Entropic Lattice Boltzmann: Study of the Implicit Subgrid scale model

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Motivations

Lattice Boltzmann Method:

- Adapted to a wide range of physical simulations
- Intrinsic scalability, well suited for HPC
- Can handle very complex (moving) geometry

Large Eddy Simulation:

- Enable cost-effective highly turbulent flow simulations
- Popular in commercial CFD softwares

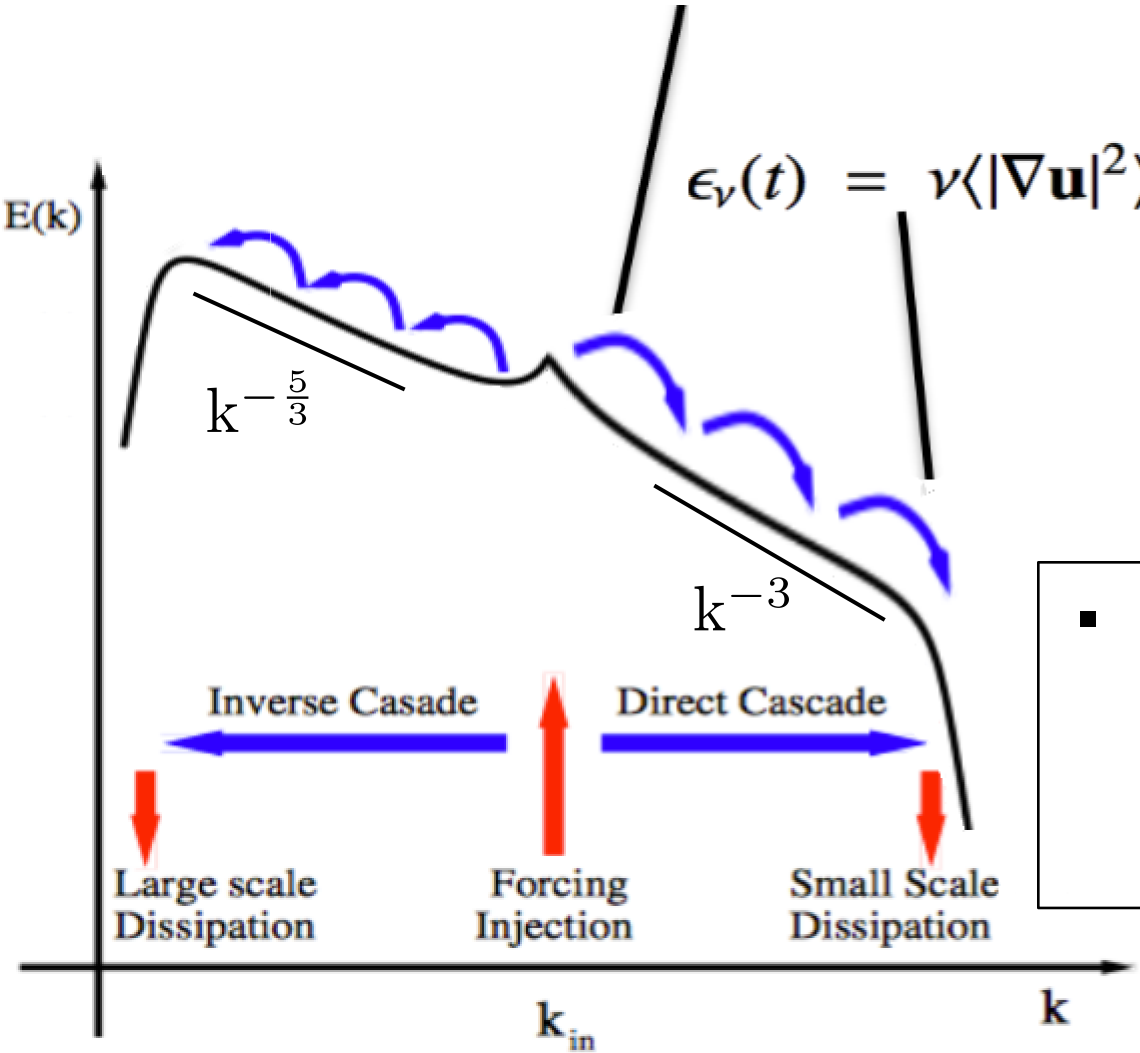
Study of a Large Eddy Simulation within the Lattice Boltzmann framework

2D Forced Homogeneous Isotropic Turbulence

$$\epsilon_{in}(t) = \langle \mathbf{u} \cdot \mathbf{f} \rangle$$

$$Re = \frac{U_{RMS}}{k_{in}\nu}$$

$$\epsilon_{\nu}(t) = \nu \langle |\nabla \mathbf{u}|^2 \rangle$$



High Reynolds

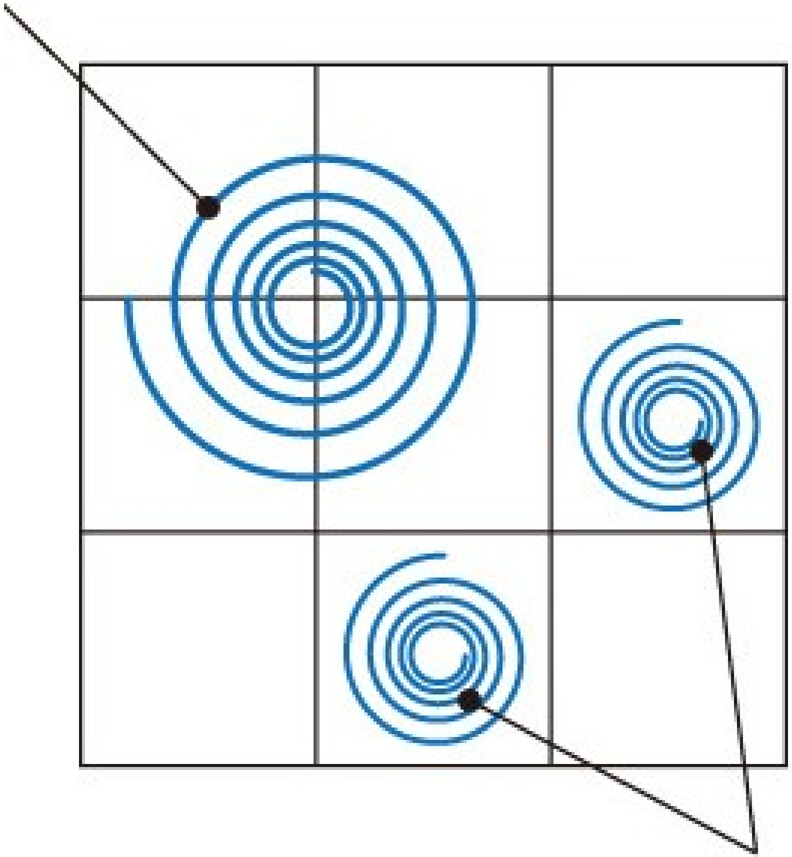
- Extended direct cascade
- Decreased smallest scales

- Direct Num. Sim. (DNS)

  All scales of the flow are solved (expensive)

(Implicit) Large Eddy Simulation (LES)

Grid scale:
Resolved



Sub-Grid Scale (SGS):
Not captured by the grid
Needs to be modeled

- Large Eddy Sim. (LES)

  All scales up to a cut-off are resolved, a SGS is used to model small scales effect

Good SGS?

- Captures small scales dissipation
- Extends the inertial range of scales
- Models intermittent transfer of energy to resolved scales (backscatter)

No SGS => small scale instabilities

Eddy viscosity SGS model

$$\partial_t \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} = -\nabla p + \nu_0 \Delta \boldsymbol{v}$$

(Navier Stokes eq.)

Filtered velocity field

$$\overline{\boldsymbol{v}}(\boldsymbol{x}, t) \equiv \int_\Omega d\boldsymbol{y}\; G(|\boldsymbol{x} - \boldsymbol{y}|)\; \boldsymbol{v}(\boldsymbol{y}, t) = \sum_{\boldsymbol{k} \in \mathbb{Z}^3} G(\boldsymbol{k})\; \hat{\boldsymbol{v}}(\boldsymbol{k}, t) e^{i\boldsymbol{k}\boldsymbol{x}}$$

$$\partial_t \overline{\boldsymbol{v}} + (\overline{\boldsymbol{v}} \cdot \nabla)\overline{\boldsymbol{v}} = -\nabla \overline{p} + \nu_0 \Delta \overline{\boldsymbol{v}} - \nabla \cdot \tau_{model}(\overline{\boldsymbol{v}}, \overline{\boldsymbol{v}})$$

Eddy viscosity model

$$\tau_{model}(\overline{\boldsymbol{v}}, \overline{\boldsymbol{v}}) = \delta\nu_e (\nabla \overline{\boldsymbol{v}} + (\nabla \overline{\boldsymbol{v}})^T) \Longrightarrow \nabla \cdot \tau_{model}(\overline{\boldsymbol{v}}, \overline{\boldsymbol{v}}) = \delta\nu_e \Delta \overline{\boldsymbol{v}}$$

$$\partial_t \overline{\boldsymbol{v}} + (\overline{\boldsymbol{v}} \cdot \nabla)\overline{\boldsymbol{v}} = -\nabla \overline{p} + (\nu_0 + \delta\nu_e) \Delta \overline{\boldsymbol{v}}$$

Example: Smagorinsky SGS

[Smagorinsky, 1963]

$$\delta\nu_e = C^S \sqrt{S_{\theta\kappa} S_{\theta\kappa}}$$

$$\mathrm{S}_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$$

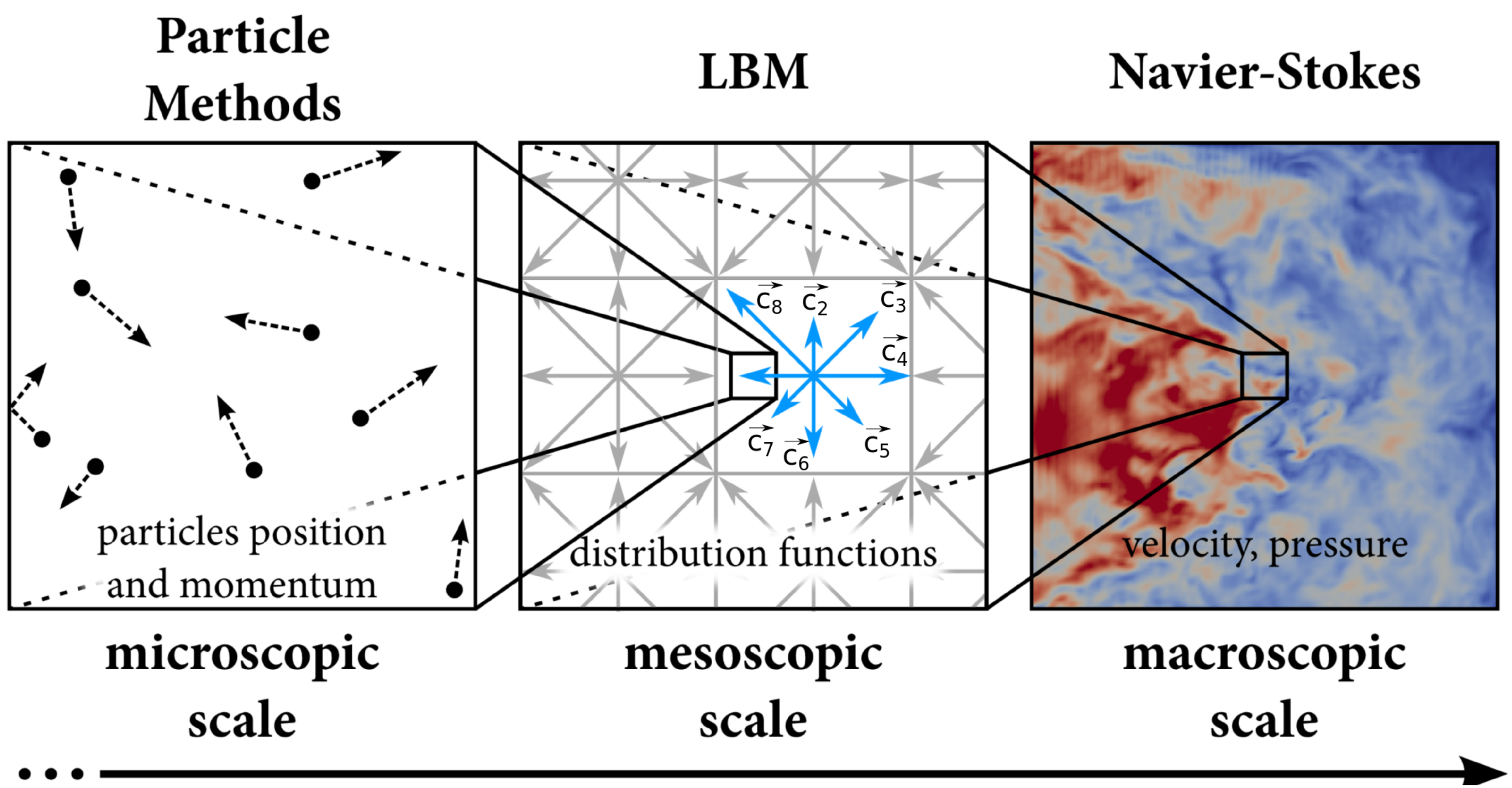
DEFINITE-POSITIVE $\Longrightarrow$ **PURELY DISSIPATIVE**

Introduction to LBM

LBM Equation with a relaxation time $\tau \equiv \tau_0$ fixed (LBGK)

$$f_i(\vec{x} + \vec{c}_i \Delta t, t + \Delta t) - f_i(\vec{x}, t) = -\frac{1}{\tau_0} \left[f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t) \right]$$

Macroscopic quantities: Density $\rho = \sum_i f_i$ Momentum $\rho \vec{u} = \sum_i f_i \vec{c}_i$



Simulation of turbulent flows with LBM

- At a fixed resolution, the Reynolds number reachable in practice is limited:

$$Re = \frac{U_{RMS}}{k_{in}\nu_0}$$

- Low Mach number approximation

$$\mathrm{u}_{RMS} \leq 10^{-1}$$

- Instabilities

$$\tau_0 \rightarrow 0.5 \;\; i.e. \;\; \nu_0 \rightarrow 0$$

$$\nu = c_s^2(\tau - 0.5)\Delta t$$

Can we get rid of those instabilities?

- Non-linear stabilization of LBM has been linked to the existence of a H-functional acting as a Lyapunov functional

How can LBM equip a H-theorem?

Entropic Lattice Boltzmann Method (ELBM)

- ELBM equation adapts the relaxation time locally $\tau_{\text{eff}} = \frac{1}{\alpha\beta}$

ELBM Equation [Karlin *et al.*, 1999]

$$f_i(x + c_i, t + 1) = f_i(x, t) + \alpha\beta \left[f_i^{eq}(x, t) - f_i(x, t) \right]$$

With $\beta = \frac{1}{2\tau_0}$ and $\alpha \equiv \alpha(\vec{x}, t)$ a free parameter

- ELBM equips a discrete H-theorem with

$$\mathrm{H}\ (\mathbf{f}) = \sum_0^{q-1} f_i \log\left(\frac{f_i}{\omega_i}\right)$$

- Defining the equilibrium distribution as the extrema of H under the constraints of mass and momentum conservation, we find for D2Q9:

$$\mathrm{f}_i^{eq}\left(\rho(\vec{x},\, t),\, \vec{u}(\vec{x},\, t)\right) = t_i\, \rho \prod_{\gamma=1}^{d} \left\{ \left(2 - \sqrt{1 + \frac{u_\gamma^2}{c_s^2}}\right) \left[\frac{\frac{2u_\gamma}{\sqrt{3}c_s} + \sqrt{1 + \frac{u_\gamma^2}{c_s^2}}}{1 - \frac{u_\gamma}{\sqrt{3}c_s}} \right]^{\frac{c_{i,\gamma}}{\sqrt{3}c_s}} \right\}$$

Entropic Lattice Boltzmann Method (ELBM)

- Setting $\mathbf{f}^{mirror}(\alpha) = \mathbf{f} - \alpha\,(\mathbf{f} - \mathbf{f}^{\mathbf{eq}})$, we have

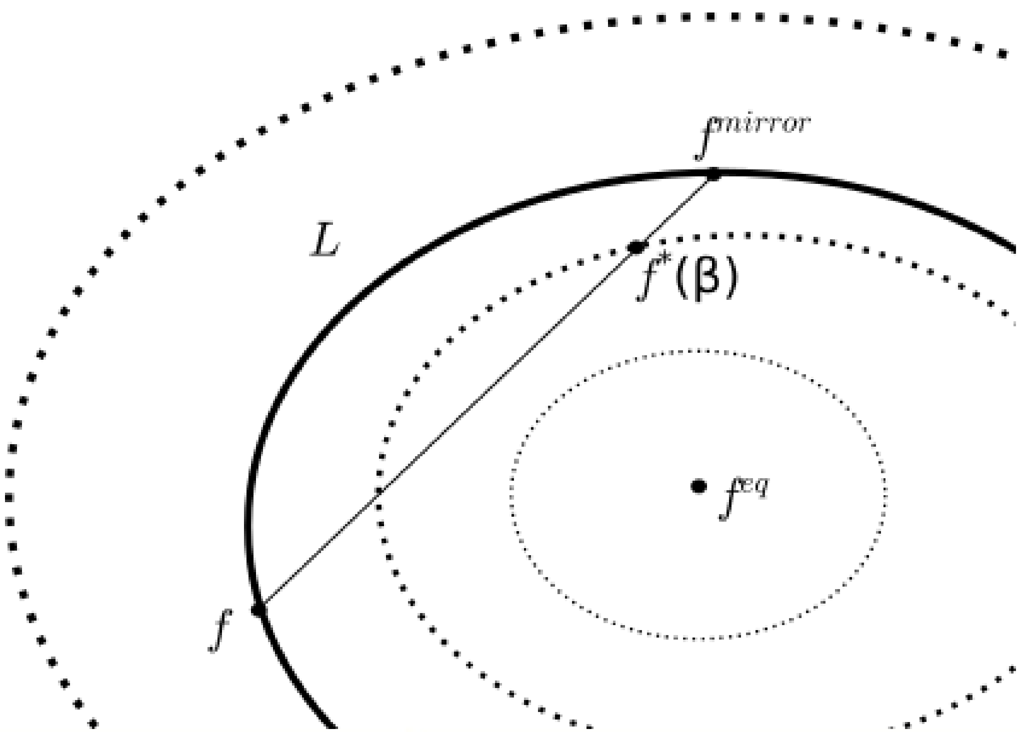
ELBM Equation [Karlin *et al.*, 1999]

$$f_i(x + c_i, t + 1) = (1 - \beta)\ f_i(x, t) + \beta\, f_i^{mirror}(x, t)$$

with $\quad 0 < \beta < 1 \ (0.5 < \tau < +\infty)$

- Calculating α locally by solving the entropic step eq.

$$H(\mathbf{f}) = H\left(\mathbf{f}^{\mathbf{mirror}}(\alpha)\right)$$



[Karlin *et. al.*, EPL, 1999]

ELBM: implicit eddy viscosity SGS model

$$\nu = c_s^2(\tau - 0.5)\Delta t$$

- ELBM is (apparently) unconditionally stable and recover N-S with

$$\nu = \nu_0 + c_s^2 \tau_0 (\frac{\alpha}{2} - 1)\Delta t$$

Measured $$\delta\nu_e^M = c_s^2 \tau_0 (\frac{\alpha}{2} - 1)\Delta t$$

- Assuming $\alpha \approx 2$, one can derive an approximation of $\nu_e^M(\vec{x}, t)$

[Malaspinas & Sagaut, PRE, 2008]

Approximated $$\delta\nu_e^A = -\frac{4c_s^2}{3}\tau_0^2 \Delta t^2 \frac{S_{\theta\kappa}S_{\kappa\gamma}S_{\gamma\theta}}{S_{\lambda\mu}S_{\lambda\mu}} \propto -\frac{Tr(S^3)}{Tr(S^2)}$$

Scale as $|\mathbf{S}|$ like the Smagorinsky SGS $\quad \mathrm{S}_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$

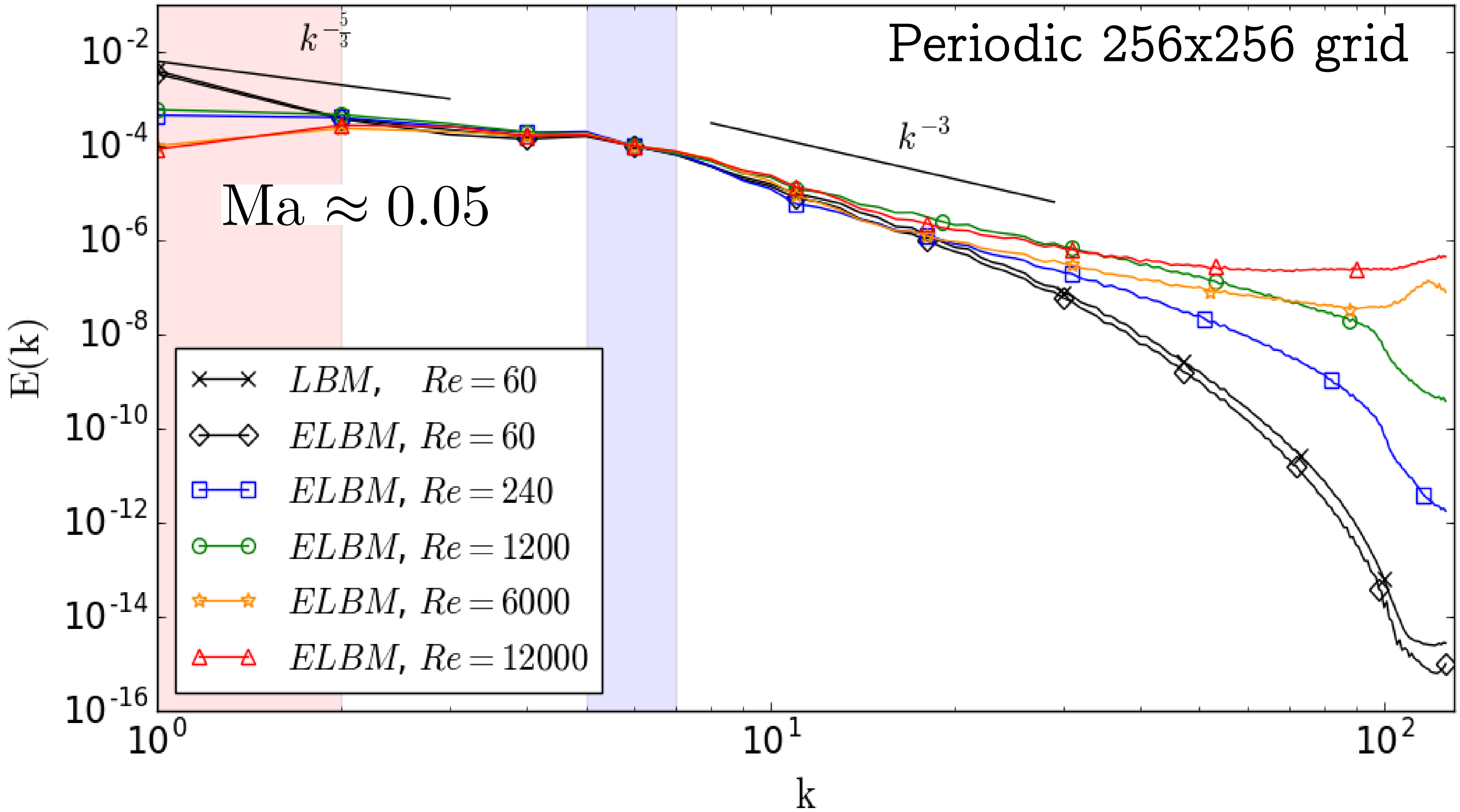
NOT DEFINITE-POSITIVE ⇨ **ALLOWS BACKSCATTER**

Objectives

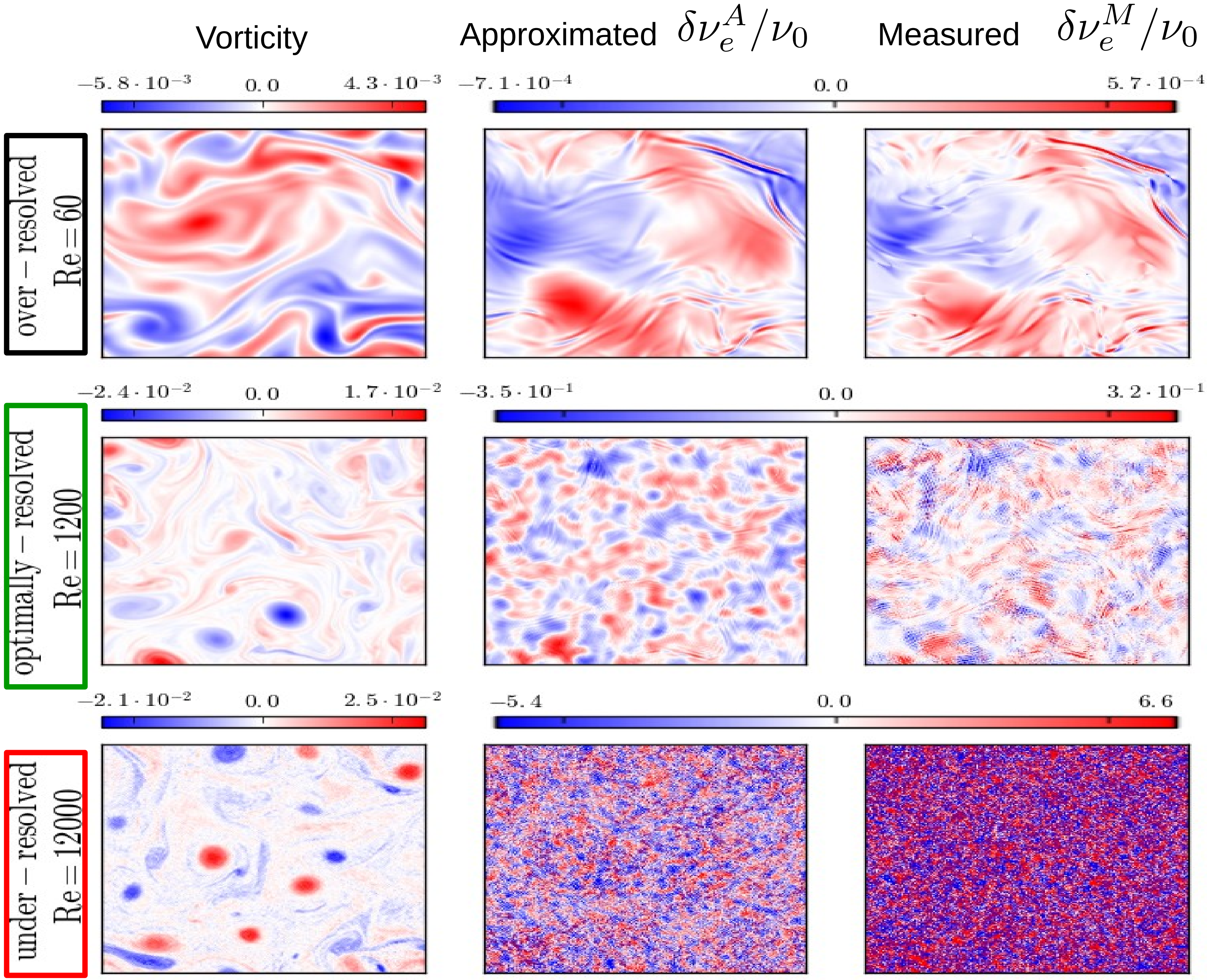
1) Numerically check if the approximated eddy viscosity is valid.

2) Is this implicit SGS an artifact of the stabilization or a physical SGS stemming from Kinetic theory?

Superposed energy spectra of the simulations

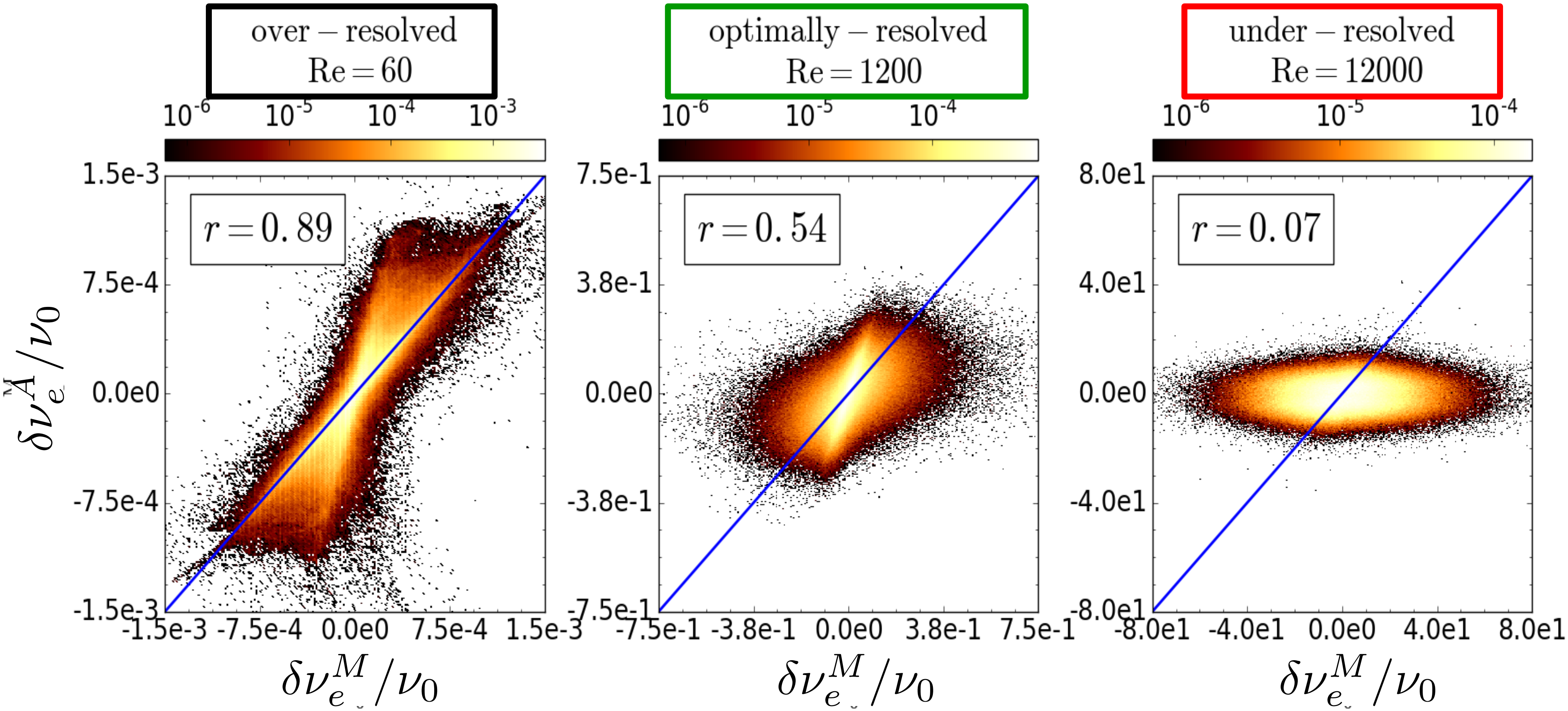


over-resolved	optimally-resolved	under-resolved
$Re = 60$	$Re = 1200$	$Re = 12000$



Vorticity
Approximated $\delta\nu_e^A/\nu_0$
Measured $\delta\nu_e^M/\nu_0$
$-5.8\cdot10^{-3}$ 0.0 $4.3\cdot10^{-3}$
$-7.1\cdot10^{-4}$ 0.0 $5.7\cdot10^{-4}$
over − resolved
Re = 60
$-2.4\cdot10^{-2}$ 0.0 $1.7\cdot10^{-2}$
$-3.5\cdot10^{-1}$ 0.0 $3.2\cdot10^{-1}$
optimally − resolved
Re = 1200
$-2.1\cdot10^{-2}$ 0.0 $2.5\cdot10^{-2}$
-5.4 0.0 6.6
under − resolved
Re = 12000

Numerical check of Malaspinas formulation



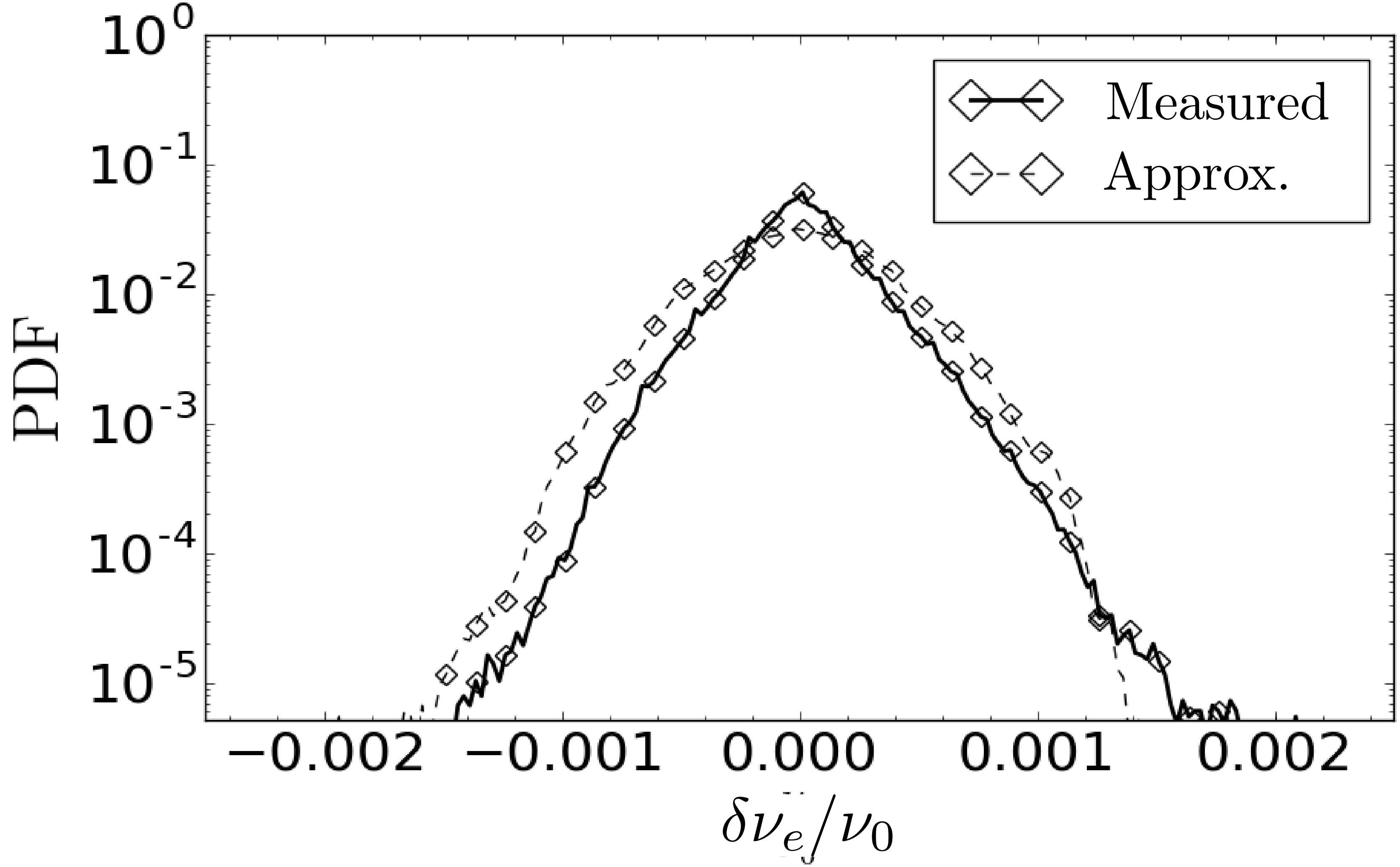
Measured eddy viscosity

$$\delta\nu_e^M(\vec{x},t) = c_s^2\tau_0\left(\frac{\alpha}{2}-1\right)\Delta t$$

Approximated eddy viscosity

$$\delta\nu_e^A(\vec{x},t) = -\frac{4c_s^2}{3}\tau_0^2\Delta t^2\frac{Tr(S^3)}{Tr(S^2)}$$

Over-resolved case



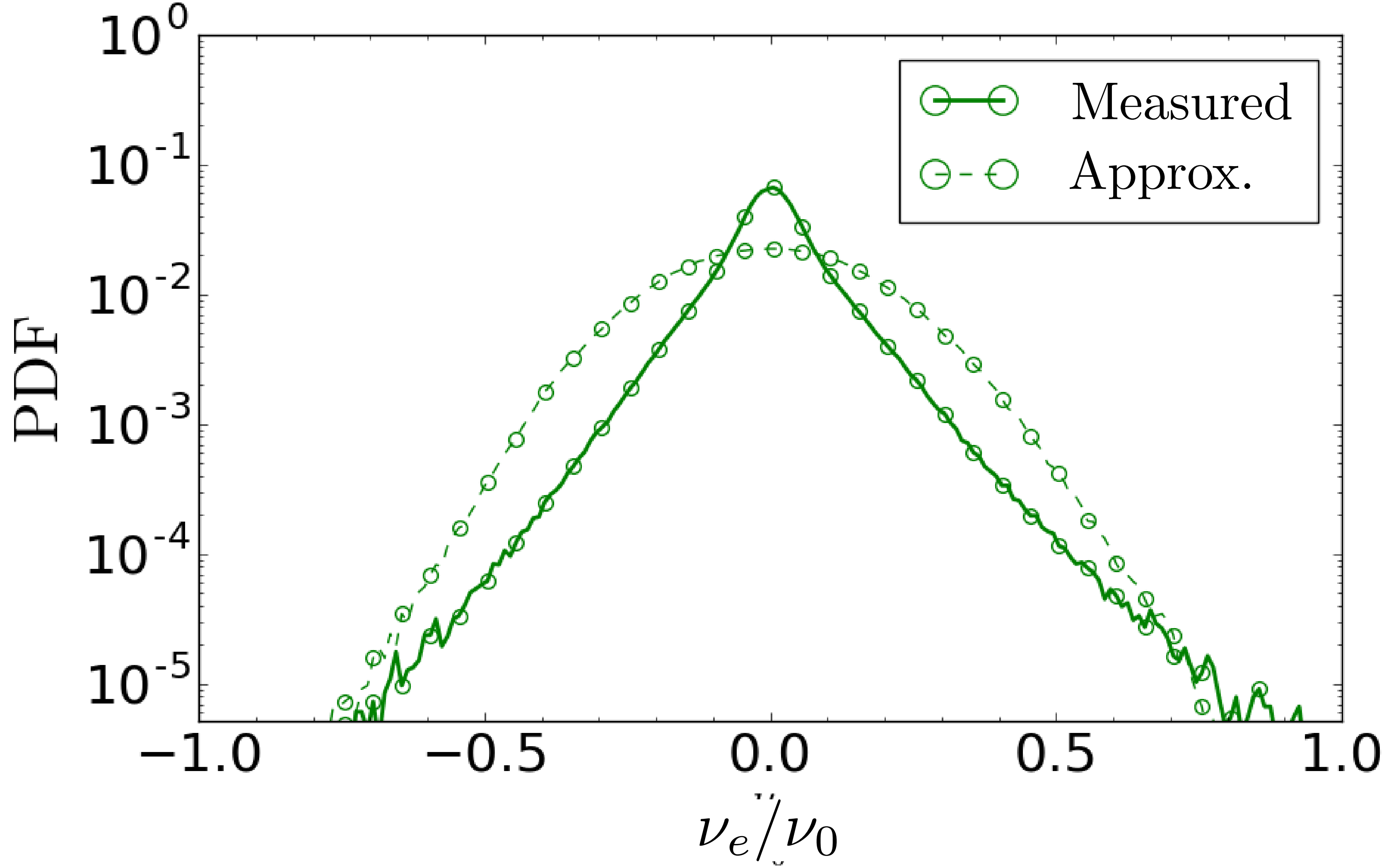
Measured eddy viscosity

$$\delta\nu_e^M(\vec{x},t) = c_s^2\tau_0(\frac{\alpha}{2}-1)\Delta t$$

Approximated eddy viscosity

$$\delta\nu_e^A(\vec{x},t) = -\frac{4c_s^2}{3}\tau_0^2\Delta t^2\frac{Tr(S^3)}{Tr(S^2)}$$

Optimally-resolved case



Measured eddy viscosity

$$\nu_e^M(\vec{x}, t) = c_s^2 \tau_0 (\frac{\alpha}{2} - 1)\Delta t$$

Approximated eddy viscosity

$$\nu_e^A(\vec{x}, t) = -\frac{4c_s^2}{3}\tau_0^2 \Delta t^2 \frac{Tr(S^3)}{Tr(S^2)}$$

Physical relevance of the implicit SGS

Averaged kinetic energy balance equation for $\nu = \nu^{eff}(\vec{x}, t) = \nu_0 + \nu_e(\vec{x}, t)$

$$\partial_t \langle \frac{\rho u_i u_i}{2} \rangle_V$$

$$= -\langle u_i \partial_i p \rangle_V - \nu_0 \langle \rho \left(\partial_j u_i + \partial_i u_j \right) \partial_j u_i \rangle_V + \nu_0 \langle \partial_j \rho u_i \left(\partial_j u_i + \partial_i u_j \right) \rangle_V$$

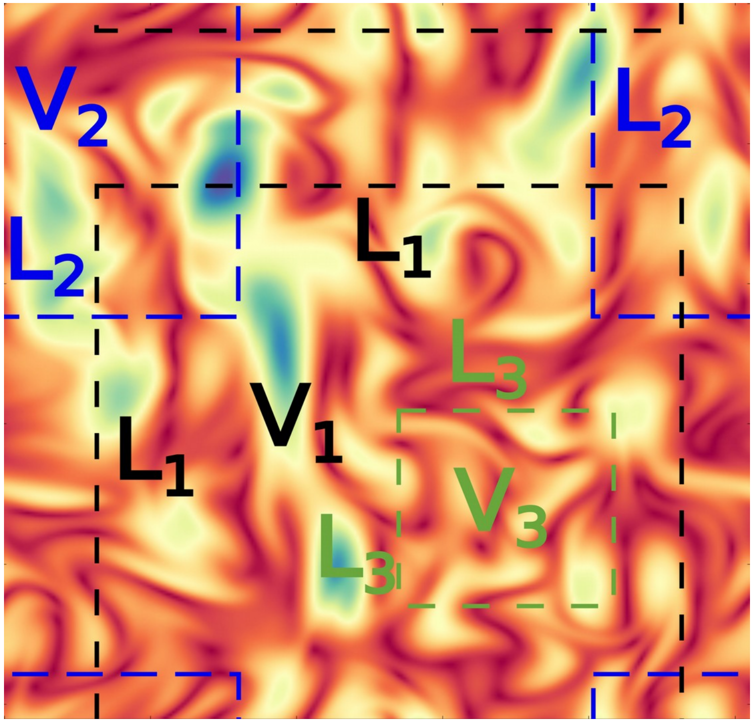
$$- \langle \partial_j \frac{\rho u_i u_i}{2} u_j \rangle_V + \langle u_i F_i \rangle_V - \langle \nu_e \rho \left(\partial_j u_i + \partial_i u_j \right) \partial_j u_i \rangle_V + \langle \partial_j \nu_e \rho u_i \left(\partial_j u_i + \partial_i u_j \right) \rangle_V$$

For a scale L, we calculate each term of the balance eq. For random sub-volumes of size

$V = L \times L$ and evaluate the hydrodynamic recovery

=> Range of validity of ELBM

[Tauzin et al., C&F, 2018]



Conclusions

- Conducted 2D Homogeneous Isotropic Turbulence simulations at increasing Reynolds number
- ELBM enables an extension of the inertial range
- The implicit turbulence models gets increasingly active with Re
- Approximated viscosity model is in fair agreement but fails to capture the skewness of the actual turbulent viscosity

Not covered in this talk

Is ELBM a mere stabilization or an implicit physical model of the sub-grid scales stemming from kinetic theory?

- Development of a tool to check numerically the balance of kinetic energy and enstrophy on sub-volumes of the computational domain
- Systematic statistical analysis of hydrodynamics recovery for Entropic LBM with the implicit SGS included

[Tauzin et al., In preparation]

Acknowledgement

Thank you for your attention
Any question?

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