

# Pseudospectral Reduction of Incompressible Two-Dimensional Turbulence

John C. Bowman and Malcolm Roberts  
University of Alberta

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[www.math.ualberta.ca/~bowman/talks](http://www.math.ualberta.ca/~bowman/talks)

# 2D Turbulence in Fourier Space

- Navier–Stokes equation for vorticity  $\omega \doteq \hat{\mathbf{z}} \cdot \nabla \times \mathbf{u}$ :

$$\frac{\partial \omega}{\partial t} + \mathbf{u} \cdot \nabla \omega = \nu \nabla^2 \omega + f.$$

- In Fourier space:

$$\frac{\partial \omega_{\mathbf{k}}}{\partial t} + \nu_{\mathbf{k}} \omega_{\mathbf{k}} = \int d\mathbf{p} \int d\mathbf{q} \frac{\epsilon_{\mathbf{k}\mathbf{p}\mathbf{q}}}{q^2} \omega_{\mathbf{p}}^* \omega_{\mathbf{q}}^* + f_{\mathbf{k}},$$

where  $\nu_{\mathbf{k}} \doteq \nu k^2$  and  $\epsilon_{\mathbf{k}\mathbf{p}\mathbf{q}} \doteq (\hat{\mathbf{z}} \cdot \mathbf{p} \times \mathbf{q}) \delta(\mathbf{k} + \mathbf{p} + \mathbf{q})$  is antisymmetric under permutation of any two indices.

- When  $\nu = f_{\mathbf{k}} = 0$ ,

enstrophy  $Z = \frac{1}{2} \sum_{\mathbf{k}} |\omega_{\mathbf{k}}|^2$  and energy  $E = \frac{1}{2} \sum_{\mathbf{k}} \frac{|\omega_{\mathbf{k}}|^2}{k^2}$  are

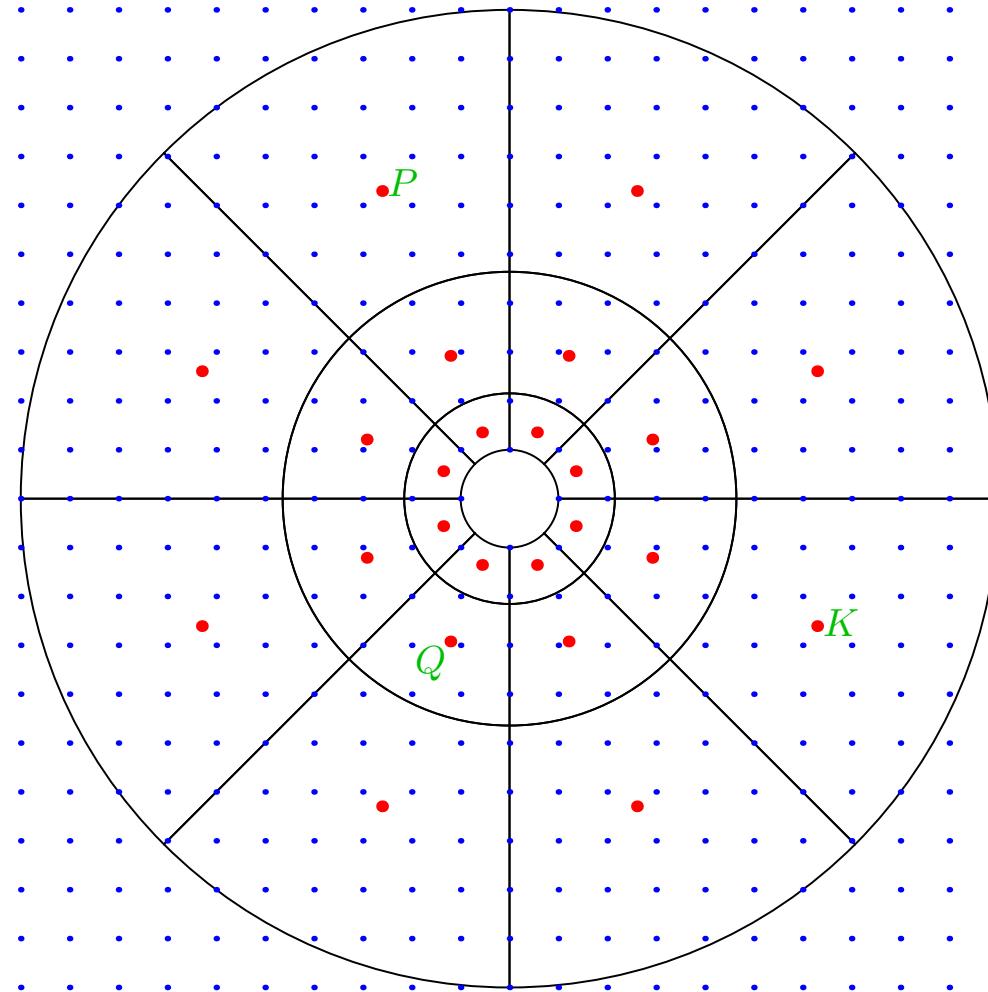
conserved:

$$\frac{\epsilon_{\mathbf{k}pq}}{q^2} \quad \text{antisymmetric in } \mathbf{k} \leftrightarrow \mathbf{p},$$

$$\frac{1}{k^2} \frac{\epsilon_{\mathbf{k}pq}}{q^2} \quad \text{antisymmetric in } \mathbf{k} \leftrightarrow \mathbf{q}.$$

# Spectral Reduction

- Introduce a coarse-grained grid indexed by  $K$ :



Wavenumber Bin Geometry ( $8 \times 3$  bins)

- Define new variables

$$\Omega_{\mathbf{K}} = \langle \omega_{\mathbf{k}} \rangle_{\mathbf{K}} \doteq \frac{1}{\Delta_{\mathbf{K}}} \int_{\Delta_{\mathbf{K}}} \omega_{\mathbf{k}} d\mathbf{k},$$

where  $\Delta_{\mathbf{K}}$  is the area of bin  $\mathbf{K}$ .

- Evolution of  $\Omega_{\mathbf{K}}$ :

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

where  $\langle f \rangle_{KPQ} = \frac{1}{\Delta_{\mathbf{K}} \Delta_{\mathbf{P}} \Delta_{\mathbf{Q}}} \int_{\Delta_{\mathbf{K}}} d\mathbf{k} \int_{\Delta_{\mathbf{P}}} d\mathbf{p} \int_{\Delta_{\mathbf{Q}}} d\mathbf{q} f$ .

- Approximate  $\omega_{\mathbf{p}}$  and  $\omega_{\mathbf{q}}$  by bin-averaged values  $\Omega_{\mathbf{P}}$  and  $\Omega_{\mathbf{Q}}$ :

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

- Define the coarse-grained enstrophy  $Z$  and energy  $E$ :

$$Z \doteq \frac{1}{2} \sum_{\mathbf{K}} |\Omega_{\mathbf{K}}|^2 \Delta_{\mathbf{K}}, \quad E \doteq \frac{1}{2} \sum_{\mathbf{K}} \frac{|\Omega_{\mathbf{K}}|^2}{K^2} \Delta_{\mathbf{K}}.$$

- Enstrophy is still conserved by the nonlinearity since

$$\left\langle \frac{\epsilon_{kpq}}{q^2} \right\rangle_{\mathbf{KPQ}} \quad \text{antisymmetric in } \mathbf{K} \leftrightarrow \mathbf{P}.$$

- But energy conservation has been lost!

$$\frac{1}{K^2} \left\langle \frac{\epsilon_{kpq}}{q^2} \right\rangle_{\mathbf{KPQ}} \quad \text{NOT antisymmetric in } \mathbf{K} \leftrightarrow \mathbf{Q}.$$

- Reinstate both desired symmetries with the modified coefficient

$$\frac{\langle \epsilon_{kpq} \rangle_{\mathbf{KPQ}}}{Q^2}.$$

# Properties

- We call the forced-dissipative version of this approximation *spectral reduction* (SR):

$$\frac{\partial \Omega_{\mathbf{K}}}{\partial t} + \langle \nu_{\mathbf{k}} \rangle_{\mathbf{K}} \Omega_{\mathbf{K}} = \sum_{\mathbf{P}, \mathbf{Q}} \Delta_{\mathbf{P}} \Delta_{\mathbf{Q}} \frac{\langle \epsilon_{\mathbf{k}pq} \rangle_{\mathbf{KPQ}}}{Q^2} \Omega_{\mathbf{P}}^* \Omega_{\mathbf{Q}}^*.$$

- SR conserves both energy and enstrophy and reduces to the exact dynamics in the limit of small bin size.
- It has the same general structure and symmetries as the original equation and in this sense may be considered a *renormalization*.
- SR obeys a Liouville Theorem; in the inviscid limit, it yields statistical-mechanical (equipartition) solutions.
- However: since the  $\delta_{\mathbf{k}+\mathbf{p}+\mathbf{q},0}$  factor in the nonlinear coefficient  $\epsilon_{\mathbf{k}pq}$  has been smoothed over, spectral reduction is no longer a convolution: pseudospectral collocation does not apply.

# Moments

- Q. How accurate is spectral reduction?
- A. For large bins, the *instantaneous* dynamics of SR is inaccurate.
- However: the equations for the *time-averaged* (or ensemble-averaged) moments predicted by SR closely approximate those of the exact bin-averaged statistics.
- E.g., time average the exact bin-averaged enstrophy equation:

$$\overline{\frac{\partial}{\partial t} \left\langle |\omega_{\mathbf{k}}|^2 \right\rangle_{\mathbf{K}}} + 2 \operatorname{Re} \left\langle \nu_{\mathbf{k}} \overline{|\omega_{\mathbf{k}}|^2} \right\rangle_{\mathbf{K}} = 2 \operatorname{Re} \sum_{\mathbf{P}, \mathbf{Q}} \Delta_{\mathbf{P}} \Delta_{\mathbf{Q}} \left\langle \frac{\epsilon_{\mathbf{k}pq}}{q^2} \overline{\omega_{\mathbf{k}}^* \omega_{\mathbf{p}}^* \omega_{\mathbf{q}}^*} \right\rangle_{\mathbf{KPQ}},$$

where the bar means time average and  $\langle \cdot \rangle_{\mathbf{K}}$  means bin average.

- Time-averaged quantities such as  $\overline{|\omega_{\mathbf{k}}|^2}$  and  $\overline{\omega_{\mathbf{k}}^* \omega_{\mathbf{p}}^* \omega_{\mathbf{q}}^*}$  are generally *smooth* functions of  $\mathbf{k}$ ,  $\mathbf{p}$ ,  $\mathbf{q}$  on the four-dimensional surface defined by the triad condition  $\mathbf{k} + \mathbf{p} + \mathbf{q} = 0$ .

- Mean Value Theorem for integrals: for some  $\xi \in K$ .

$$\overline{|\Omega_K|^2} = \overline{|\omega_\xi|^2} \approx \overline{|\omega_k|^2} \quad \forall k \in K.$$

- To good accuracy these statistical moments may therefore be evaluated at the characteristic wavenumbers  $K, P, Q$ :

$$\overline{\frac{\partial}{\partial t} |\Omega_K|^2} + 2 \operatorname{Re} \langle \nu_k \rangle_K \overline{|\Omega_K|^2} = 2 \operatorname{Re} \sum_{P,Q} \Delta_P \Delta_Q \left\langle \frac{\epsilon_{kpq}}{q^2} \right\rangle_{KPKQ} \overline{\Omega_K^* \Omega_P^* \Omega_Q^*}.$$

- To the extent that the wavenumber magnitude  $q$  varies slowly over a bin:

$$\overline{\frac{\partial}{\partial t} |\Omega_K|^2} + 2 \operatorname{Re} \langle \nu_k \rangle_K \overline{|\Omega_K|^2} = 2 \operatorname{Re} \sum_{P,Q} \Delta_P \Delta_Q \frac{\langle \epsilon_{kpq} \rangle_{KPKQ}}{Q^2} \overline{\Omega_K^* \Omega_P^* \Omega_Q^*}.$$

- But this is precisely the time-average of the SR equation!

# Noncanonical Hamiltonian Formulation

- Underlying *noncanonical* Hamiltonian formulation for inviscid 2D vorticity equation:

$$\dot{\omega}_{\mathbf{k}} = \int d\mathbf{q} J_{\mathbf{k}\mathbf{q}} \frac{\delta H}{\delta \omega_{\mathbf{q}}},$$

where

$$H \doteq \frac{1}{2} \int d\mathbf{k} \frac{|\omega_{\mathbf{k}}|^2}{k^2},$$

$$J_{\mathbf{k}\mathbf{q}} \doteq \int d\mathbf{p} \epsilon_{\mathbf{k}\mathbf{p}\mathbf{q}} \omega_{\mathbf{p}}^*.$$

- Leads to inviscid Navier–Stokes equation:

$$\frac{\partial \omega_{\mathbf{k}}}{\partial t} + \nu_{\mathbf{k}} \omega_{\mathbf{k}} = \int d\mathbf{p} \int d\mathbf{q} \frac{\epsilon_{\mathbf{k}\mathbf{p}\mathbf{q}}}{q^2} \omega_{\mathbf{p}}^* \omega_{\mathbf{q}}^*.$$

# Liouville Theorem

- Navier–Stokes:

$$J_{\mathbf{k}\mathbf{q}} \doteq \int d\mathbf{p} \epsilon_{kpq} \omega_p^*$$

$$\Rightarrow \int d\mathbf{k} \frac{\delta \dot{\omega}_{\mathbf{k}}}{\delta \omega_{\mathbf{k}}} = \int d\mathbf{k} \int d\mathbf{q} \underbrace{\frac{\delta J_{\mathbf{k}\mathbf{q}}}{\delta \omega_{\mathbf{k}}}}_{\epsilon_{\mathbf{k}(-\mathbf{k})\mathbf{q}}=0} \frac{\delta H}{\delta \omega_{\mathbf{q}}} + J_{\mathbf{k}\mathbf{q}} \frac{\delta^2 H}{\delta \omega_{\mathbf{k}} \delta \omega_{\mathbf{q}}} = 0.$$

- Spectral Reduction:

$$J_{\mathbf{K}\mathbf{Q}} \doteq \sum_{\mathbf{P}} \Delta_{\mathbf{P}} \langle \epsilon_{kpq} \rangle_{\mathbf{K}\mathbf{P}\mathbf{Q}} \Omega_{\mathbf{P}}^*$$

$$\Rightarrow \sum_{\mathbf{K}} \frac{\partial \dot{\Omega}_{\mathbf{K}}}{\partial \Omega_{\mathbf{K}}} = \sum_{\mathbf{K}, \mathbf{Q}} \underbrace{\frac{\partial J_{\mathbf{K}\mathbf{Q}}}{\partial \Omega_{\mathbf{K}}}}_{\langle \epsilon_{kpq} \rangle_{\mathbf{K}(-\mathbf{K})\mathbf{Q}}=0} \frac{\partial H}{\partial \Omega_{\mathbf{Q}}} + J_{\mathbf{K}\mathbf{Q}} \frac{\partial^2 H}{\partial \Omega_{\mathbf{K}} \partial \Omega_{\mathbf{Q}}} = 0.$$

# Statistical Equipartition

- For *mixing* dynamics, the Liouville Theorem and the coarse-grained invariants

$$E \doteq \frac{1}{2} \sum_{\mathbf{K}} \frac{|\Omega_{\mathbf{K}}|^2}{K^2} \Delta_{\mathbf{K}}, \quad Z \doteq \frac{1}{2} \sum_{\mathbf{K}} |\Omega_{\mathbf{K}}|^2 \Delta_{\mathbf{K}},$$

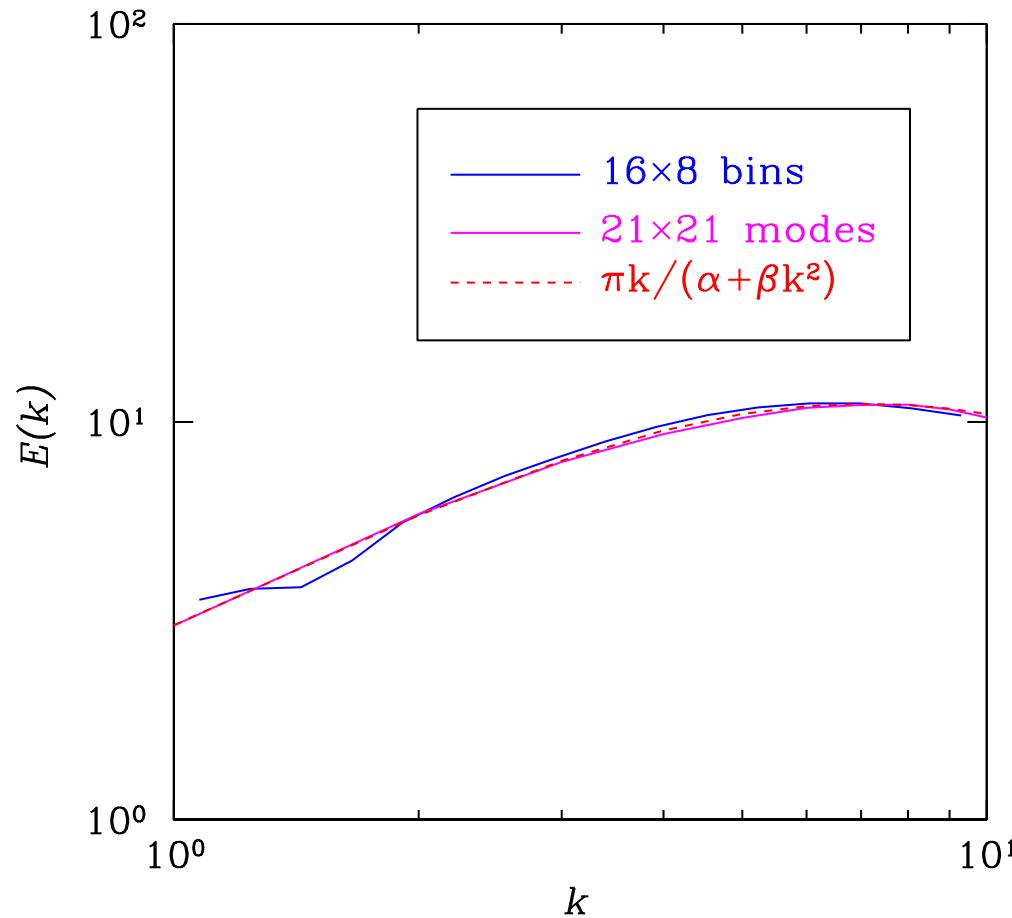
lead to statistical equipartition of  $(\alpha/K^2 + \beta) |\Omega_{\mathbf{K}}|^2 \Delta_{\mathbf{K}}$ .

- This is the correct equipartition only for **uniform bins**.
- However, for nonuniform bins, a rescaling of time by  $\Delta_{\mathbf{K}}$ ,

$$\boxed{\frac{1}{\Delta_{\mathbf{K}}} \frac{\partial \Omega_{\mathbf{K}}}{\partial t} + \langle \nu_{\mathbf{k}} \rangle_{\mathbf{K}} \Omega_{\mathbf{K}} = \sum_{P,Q} \Delta_P \Delta_Q \frac{\langle \epsilon_{kpq} \rangle_{KPQ}}{Q^2} \Omega_P^* \Omega_Q^*,}$$

yields the correct inviscid equipartition:  $\left\langle |\Omega_{\mathbf{K}}|^2 \right\rangle = \left( \frac{\alpha}{K^2} + \beta \right)^{-1}$ .

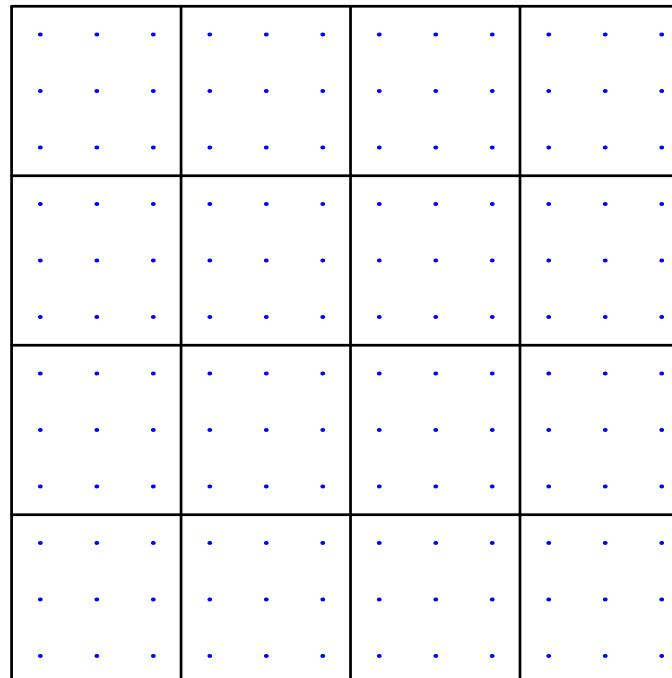
- Unfortunately, the rescaled spectral reduction equations are hopelessly stiff.



Relaxation of rescaled spectral reduction to equipartition.

# Spectral Reduction on a Lattice

- Reluctantly, we accept the fact that each bin must contain the same number of modes.
- Imposing uniform bins has an important advantage: it affords a pseudospectral implementation of spectral reduction!
- Consider spectral reduction on a coarse-grained lattice, with  $r \times r$  modes per rectangular bin (here  $r = 3$ ):



- The bin-averaging operations become:

$$\langle f_{\mathbf{k}} \rangle_{\mathbf{K}} \doteq \frac{1}{r^2} \sum_{\mathbf{k} \in \mathbf{K}} f_{\mathbf{k}},$$

$$\langle f_{\mathbf{k}pq} \rangle_{\mathbf{KPQ}} \doteq \frac{1}{r^6} \sum_{\mathbf{k} \in \mathbf{K}} \sum_{\mathbf{p} \in \mathbf{P}} \sum_{\mathbf{q} \in \mathbf{Q}} f_{\mathbf{k}pq}.$$

- Uniform discrete spectral reduction:

$$\frac{\partial \Omega_{\mathbf{K}}}{\partial t} + \langle \nu_{\mathbf{k}} \rangle_{\mathbf{K}} \Omega_{\mathbf{K}} = r^4 \sum_{\mathbf{P}, \mathbf{Q}} \frac{1}{Q^2} \langle \epsilon_{\mathbf{k}pq} \rangle_{\mathbf{KPQ}} \Omega_{\mathbf{P}}^* \Omega_{\mathbf{Q}}^* + F_{\mathbf{K}} \xi(t).$$

- Let  $\xi(t)$  be a unit Gaussian stochastic white-noise process and choose  $F_{\mathbf{K}} = 2\epsilon_Z \frac{f_K}{\sqrt{\sum_{\mathbf{K}} |f_K|^2}}$  to inject on average  $\epsilon_Z$  units of enstrophy Novikov [1964].

# Discrete Fast Fourier Transform

- Define the *Nth primitive root of unity*:

$$\zeta_N = \exp\left(\frac{2\pi i}{N}\right).$$

- The fast Fourier transform (FFT) method exploits the properties that  $\zeta_N^r = \zeta_{N/r}$  and  $\zeta_N^N = 1$ .

# FFT of a Piecewise Constant Function

- Suppose  $N = rM$  and  $f_{rK+\ell} = F_K$  for  $\ell = 0, 1, \dots, r-1$  and  $K = 0, 1, \dots, M-1$ .
- For  $J = 0, \dots, M-1$  and  $s = 0, \dots, r-1$  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

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

$$\hat{F}_J \doteq \sum_{K=0}^{M-1} \zeta_M^{JK} F_K.$$

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

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

# 1D Coarse-Grained Convolution

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

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

in terms of the spatial weight factors  $W_J \doteq \sum_{s=0}^{r-1} |S_{J,s}|^2 S_{J,s}$ .

- Similarly, the bin-averaged Fourier transform of  $F_K$  weighted by  $\ell$  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

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

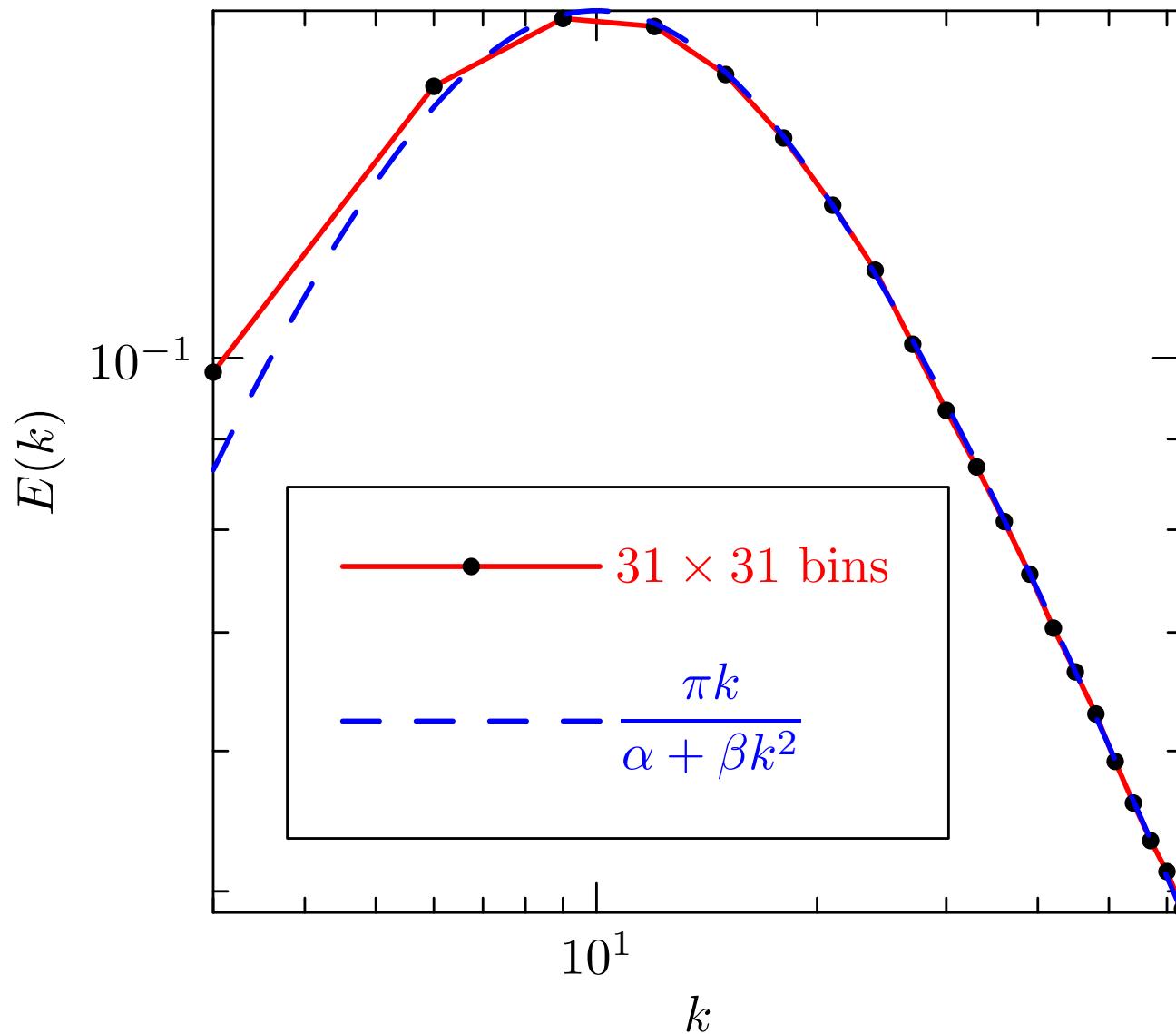
- Let  $W'_J \doteq \sum_{s=0}^{r-1} |S_{J,s}|^2 T_{J,s}$ .

# Pseudospectral reduction

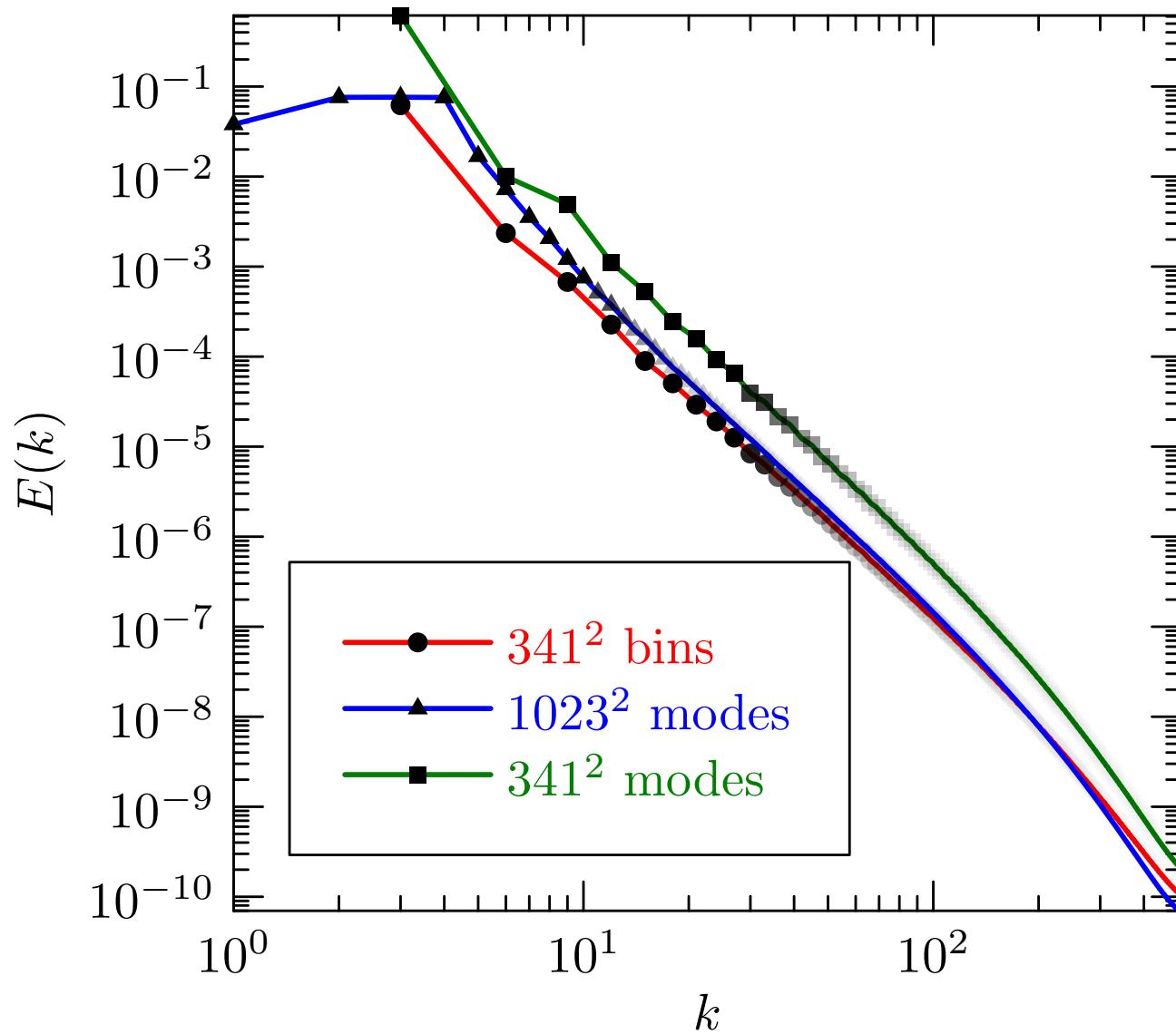
- In terms of  $F^0 \doteq K_x \Omega_{\mathbf{K}}$ ,  $F^1 \doteq K_y \Omega_{\mathbf{K}}$ ,  $F^2 \doteq \Omega_{\mathbf{K}}$ ,  $G^0 \doteq K_x K^{-2} \Omega_{\mathbf{K}}$ ,  $G^1 \doteq K_y K^{-2} \Omega_{\mathbf{K}}$ , and  $G^2 \doteq K^{-2} \Omega_{\mathbf{K}}$ :

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

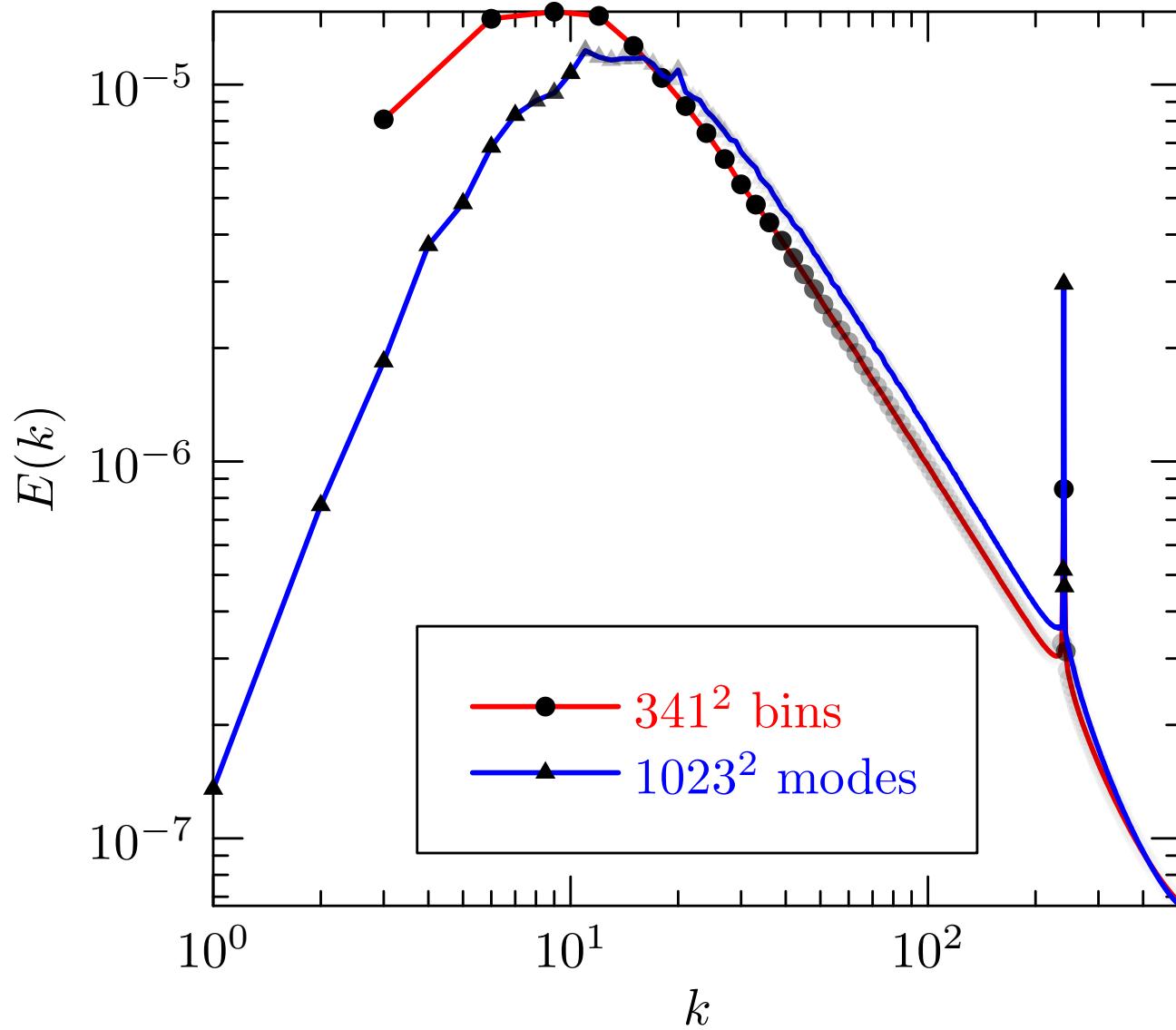
- Computational complexity is  $\mathcal{O}(N \log N)$ , with a coefficient  $7/5 = 1.4$  times greater than for pseudospectral collocation.



Inviscid equipartition of a  $31 \times 31$  pseudospectrally reduced simulation with radix  $r = 3$ .



Direct cascade.



Inverse cascade.

# Implicit Dealiasing

- Over 40 years ago, Orszag pointed out the importance of dealiasing pseudospectral convolutions:
  - Convolution is **linear**.
  - Discrete Fourier transform is **cyclic**.
- In 2D, implicit dealiasing [Bowman & Roberts 2011] uses 2/3 of the memory and half of the computation time compared to explicit (2/3 rule) zero padding.
- Our efficient FFTW++ library was generalized to support implicitly dealiased 2D coarse-grained Hermitian convolutions:  
<http://fftwpp.sourceforge.net>
- Writing a high-performance dealiased pseudospectral code is now a relatively straightforward exercise.

# Parallelization

- Our implicit convolution routines have been multithreaded for shared-memory architectures.
- Parallel generalized slab/pencil model implementations have also been developed for distributed-memory architectures (available in svn repository and upcoming 1.14 release).
- The key bottleneck is the distributed matrix transpose.
- We have compared several distributed matrix transpose algorithms, both blocking and nonblocking, under both pure MPI and hybrid MPI/OpenMP architectures.
- One advantage of hybrid MPI/OpenMP over pure MPI for matrix transposition is that it yields a larger communication block size.

# Conclusions

- Spectral reduction reduces the number of degrees of freedom that must be explicitly evolved in turbulence simulations.
- One can evolve a turbulent system for thousands of eddy turnover times to obtain energy spectra smooth enough to compare with theory.
- Recognizing that spectral reduction yields inviscid equipartition spectra only with uniform binning, we developed an efficient FFT-based implementation, called pseudospectral reduction.
- Even with uniform binning, the resulting energy spectrum is much more accurate than what results from simply using a smaller spatial domain (larger mode spacing).
- Spectral reduction could be used to develop a reliable dynamic subgrid model by coupling a pseudospectrally reduced subgrid model to a large-eddy simulation [Roberts 2011].

# Asymptote: 2D & 3D Vector Graphics Language



Andy Hammerlindl, John C. Bowman, Tom Prince

<http://asymptote.sf.net>

(freely available under the GNU public license)

# Asymptote Lifts T<sub>E</sub>X to 3D

$$\int_{-\infty}^{+\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$$

<http://asymptote.sf.net>

Acknowledgements: Orest Shardt (U. Alberta)

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