Lattice Boltzmann and Pseudo-Spectral Methods for Decaying Homogeneous Isotropic Turbulence

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Outline

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   - Theory of LBE
   - D3Q19 LBE Model
2. Results
   - A Vortex Ring Impacting a Flat Plate
   - DNS for Turbulence: LBE vs. Pseudo-Spectral Method
3. Conclusions and Future Work

Hierarchy of Scales and PDEs

Macroscopic Scale

$$\rho D_t \boldsymbol{u} = -\boldsymbol{\nabla} p + \frac{1}{\mathrm{Re}} \boldsymbol{\nabla}\cdot\sigma$$

$$D_t = \partial_t + \boldsymbol{u}\cdot\boldsymbol{\nabla}$$

$$\sigma = \frac{\rho\nu}{2}[(\boldsymbol{\nabla}\boldsymbol{u})+(\boldsymbol{\nabla}\boldsymbol{u})^{\dagger}] + \frac{2\rho\zeta}{D}\mathsf{I}(\boldsymbol{\nabla}\cdot\boldsymbol{u})$$

$$\mathrm{Re}_{\delta} = \frac{UL}{\nu} \sim \frac{\mathrm{Ma}}{\mathrm{Kn}}$$

$$\nu \approx 10^{-6} - 10^{-4}\ (\mathrm{m}^2/\mathrm{s})$$

$\mathrm{Kn} \approx 0$ $\quad$ $\mathrm{Ma} < 10^2$

$$L \geq 10^{-5}(\mathrm{m}) = 10(\mu\mathrm{m})$$

$$T \geq 10^{-4}(\mathrm{s})$$

$$N \geq N_A \approx 6.02 \cdot 10^{23}$$

Hierarchy of Scales and PDEs

Microscopic Scale

$$\dot{q}_k = \frac{\partial H}{\partial p_k},\ \dot{p}_k = -\frac{\partial H}{\partial q_k}$$

$$H = \sum_{k=1}^{(D+K)N} p_k^2 + V$$

$$i\hbar\dot{\psi} = \mathcal{H}\psi$$

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\boldsymbol{\nabla}_j^2 + V$$

$$h \approx 6.62 \cdot 10^{-34}(\mathrm{J}\cdot\mathrm{s})$$

$$c \approx 2.99 \cdot 10^{8}(\mathrm{m/s})$$

$$a \approx 5\cdot 10^{-11}(\mathrm{m})$$

$$t_a \approx 2.41\cdot 10^{-17}(\mathrm{s})$$

$$m \approx 10^{-27}(\mathrm{kg})$$

$$N = 1,\, 2,\, \ldots,\, N_0$$

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Mesoscopic Scale

$$\partial_t f + \boldsymbol{\xi}\cdot\boldsymbol{\nabla} f = \frac{1}{\varepsilon}Q(f, f)$$

$$f = f(\boldsymbol{x}, \boldsymbol{\xi}, t)$$

$$\varepsilon = \mathrm{Kn} = \frac{\ell}{L}, \; \mathrm{Ma} = \frac{U}{c_s}$$

$k_B \approx 1.38 \cdot 10^{-23}(\mathrm{J/°K})$

$\ell \approx 10^2 - 10^3$ (Å)

$\approx 10 - 100$ (nm)

$\tau \approx 10^{-10}(\mathrm{s})$

$c_s \approx 300$ (m/s)

$N \gg 1$

Macroscopic Scale

$$\rho D_t \boldsymbol{u} = -\boldsymbol{\nabla} p + \frac{1}{\mathrm{Re}}\boldsymbol{\nabla}\cdot\sigma$$

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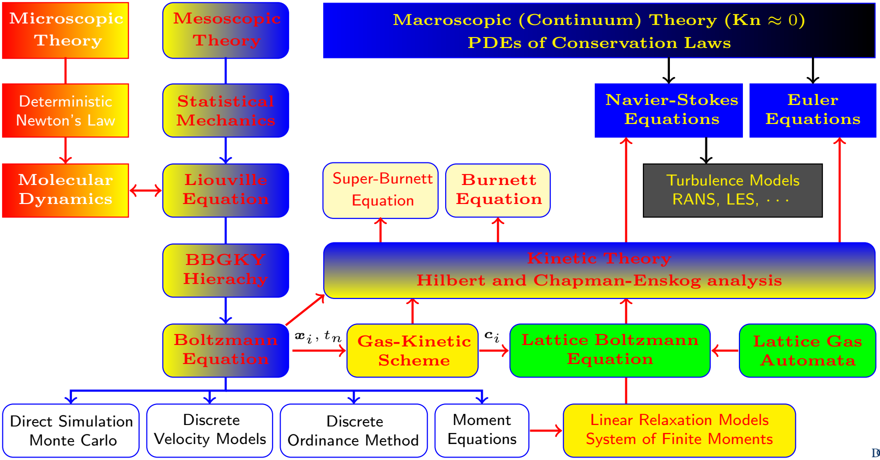
Micro-, Meso-, Macro-Descriptions of Fluids

$$\text{Knudsen Number Kn} := \frac{\ell}{L} = \frac{\text{Mean Free Path}}{\text{Characteristic Hydrodynamic Length}}$$



In the Course of Hydrodynamic Events ...

Ma (Mach) and Kn (Knudsen) characterize nonequilibrium

Van Karmen relation based on Navier-Stokes equation ($\mathrm{Kn}=O(\varepsilon)$): $\mathrm{Ma}=\mathrm{Re}\cdot\mathrm{Kn}$

	$\mathrm{Re}\ll 1$	$\mathrm{Re}\approx 1$	$\mathrm{Re}\gg 1$
$\mathrm{Ma}\ll 1$	Stokes Flows $\mathrm{Ma}=O(\varepsilon^2)$, $\mathrm{Re}=O(\varepsilon)$	Incompressible Navier-Stokes Flows $\mathrm{Ma}=O(\varepsilon)$, $\mathrm{Re}=O(1)$	Incompressible Navier-Stokes Flows $\mathrm{Ma}=O(\varepsilon^{1-\alpha})$, $\mathrm{Re}=O(\varepsilon^{-\alpha})$
$\mathrm{Ma}\approx 1$			Sub/Transonic Flows $\mathrm{Ma}=O(1)$, $\mathrm{Re}=O(\varepsilon^{-1})$
$\mathrm{Ma}\gg 1$			Super/Hypersonic Flows $\mathrm{Ma}=O(\varepsilon^{-1})$, $\mathrm{Re}=O(\varepsilon^{-2})$

With the framework of kinetic theory (Boltzmann equation)

Hydrodynamics	Slip Flow	Transitional	Free Molecular
$\mathrm{Kn}<10^{-3}$	$10^{-3}<\mathrm{Kn}<10^{-1}$	$10^{-1}<\mathrm{Kn}<10$	$10<\mathrm{Kn}$

A Priori Derivation of Lattice Boltzmann Equation

The Boltzmann Equation for $f := f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ with BGK approximation:

$$\partial_t f + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} f = \int [f_1' f_2' - f_1 f_2] d\mu \approx \mathcal{L}(f, f) \approx -\frac{1}{\lambda}[f - f^{(0)}] \tag{1}$$

The Boltzmann-Maxwellian equilibrium distribution function:

$$f^{(0)} = \rho\,(2\pi\theta)^{-D/2} \exp\left[-\frac{(\boldsymbol{\xi} - \boldsymbol{u})^2}{2\theta}\right], \quad \theta := RT \tag{2}$$

The macroscopic variables are the first few moments of f and $f^{(0)}$:

$$\rho = \int f d\boldsymbol{\xi} = \int f^{(0)} d\boldsymbol{\xi}\,, \tag{3a}$$

$$\rho \boldsymbol{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi} = \int \boldsymbol{\xi} f^{(0)} d\boldsymbol{\xi}\,, \tag{3b}$$

$$\rho \varepsilon = \frac{1}{2} \int (\boldsymbol{\xi} - \boldsymbol{u})^2 f d\boldsymbol{\xi} = \frac{1}{2} \int (\boldsymbol{\xi} - \boldsymbol{u})^2 f^{(0)} d\boldsymbol{\xi}\,. \tag{3c}$$

Integral Solution of Continuous Boltzmann Equation

Rewrite the Boltzmann BGK Equation in the form of ODE:

$$D_t f + \frac{1}{\lambda} f = \frac{1}{\lambda} f^{(0)} , \qquad D_t := \partial_t + \boldsymbol{\xi} \cdot \nabla . \tag{4}$$

Integrate Eq. (4) over a time step δ_t along characteristics:

$$\begin{aligned} f(\boldsymbol{x} + \boldsymbol{\xi}\delta_t, \boldsymbol{\xi}, t + \delta_t) &= e^{-\delta_t/\lambda} f(\boldsymbol{x}, \boldsymbol{\xi}, t) \\ &+ \frac{1}{\lambda} e^{-\delta_t/\lambda} \int_0^{\delta_t} e^{t'/\lambda} f^{(0)}(\boldsymbol{x} + \boldsymbol{\xi} t', \boldsymbol{\xi}, t + t') \, dt' . \end{aligned} \tag{5}$$

By Taylor expansion, and with $\tau := \lambda/\delta_t$, we obtain:

$$f(\boldsymbol{x} + \boldsymbol{\xi}\delta_t, \boldsymbol{\xi}, t + \delta_t) - f(\boldsymbol{x}, \boldsymbol{\xi}, t) = -\frac{1}{\tau} [f(\boldsymbol{x}, \boldsymbol{\xi}, t) - f^{(0)}(\boldsymbol{x}, \boldsymbol{\xi}, t)] + \mathcal{O}(\delta_t^2) . \tag{6}$$

Note that a *finite-volume* scheme or higher-order schemes can also be formulated based upon the integral solution.

Passage to Lattice Boltzmann Equation

Three necessary steps to derive LBE:[1,2]

1. Low Mach number expansion of the distribution functions;
2. Discretize $\boldsymbol{\xi}$-space with necessary and min. number of $\boldsymbol{\xi}_\alpha$;
3. Discretization of $\boldsymbol{x}$ space according to $\{\boldsymbol{\xi}_\alpha\}$.

Low Mach Number ($\boldsymbol{u} \approx 0$) Expansion of the distribution functions $f^{(0)}$ and f up to $\mathcal{O}(\boldsymbol{u}^2)$ is sufficient to derive the Navier-Stokes equations:

$$f^{(\text{eq})} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left[-\frac{\boldsymbol{\xi}^2}{2\theta}\right] \left\{1 + \frac{\boldsymbol{\xi}\cdot\boldsymbol{u}}{\theta} + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})^2}{2\theta^2} - \frac{\boldsymbol{u}^2}{2\theta}\right\} + \mathcal{O}(\boldsymbol{u}^3)\,. \tag{7a}$$

$$f = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left[-\frac{\boldsymbol{\xi}^2}{2\theta}\right] \sum_{n=0}^{2} \frac{1}{n!} \mathsf{a}^{(n)}(\boldsymbol{x},\, t) : \mathsf{H}^{(n)}(\boldsymbol{\xi})\,, \tag{7b}$$

where $\mathsf{a}^{(0)} = 1$, $\mathsf{a}^{(1)} = \boldsymbol{u}$, $\mathsf{a}^{(2)} = \boldsymbol{u}\boldsymbol{u} - (\theta - 1)\mathsf{I}$, and $\{\mathsf{H}^{(n)}(\boldsymbol{\xi})\}$ are generalized Hermite polynomials.

[1] X. He and L.-S. Luo, *Phys. Rev. E* **55**:R6333 (1997); *ibid* **56**:6811 (1997).

[2] X. Shan and X. He, *Phys. Rev. Lett.* **80**:65 (1998).

Discretization and Conservation Laws

The conservation laws are preserved exactly, if the hydrodynamic moments (ρ, $\rho\boldsymbol{u}$, and $\rho\epsilon$) are evaluated exactly:

$$I = \int \boldsymbol{\xi}^m f^{(\text{eq})} d\boldsymbol{\xi} = \int \exp(-\boldsymbol{\xi}^2/2\theta)\psi(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad (8)$$

where $0 \leq m \leq 3$, and $\psi(\boldsymbol{\xi})$ is a polynomial in $\boldsymbol{\xi}$. The above integral can be evaluated by quadrature:

$$I = \int \exp(-\boldsymbol{\xi}^2/2\theta)\psi(\boldsymbol{\xi}) d\boldsymbol{\xi} = \sum_j W_j \exp(-\boldsymbol{\xi}_j^2/2\theta)\psi(\boldsymbol{\xi}_j) \quad (9)$$

where $\boldsymbol{\xi}_j$ and W_j are the abscissas and the weights. Then

$$\rho = \sum_\alpha f_\alpha^{(\text{eq})} = \sum_\alpha f_\alpha, \qquad \rho\boldsymbol{u} = \sum_\alpha \boldsymbol{\xi}_\alpha f_\alpha^{(\text{eq})} = \sum_\alpha \boldsymbol{\xi}_\alpha f_\alpha, \quad (10)$$

where $f_\alpha := f_\alpha(\boldsymbol{x}, t) := W_\alpha f(\boldsymbol{x}, \boldsymbol{\xi}_\alpha, t)$, and $f_\alpha^{(\text{eq})} := W_\alpha f^{(\text{eq})}(\boldsymbol{x}, \boldsymbol{\xi}_\alpha, t)$.

The quadrature must preserve the conservation laws *exactly*!

Example: 9-bit LBE Model with Square Lattice

In two-dimensional Cartesian (momentum) space, set

$$\psi(\boldsymbol{\xi}) = \xi_x^m \xi_y^n,$$

the integral of the moments can be given by

$$I = (\sqrt{2\theta})^{(m+n+2)} I_m I_n, \qquad I_m = \int_{-\infty}^{+\infty} e^{-\zeta^2} \zeta^m d\zeta, \tag{11}$$

where $\zeta = \xi_x/\sqrt{2\theta}$ or $\xi_y/\sqrt{2\theta}$.
The second-order Hermite formula ($k = 2$) is the *optimal* choice to evaluate I_m for the purpose of deriving the 9-bit model, *i.e.*,

$$I_m = \sum_{j=1}^{3} \omega_j \zeta_j^m.$$

Note that the above quadrature is *exact* up to $m = 5 = (2k + 1)$.

Discretization of Velocity $\boldsymbol{\xi}$-Space (9-bit Model)

The three abscissas in momentum space (ζ_j) and the corresponding weights (ω_j) are:

$$\begin{array}{lll} \zeta_1 = -\sqrt{3/2}\,, & \zeta_2 = 0\,, & \zeta_3 = \sqrt{3/2}\,, \\ \omega_1 = \sqrt{\pi}/6\,, & \omega_2 = 2\sqrt{\pi}/3\,, & \omega_3 = \sqrt{\pi}/6\,. \end{array} \tag{12}$$

Then, the integral of moments becomes:

$$I = 2\theta \left[\omega_2^2 \psi(\mathbf{0}) + \sum_{\alpha=1}^{4} \omega_1 \omega_2 \psi(\boldsymbol{\xi}_\alpha) + \sum_{\alpha=5}^{8} \omega_1^2 \psi(\boldsymbol{\xi}_\alpha) \right] , \tag{13}$$

where

$$\boldsymbol{\xi}_\alpha = \begin{cases} (0,\, 0) & \alpha = 0, \\ (\pm 1,\, 0)\sqrt{3\theta},\ (0,\, \pm 1)\sqrt{3\theta}, & \alpha = 1 - 4, \\ (\pm 1,\, \pm 1)\sqrt{3\theta}, & \alpha = 5 - 8. \end{cases} \tag{14}$$

Discretization of Velocity $\boldsymbol{\xi}$-Space (9-bit Model)

Identifying

$$W_\alpha = (2\pi\,\theta)\,\exp(\boldsymbol{\xi}_\alpha^2/2\theta)\,w_\alpha\,, \tag{15}$$

with $c := \delta_x/\delta_t = \sqrt{3\theta}$, or $c_s^2 = \theta = c^2/3$, δ_x is the lattice constant, then:

$$\begin{aligned} f_\alpha^{(\mathrm{eq})}(\boldsymbol{x},\,t) &= W_\alpha\, f^{(\mathrm{eq})}(\boldsymbol{x},\,\boldsymbol{\xi}_\alpha,\,t) \\ &= w_\alpha\,\rho\left\{1 + \frac{3(\boldsymbol{c}_\alpha\cdot\boldsymbol{u})}{c^2} + \frac{9(\boldsymbol{c}_\alpha\cdot\boldsymbol{u})^2}{2c^4} - \frac{3\boldsymbol{u}^2}{2c^2}\right\}, \end{aligned} \tag{16}$$

where weight coefficient w_α and discrete velocity $\boldsymbol{c}_\alpha$ are:

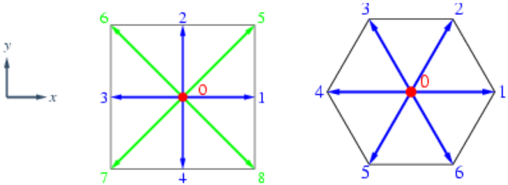
$$w_\alpha = \begin{cases} 4/9, \\ 1/9, \\ 1/36, \end{cases} \quad \boldsymbol{c}_\alpha = \boldsymbol{\xi}_\alpha = \begin{cases} (0,\,0), & \alpha = 0\,, \\ (\pm1,\,0)\,c,\ (0,\,\pm1)\,c, & \alpha = 1-4, \\ (\pm1,\,\pm1)\,c, & \alpha = 5-8. \end{cases} \tag{17}$$

With $\{\boldsymbol{c}_\alpha|\alpha = 0,\,1,\,\ldots,\,8\}$, a square lattice structure is constructed in the physical space.

Discretized 2D Velocity Space (9-bit)

With Cartesian coordinates in $\boldsymbol{\xi}$-space, a 2D square lattice is obtained:

$$\boldsymbol{c}_\alpha = \begin{cases} (0,\, 0), & \alpha = 0\,, \\ (\pm 1,\, 0)\, c,\ (0,\, \pm 1)\, c, & \alpha = 1 - 4, \\ (\pm 1,\, \pm 1)\, c, & \alpha = 5 - 8. \end{cases}$$



If spherical coordinates are used, a 2D triangular lattice is obtained.

$$\boldsymbol{c}_\alpha = \begin{cases} (0,\, 0), & \alpha = 0\,, \\ (\cos((\alpha - 1)\pi/3),\, \sin((\alpha - 1)\pi/3))\, c, & \alpha = 1 - 6. \end{cases}$$

D3Q19 MRT-LBE Model

$$\mathbf{f}(\boldsymbol{x}_j + \boldsymbol{c}\delta t,\, t_n + \delta t) = \mathbf{f}(\boldsymbol{x}_j,\, t_n) - \mathsf{M}^{-1} \cdot \mathsf{S} \cdot \left[\mathbf{m} - \mathbf{m}^{(\mathrm{eq})}\right], \tag{18}$$

$$e^{(\mathrm{eq})} = -11\delta\rho + \frac{19}{\rho_0}\boldsymbol{j}\cdot\boldsymbol{j}, \quad \epsilon^{(\mathrm{eq})} = 3\delta\rho - \frac{11}{2\rho_0}\boldsymbol{j}\cdot\boldsymbol{j}, \tag{19a}$$

$$(q_x^{(\mathrm{eq})},\, q_y^{(\mathrm{eq})},\, q_z^{(\mathrm{eq})}) = -\frac{2}{3}(j_x,\, j_y,\, j_z), \tag{19b}$$

$$p_{xx}^{(\mathrm{eq})} = \frac{1}{3\rho_0}\left[2j_x^2 - (j_y^2 + j_z^2)\right], \quad p_{ww}^{(\mathrm{eq})} = \frac{1}{\rho_0}\left[j_y^2 - j_z^2\right], \tag{19c}$$

$$p_{xy}^{(\mathrm{eq})} = \frac{1}{\rho_0}j_x j_y, \quad p_{yz}^{(\mathrm{eq})} = \frac{1}{\rho_0}j_y j_z, \quad p_{xz}^{(\mathrm{eq})} = \frac{1}{\rho_0}j_x j_z, \tag{19d}$$

$$\pi_{xx}^{(\mathrm{eq})} = -\frac{1}{2}p_{xx}^{(\mathrm{eq})}, \quad \pi_{ww}^{(\mathrm{eq})} = -\frac{1}{2}p_{ww}^{(\mathrm{eq})}, \tag{19e}$$

$$m_x^{(\mathrm{eq})} = m_y^{(\mathrm{eq})} = m_z^{(\mathrm{eq})} = 0, \tag{19f}$$

where $\delta\rho$ is the density fluctuation, $\rho = \rho_0 + \delta\rho$ and $\rho_0 = 1$.

D3Q19 MRT-LBE Model (cont.)

Conserved quantities:

$$\delta\rho = \sum_{i=0}^{Q-1} f_i, \quad \boldsymbol{j} = \rho_0 \boldsymbol{u} = \sum_{i=0}^{Q-1} f_i \boldsymbol{c}_i,$$

Transport coefficients and the speed of sound:

$$\nu = \frac{1}{3}\left(\frac{1}{s_\nu} - \frac{1}{2}\right), \quad \zeta = \frac{(5 - 9c_s^3)}{9}\left(\frac{1}{s_e} - \frac{1}{2}\right), \quad c_s^2 = \frac{1}{3} c\delta x,$$

where $c := \delta x/\delta t$.
The transform between the discrete distribution functions $\mathbf{f} \in \mathbb{V} = \mathbb{R}^Q$ and the moments $\mathbf{m} \in \mathbb{M} = \mathbb{R}^Q$:

$$\mathbf{m} = \mathsf{M} \cdot \mathbf{f}, \qquad \mathbf{f} = \mathsf{M}^{-1} \cdot \mathbf{m}.$$

Note that M^{-1} is related $\mathsf{M}^\dagger$.

Implement LBE Computation

Implementation:

1. Initialize $\boldsymbol{u}_0(\boldsymbol{x}_j)$, $\rho_0(\boldsymbol{x}_j) = 1$ or a consistent solution from $\boldsymbol{u}_0$;
2. Initialize $\mathbf{f}(\boldsymbol{x}_j, t_0) = \mathbf{f}^{(\text{eq})}(\rho_0, \boldsymbol{u}_0)$
3. Advection: $\mathbf{f}(\boldsymbol{x}_j, t_0) \longrightarrow \mathbf{f}(\boldsymbol{x}_j + \boldsymbol{c}\delta_t, t_0 + \delta_t)$
4. Collision:
    - Compute moments $\mathbf{m} = \mathsf{M} \cdot \mathbf{f}$ and their equilibria $\mathbf{m}^{(\text{eq})}$;
    - Relaxation: $\mathbf{m}^* = -\mathsf{S} \cdot [\mathbf{m} - \mathbf{m}^{(\text{eq})}]$;
    - Go back to velocity space: $\mathbf{f}^* = \mathbf{f} + \mathsf{M}^{-1} \cdot \mathbf{m}^*$;
5. Go to Advection . . .

Features of LBE:

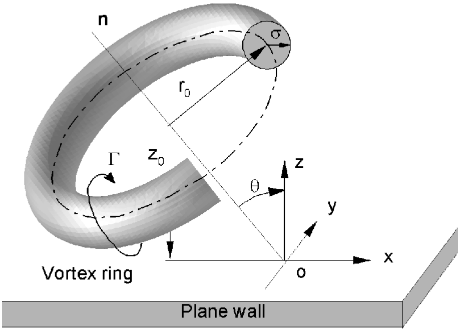
- A 2nd-order central-finite difference scheme;
- Larger stencil $\longrightarrow$ isotropy (2nd order);
- No stagger grid needed for incompressible Navier-Stokes equation;
- Related to “artificial compressibility” method;

A vortex ring impacting a flat plate

For a vortex ring of initial circulation Γ, radius r_0, and core radius σ, the initial velocity is:

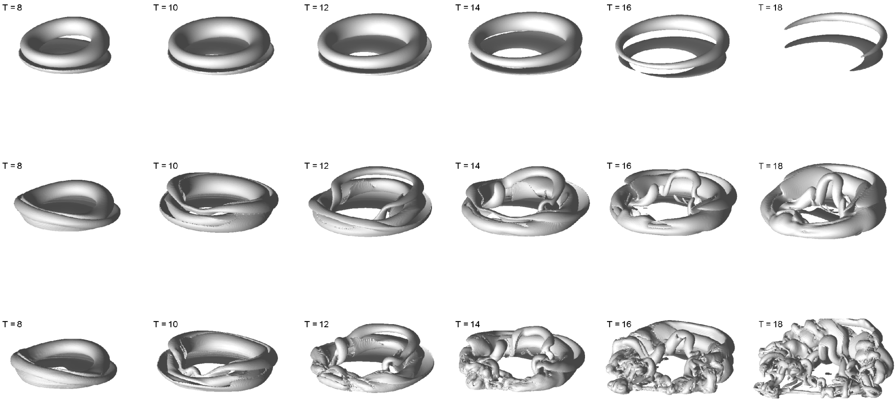
$$\boldsymbol{u}_0 = \frac{\Gamma}{2\pi r}\left(1 - e^{-(r/\sigma)^2}\right)\hat{\boldsymbol{n}} \quad (20)$$

where r is the distance from the core center, $\sigma/r_0 = 0.21$.
The domain size is $L \times W \times H = 12r_0 \times 12r_0 \times 7r_0$.
The resolution is $r_0 = 30\delta_x$, $N_x \times N_y \times N_z = 360 \times 360 \times 210$.

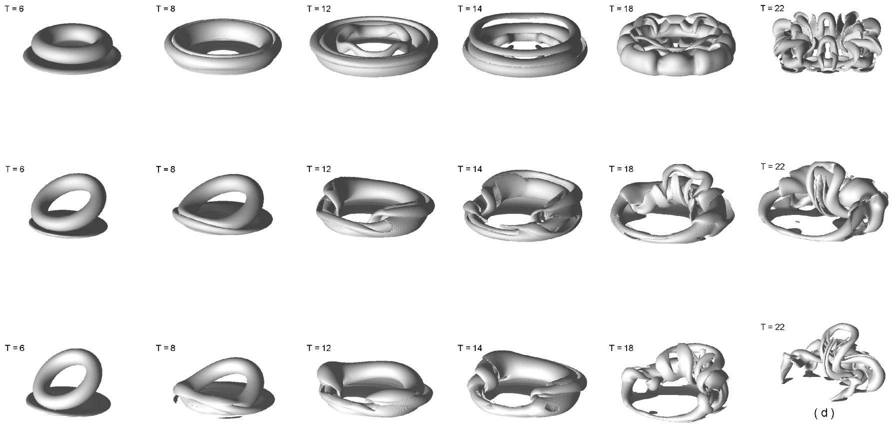


The Reynold number is $\mathrm{Re} = 2r_0U_s/\nu$, $U_s = (\Gamma/4\pi r_0)[\ln(8r_0/\sigma) - 1/4]$ is the initial translational speed of the ring.

Vortex structure: Re = 100, 500, 1,000; $\theta = 20°$



Vortex structure: $\theta = 0, 30°, 40°$; Re = 500



Motivation

1. *What is a DNS of turbulence*?
   - Numerical methods without explicit turbulence modeling?
   - Schemes which *demonstrably* resolve everything up to the smallest dynamically relevant scale?

   In the latter sense, spectral-type methods are the only ones completely true to this meaning of "DNS" we know of.

2. What is the best way to construct a good (high-order) numerical scheme for DNS/CFD?

We will compare the LBE method, a second-order method, with a pseudo-spectral method, an exponentially accurate and the *de facto* method for homogeneous turbulence.

Decaying Homogeneous Isotropic Turbulence

The decaying homogeneous isotropic turbulence is the solution of the *incompressible* Navier-Stokes equation

$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla} p + \nu \nabla^2 \boldsymbol{u}, \quad \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0, \quad \boldsymbol{x} \in [0,\, 2\pi]^3, \tag{21}$$

with periodic boundary conditions. The initial velocity satisfies a given initial energy spectrum $E_0(k)$

$$E_0(k) := E(k,\, t=0) = Ak^4 e^{-0.14k^4}, \quad k \in [k_a,\, k_b]. \tag{22}$$

The initial velocity $\boldsymbol{u}_0$ can be given by Rogallo procedure:

$$\tilde{\boldsymbol{u}}_0(\boldsymbol{k}) = \frac{\alpha k k_2 + \beta k_1 k_3}{k\sqrt{k_1^2 + k_2^2}} \hat{\boldsymbol{k}}_1 + \frac{\beta k_2 k_3 - \alpha k_1 k}{k\sqrt{k_1^2 + k_2^2}} \hat{\boldsymbol{k}}_2 - \frac{\beta\sqrt{k_1^2 + k_2^2}}{k} \hat{\boldsymbol{k}}_3, \tag{23}$$

where $\alpha = \sqrt{E_0(k)/4\pi k^2} e^{\imath\theta_1} \cos\phi$, $\beta = \sqrt{E_0(k)/4\pi k^2} e^{\imath\theta_2} \sin\phi$, $\imath := \sqrt{-1}$, and θ_1, θ_2, $\phi \in [0,\, 2\pi]$ are uniform random variables.

Low-Order Turbulence Statistics

The energy and the compensated spectra:

$$E(\boldsymbol{k}, t) := \frac{1}{2}\tilde{\boldsymbol{u}}(\boldsymbol{k}, t) \cdot \tilde{\boldsymbol{u}}^{\dagger}(\boldsymbol{k}, t), \quad \Psi(k) := \tilde{\varepsilon}(k)^{-2/3} k^{5/3} E(k), \tag{24}$$

And the *pressure spectrum* $P(\boldsymbol{k}, t)$. Low-order moments of $E(\boldsymbol{k}, t)$:

$$K(t) := \int d\boldsymbol{k}\, E(k, t), \quad \Omega(t) := \int d\boldsymbol{k}\, k^2 E(k, t) \tag{25a}$$

$$\varepsilon(t) := 2\nu\Omega(t), \quad \eta := \sqrt[4]{\nu^3/\varepsilon} \tag{25b}$$

$$S_{u_i}(t) = \frac{\langle(\partial_i u_i)^3\rangle}{\langle(\partial_i u_i)^2\rangle^{3/2}}, \qquad S_u(t) = \frac{1}{3}\sum_i S_{u_i} \tag{25c}$$

$$F_{u_i}(t) = \frac{\langle(\partial_i u_i)^4\rangle}{\langle(\partial_i u_i)^2\rangle^{2}}, \qquad F_u(t) = \frac{1}{3}\sum_i F_{u_i} \tag{25d}$$

We will also compare *instantaneous flows fields* $\boldsymbol{u}(\boldsymbol{x}, t)$ and $\boldsymbol{\omega}(\boldsymbol{x}, t)$.

Pseudo-Spectral Method

The pseudo-spectral (PS) method solve the Navier-Stokes equation in the Fourier space $\boldsymbol{k}$, i.e.,

$$\boldsymbol{u}(\boldsymbol{x}, t) = \sum_{\boldsymbol{k}} \tilde{\boldsymbol{u}}(\boldsymbol{k}, t) e^{\imath \boldsymbol{k}\cdot\boldsymbol{x}}, \quad -N/2+1 \leq k_\alpha \leq N/2.$$

- The nonlinear term $\boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u}$ computed in physical space $\boldsymbol{x}$ by inverse Fourier-transform $\tilde{\boldsymbol{u}}$ and $\boldsymbol{k}\tilde{\boldsymbol{u}}$ to $\boldsymbol{x}$ for form the nonlinear term; and it is transformed back to $\boldsymbol{k}$ space;
- De-aliasing: $\tilde{\boldsymbol{u}}(\boldsymbol{k}, t) = \boldsymbol{0} \ \forall \|\boldsymbol{k}\| \geq N/6$;
- Time matching: second-order Adams-Bashforth scheme:

$$\frac{\tilde{\boldsymbol{u}}(t+\delta t) - \tilde{\boldsymbol{u}}(t)}{\delta t} = -\frac{3}{2}\tilde{T}(t) + \frac{1}{2}\tilde{T}(t-\delta t) e^{-\nu k^2 \delta t},$$

where $\tilde{T} := \mathcal{F}[\boldsymbol{\omega} \times \boldsymbol{u}] - (\mathcal{F}[\boldsymbol{\omega} \times \boldsymbol{u}] \cdot \hat{\boldsymbol{k}})\hat{\boldsymbol{k}}$.

Parameters in DNS

Use $N^3 = 128^3$ and $[k_a,\, k_b] = [3,\, 8]$.
In LBE: $\nu = 1/600\,(c\delta x)$, $c := \delta x/\delta t = 1$, $\mathrm{Ma}_{\max} = \|\boldsymbol{u}_0\|_{\max}/c_s \le 0.15$, $A = 1.4293 \cdot 10^{-4}$ in $E_0(k)$, and $K_0 \approx 1.0130 \cdot 10^{-2}$, $u_0' \approx 8.2181 \cdot 10^{-2}$.
The time t is normalized by the turbulence turn-over time $t_0 = K_0/\varepsilon_0$.
In SP method, $K_0 = 1$ and $u_0' = \sqrt{2/3}$.

Method	L	δx	u_0'	δt	ν	$\delta t'$
LBE	2π	$2\pi/N$	$\sqrt{2K_0/3}$	$2\pi/N$	ν	$2\pi/Nt_0$
PS	2π	$2\pi/N$	$\sqrt{2/3}$	$2\pi\sqrt{K_0}/N$	$\nu/\sqrt{K_0}$	$2\pi/Nt_0$

The Taylor microscale Reynolds number:

$$\mathrm{Re}_\lambda := \frac{u'\lambda}{\nu}, \quad \lambda := \sqrt{\frac{15}{2\Omega}}u' := \sqrt{\frac{15\nu}{\varepsilon}}u' \tag{26}$$

The resolution criterion:

$$\text{SP: } N \sim 0.4\mathrm{Re}_\lambda^{3/2}, \quad \eta/\delta x \ge 1/2.1, \quad N = 128 \to \mathrm{Re}_\lambda = 46.78$$

$$\text{LBE: } \eta k_{\max} = \eta/\delta x \ge 1, \quad N = 128 \to \mathrm{Re}_\lambda = 24.35.$$

Initial Conditions

For the psuedo-spectral method:

- Generate $\tilde{\boldsymbol{u}}_0(\boldsymbol{k})$ in $\boldsymbol{k}$-space with a given $E_0(k)$ (Rogallo's procedure) with $K_0 = 1$ and $u' = \sqrt{3/2}$;
- The initial pressure p_0 is obtained by solving the Poisson equation in $\boldsymbol{k}$-space.

For the LBE method:

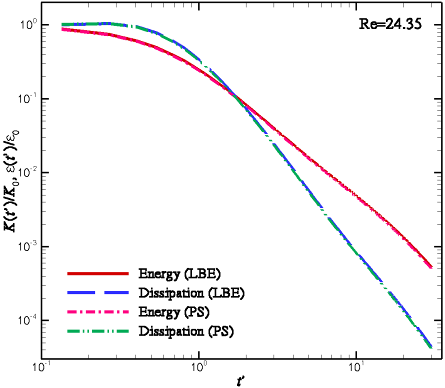
- Use the initial velocity $\boldsymbol{u}_0$ as in PS method except a scaling factor so that $\mathrm{Ma}_{\mathrm{max}} = 0.15$;
- The pressure p_0 is obtained by an iterative procedure with a given $\boldsymbol{u}_0$.[3]

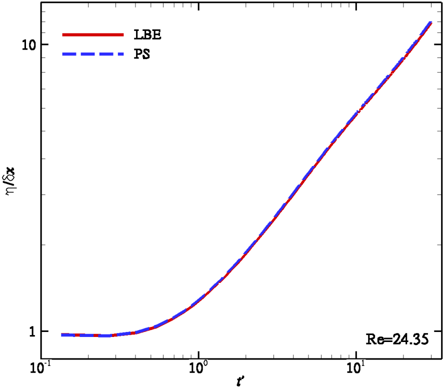
[3] R. Mei, L.-S. Luo, P. Lallemand, and D. d'Humières, Computers & Fluids **35**(8/9):855–862 (2006).

$K(t')/K_0$, $\varepsilon(t')/\varepsilon_0$, and $\eta(t')/\delta x$

$$K(t') := \int d\boldsymbol{k} E(\boldsymbol{k},\, t'), \quad \varepsilon(t') := 2\nu \int d\boldsymbol{k} k^2 E(\boldsymbol{k},\, t'), \quad \eta(t') := \sqrt[4]{\nu^3/\varepsilon(t')}$$

$\mathrm{Re}_\lambda = 24.37$, $\nu = 1/600$, $\eta_0/\delta x \approx 1.036$.

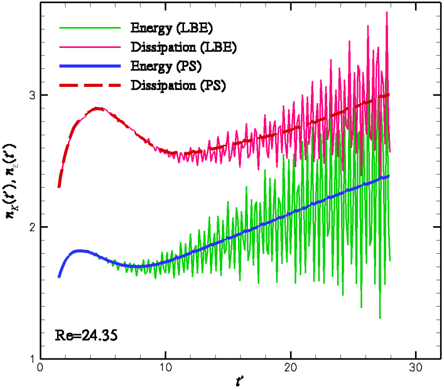


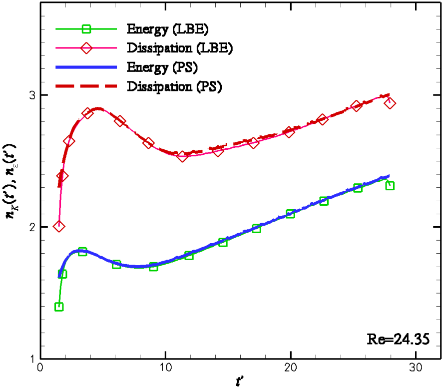


Decaying exponent n

$$K(t')/K_0 \sim (t'/t_0)^{-n}, \quad \varepsilon(t')/\varepsilon_0 \sim (t'/t_0)^{-(n+1)}$$

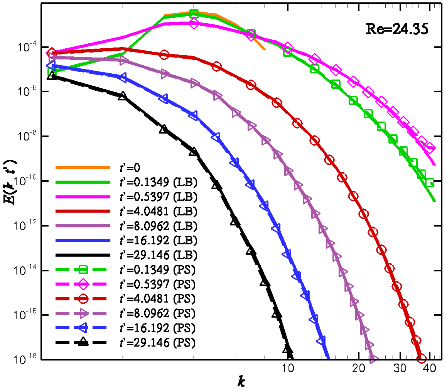
$$n_K = \frac{\ln K(t_i) - \ln K(t_j)}{\ln t_j - \ln t_i}, \quad n_\varepsilon + 1 = \frac{\ln \varepsilon(t_i) - \ln \varepsilon(t_j)}{\ln t_j - \ln t_i}$$

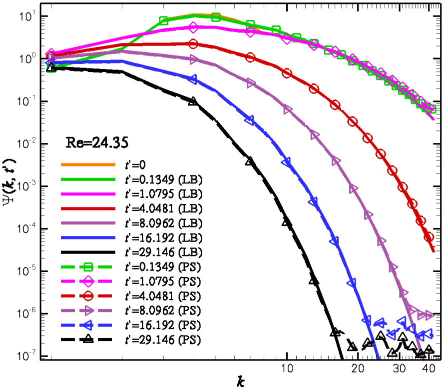




Energy and compensated spectra

$$E(k,\, t') := \frac{1}{2}\tilde{\boldsymbol{u}}(\boldsymbol{k},\, t')\cdot\tilde{\boldsymbol{u}}(\boldsymbol{k},\, t')^{\dagger}, \quad \Psi(k,\, t') := k^{5/3}\varepsilon^{-2/3}E(k,\, t')$$





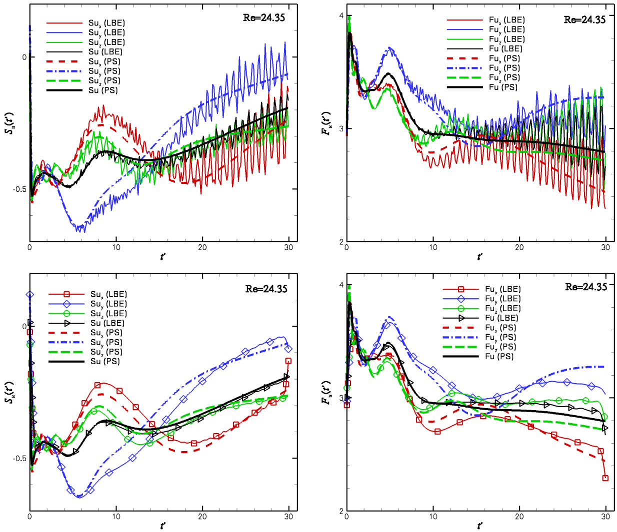
Skewness S_u and Flatness F_u

$$S_{u_\alpha}(t') := \frac{\langle (\partial_\alpha u_\alpha)^3 \rangle}{\langle (\partial_\alpha u_\alpha)^2 \rangle^{3/2}}$$

$$S_u := \frac{1}{3} \sum_\alpha S_{u_\alpha}$$

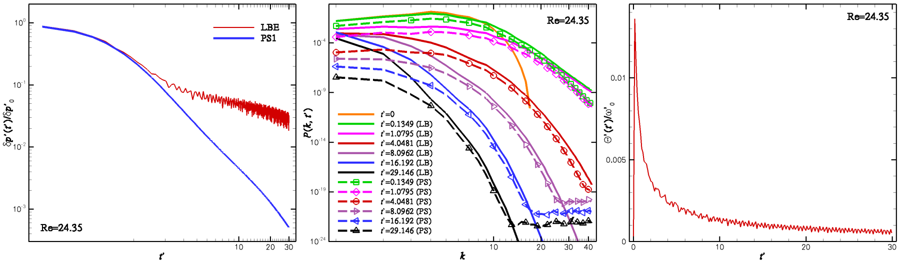
$$F_{u_\alpha}(t') := \frac{\langle (\partial_\alpha u_\alpha)^4 \rangle}{\langle (\partial_\alpha u_\alpha)^2 \rangle^2}$$

$$F_u := \frac{1}{3} \sum_\alpha F_{u_\alpha}$$



Acoustics, $\mathrm{Re}_\lambda = 24.37$

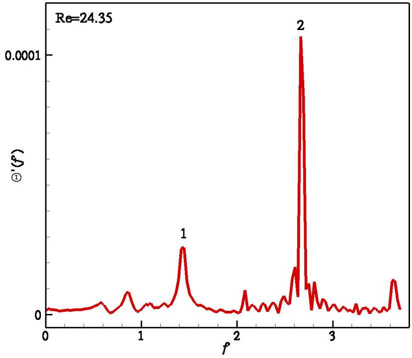
From left to right: the rms pressure $\delta p'(t')/\delta p'_0$, the pressure spectra $P(k, t')$, and the velocity divergence $\Theta'(t')/\omega'_0$:

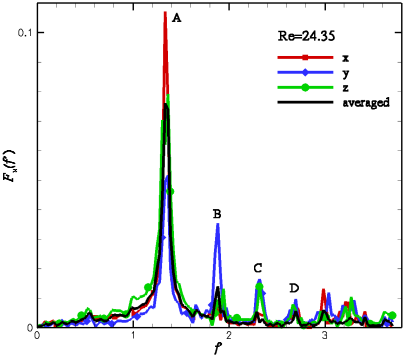


Acoustics, $\mathrm{Re}_\lambda = 24.37$ (cont.)

The Fourier transform of the fluctuating parts of $\Theta'(t')$ and $F_u(t')$. The normalized basic frequency is:

$$f'_s = \frac{\tau_0}{T} = \frac{K_0}{\varepsilon_0}\frac{c_s}{L} \approx 1.344$$

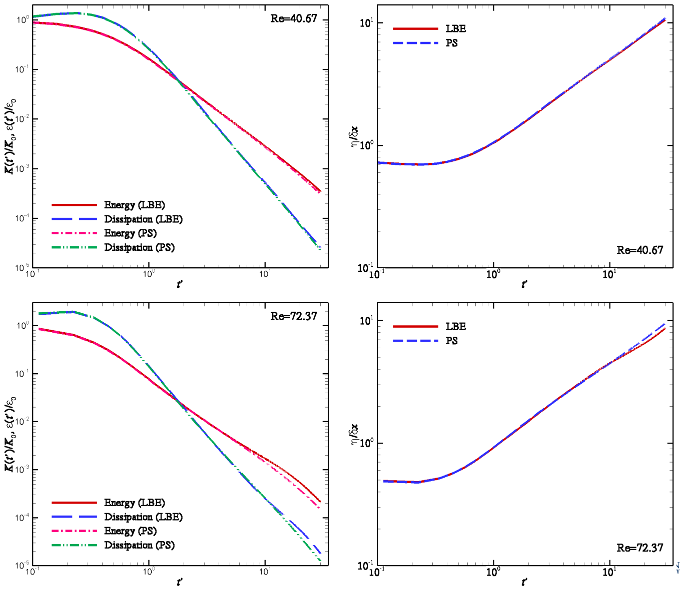




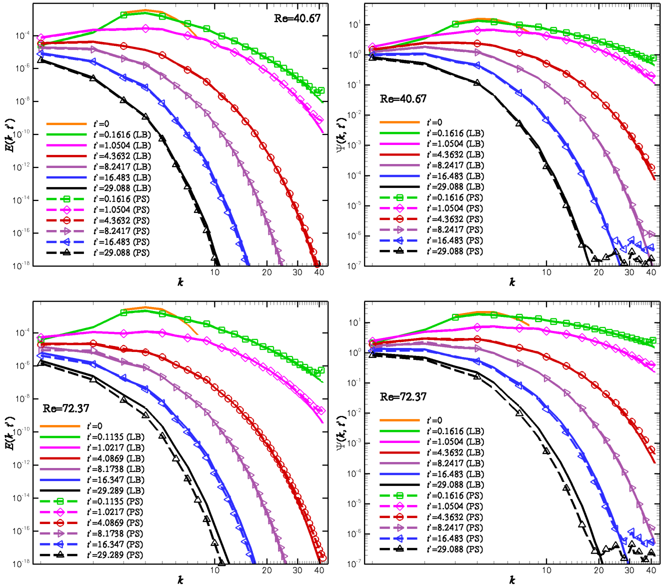
$K(t')/K_0$, $\varepsilon(t')/\varepsilon_0$, and $\eta(t')/\delta x$

$\mathrm{Re}_\lambda = 40.67$
$\nu = 1/1000$
$\dfrac{\eta_0}{\delta x} = \sqrt{3/5} \approx 0.77$

$\mathrm{Re}_\lambda = 72.37$
$\nu = 1/1800$
$\dfrac{\eta_0}{\delta x} = \sqrt{1/3} \approx 0.55$

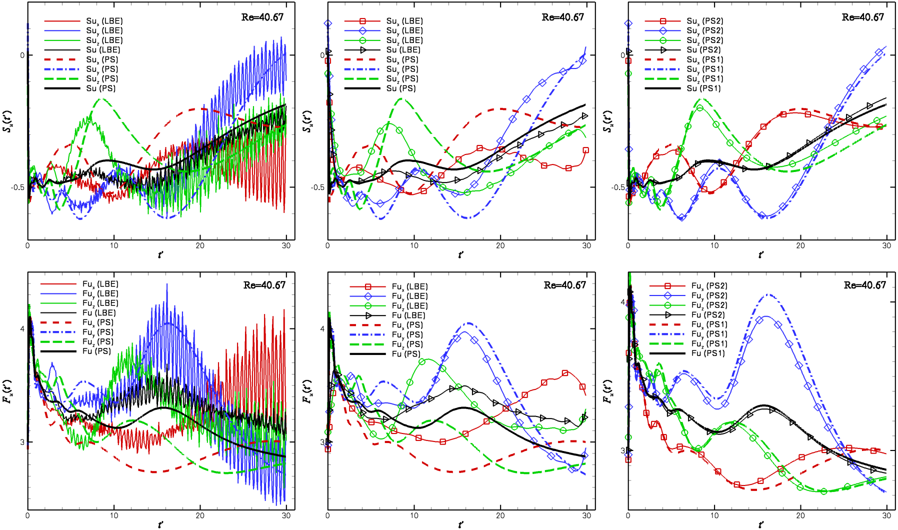


Energy and compensated spectra



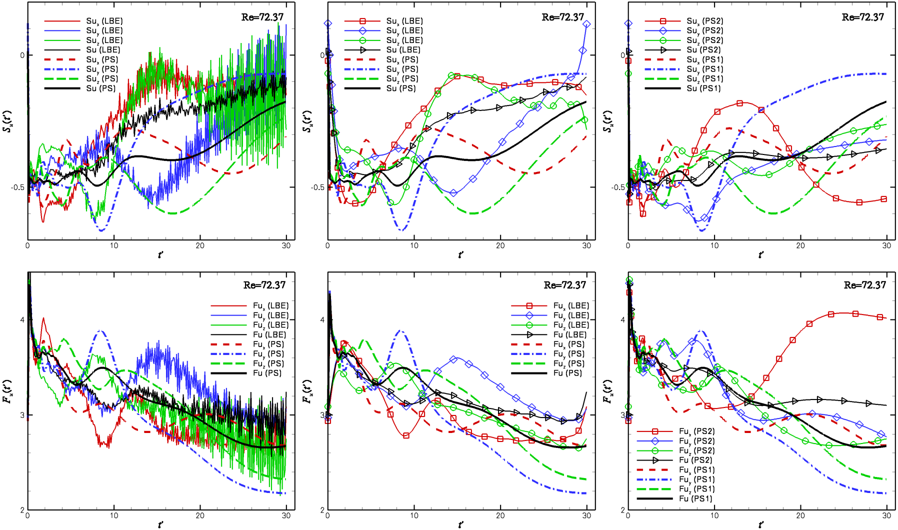
Skewness S_u and Flatness F_u at $\mathrm{Re}_\lambda = 40.67$

Fron left to right: LBE and averaged-LBE vs. PS1, and PS1 vs. PS2

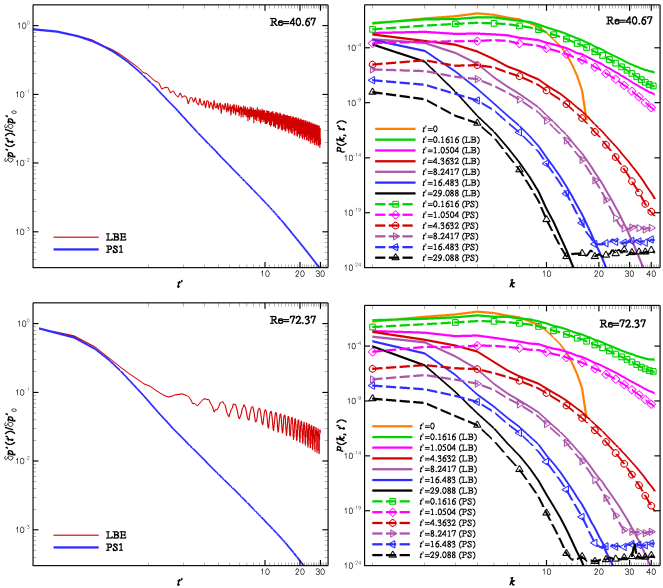


Skewness S_u and Flatness F_u at $\mathrm{Re}_\lambda = 72.37$

Fron left to right: LBE and averaged-LBE vs. PS1, and PS1 vs. PS2

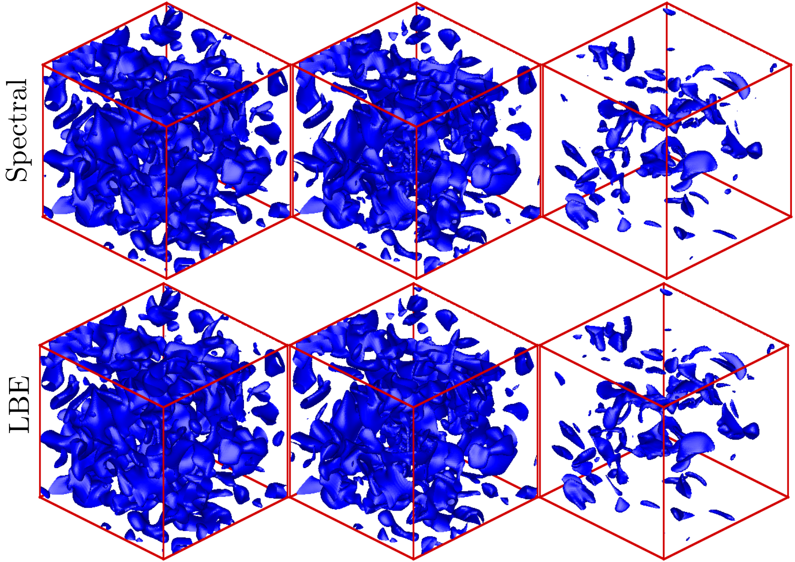


$\mathrm{Re}_\lambda = 40.67$ and 72.37, $P(k,\, t')$



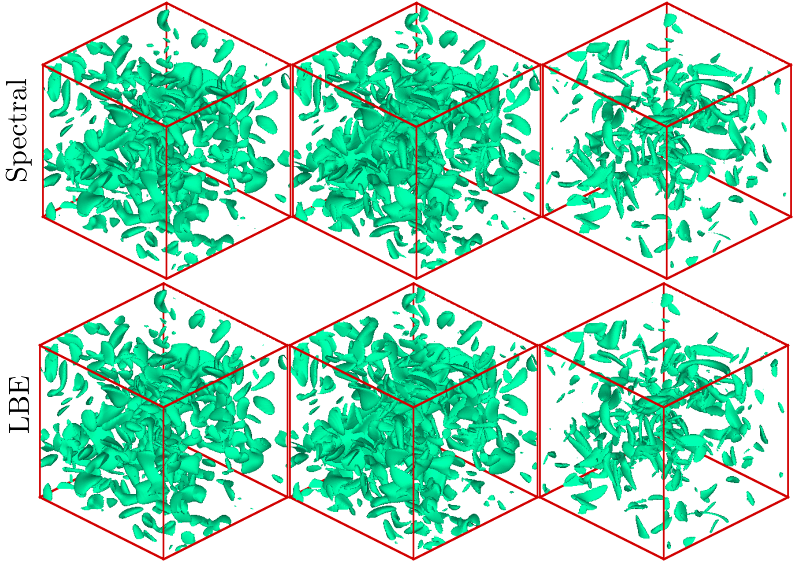
Velocity Iso-surface in 3D, $\mathrm{Re}_\lambda = 24.37$

LBE vs. PS1 (equal δt): $t' = 0.1348$, 0.2359, 0.573; $\|\boldsymbol{u}(t')/u'\| = 2.0$



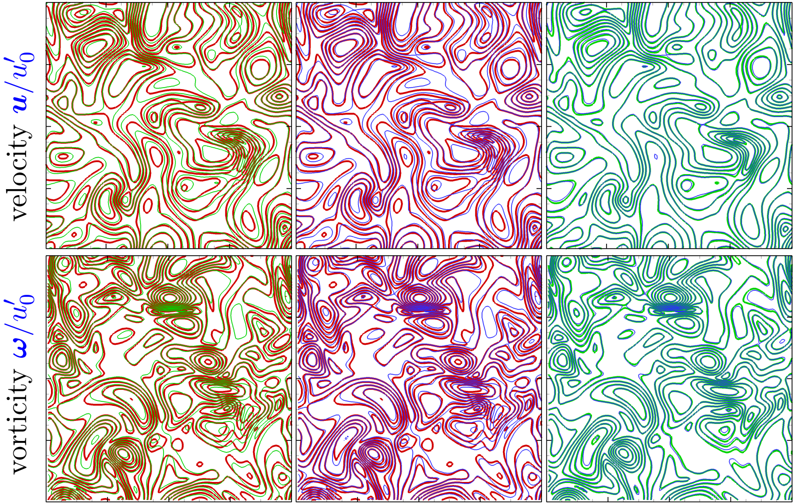
Vorticity Iso-surface in 3D, $Re_\lambda = 24.37$

LBE vs. PS1 (equal δt): $t' = 0.1348, 0.2359, 0.573$; $\|\boldsymbol{\omega}(t')/u'\| = 13.0$



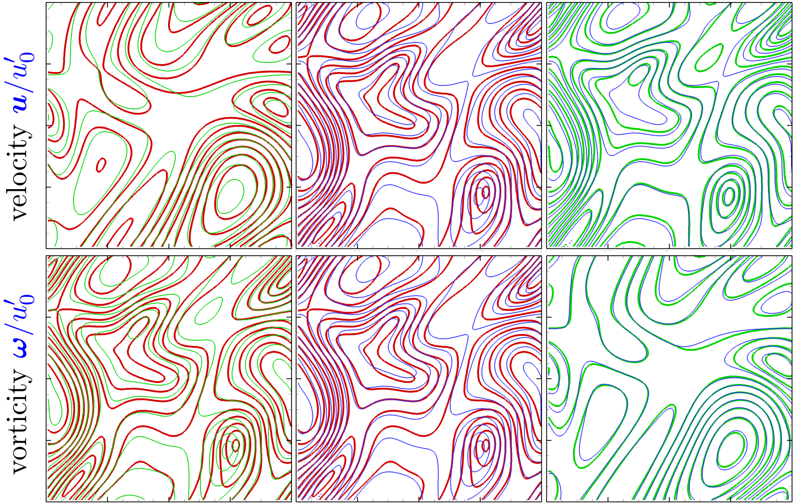
$\|\boldsymbol{u}(t')/u'\|$ and $\|\boldsymbol{\omega}(t')/u'\|$ at $\mathrm{Re}_\lambda = 24.37$, $t' = 4.048$

LBE vs. PS1 (equal δt) and PS2 ($\delta t/3$), PS1 vs. PS2



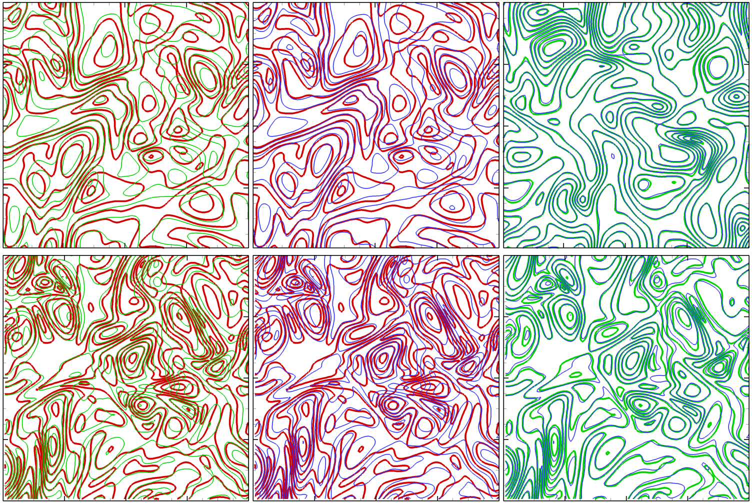
$\|\boldsymbol{u}(t')/u'\|$ and $\|\boldsymbol{\omega}(t')/u'\|$ at $\mathrm{Re}_\lambda = 24.37$, $t' = 29.949$

LBE vs. PS1 (equal δt) and PS2 ($\delta t/3$), PS1 vs. PS2



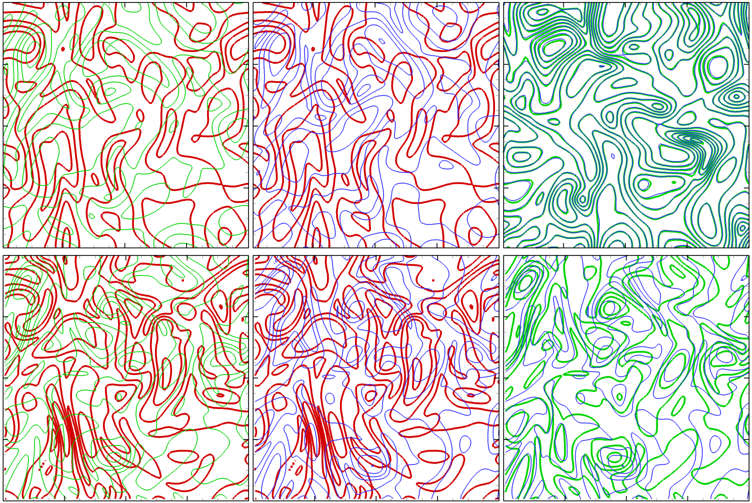
$\|\boldsymbol{u}(t')/u'\|$ and $\|\boldsymbol{\omega}(t')/u'\|$ at $\mathrm{Re}_\lambda = 40.67$, $t' = 4.363$

LBE vs. PS1 (equal δt) and PS2 ($\delta t/3$), PS1 vs. PS2.



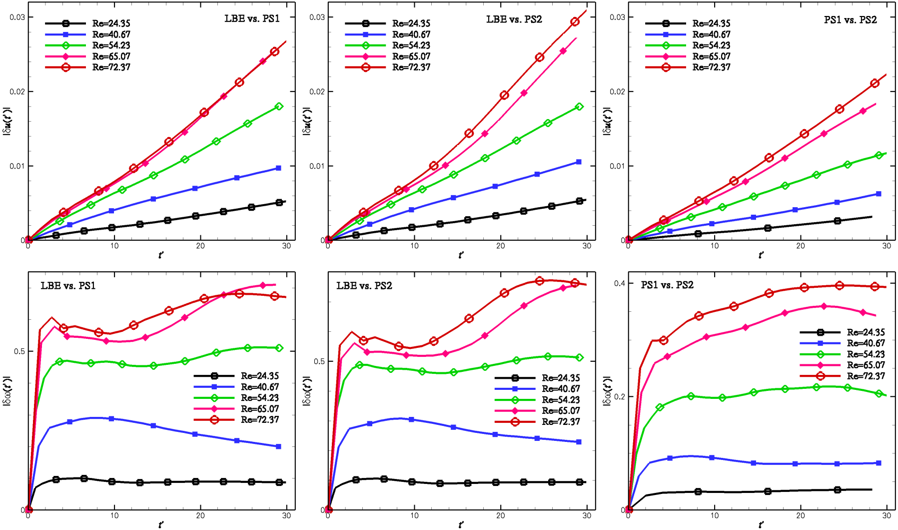
$\|\boldsymbol{u}(t')/u'\|$ and $\|\boldsymbol{\omega}(t')/u'\|$ at $\mathrm{Re}_\lambda = 72.37$, $t' = 4.086$

LBE vs. PS1 (equal δt) and PS2 ($\delta t/3$), PS1 vs. PS2.

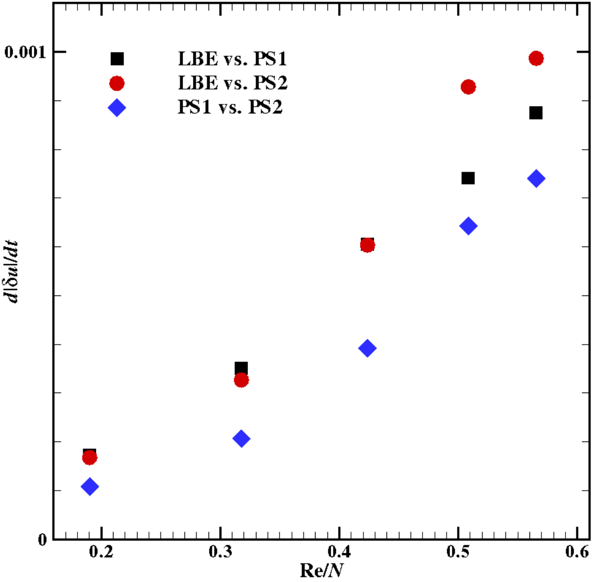


L^2 $\|\delta \boldsymbol{u}(t')\|$ and $\|\delta \boldsymbol{\omega}(t')\|$

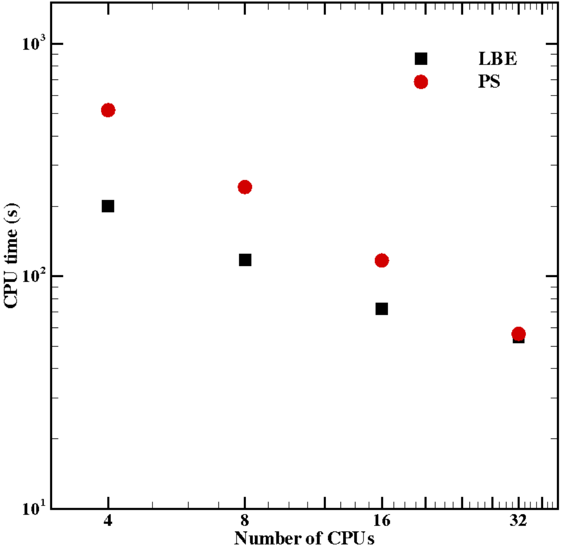
LBE vs. PS1 (equal δt) and PS2 ($\delta t/3$), PS1 vs. PS2.



Re_λ Dependence of $d\|\delta\boldsymbol{u}(t')\|/dt'$



Efficiency and Performace



Conclusions

For DNS of the decaying homogeneous isotropic turbulence:

- When flow is *well resolved*, the LBE can yield accurate low-order statistical quantities: $K(t)$, $\varepsilon(t)$, $S_u(t)$, $F_u(t)$, $E(k, t)$, $\Psi(k, t)$;
- The LBE is not accurate for the pressure spectra $P(k, t)$, because it does not solve the Poisson equation accurately;
- The LBE can accurately compute velocity and vorticity fields;
- The difference between the velocity fields obtained by the LBE and PS methods grows linearly in time, and the grow-rate depends linearly on the grid Reynolds number $\mathrm{Re}_\lambda^* := \mathrm{Re}_\lambda / N$;
- LBE requires twice the resolution in each dimension as that of PS;
- LBE has low-dissipation and low-dispersion, and is isotropic.

Given the *formal* accuracy of LBE is of $O(\delta x^2)$ and $O(\delta t)$, it is a *surprisingly* good scheme for DNS of turbulence.

Future Work

- High-order LBE schemes (Dubois and Lallemand);
- Stability analysis (Ginzburg and d'Humières);
- Numerical analysis (Dubouis, Junk *et al.*);
- LBE-LES (Krafczyk, Sagaut *et al.*);
- Better theory/models of multi-component/phase fluids;
- Extended hydrodynamics (finite Kn effects, *etc.*);
- Good propagada: Go to ICMMES, `http://www.icmmes.org`