_N^{J\ell} \zeta_r^{s\ell}.$$

Using these definitions, the spatial weight factors W and W' appearing in Eq. (5) can then be constructed. We have recently expanded our efficient `FFTW++` [19, 20] library to include an implicitly dealiased version of the resulting 2D coarse-grained Hermitian convolution.

5. Comparison against full dynamics

Because pseudospectral reduction conserves both energy and enstrophy and satisfies Liouville's theorem, with uniform binning one expects inviscid

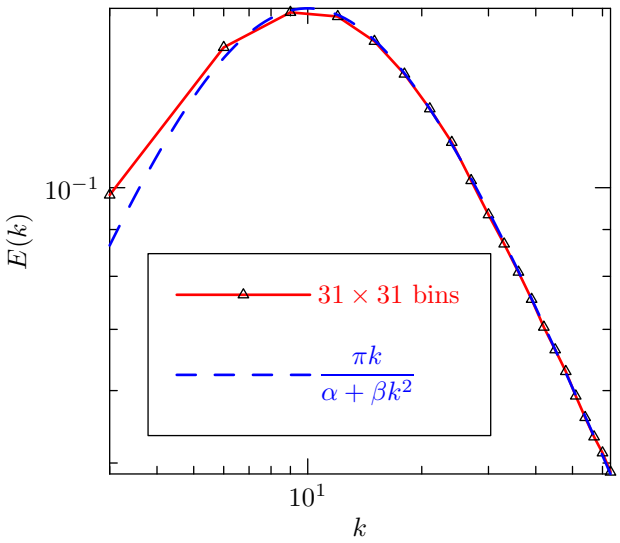

Figure 1: Inviscid equipartition of a 31×31 pseudospectrally reduced simulation with radix $r = 3$ to the theoretically expected curve $\pi k/(\alpha+\beta k^2)$, where the constants α and β are Lagrange multipliers.

equipartition solutions of the form illustrated in Fig. 1. This represents a nontrivial test of the nonlinear dynamical interactions.

In Fig. 2, we compare the direct cascade predicted by a radix $r = 3$ pseudospectrally reduced simulation using 85×85 bins with the energy spectrum for a full 255×255 simulation. Here, the forcing is band-limited to wavenumbers in $[3.5, 4.5]$, the injection rate is $\epsilon_Z = 1$, and $\nu_{\boldsymbol{k}} = 0.0002k^2 + 0.15$. We observe that pseudospectral reduction captures the inertial-range and dissipation dynamics reasonably well, doing much better than the naive decimation obtained by simply dropping all modes with wavenumber coordinates that are not multiples of 3.

In Fig. 3, we demonstrate that a radix $r = 3$ pseudospectrally reduced simulation with 85×85 bins closely approximates the inverse cascade obtained with a full 255×255 simulation. Here, the forcing is band-limited to wavenumbers in $[59.5, 60.5]$, the injection rate is $\epsilon_Z = 1$, and $\nu_{\boldsymbol{k}} = 1.5 \times 10^{-5}k^2 + 0.03$.

We should point out that, in contrast to the situation for conventional zero-padded Hermitian convolutions, the optimal sizes for implicitly dealiased Hermitian convolutions are one less than a power of two. The resolutions for

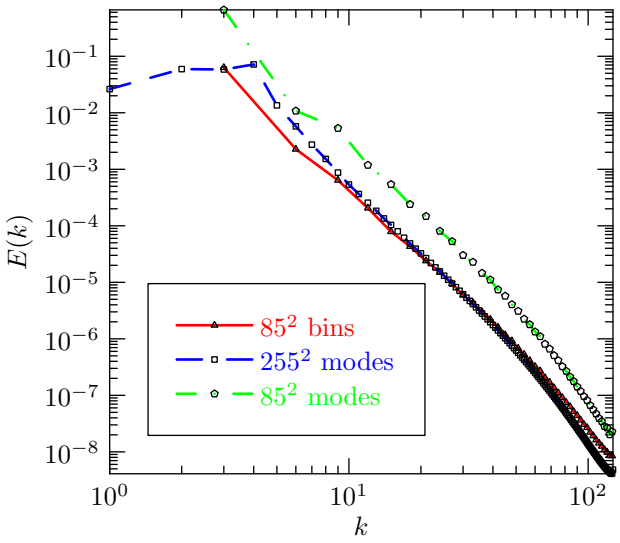

Figure 2: Comparison of the direct cascades obtained for a pseudospectrally reduced simulation with 85×85 bins, a pseudospectral simulation with 255×255 modes, and a "poor-man's" decimation using 85×85 modes and a mode spacing of 3.

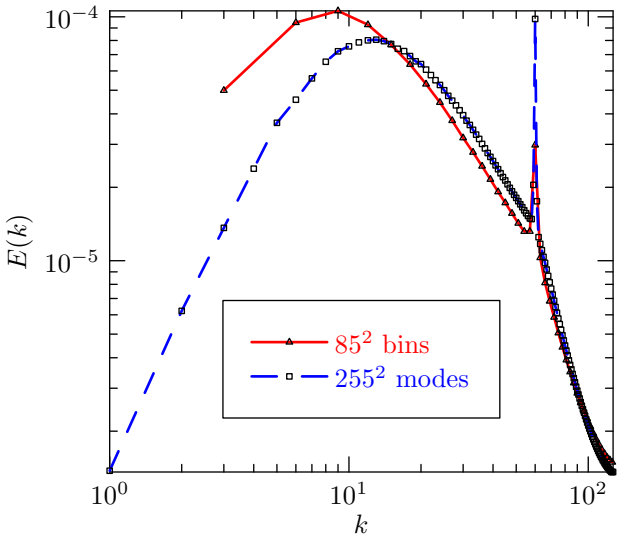

Figure 3: Comparison of the inverse cascades obtained for a pseudospectrally reduced simulation with 85×85 bins and a pseudospectral simulation with 255×255 modes.

the pseudospectral reduction approximations in Figs. 2 and 3 were chosen to match the full simulations but are actually suboptimal: a 127×127 pseudospectral reduction simulation affords a maximum truncation wavenumber almost 50% higher but runs only about 14% slower!

6. Conclusions

In this work, one of the two outstanding issues with spectral reduction is addressed, namely the need for a pseudospectral formulation. Recognizing that spectral reduction yields correct inviscid equipartition spectra only with uniform binning and restricting our attention to this case only, an efficient FFT-based implementation, which we call pseudospectral reduction, is proposed.

Even with uniform binning, we have seen that the resulting energy spectrum is much closer to the predictions of the full dynamics than, say, the spectrum obtained by simply using a smaller spatial domain (larger mode spacing). This is because spectral reduction incorporates fine-scale geometrical interactions in the form of renormalized nonlinear coupling coefficients. This distinction suggests that spectral reduction could be used to develop a reliable dynamic subgrid model. With this in mind, an ongoing project is underway [21] to develop a means of coupling such a pseudospectrally reduced subgrid model to the larger-scale dynamics of a fully resolved grid.

Acknowledgments

Both authors would like to thank the Kavli Institute for Theoretical Physics for its hospitality at the recent workshop, "The Nature of Turbulence", where the ideas in this work were conceived and implemented. Additional financial support for this work was generously provided by the Natural Sciences and Engineering Research Council of Canada.

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