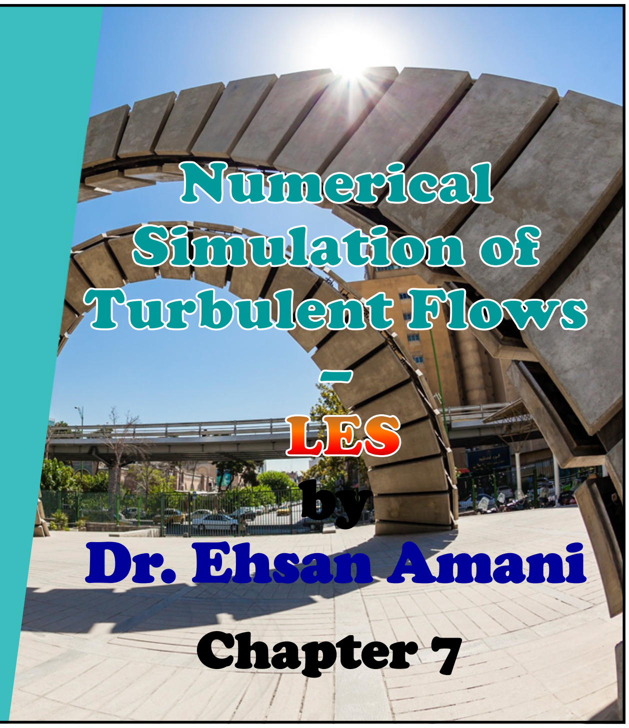

VII.1 Numerics of spectral methods

Series expansion

- An infinite sequence of orthogonal functions $\{\phi_k\}$

$$f(x) = \sum_{k=-\infty}^{+\infty} \tilde{f}_k \phi_k \qquad (7.1)$$

- Can the series be approximated by a few terms?
- Spectral accuracy: The k[th] coefficient decays fast enough for $|k| \geq m$; m is not-a-very-large integer.
  - For periodic functions: Fourier series
  - For non-periodic functions: Chebyshev series, …

Chap 7 By E. Amani

VII.1 Numerics of spectral methods

The Fourier system

Lecture: 7.1.1

- Fourier series expansion:

$$Sf = \sum_{k=-\infty}^{+\infty} \tilde{f}_k \phi_k = \sum_{k=-\infty}^{+\infty} \underbrace{\tilde{f}_k}_{\text{Fourier coefficient}} \underbrace{e^{ikx}}_{\text{Fourier mode}} = f(x) \qquad (7.5)$$

Wave number (k)

- Fourier transform:

$$\tilde{f}_k = \frac{1}{2\pi}\int_0^{2\pi} f(x) e^{-ikx} dx = \mathcal{F}\{f(x)\} \qquad (7.6)$$

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VII.1 Numerics of spectral methods

The Fourier system

- Fourier transform:

$$\underbrace{f(x); x \in \mathbb{R}(0,2\pi)}_{\text{Physical space (continuous)}} \xrightarrow{\text{Fourier transform}} \underbrace{\tilde{f}_k; k \in \mathbb{Z}(-\infty,+\infty)}_{\text{Wavenumber space (discrete)}}$$

$$\underbrace{f(t); t \in \mathbb{R}(0,2\pi)}_{\text{Time domain (continuous)}} \xrightarrow{\text{Fourier transform}} \underbrace{\tilde{f}_\omega; \omega \in \mathbb{Z}(-\infty,+\infty)}_{\text{Frequency domain (discrete)}}$$

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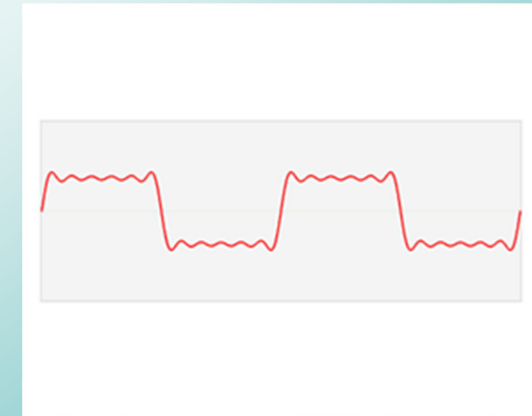
VII.1 Numerics of spectral methods

The Fourier system

Fourier transform decomposes a function into different modes; waves of different wavenumbers and amplitudes. ►



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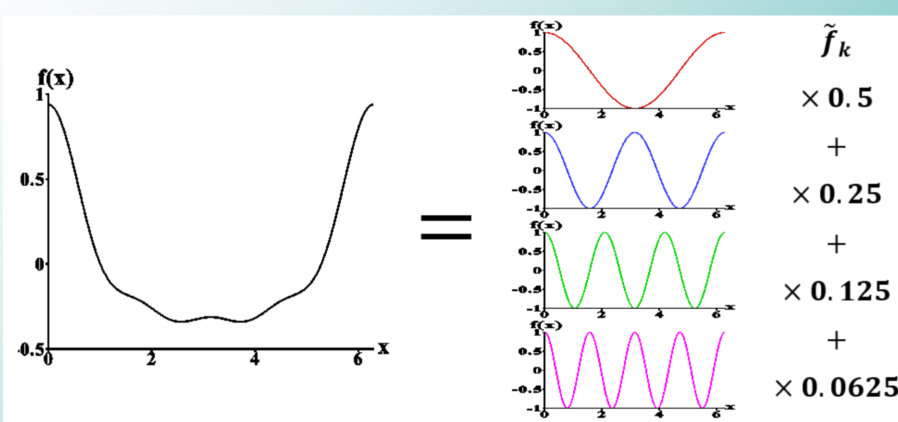
VII.1 Numerics of spectral methods

The Fourier system



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VII.1 Numerics of spectral methods

The Fourier system

- An important property: If $f(x)$ is real-valued

$$\tilde{f}_{-k} = \left(\tilde{f}_k\right)^* \qquad (7.7)$$

- Fourier cosine and sine transforms:

$$\tilde{a}_k = \frac{1}{2\pi}\int_0^{2\pi} f(x)\cos(kx)dx$$
$$\tilde{b}_k = \frac{1}{2\pi}\int_0^{2\pi} f(x)\sin(kx)dx \qquad (7.8)$$

- Relation between Fourier transforms:

$$\tilde{f}_k = \tilde{a}_k - i\tilde{b}_k \qquad (7.9)$$

- For a smooth periodic function, the Fourier series expansion possesses the "spectral accuracy" property

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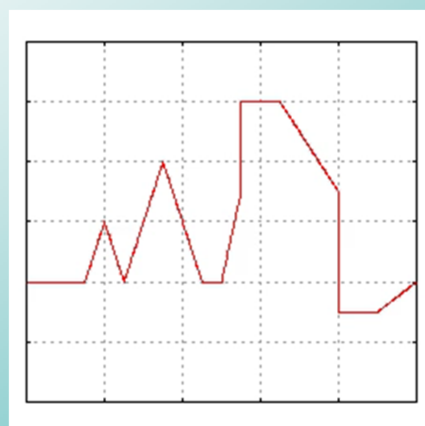
VII.1 Numerics of spectral methods

The Fourier system

Fourier transform decomposes a function into different modes; waves of different wavenumbers and amplitudes. ►



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VII.1 Numerics of spectral methods

The Fourier system

- N[th]-order truncated Fourier series:

$$P_N f = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \tilde{f}_k e^{ikx} = f(x) + \underbrace{T_N}_{\text{Truncation error}} \qquad (7.10)$$

$$\tilde{f}_k = \frac{1}{2\pi}\int_0^{2\pi} f(x)e^{-ikx}dx = \mathcal{F}\{f(x)\}$$

- What if the values of $f(x)$ are known at discrete points (a computational grid) rather than $x \in \mathbb{R}(0,2\pi)$?

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VII.1 Numerics of spectral methods

Discrete Fourier series

⇨ **Lecture Notes:7.1.2**

- The discrete Fourier series:

$$I_N f(x_j) = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \underbrace{\hat{f}_k}_{\text{Discrete Fourier coefficient}} e^{ikx_j} = f(x_j) = f_j \qquad j = 0,1,2,\dots,N-1 \quad (7.12)$$

- The Discrete Fourier Transform (DFT):

$$\hat{f}_k = \frac{1}{N}\sum_{j=0}^{N-1} f_j e^{-ikx_j} = \mathcal{F}_N\{f_j\} \qquad k = -\frac{N}{2},\dots,\frac{N}{2}-1 \quad (7.15)$$

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VII.1 Numerics of spectral methods

Discrete Fourier series

- DFT:

$$\underbrace{f_j}_{\text{Physical space (discrete)}};x_j = jh, j \in \mathbb{Z}(0, N-1) \xrightarrow{\text{DFT}} \underbrace{\hat{f}_k}_{\text{Wavenumber space (discrete)}}; k \in \mathbb{Z}(-\tfrac{N}{2}, \tfrac{N}{2}-1)$$

- An important property: If $f(x)$ is real-valued

$$\hat{f}_{-k} = \left(\hat{f}_k\right)^* \qquad (7.16)$$

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VII.1 Numerics of spectral methods

Discrete Fourier series

- Extension to general case of period length L:
  - Base function definition:

$$\phi(x) = e^{i\overbrace{\left(\frac{2\pi}{L}\right)k}^{\omega_k \text{ is the wavenumber}}x} \qquad (7.17)$$

  - It can be shown that all previous relations are valid, replacing π with L, and k with $\left(\frac{2\pi}{L}\right)k$.
  - For instance, in Eq. (7.12):

$$x_j = jh = j\left(\frac{L}{N}\right);$$

$$f_j = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \hat{f}_k e^{i\left(\frac{2\pi}{L}\right)kj\left(\frac{L}{N}\right)} = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \hat{f}_k e^{ik\overbrace{\left(\frac{2\pi}{N}\right)}^{\text{Like when } x_j \in \mathbb{R}(0,2\pi)}j}$$

This is why DFT subroutines do not get L

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VII.1 Numerics of spectral methods

Discrete Fourier series

- Extension to general case of period length L:
  - Eqs. (7.12) and (7.15) are valid for the period length L
  - For derivatives of f, a modification is required as will be shown later
- DFT requires $O(N^2)$ operations
- In practice, a more efficient algorithm, called Fast Fourier Transform (FFT), is incorporated in computations that reduces the computational cost to $O(N \log_2 N)$
- Suggested reading: [3] (sections 6.1-6.3)

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Aliasing

Aliasing error

- Image processing
  - moiré pattern

Reducing resolution

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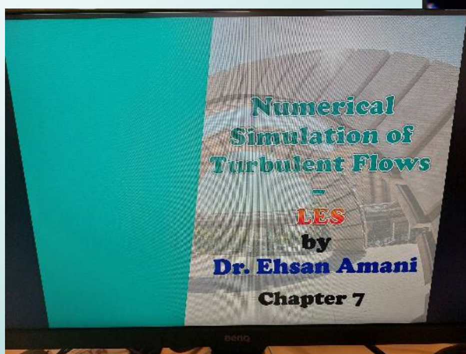
Aliasing

Aliasing error

- Image processing
  - moiré pattern



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Aliasing

Aliasing error

- Numerical analysis
  - The discrete representation induces another error, called the aliasing error:

$$P_N f = \underbrace{Sf}_{=f(x)} + T_N$$

Truncation error

$$I_N f = P_N f + R_N = Sf + T_N + R_N \qquad (7.18)$$

Aliasing error

⇨ **Lecture Notes: 7.1.4**

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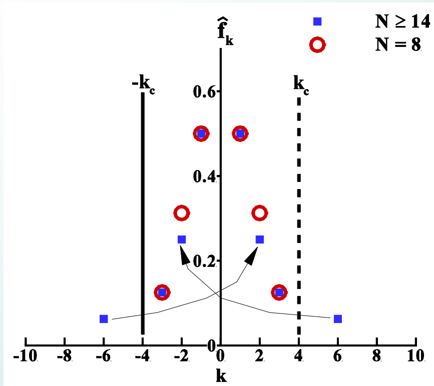
Aliasing

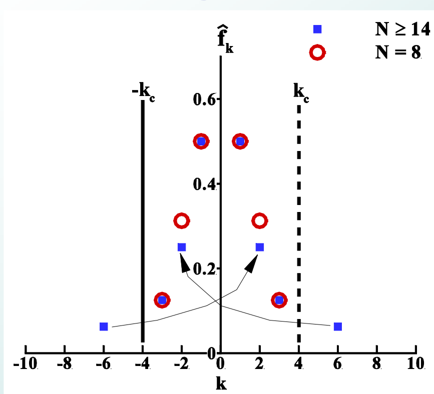
$f(x) = \cos x + \frac{1}{2}\cos 2x + \frac{1}{4}\cos 3x + \frac{1}{8}\cos 6x$



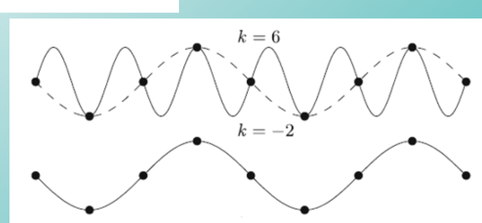
▲ Discrete Fourier coefficients of $f(x)$ on $N = 8$ grid and on a grid with $N \geq 14$.

Aliasing

$f(x) = \cos x + \frac{1}{2}\cos 2x + \frac{1}{4}\cos 3x + \frac{1}{8}\cos 6x$

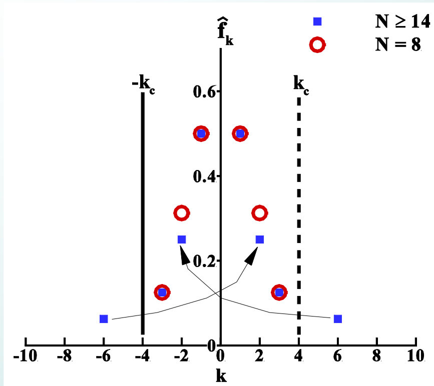


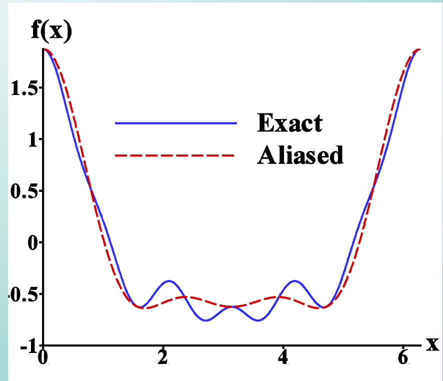
on $N = 8$ grid, the modes $k = 6$ and $k = -2$ are indistinguishable. ►

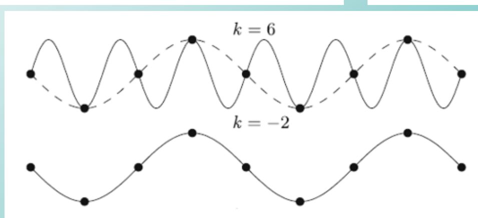


Aliasing

$$f(x) = \cos x + \tfrac{1}{2}\cos 2x + \tfrac{1}{4}\cos 3x + \tfrac{1}{8}\cos 6x$$







▲ The inverse transforms of exact ($N \geq 14$) and aliased ($N = 8$) Fourier coefficients of $f(x)$.

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Aliasing

Aliasing error

- The aliasing error is of Nth order and can be omitted in the conventional discretization schemes
- In spectral discretization, the aliasing error can contaminate the solution in the presence of non-linear terms and have to be controlled.
- In general, all modes k' ($|k'| > \frac{N}{2}$) alias the mode k ($|k| \leq \frac{N}{2}$) where:

$$k' + mN = k; \quad m = \pm 1, \pm 2, \ldots$$

  - Proof: See file “chap7-proofs.pdf”
  - In the previous example:

$$-6 + 1 \times 8 = 2$$

$$+6 + (-1) \times 8 = -2$$

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Aliasing

Discrete Fourier transform of a product

- The simplest non-linear case: $H(x) = f(x)g(x)$
- Example: Consider $f(x) = \sin(2x)$ and $g(x) = \sin(3x)$ on a grid $N = 8$.
  - Each function is represented on $N = 8$ grid without aliasing:

$$|k| = 2 < \frac{8}{2} = 4:\ \hat{f}_k = \begin{cases} -i/2 & ; k = 2 \\ +i/2 & ; k = -2 \\ 0 & ; \text{otherwise} \end{cases}$$

$$|k| = 3 < \frac{8}{2} = 4:\ \hat{g}_k = \begin{cases} -i/2 & ; k = 3 \\ +i/2 & ; k = -3 \\ 0 & ; \text{otherwise} \end{cases}$$

  - Using the trigonometric relation:
    $H(x) = f(x)g(x) = \sin(2x)\sin(3x) = 0.5[\cos(x) - \cos(5x)]$
  - The product cannot be presented on $N = 8$ grid and generates aliasing error. $|k| = 5 > \frac{8}{2} = 4$

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Aliasing

Discrete Fourier transform of a product

- The convolution sum (proof: “chap7-proofs.pdf”):

$$\hat{H}_m = \sum_{\substack{k=-\frac{N}{2} \\ |m-k|\le\frac{N}{2}}}^{\frac{N}{2}-1} \hat{f}_k \hat{g}_{m-k} \qquad m = -\frac{N}{2}, \dots, \frac{N}{2} - 1 \qquad (7.22)$$

  - Needs $O(N^2)$ operations
  - More efficient algorithms?

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Aliasing

Pseudo-spectral transform – padding method

- Requires $O(N\log_2 N)$ operations
- Uses more grid points $M = 3N/2$ temporarily to avoid aliasing
- Philosophy: Using a finer grid, allowing the high wavenumbers generated by the non-linearity to appear and not to alias the modes with $|k| \le N/2$. Then, these high wavenumbers are filtered out.
- Steps:
  1. Transform $\hat{f}_k$ and $\hat{g}_k$ to physical space on M grid nodes using inverse FFT:

$$\hat{f}_k, \hat{g}_k \xrightarrow{\text{Inverse FFT}} f_j, g_j \qquad j = 0,1,\dots,M-1$$

$$M = 2N:\quad \underbrace{-\frac{M}{2},\dots,}_{\hat{f}_k = \hat{g}_k = 0}\ \underbrace{-\frac{N}{2}}_{0},\dots,\frac{N}{2}-1,\underbrace{\dots,\frac{M}{2}-1}_{\hat{f}_k = \hat{g}_k = 0}$$

(Nyquist is set to zero)

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Aliasing

Pseudo-spectral transform – padding method

- Requires $O(N\log_2 N)$ operations
- Uses more grid points $M = 3N/2$ temporarily to avoid aliasing
- Steps:
  1. Transform $\hat{f}_k$ and $\hat{g}_k$ to physical space on M grid nodes using inverse FFT
  2. Compute H_j on the fine grid:

$$H_j = f_j g_j \qquad ; j = 0,1,\dots,M-1$$

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Aliasing

Pseudo-spectral transform – padding method

- Requires $O(N \log_2 N)$ operations
- Uses more grid points $M = 3N/2$ temporarily to avoid aliasing
- Steps:
  1. Transform $\hat{f}_k$ and $\hat{g}_k$ to physical space on M grid nodes using inverse FFT
  2. Compute H_j on the fine grid
  3. Compute $\widehat{H}_k$ using FFT:

$$\underset{j=0,1,\dots,M-1}{H_j} \xrightarrow{\text{FFT}} \underset{k=-\frac{M}{2},\dots,\frac{M}{2}-1}{\widehat{H}_k}$$

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Aliasing

Pseudo-spectral transform – padding method

- Requires $O(N \log_2 N)$ operations
- Uses more grid points $M = 3N/2$ temporarily to avoid aliasing
- Steps:
  1. Transform $\hat{f}_k$ and $\hat{g}_k$ to physical space on M grid nodes using inverse FFT
  2. Compute H_j on the fine grid
  3. Compute $\widehat{H}_k$ using FFT
  4. Keep $\widehat{H}_k$ on the coarse grid and discard the others:

0 (Nyquist is set to zero)

$$\widehat{H}_k:\quad k = \underbrace{-\frac{M}{2},\dots,}\overbrace{-\frac{N}{2},\dots,\frac{N}{2}-1}^{\text{kept}},\underbrace{\dots,\frac{M}{2}-1}$$

Now these frequencies include aliasing error (discarded)

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Aliasing

DeAliasing of non-linear terms

- DNS of turbulent power-law fluid flows

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Dynamic subgrid-scale LES model for turbulent non-Newtonian flows: A priori and a posteriori analyses of Burgers turbulence

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Aliasing

DeAliasing of non-linear terms

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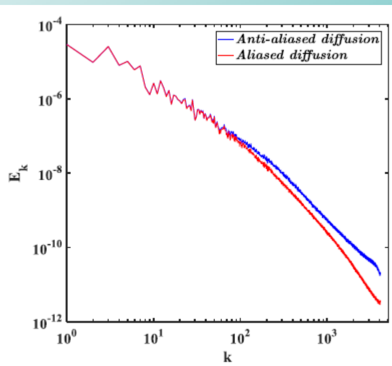

Fig. 1. DNS of NNSBE: The energy spectrum function versus wavenumber for $n = 0.2$. The spectrum is time-averaged over $50 < t < 100$.

VII.1 Numerics of spectral methods

Transform of derivatives

Lecture Notes: 7.1.7

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VII.1 Numerics of spectral methods

Higher dimensions

- $f(x, y)$ which is periodic in x or y is treated like before, the dependence on the other variable is implied.
- $f(x, y)$ which is periodic in both x and y (two-time Fourier transforming):

$$f_{m,l} = f(x_m, y_l) = \sum_{k_1=-\frac{N_1}{2}}^{\frac{N_1}{2}-1} \sum_{k_2=-\frac{N_2}{2}}^{\frac{N_2}{2}-1} \hat{f}_{k_1,k_2} e^{ik_1x_m} e^{ik_2y_l} \qquad \begin{array}{r} m = 0,1, \dots, N_1 - 1 \\ l = 0,1, \dots, N_2 - 1 \end{array} \quad (7.27)$$

$$\hat{f}_{k_1,k_2} = \frac{1}{N_1}\frac{1}{N_2} \sum_{m=0}^{N_1-1} \sum_{l=0}^{N_2-1} f_{m,l} e^{-ik_1x_m} e^{-ik_2y_l} \qquad \begin{array}{r} k_1 = -\frac{N_1}{2}, \dots, \frac{N_1}{2} - 1 \\ k_2 = -\frac{N_2}{2}, \dots, \frac{N_2}{2} - 1 \end{array} \quad (7.28)$$

- For real-valued f:

$$\hat{f}_{-k_1,-k_2} = \left(\hat{f}_{k_1,k_2}\right)^* \quad (7.29)$$

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VII.1 Numerics of spectral methods

Higher dimensions

- In three dimensions, and for a vector quantity:

$$\vec{f}(\vec{x}) = \sum_{\vec{k}} \vec{\hat{f}}_{\vec{k}} e^{i\vec{k}.\vec{x}} \qquad (7.30)$$

$$\vec{x} = (x_1, x_2, x_3) = x_i \hat{e}_i$$

$$\vec{k} = (k_1, k_2, k_3) = k_i \hat{e}_i \qquad (7.31)$$

$$\sum_{\vec{k}} \rightarrow \sum_{k_1} \sum_{k_2} \sum_{k_3}$$

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VII.1 Numerics of spectral methods

Numerical solution of differential equations

- Linear advection-diffusion equation:

⇨ **Lecture Notes: 7.1.8**

- Non-linear Burgers equation

⇨ **Lecture Notes: 7.1.9**

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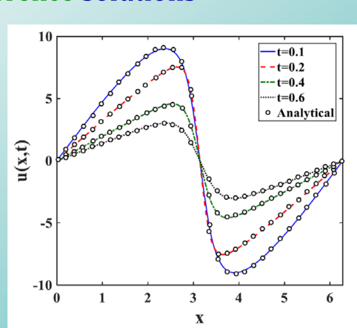
Hands-on practice

- **HW#5:**
  - Using "pyBurgers.py" and python FFT packages for numerical analysis
  - Solving linear and non-linear equations using spectral methods
  - Comparing spectral and conventional 2nd- and 4th-order finite difference solutions



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Project#2: *A posteriori* study

1D Stochastic Forced Burgers Equation (1DFSBE)

- Energy spectrum (you can do Q11)

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VII.2 Spectral description of turbulence

Fourier series representation

- The velocity field is periodic in a box of length $L > L_{11}$:

$$\vec{U}(\vec{x},t) = \vec{U}(\vec{x} + \vec{N}L, t)$$

Integer vector

$$\vec{N} = n_1\hat{e}_1 + n_2\hat{e}_2 + n_3\hat{e}_3 = n_i\hat{e}_i$$

- Using Eqs. (7.5) and (7.30)

$$\vec{U}(\vec{x},t) = \sum_{\vec{k}} \hat{\vec{U}}(\vec{k},t)e^{i\vec{k}.\vec{x}} \qquad (7.44)$$

$$\vec{x} = x_i\hat{e}_i \qquad \vec{k} = \frac{2\pi}{L}\vec{N} = \frac{2\pi}{L}n_i\hat{e}_i, n_i = 0, \pm1, \dots, \pm\infty \qquad (7.45)$$

Wavenumber vector $\quad k = |\vec{k}|$

- Note: In section VII.2, the notation $\hat{U}$ is used instead of $\tilde{U}$, to be consistent with reference [1]

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VII.2 Spectral description of turbulence

Fourier series representation

- Note: For non-periodic cases, the wavenumber space becomes continuous:

$$L \to \infty;\ \Delta k = k_{i,n+1} - k_{i,n} = \frac{2\pi}{L} \to 0$$

- The volume-averaging operator over the cube $0 \leq x_i \leq L$:

$$\left\langle \vec{f}(\vec{x}) \right\rangle_L = \frac{1}{L^3}\int_0^L\int_0^L\int_0^L \vec{f}(\vec{x})dx_1dx_2dx_3 \qquad (7.46)$$

- The orthogonality property:

$$\left\langle e^{i\vec{k}.\vec{x}}e^{-i\vec{k}'.\vec{x}} \right\rangle_L = \delta_{\vec{k},\vec{k}'} \qquad (7.47)$$

- Exercise: Using Eq. (7.4) (replacing 2π with L) verify Eq. (7.47)

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VII.2 Spectral description of turbulence

Fourier series representation

- Using the orthogonality property, Eq. (7.47), the Fourier coefficients are obtained as:

$$\hat{\vec{U}}(\vec{k},t) \equiv \mathcal{F}_L\{\vec{U}(\vec{x},t)\} = \left\langle \vec{U}(\vec{x},t)e^{-i\vec{k}.\vec{x}} \right\rangle_L = \frac{1}{L^3}\iiint_0^L \vec{U}(\vec{x},t)e^{-i\vec{k}.\vec{x}}dx_1dx_2dx_3 \quad (7.48)$$

- Hereafter, the dependence on t is implied.

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VII.2 Spectral description of turbulence

Fourier series representation

- Exercise: Prove the following relations:

$$\hat{A}(\vec{k}) \equiv \mathcal{F}_L\{A(\vec{x})\}$$

A → **Scalar, vector, or tensor**

$$\hat{A}(-\vec{k}) \equiv \hat{A}^*(\vec{k})$$

Each component of $\hat{A}^*$ is the complex conjugate of the same component of $\hat{A}$

$$\mathcal{F}_L\left\{\frac{\partial A(\vec{x})}{\partial x_j}\right\} = ik_j\hat{A}(\vec{k})$$

$$\mathcal{F}_L\{\nabla.A(\vec{x})\} = i\vec{k}.\hat{A}(\vec{k}) \qquad \mathcal{F}_L\{\nabla \times A(\vec{x})\} = i\vec{k} \times \hat{A}(\vec{k})$$

$$\mathcal{F}_L\{\nabla^2 A(\vec{x})\} = -k^2\hat{A}(\vec{k}) \qquad \mathcal{F}_L\{\nabla A(\vec{x})\} = i\vec{k}\hat{A}(\vec{k})$$

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VII.2 Spectral description of turbulence

The Navier-Stokes equations in the Fourier space

Lecture Notes: 7.2.2

The kinetic energy of Fourier modes

Lecture Notes: 7.2.3

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VII.2 Spectral description of turbulence

The energy spectrum function

- Theoretical turbulence literature: Integral Fourier transform

$$\vec{\hat{U}}(\vec{k}) \equiv \mathcal{F}\{\vec{U}(\vec{x})\} = \frac{1}{(2\pi)^3} \iiint_{-\infty}^{+\infty} \vec{U}(\vec{x}) e^{-i\vec{k}.\vec{x}} d\vec{x} \qquad (7.71)$$

$$\vec{U}(\vec{x}) = \mathcal{F}^{-1}\left\{\vec{\hat{U}}(\vec{k})\right\} = \iiint_{-\infty}^{+\infty} \vec{\hat{U}}(\vec{k}) e^{i\vec{k}.\vec{x}} d\vec{k} \qquad (7.72)$$

- Non-periodic function, continuous real-valued wavenumber component k_i

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VII.2 Spectral description of turbulence

The energy spectrum function

- For flow in a finite domain $D \in L^3$, both $\mathcal{F}$ and $\mathcal{F}_L$ can be defined.
- $\mathcal{F}$ is usually used in theoretical discussions
- $\mathcal{F}_L$ is usually used in numerical calculations
- The relation between $\mathcal{F}$ and $\mathcal{F}_L$ (proof: Lesieur, Turbulence in fluids, section 5.1):

$$\underbrace{\underset{\text{continuous}}{\hat{\vec{U}}(\vec{k})}}_{\mathcal{F}\{\vec{U}(\vec{x})\}} = \sum_{\vec{k}'} \delta(\vec{k}-\vec{k}')\underbrace{\underset{\text{discrete}}{\hat{\vec{U}}(\vec{k}')}}_{\mathcal{F}_L\{\vec{U}(\vec{x})\}} \qquad (7.72)'$$

VII.2 Spectral description of turbulence

The energy spectrum function

- A unified energy spectrum function for periodic and non-periodic cases:

$$E(k) = \sum_{\vec{k}'} \delta(k'-k)\hat{E}(\vec{k}') \qquad (7.80)'$$

- It can be shown that (proof: "chap7-proofs.pdf"):

$$\underbrace{\phi_{ij}(\vec{k})}_{\text{Velocity spectrum function}} \equiv \mathcal{F}\{R_{ij}(\vec{r})\} = \sum_{\vec{k}'} \delta(\vec{k}-\vec{k}')\underbrace{\hat{R}_{ij}(\vec{k}')}_{\mathcal{F}_L\{R_{ij}(\vec{r})\}} \qquad (7.73)'$$

$$E(k) = \iiint_{-\infty}^{+\infty} \tfrac{1}{2}\phi_{ii}(\vec{k}')\delta(k'-k)d\vec{k}' \qquad (7.81)$$

$$k = \int_0^\infty E(k)dk \quad (7.82) \qquad \varepsilon = \int_0^\infty 2\nu k^2 E(k)dk \quad (7.83)$$

VII.2 Spectral description of turbulence

Kolmogorov spectra

- The first similarity hypothesis (for scales $l \ll l_0\sim$ or $l < l_{EI}\sim\frac{1}{6}L_{11}$):

$$E(k)=f(k,\varepsilon,\nu);\quad k\gg k_0=\frac{2\pi}{l_0}\ \textbf{or}\ k>k_{EI}=\frac{2\pi}{l_{EI}}$$

- Exercise: knowing $\eta=(\nu^3/\varepsilon)^{1/4}$ and using a dimensional analysis, show that:

$$E(k)=(\varepsilon\nu^5)^{1/4}\varphi(k\eta)\quad \overset{k>k_{EI}}{(7.91)}\quad \textbf{or}\quad E(k)=\varepsilon^{2/3}k^{-5/3}\psi(k\eta)\quad \overset{k>k_{EI}}{(7.92)}$$

Kolmogorov spectrum function

compensated Kolmogorov spectrum function

$$\psi(k\eta)=(k\eta)^{5/3}\varphi(k\eta)$$

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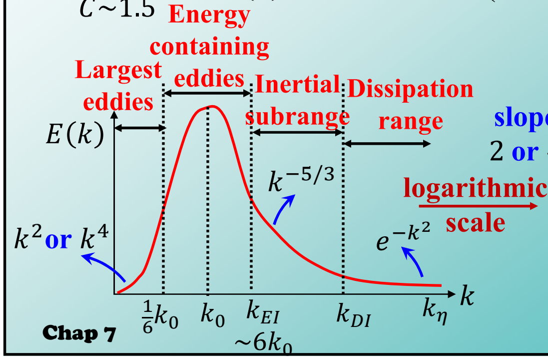
VII.2 Spectral description of turbulence

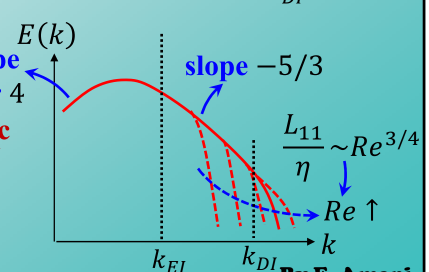
Kolmogorov spectra

- The second similarity hypothesis (for scales $l_0 \ll l \ll \eta$ or $60\eta\sim l_{DI} < l < l_{EI}$):

Kolmogorov constant experiment: $C\sim1.5$

$$E(k)=C\varepsilon^{2/3}k^{-5/3}\quad (7.93)\quad k_0\ll k\ll k_\eta=\frac{2\pi}{\eta}\ \textbf{or}\ k_{EI}<k<k_{DI}=\frac{2\pi}{l_{DI}}$$





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VII.2 Spectral description of turbulence

Kolmogorov spectra

- Pao's model spectrum:

$$E(k) = f_L(kL) C \varepsilon^{2/3} k^{-5/3} f_\eta(k\eta) \qquad (7.94)$$

$$f_L(kL) = \left(\frac{kL}{[(kL)^2 + c_L]^{1/2}}\right)^{\frac{5}{3}+p_0} \quad ; p_0 = 2 \text{ or } 4 \qquad c_L = 6.78$$

$$f_\eta(k\eta) = \exp(-\beta (k\eta)^{4/3}) \quad ; \beta = \frac{3}{2}C$$

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VII.3 LES in spectral space

Spectral representation of filtering

- Comparing Eq. (6.1) and Eq. (D.15) (appendix D [1]):

$$\underbrace{\hat{\overline{\vec{U}}}(\vec{k})}_{\mathcal{F}_L\{\overline{\vec{U}}(\vec{x})\}} = \underbrace{\hat{G}(\vec{k})}_{\text{Transfer function}} \underbrace{\hat{\vec{U}}(\vec{k})}_{\mathcal{F}_L\{\vec{U}(\vec{x})\}} \qquad (7.95)$$

$$\hat{G}(\vec{k}) = L^3 \mathcal{F}_L\{G(\vec{r})\} = \iiint_0^L G(\vec{r}) e^{-i\vec{k}.\vec{r}} d\vec{r}$$

- Note that:

$$\hat{G}(0) = \iiint_0^L G(\vec{r}) d\vec{r} = 1 \qquad (7.96)$$

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VII.3 LES in spectral space

Filter types

- The sharp spectral (cut-off) filter:

$$\hat{G}(\vec{k}) = H(k_c - |\vec{k}|) \qquad (7.97)$$

Cut-off wavenumber

- Isotropic
- Filter width:

Number of modes

$$k_c = \frac{2\pi}{L}\frac{N_c}{2} = \pi\frac{N_c}{L} = \frac{\pi}{\Delta} \longrightarrow \Delta = \frac{\pi}{k_c}$$

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VII.3 LES in spectral space

Filter types

Name	Filter function	Transfer function
General	$G(r)$	$\widehat{G}(\kappa) \equiv \int_{-\infty}^{\infty} e^{i\kappa r} G(r)\,\mathrm{d}r$
Box	$\frac{1}{\Delta}H(\frac{1}{2}\Delta - \vert r\vert)$	$\frac{\sin(\frac{1}{2}\kappa\Delta)}{\frac{1}{2}\kappa\Delta}$
Gaussian	$\left(\frac{6}{\pi\Delta^2}\right)^{1/2}\exp\left(-\frac{6r^2}{\Delta^2}\right)$	$\exp\left(-\frac{\kappa^2\Delta^2}{24}\right)$
Sharp spectral	$\frac{\sin(\pi r/\Delta)}{\pi r}$	$H(\kappa_c - \vert\kappa\vert)$, $\kappa_c \equiv \pi/\Delta$
Cauchy	$\frac{a}{\pi\Delta[(r/\Delta)^2 + a^2]}$, $a = \frac{\pi}{24}$	$\exp(-a\Delta\vert\kappa\vert)$
Pao		$\exp\left(-\frac{\pi^{2/3}}{24}(\Delta\vert\kappa\vert)^{4/3}\right)$

◄ Table 13.2 [1], filters formula in physical space

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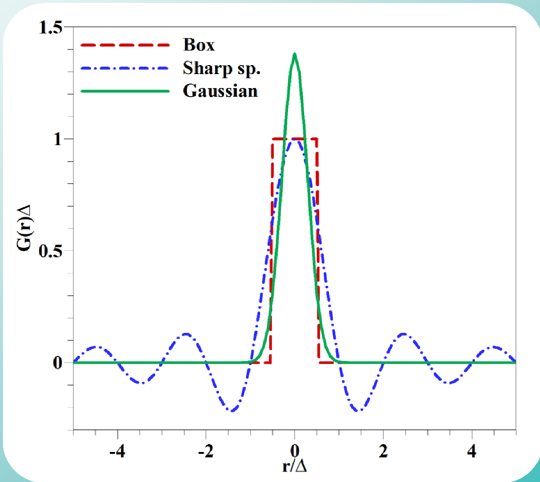
VII.3 LES in spectral space

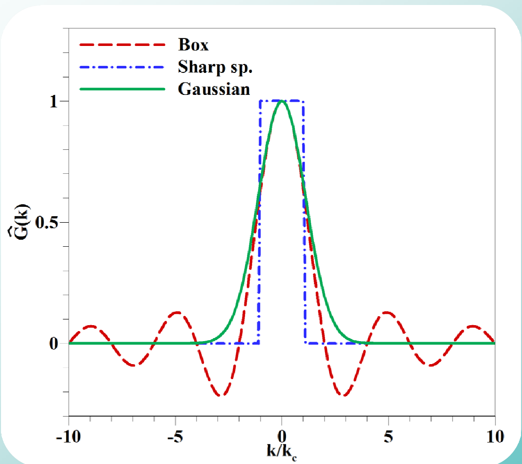
Filter types

Representation of filters in physical space. Solid line: Gaussian filter, dashed line: box filter, dash-dotted: sharp spectral filter. ▶



VII.3 LES in spectral space

Filter types



◀ **Representation of filters in spectral space. Solid line: Gaussian filter, dashed line: box filter, dash-dotted: sharp spectral filter.**

VII.3 LES in spectral space

The filtered fluctuations and energy spectrum:

- Remember

Resolved part of fluctuation **Similarly**

$$u_i \equiv U_i - \langle U_i \rangle \qquad \bar{u}_i \equiv \bar{U}_i - \langle \bar{U}_i \rangle \quad (6.19)$$

$$R_{ij}(\vec{r}) \equiv \langle u_i(\vec{x}) u_j(\vec{x}+\vec{r}) \rangle \qquad R_{ij}^R(\vec{r}) \equiv \langle \bar{u}_i(\vec{x}) \bar{u}_j(\vec{x}+\vec{r}) \rangle \quad (6.20)$$

$$\hat{R}_{ij}(\vec{k}) \equiv \mathcal{F}_L\{R_{ij}(\vec{r})\} = \langle \hat{u}_i^*(\vec{k}) \hat{u}_j(\vec{k}) \rangle \qquad \hat{R}_{ij}^R(\vec{k}) \equiv \mathcal{F}_L\{R_{ij}^R(\vec{r})\} = \langle \hat{\bar{u}}_i^*(\vec{k}) \hat{\bar{u}}_j(\vec{k}) \rangle \quad (7.97)'$$

$$\mathcal{F}_L \qquad \mathcal{F}$$

$$\phi_{ij}(\vec{k}) \equiv \mathcal{F}\{R_{ij}(\vec{r})\} = \langle \hat{u}_i^*(\vec{k}) \hat{u}_j(\vec{k}) \rangle \qquad \phi_{ij}^R(\vec{k}) \equiv \mathcal{F}\{R_{ij}^R(\vec{r})\} = \langle \hat{\bar{u}}_i^*(\vec{k}) \hat{\bar{u}}_j(\vec{k}) \rangle \quad (7.98)$$

$$\hat{E}(\vec{k}) = \tfrac{1}{2} \hat{R}_{ii}(\vec{k}) \qquad \hat{E}^R(\vec{k}) = \tfrac{1}{2} \hat{R}_{ii}^R(\vec{k}) \quad (7.97)''$$

$$E(k) = \sum_{\vec{k}'} \delta(k'-k) \hat{E}(\vec{k}') \qquad E^R(k) = \sum_{\vec{k}'} \delta(k'-k) \hat{E}^R(\vec{k}') \quad (7.97)'''$$

In Ref. [1], E^R is denoted by $\bar{E}$

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VII.3 LES in spectral space

The filtered fluctuations and energy spectrum:

- Remember

Resolved part of fluctuation **Similarly**

$$u_i \equiv U_i - \langle U_i \rangle \qquad \bar{u}_i \equiv \bar{U}_i - \langle \bar{U}_i \rangle \quad (6.19)$$

$$R_{ij}(\vec{r}) \equiv \langle u_i(\vec{x}) u_j(\vec{x}+\vec{r}) \rangle \qquad R_{ij}^R(\vec{r}) \equiv \langle \bar{u}_i(\vec{x}) \bar{u}_j(\vec{x}+\vec{r}) \rangle \quad (6.20)$$

$$\hat{R}_{ij}(\vec{k}) \equiv \mathcal{F}_L\{R_{ij}(\vec{r})\} = \langle \hat{u}_i^*(\vec{k}) \hat{u}_j(\vec{k}) \rangle \qquad \hat{R}_{ij}^R(\vec{k}) \equiv \mathcal{F}_L\{R_{ij}^R(\vec{r})\} = \langle \hat{\bar{u}}_i^*(\vec{k}) \hat{\bar{u}}_j(\vec{k}) \rangle \quad (7.97)'$$

$$\mathcal{F}_L \qquad \mathcal{F}$$

$$\phi_{ij}(\vec{k}) \equiv \mathcal{F}\{R_{ij}(\vec{r})\} = \langle \hat{u}_i^*(\vec{k}) \hat{u}_j(\vec{k}) \rangle \qquad \phi_{ij}^R(\vec{k}) \equiv \mathcal{F}\{R_{ij}^R(\vec{r})\} = \langle \hat{\bar{u}}_i^*(\vec{k}) \hat{\bar{u}}_j(\vec{k}) \rangle \quad (7.98)$$

$$\hat{E}(\vec{k}) = \tfrac{1}{2} \hat{R}_{ii}(\vec{k}) \qquad \hat{E}^R(\vec{k}) = \tfrac{1}{2} \hat{R}_{ii}^R(\vec{k}) \quad (7.97)''$$

$$E(k) = \sum_{\vec{k}'} \delta(k'-k) \hat{E}(\vec{k}') \qquad E^R(k) = \sum_{\vec{k}'} \delta(k'-k) \hat{E}^R(\vec{k}') \quad (7.97)'''$$

$$k = \tfrac{1}{2}\langle u_i u_i \rangle = \int_0^\infty E(k)\,dk \qquad k^R = \tfrac{1}{2}\langle \bar{u}_i \bar{u}_i \rangle = \int_0^\infty E^R(k)\,dk \quad (7.99)''$$

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VII.3 LES in spectral space

The filtered fluctuations and energy spectrum:

- Exercise: For homogeneous flow and homogeneous filters, show that:

$$\hat{R}_{ij}^{R}(\vec{k}) = \left|\hat{G}(\vec{k})\right|^2 \hat{R}_{ij}(\vec{k}) = \hat{G}^2(\vec{k})\hat{R}_{ij}(\vec{k}) \qquad (7.98)^{(5)}$$

and for isotropic filter:

$$E^R(k) = \hat{G}^2(k)E(k) \qquad (7.99)'$$

- Remember:

$$k^{SFS} = k - k^R \qquad (6.50)$$

- Exercise: Show that:

$$k^{SFS} = \int_0^\infty \left(1 - \hat{G}^2(k)\right) E(k)dk \qquad (7.99)^{(4)}$$

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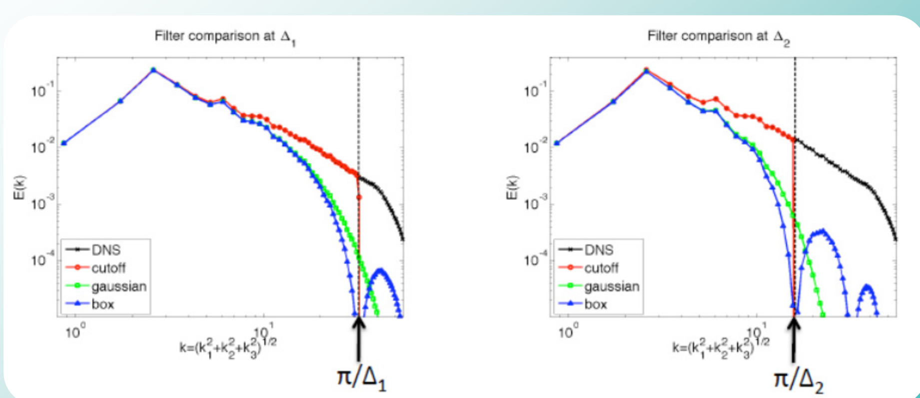
VII.3 LES in spectral space

Filtered energy spectrum



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VII.3 LES in spectral space

Filtered equations

- Remember: Assuming a periodic velocity field of period length length L:

$$\frac{d\vec{\hat{U}}(\vec{k})}{dt} + \nu k^2 \vec{\hat{U}}(\vec{k}) = -\underline{P}.\vec{\hat{G}} \qquad (7.57)$$

$$\underline{P} = \underline{I} - \frac{\vec{k}\vec{k}}{k^2} \qquad (7.52)$$

$$\vec{\hat{G}} = -i\vec{k}.\sum_{\vec{k}'} \vec{\hat{U}}(\vec{k}')\vec{\hat{U}}(\vec{k}-\vec{k}') = -i\vec{k}.\sum_{\vec{k}'}\sum_{\vec{k}''} \delta_{\vec{k},\vec{k}'+\vec{k}''} \vec{\hat{U}}(\vec{k}')\vec{\hat{U}}(\vec{k}'') \qquad (7.55)$$

- The pressure variable is removed and the continuity equation is decoupled in the spectral space
- Filtering in spectral space: The multiplication of Eq. (7.57) by the transfer function

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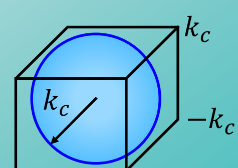
VII.3 LES in spectral space

Filtered equations

- Assuming the isotropic sharp spectral filter $\hat{G}(\vec{k}) = H(k_c - k)$:

Closure problem ⟵ Triad Interaction (TI)

$$\begin{cases} \left(\frac{d}{dt} + \nu k^2\right)\hat{\bar{U}}_j(\vec{k}) = -ik_l P_{jk}(\vec{k}) \overbrace{\sum_{\vec{k}'}\sum_{\vec{k}''} \delta_{\vec{k},\vec{k}'+\vec{k}''} H(k_c - k)\hat{U}_k(\vec{k}')\hat{U}_l(\vec{k}'')}^{\text{Triad Interaction (TI)}}; \\ k_i = \frac{2\pi}{L} n_i, n_i = 0, \pm 1, \dots, -\frac{N_c}{2}, n_1^2 + n_2^2 + n_3^2 \le N_c^2 = \left(\frac{L}{\pi} k_c\right)^2 \qquad (7.100a) \\ \hat{\bar{U}}_j(\vec{k}) = 0; \ \text{otherwise} \qquad (7.100b) \end{cases}$$



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VII.3.3 SGS modeling

The filtered rate of strain

- The filtered rate of strain tensor:

$$\bar{s}_{ij} = \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) \qquad (7.101)$$

- The characteristic rate of strain:

$$\bar{s} = \left(2\bar{s}_{ij}\bar{s}_{ij}\right)^{1/2} \qquad (7.102)$$

- Note: For isotropic turbulence $\bar{u}_i = \bar{U}_i$ and $\bar{s}_{ij} = \bar{S}_{ij}$.
- Remember, Eq. (3.15) and (7.83):

Similarly

$$\varepsilon = 2\nu\langle s_{ij}s_{ij}\rangle \cong \int_0^\infty 2\nu k^2 E(k)dk \qquad \langle \varepsilon_f\rangle \equiv 2\nu\langle \bar{s}_{ij}\bar{s}_{ij}\rangle \cong \int_0^\infty 2\nu k^2 E^R(k)dk \qquad (7.103)$$

$$\left\langle \bar{s}^2\right\rangle \equiv 2\langle \bar{s}_{ij}\bar{s}_{ij}\rangle \cong 2\int_0^\infty k^2 E^R(k)dk = 2\int_0^\infty k^2 \hat{G}^2(k)E(k)dk \qquad (7.104)$$

Isotropic filter

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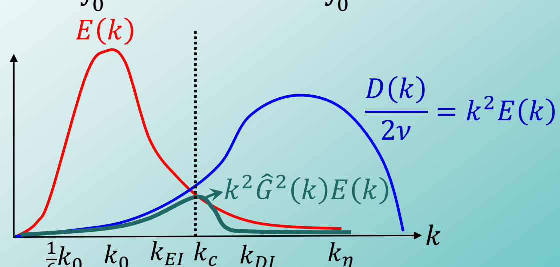
VII.3.3 SGS modeling

The filtered rate of strain

$$\left\langle \bar{s}^2\right\rangle \equiv 2\langle \bar{s}_{ij}\bar{s}_{ij}\rangle \cong 2\int_0^\infty k^2 E^R(k)dk = 2\int_0^\infty k^2 \hat{G}^2(k)E(k)dk \qquad (7.104)$$



- Therefore, the contributions to $\left\langle \bar{s}^2\right\rangle$ are predominantly from wavenumbers around k_c.
- Assuming high Re, and k_c being in the inertial subrange, Eq. (7.104) can be approximated by $E(k)$ in this range, Eq. (7.93)

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VII.3.3 SGS modeling

The filtered rate of strain

$$\left\langle \bar{\mathcal{S}}^2 \right\rangle \sim 2\int_0^\infty k^2 \hat{G}^2(k)\left[C\varepsilon^{2/3}k^{-5/3}\right]dk = a_f C\varepsilon^{2/3}\Delta^{-4/3} \qquad (7.105)$$

Dependence on filter type

Dependence on filter width

$$a_f = 2\int_0^\infty (k\Delta)^{1/3}\hat{G}^2(k)\Delta dk \qquad (7.106)$$

- Exercise: Using the appropriate relations for $\hat{G}(k)$, show that:

$$a_f = \begin{cases} 6.90 & ;\text{ for sharp spectral filter} \\ 7.10 & ;\text{ for Gaussian filter} \end{cases} \qquad (7.107)$$

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VII.3.3 SGS modeling

Determining the Smagorinsky constant

- Assuming isotropic turbulence, high Re, and the filter width in the inertial subrange:

$$\varepsilon \sim \langle \mathcal{P}_r \rangle = \left\langle -\tau_{ij}^r \bar{S}_{ij} \right\rangle \xrightarrow{\text{Eq. (6.40)}} = \left\langle 2\nu_r \bar{S}_{ij}\bar{S}_{ij} \right\rangle = \left\langle \nu_r \bar{\mathcal{S}}^2 \right\rangle \xrightarrow{\text{Eq. (6.48)}} = l_S^2 \left\langle \bar{\mathcal{S}}^3 \right\rangle \longrightarrow$$

$$l_S = \left(\frac{\varepsilon}{\left\langle \bar{\mathcal{S}}^3 \right\rangle}\right)^{1/2} = \frac{\varepsilon^{1/2}}{\left\langle \bar{\mathcal{S}}^2 \right\rangle^{3/4}} \left(\frac{\left\langle \bar{\mathcal{S}}^2 \right\rangle^{3/4}}{\left\langle \bar{\mathcal{S}}^3 \right\rangle^{1/2}}\right) \qquad (7.110)$$

- Assuming $\left\langle \bar{\mathcal{S}}^2 \right\rangle$ from the approximation (7.105) and

$$\left\langle \bar{\mathcal{S}}^3 \right\rangle \sim \left\langle \bar{\mathcal{S}}^2 \right\rangle^{3/2} : \quad l_S = \frac{\Delta}{\left(C a_f\right)^{4/3}} \qquad (7.111) \longrightarrow$$

$$C_S = \frac{l_S}{\Delta} = \left(C a_f\right)^{-4/3} \qquad (7.112)$$

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VII.3.3 SGS modeling

Determining the Smagorinsky constant

- For the sharp spectral filter, $a_f = 6.90$, and $C \sim 1.5$:

$$C_S = \left(C a_f\right)^{-4/3} \approx 0.17 \qquad (7.112)'$$

- Recommended values:

$$C_S \sim 0.1 - 0.17 \longrightarrow C_{DS} \sim C_S^2 \sim 0.01 - 0.03$$

- Exercise: Compare these values with the value obtained for the dynamic Smagorinsky constant for the **1DFSBE** in project#2.

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VII.3.3 SGS modeling

Modeling in spectral space

- The closure problem: Triad Interaction

$$TI = \sum_{\vec{k}'} \sum_{\vec{k}''} \delta_{\vec{k},\vec{k}'+\vec{k}''} H(k_c - k) \widehat{U}_k(\vec{k}') \widehat{U}_l(\vec{k}'') = \mathcal{F}_L\{\overline{U_k U_l}\} \qquad (7.113)$$

- Another reason for the superiority of Germano's decomposition:
  - Exercise: Assuming sharp spectral filter ($\overline{\overline{U}} = \overline{U}$), Eq. (6.61) is simplified to:

$$\overline{U_i U_j} \equiv \overline{\overline{U}_i \overline{U}_j} + \tau_{ij}^k, \tau_{ij}^k = \overline{\overline{U}_i U_j'} + \overline{\overline{U}_j U_i'} + \overline{U_i' U_j'} \qquad (7.114)$$

vs.

$$\overline{U_i U_j} \equiv \overline{U}_i \overline{U}_j + \tau_{ij}^R \qquad (6.30)$$

  - $\overline{U_i U_j}$ contains no wavenumber $k > k_c$
  - $\overline{U}_i \overline{U}_j$ contains wavenumbers $k_c < k < 2k_c$
  - τ_{ij}^R should cancel out wavenumbers $k_c < k < 2k_c$ with the data available for $k < k_c$, a toll order! This issue is removed by modeling τ_{ij}^k, see Eq. (7.114)

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VII.3.3 SGS modeling

Modeling in spectral space

- The closure problem: Triad Interaction (TI)

$$TI = \sum_{\vec{k}'}\sum_{\vec{k}''} \delta_{\vec{k},\vec{k}'+\vec{k}''} H(k_c - k)\widehat{U}_k(\vec{k}')\widehat{U}_l(\vec{k}'') = \mathcal{F}_L\{\overline{U_k U_l}\} \qquad (7.113)$$

- Indirect approach: Using a SGS model in physical space for $\overline{U_k U_l}$ and Fourier transform the result, like in “pyBurgers.py”
- Direct approach: Modeling TI directly in the spectral space

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VII.3.3 SGS modeling

Direct SGS modeling in the spectral space

- Using decomposition Eq. (7.114) in Eq. (7.100a):

$$\left(\frac{d}{dt} + \nu k^2\right)\widehat{\overline{U}}_j(\vec{k}) = \underbrace{F_j^{<}(\vec{k})}_{\text{Resolved TI}} + \underbrace{F_j^{>}(\vec{k})}_{\text{Unresolved TI}} \qquad (7.115)$$

$$F_j^{<}(\vec{k}) = -ik_l P_{jk}(\vec{k}) \overbrace{\sum_{\substack{\vec{k}' \\ (k',k''<k_c)}}\sum_{\vec{k}''} \delta_{\vec{k},\vec{k}'+\vec{k}''} H(k_c - k)\widehat{\overline{U}}_k(\vec{k}')\widehat{\overline{U}}_l(\vec{k}'')}^{\mathcal{F}_L\left\{\overline{\overline{U}_k \overline{U}_l}\right\}} \qquad (7.116)$$

$$F_j^{>}(\vec{k}) = -ik_l P_{jk}(\vec{k}) \overbrace{\sum_{\substack{\vec{k}' \\ (\max(k',k'')\geq k_c)}}\sum_{\vec{k}''} \delta_{\vec{k},\vec{k}'+\vec{k}''} H(k_c - k)\widehat{U}_k(\vec{k}')\widehat{U}_l(\vec{k}'')}^{\mathcal{F}_L\left\{\tau_{ij}^{k}\right\}} \qquad (7.117)$$

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VII.3.3 SGS modeling

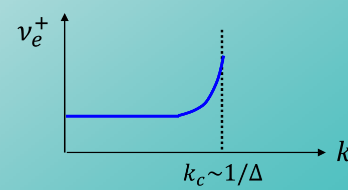
Direct SGS modeling in the spectral space

- Using a direct spectral model, e.g., spectral eddy-viscosity model for $F_j^{>}(\vec{k})$:

$$F_j^{>}(\vec{k}) = -\nu_e k^2 \widehat{\overline{U}}_j(\vec{k}) \qquad (7.118)$$

$$\nu_e = \nu_e^{+}\sqrt{\frac{E(k_c)}{k_c}} \qquad (7.119)$$

$$\nu_e^{+} = C^{-3/2}\{a + b\exp[-d(k_c/k)^p]\} \qquad (7.120)$$



- Model constants: For 3D flows:

$$C = 1.5, a = 0.441, b = 15.2, d = 3.03, p = 1 \qquad (7.121)$$

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