Transparent boundary conditions as dissipative closures

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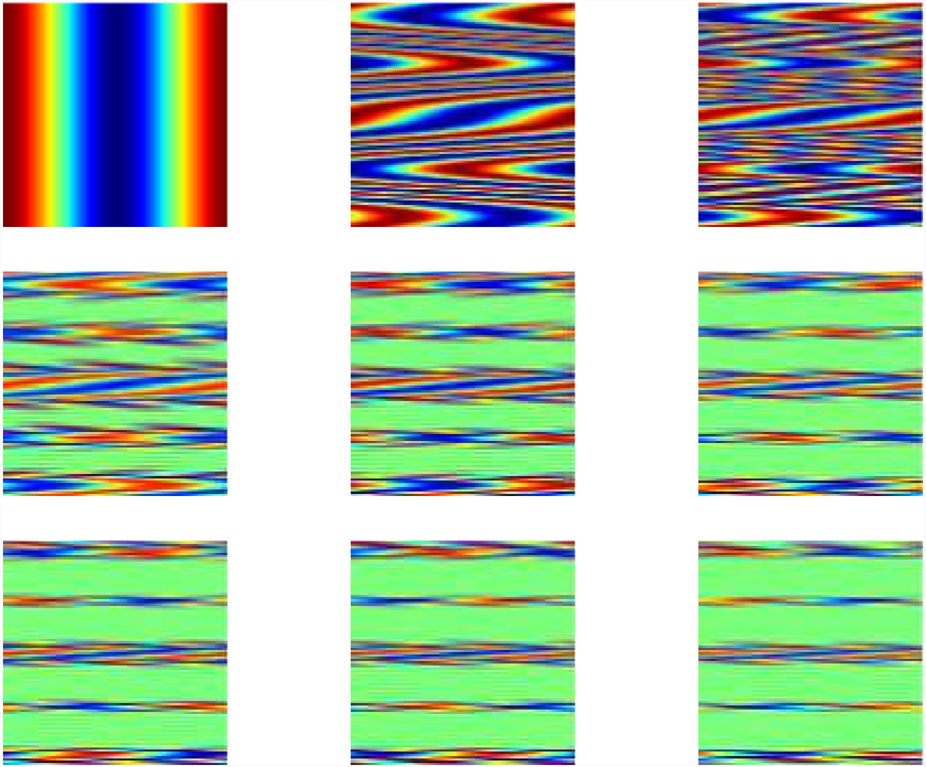
Overview

- Motivation
- Dispersive lattice waves in Fourier space
- Transparent boundary conditions
- Steady shear flows
- Unsteady shear flows



Simple example: Tracer in a shear flow

1. Motivation

- Even simple flows induce complex tracer fields
  (stretching in shear regions, "chaotic mixing")
- Some complex flows have simple velocity fields
  (potential vorticity controlled flows in GFD)
  E.g.: *quasigeostrophic equations*

$$\partial_t q + \boldsymbol{u} \cdot \boldsymbol{\nabla} q = 0 \,,$$
$$q = (1 - \Delta)\psi \,,$$
$$\boldsymbol{u} = \boldsymbol{\nabla}^\perp \psi$$

- Observation: Interaction in Fourier space is predominantly local
  Can we take advantage of this?
- Model: Passive advection

$$\partial_t \theta + \boldsymbol{u} \cdot \boldsymbol{\nabla} \theta = 0$$

  where $\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$.

2. The necessity of dissipation

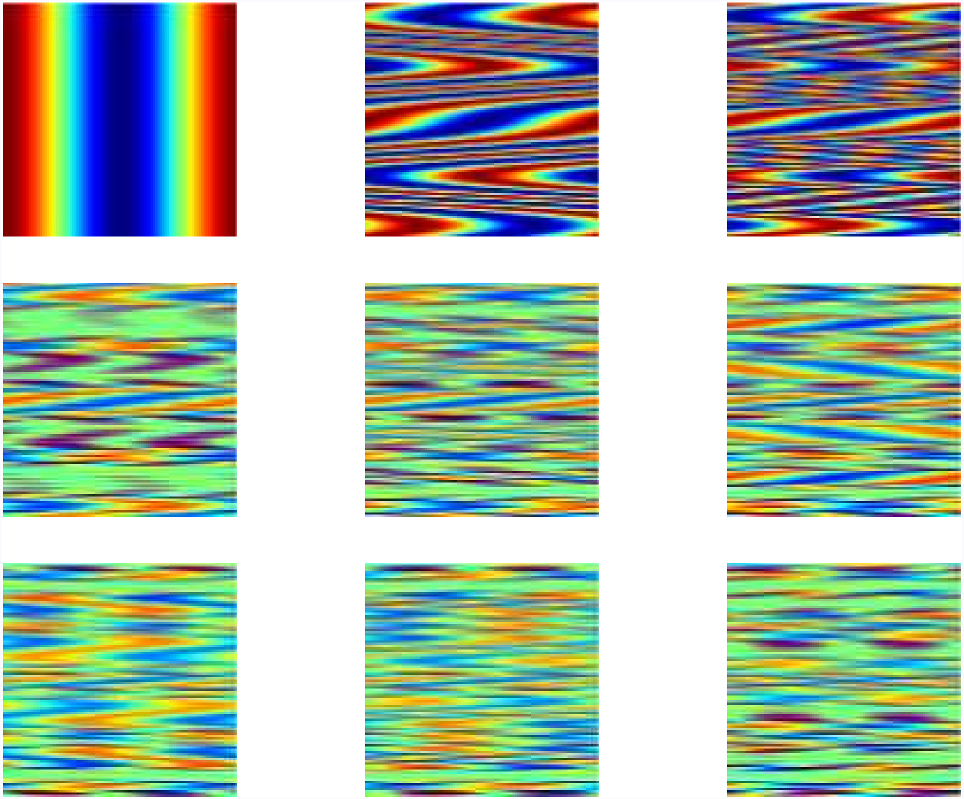
Fourier-Galerkin projection of advection equation:

$$\partial_t \theta_m + \mathbb{P}_m(\boldsymbol{u}_m \cdot \boldsymbol{\nabla} \theta_m) = 0$$

This finite dimensional truncation is conservative:

$$\begin{aligned}
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbb{P}_m\theta\|^2 &= \langle \mathbb{P}_m\theta, \partial_t\theta\rangle \\
&= \langle \mathbb{P}_m\theta, \boldsymbol{u}\cdot\boldsymbol{\nabla}\mathbb{P}_m\theta\rangle \\
&= \frac{1}{2}\langle \boldsymbol{\nabla}\cdot\boldsymbol{u}, (\mathbb{P}_m\theta)^2\rangle \\
&= 0
\end{aligned}$$

Is this what we want?



Galerkin truncation

3. Large eddy simulation

Filtered fields

$$\overline{\theta} = G * \theta \,, \qquad \overline{\boldsymbol{u}} = G * \boldsymbol{u}$$

with suitable mollifier G

Filtered equation

$$\partial_t \overline{\theta} + \overline{\boldsymbol{u}} \cdot \boldsymbol{\nabla} \overline{\theta} = \overline{\boldsymbol{u}} \cdot \boldsymbol{\nabla} \overline{\theta} - \overline{\boldsymbol{u} \cdot \boldsymbol{\nabla} \theta} \equiv \boldsymbol{\nabla} \cdot \boldsymbol{\tau} \,,$$

Closure problem

Find subgrid model

$$\boldsymbol{\tau} = \boldsymbol{\tau}(\overline{\theta}, \overline{\boldsymbol{u}})$$

Example: Classical Smagorinski closure for 3D turbulence

$$\boldsymbol{\tau} - \tfrac{1}{3} \boldsymbol{I} \ \mathrm{Tr} \, \boldsymbol{\tau} \equiv -2 \, \nu_{\mathrm{eddy}}(|\mathrm{Def} \, \boldsymbol{u}|) \ \mathrm{Def} \, \boldsymbol{u} \,,$$

with deformation tensor $\mathrm{Def} \, \boldsymbol{u} = \tfrac{1}{2} \, (\boldsymbol{\nabla} \boldsymbol{u} + \boldsymbol{\nabla} \boldsymbol{u}^T)$

4. $1\frac{1}{2}$-D toy model: Shear flows

Consider

$$\partial_t \theta + \boldsymbol{u} \cdot \boldsymbol{\nabla} \theta = 0$$

on the doubly periodic domain $\mathbb{T}^2 \equiv [0, 2\pi]^2$ with a velocity field

$$\boldsymbol{u}(\boldsymbol{x}) = \begin{pmatrix} u(y) \\ 0 \end{pmatrix}$$

Exact solution

If u is constant in time

$$\theta(x, y, t) = \theta(x - tu(y), y, 0)$$

Fourier representation

$$\partial_t \theta_{kl} + \mathrm{i}k \sum_{m+n=l} u_m \, \theta_{kn} = 0$$

5. Lattice ODEs

$$\dot{\theta}_l = \sum_{j=-M}^{M} c_j \, \theta_{l-j} \qquad \text{with} \qquad c_{-j} = -\bar{c}_j$$

Dispersion relation

Inserting the normal mode ansatz $\theta_l = \kappa^l \, \mathrm{e}^{\mathrm{i}\omega t} \equiv \mathrm{e}^{\mathrm{i}\omega t - \mathrm{i}l\xi}$, we get

$$\omega(\xi) = -\mathrm{i} \sum_{j=-M}^{M} c_j \, \kappa^j$$

where $\kappa = \kappa(\xi) = \exp(\mathrm{i}\xi)$.

Note: This formula is essentially the inverse Fourier transform for the velocity field. Thus, up to scaling constants,

$$\omega(\xi) = u(x)$$

New problem statement

Find transparent boundary conditions for dispersive lattice waves!

6. History

- Dispersive lattice wave is classical in Physics
  (Brilluin and many others)
- Study of finite difference schemes for advection equations
  (Vichnevetsky *et al.*, 1975+; Trefethen, 1982)
- High order numerically nonreflecting boundary conditions
  (Colonius, 1997; Rowley and Colonius, 2000)
- LES as numerically nonreflecting boundary conditions
  (Colonius and Ran, 2002)

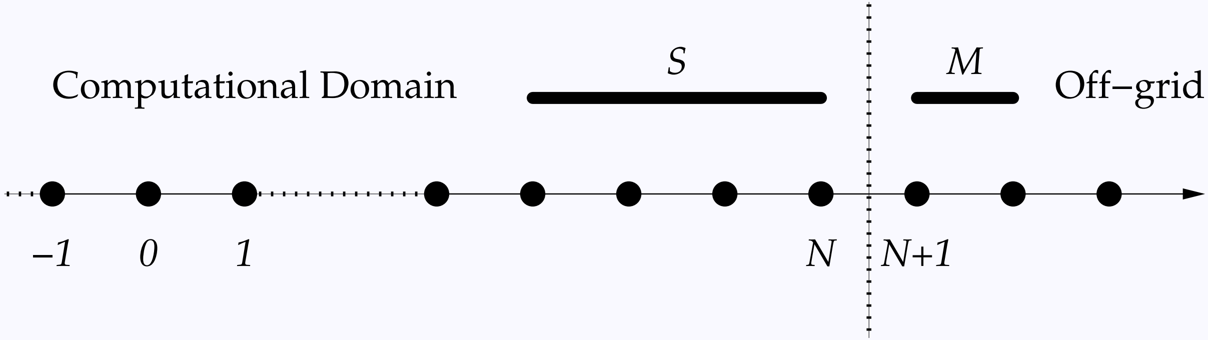
What is different here?

- No small parameter
  (Finite difference schemes have h as small parameter; need to look at dispersion relation only near the origin.)
- Isotropy in lattice wave number (= physical space!)

7. Transparent Boundary conditions

Idea

- Find linear map that extrapolates outgoing lattice waves
- Need M off-grid nodes for closure
- Stencil of extrapolation operator $S \ll N$



8. Background: Group velocity

General solution

$$\theta_l(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}\omega(\xi)t - \mathrm{i}\xi l}\,\theta(\xi,0)\,\mathrm{d}\xi$$
$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}l(\omega(\xi)t/l - \xi)}\,\theta(\xi,0)\,\mathrm{d}\xi$$

Stationary phase condition

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\omega(\xi)\frac{t}{l} - \xi\right) = 0$$

Thus, we obtain the well-known expression for the *group velocity*

$$\omega'(\xi) = \frac{l}{t}$$

9. Construction of the extrapolation operator

Step 1: Choose outgoing modes

Let $\xi_1, \dots, \xi_S$ be a set of wavenumbers with $\omega'(\xi_j) > 0$ (< 0 at left boundary). Set

$$\underbrace{\boldsymbol{v}_j = (\mathrm{e}^{\mathrm{i}\xi_j}, \dots, \mathrm{e}^{\mathrm{i}S\xi_j})}_{\text{on-grid sample}}, \qquad \underbrace{\boldsymbol{w}_j = (\mathrm{e}^{\mathrm{i}(S+1)\xi_j}, \dots, \mathrm{e}^{\mathrm{i}(S+M)\xi_j})}_{\text{off-grid extrapolation}}$$

Step 2: Compute coefficients

Solve linear system

$$\sum_{j=1}^{S} z_j \, \boldsymbol{v}_j = (\theta_1, \dots, \theta_S)$$

Step 3: Extrapolation

Set

$$(\theta_{S+1}, \dots, \theta_{S+M}) = \sum_{j=1}^{S} z_j \, \boldsymbol{w}_j$$

10. If $S_{\text{smpl}} > S$: Take least norm solution

Step 2: Compute coefficients

$$\text{Minimize } \boldsymbol{z}^T W \boldsymbol{z} \quad \text{subject to } \sum_{j=1}^{S_{\text{smpl}}} z_j \, \boldsymbol{v}_j = (\theta_1, \ldots, \theta_S)$$

where

$$W = \operatorname{diag}\left(|\omega'(\xi_1)|^{-1}, \ldots, |\omega'(\xi_{S^{\text{smpl}}})|^{-1} \right) ,$$

Step 3: Extrapolation

Set

$$(\theta_{S+1}, \ldots, \theta_{S+M}) = \sum_{j=1}^{S_{\text{smpl}}} z_j \, \boldsymbol{w}_j$$

11. Choice of sample waves numbers

Take maximum group velocity waves

- This is a different view of Colonius' procedure
- Requires knowledge of maxima, some monotonicity

Equidistant sampling

- Sort samples into right-going and left-going
- Right/left boundary stencil may be of different size

Equidistant oversampling

- Compute least-norm solution weighted with inverse group velocity
- This guarantees time-continuity of boundary conditions
- Stencil size easily controlled

12. Generalized reflection coefficients

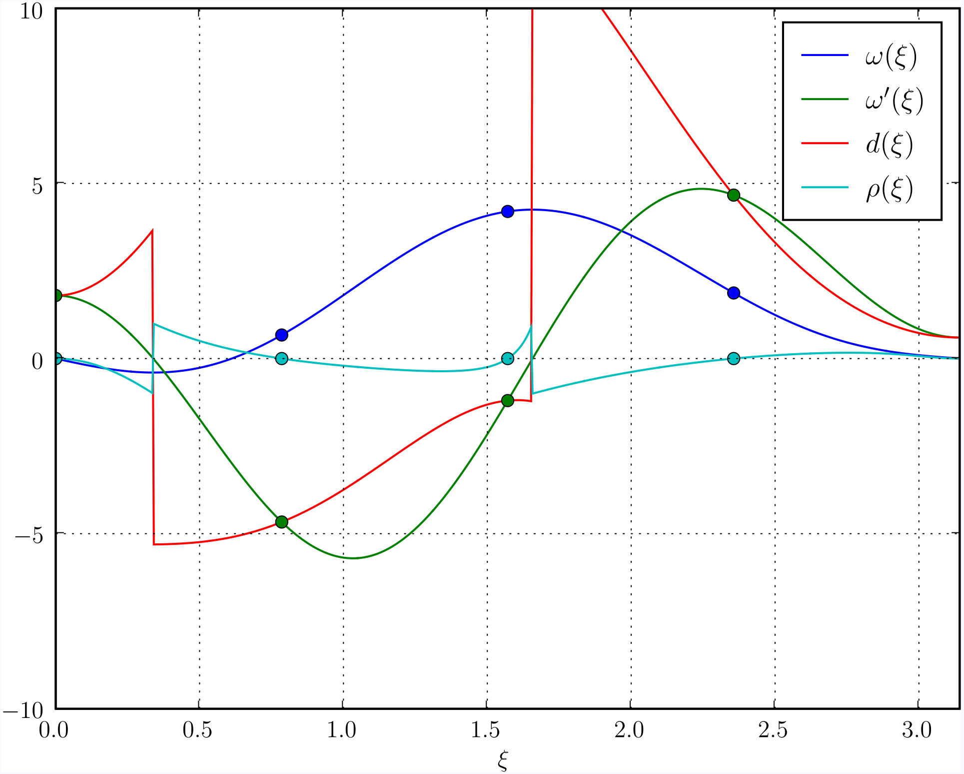
Classical reflection coefficients

- Amplitude ration of incoming to outgoing mode
- Here: generally multiple in/outgoing modes

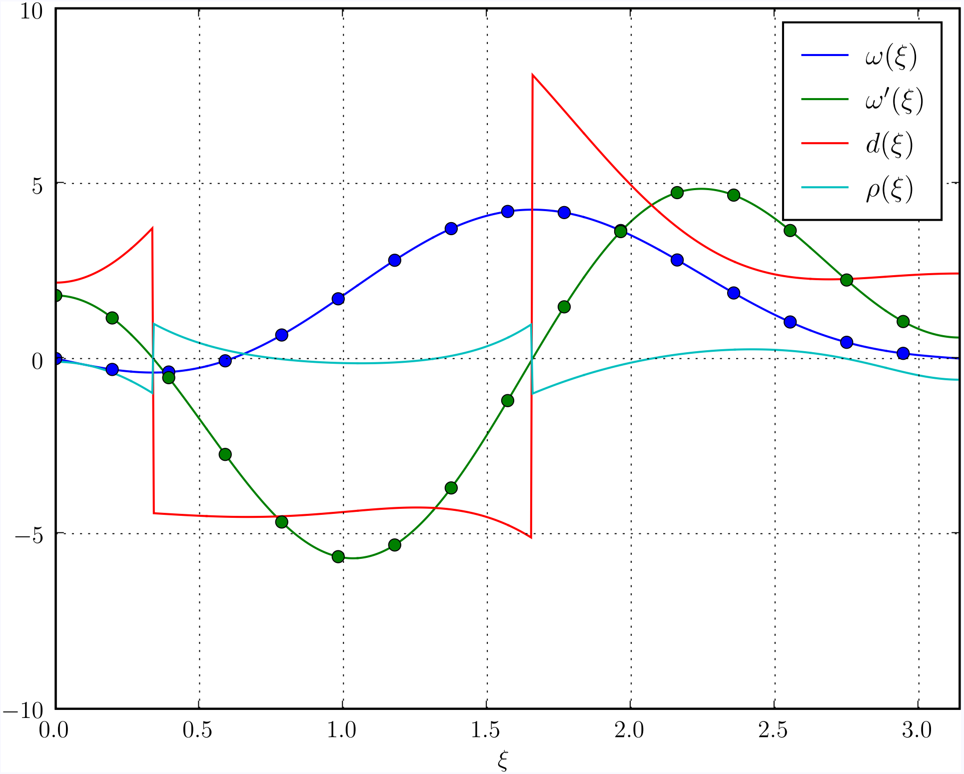
Energy dissipation rate error as reflection coefficient

- Exact normalized energy dissipation rate: group velocity $\omega'(\xi)$
- Numerical normalized energy dissipation rate $d(\xi)$ can be computed
- Define relative dissipation rate error

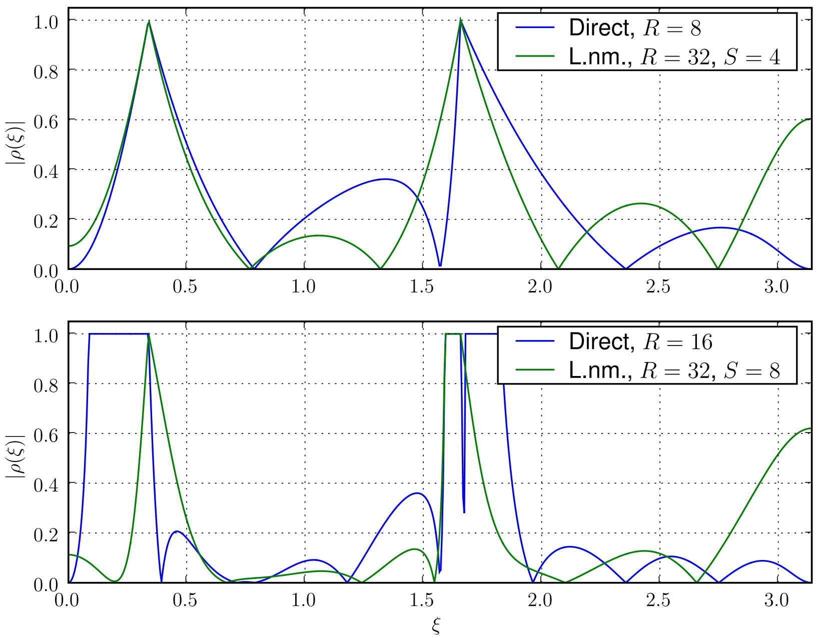
$$\rho(\xi) = \frac{\omega'(\xi) - d(\xi)}{|\omega'(\xi)| + |d(\xi)|}$$



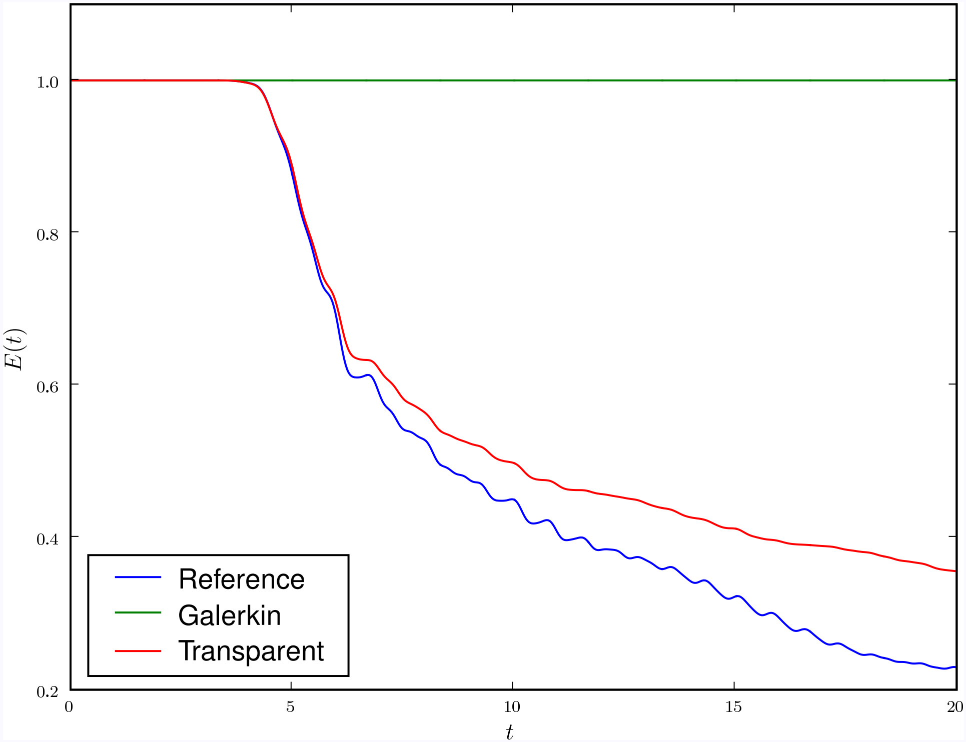
10
5
0
−5
−10
0.0
0.5
1.0
1.5
2.0
2.5
3.0
ξ
ω(ξ)
ω′(ξ)
d(ξ)
ρ(ξ)



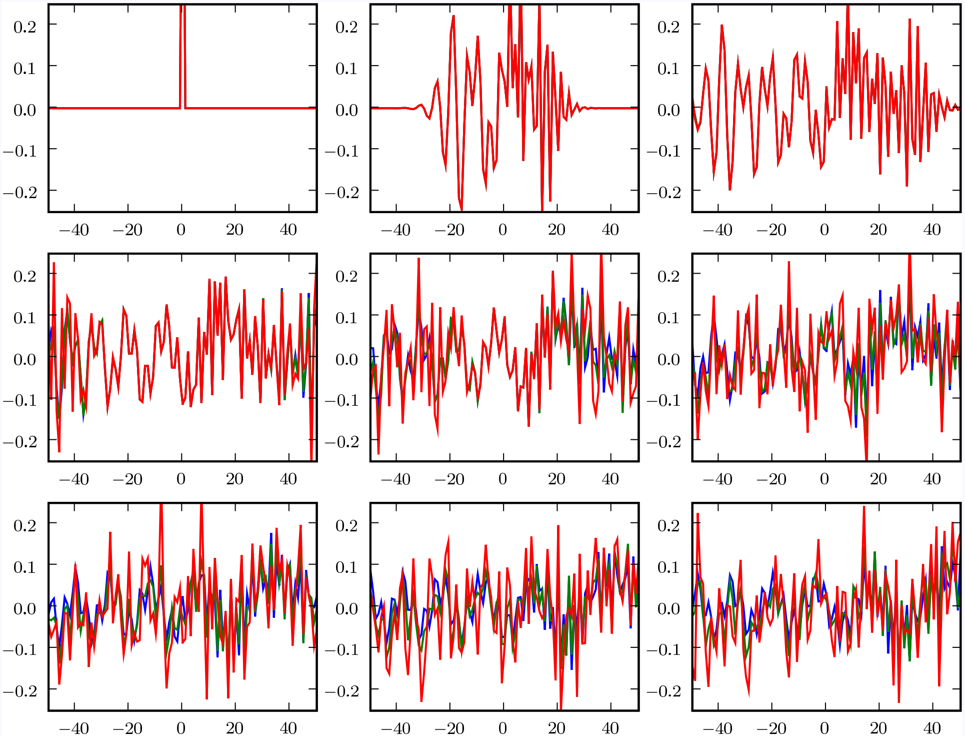
10
5
0
−5
−10
0.0
0.5
1.0
1.5
2.0
2.5
3.0
ξ
$\omega(\xi)$
$\omega'(\xi)$
$d(\xi)$
$\rho(\xi)$

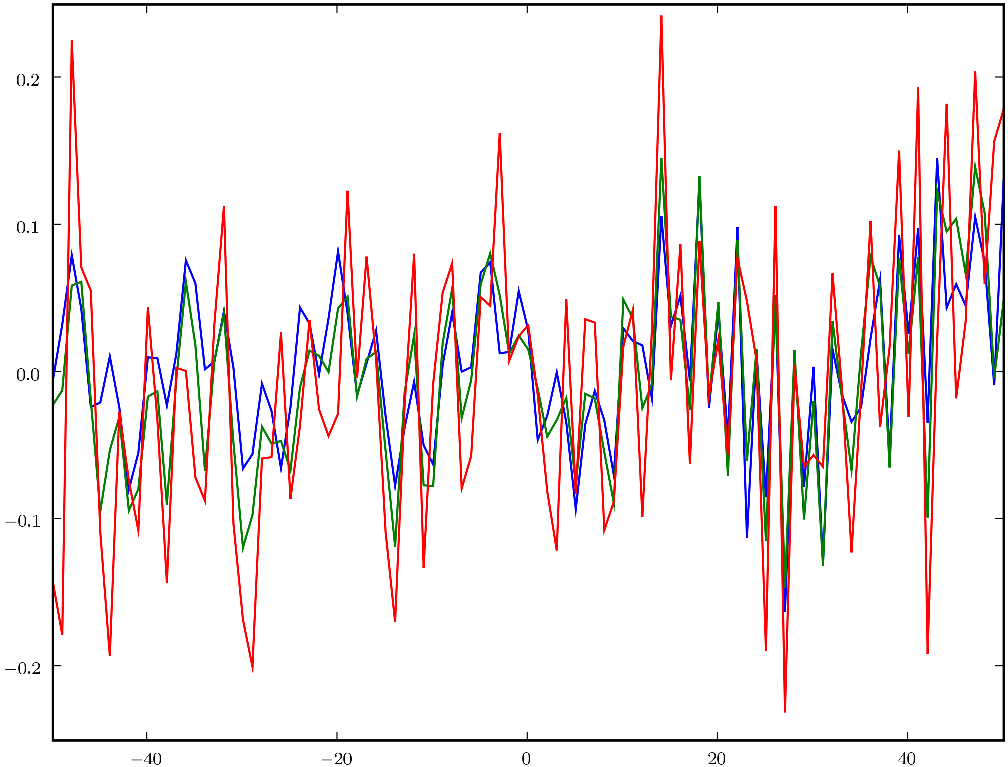


Direct, $R = 8$
L.nm., $R = 32$, $S = 4$
$|\rho(\xi)|$
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Direct, $R = 16$
L.nm., $R = 32$, $S = 8$
$|\rho(\xi)|$
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
ξ

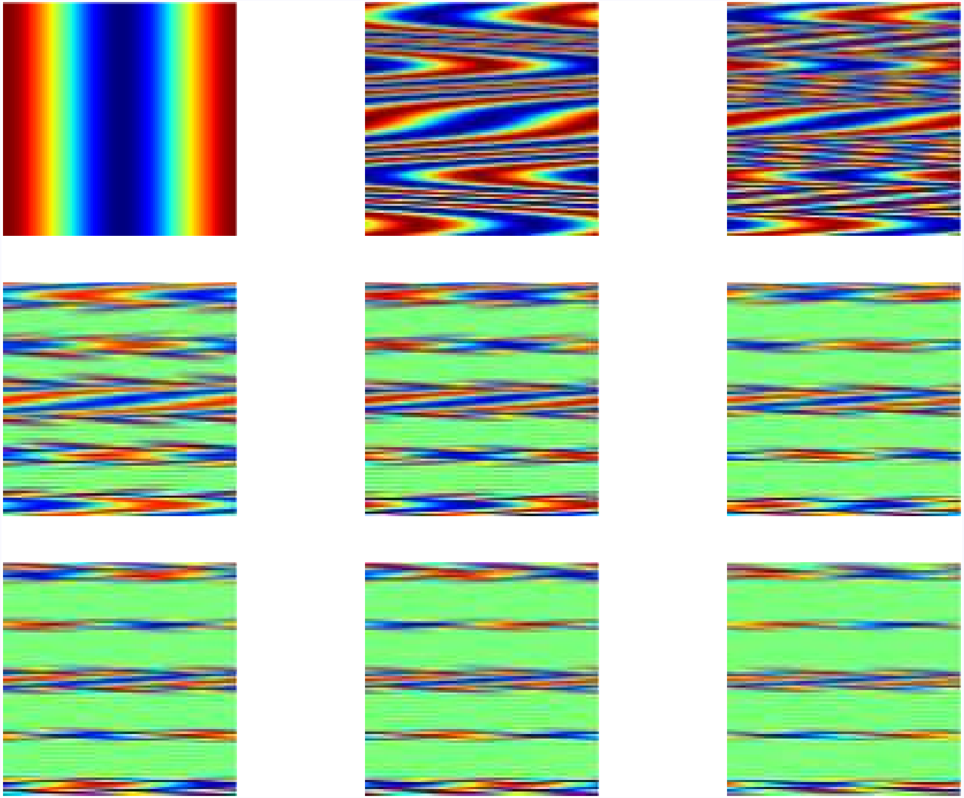


1.0
0.8
0.6
0.4
0.2
E(t)
0
5
10
15
20
t
Reference
Galerkin
Transparent

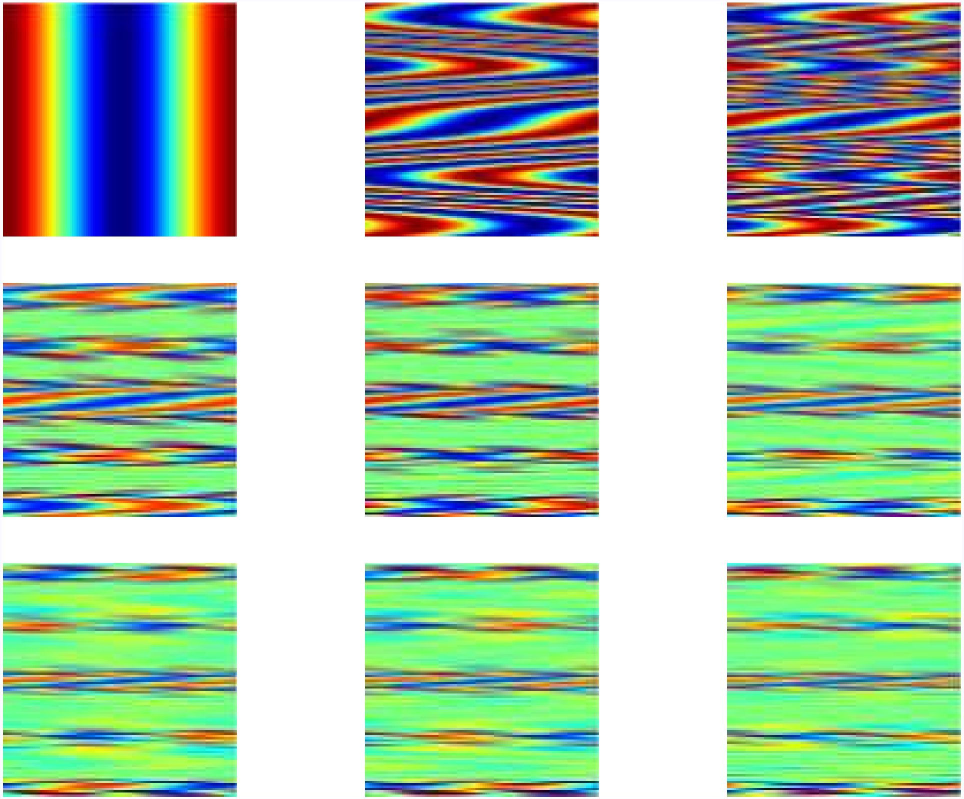

0.2
0.1
0.0
−0.1
−0.2
−40
−20
0
20
40



0.2
0.1
0.0
−0.1
−0.2
−40
−20
0
20
40



Reference solution



With transparent boundary conditions

13. Unsteady velocity fields

Ornstein–Uhlenbeck process

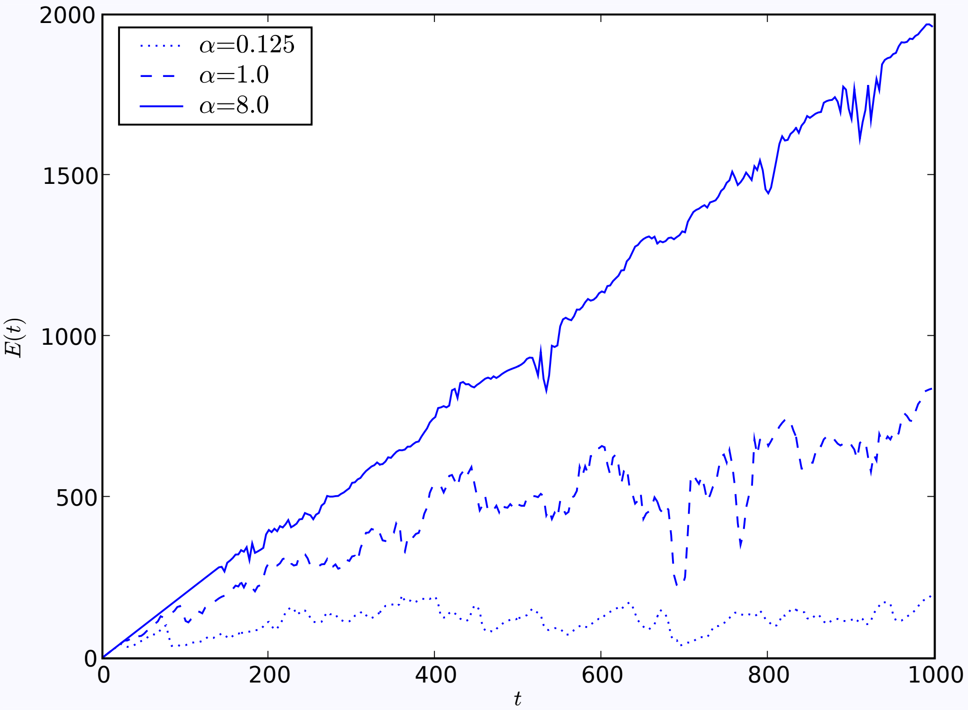
$$\mathrm{d}c(t) = -\alpha\, c(t)\, \mathrm{d}t + \sqrt{2\beta}\, \mathrm{d}W(t)$$

Properties

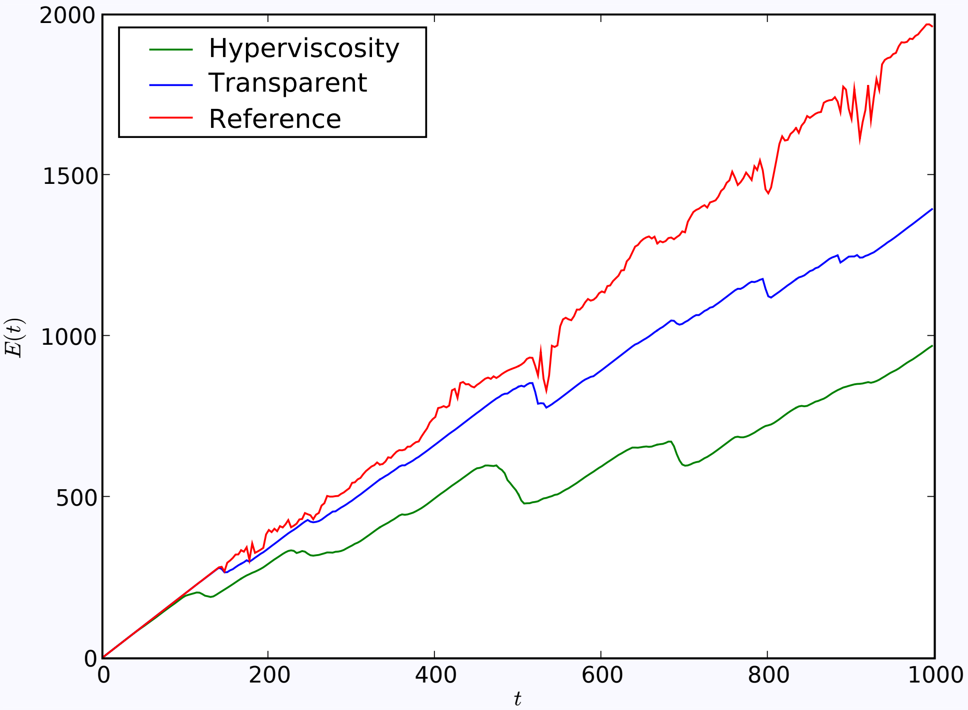
- Stationary
- Gaussian
- Covariance $\beta/\alpha\, \mathrm{e}^{-\alpha s}$
- Sum of two OU processes with identical α is again OU

Synthetic unsteady velocity fields

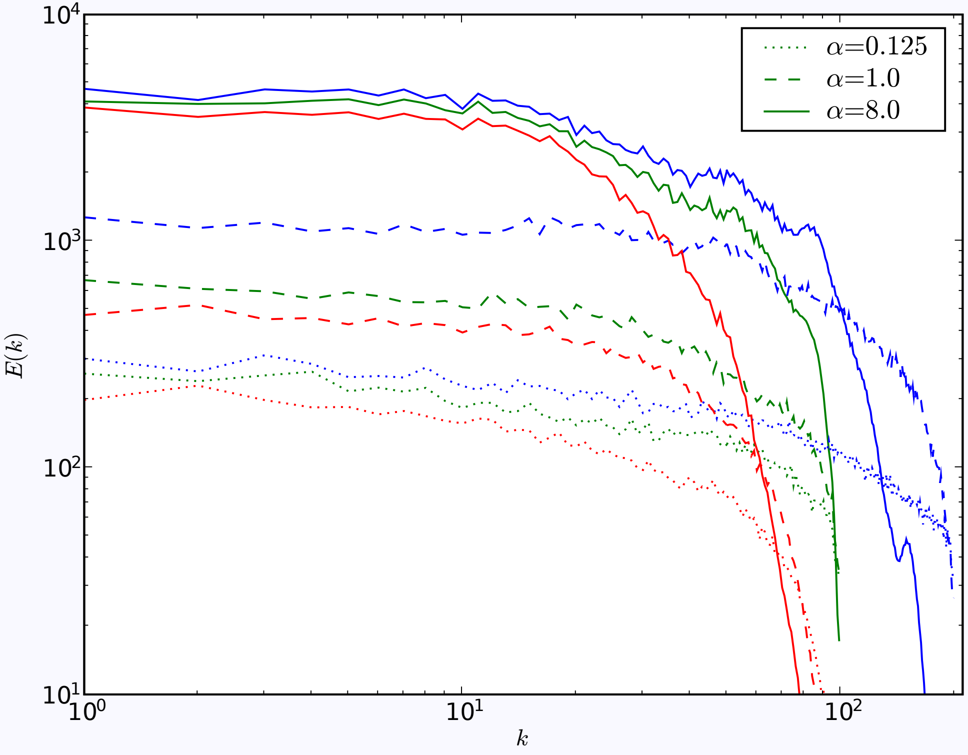
- Let Fourier coefficients of $\boldsymbol{u}$ follow independent OU processes
- Wave packets perform random walk on Fourier lattice
- Transparent boundary condition: “Once out, always out”



2000
1500
1000
500
0
0
200
400
600
800
1000
t
$E(t)$
α=0.125
α=1.0
α=8.0



Hyperviscosity
Transparent
Reference
2000
1500
1000
500
0
0
200
400
600
800
1000
$E(t)$
t



10^4
10^3
10^2
10^1
10^0
10^1
10^2
$E(k)$
k
α=0.125
α=1.0
α=8.0

14. Outlook

- 2D, 3D: Lattice wave picture only approximate, locally for $|\boldsymbol{k}| \gg 1$
- Memory effects?
- Non-compact velocity support in Fourier space
- Efficient implementation…