Entropic Lattice Boltzmann: Study of the Implicit Subgrid scale model for 3D Homogeneous Isotropic Turbulence

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This project has received funding from the European Union's Horizon 2020
research and innovation programme under grant agreement No' 642069
and was conducted within the activity of ERC Grant No' 339032

Motivations

Simulations of highly turbulent flows is challenging

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

- Turbulence is a multi-scale phenomenon
- Direct Numerical Simulations requires all scales to be solved (expensive)

Lattice Boltzmann Method:

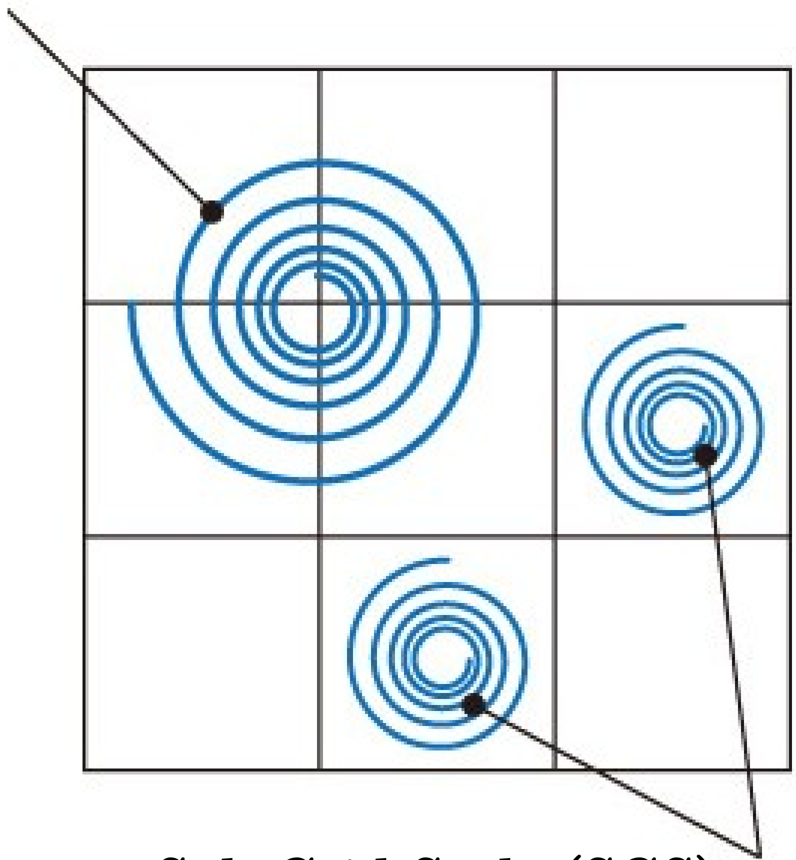
- Intrinsic scalability, well suited for HPC
- Adapted to a wide range of physical simulations
- Can handle very complex (moving) geometry

Large Eddy Simulation:

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

Large Eddy Simulation (LES)

Grid scale:
Resolved



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

- Large Eddy Simulations

  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

LES with eddy viscosity SGS model

(Navier Stokes eq.) $\partial_t \boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v} = -\nabla p + \nabla\cdot 2\nu_0 \boldsymbol{S}$

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

Filtered velocity field

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

(Filtered N-S eq.) $\partial_t\overline{\boldsymbol{v}} + (\overline{\boldsymbol{v}}\cdot\nabla)\overline{\boldsymbol{v}} = -\nabla\overline{p} + \nabla\cdot 2\nu_0\overline{\boldsymbol{S}} - \nabla\cdot\tau_{model}(\overline{\boldsymbol{v}},\overline{\boldsymbol{v}})$

Eddy viscosity model

$\tau_{model}(\overline{\boldsymbol{v}},\overline{\boldsymbol{v}}) = 2\delta\nu_e\overline{\boldsymbol{S}}$ ⇒ $\partial_t\overline{\boldsymbol{v}} + (\overline{\boldsymbol{v}}\cdot\nabla)\overline{\boldsymbol{v}} = -\nabla\overline{p} + \nabla\cdot 2(\nu_0+\delta\nu_e)\overline{\boldsymbol{S}}$

Example: Smagorinsky SGS [Smagorinsky, 1963]

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

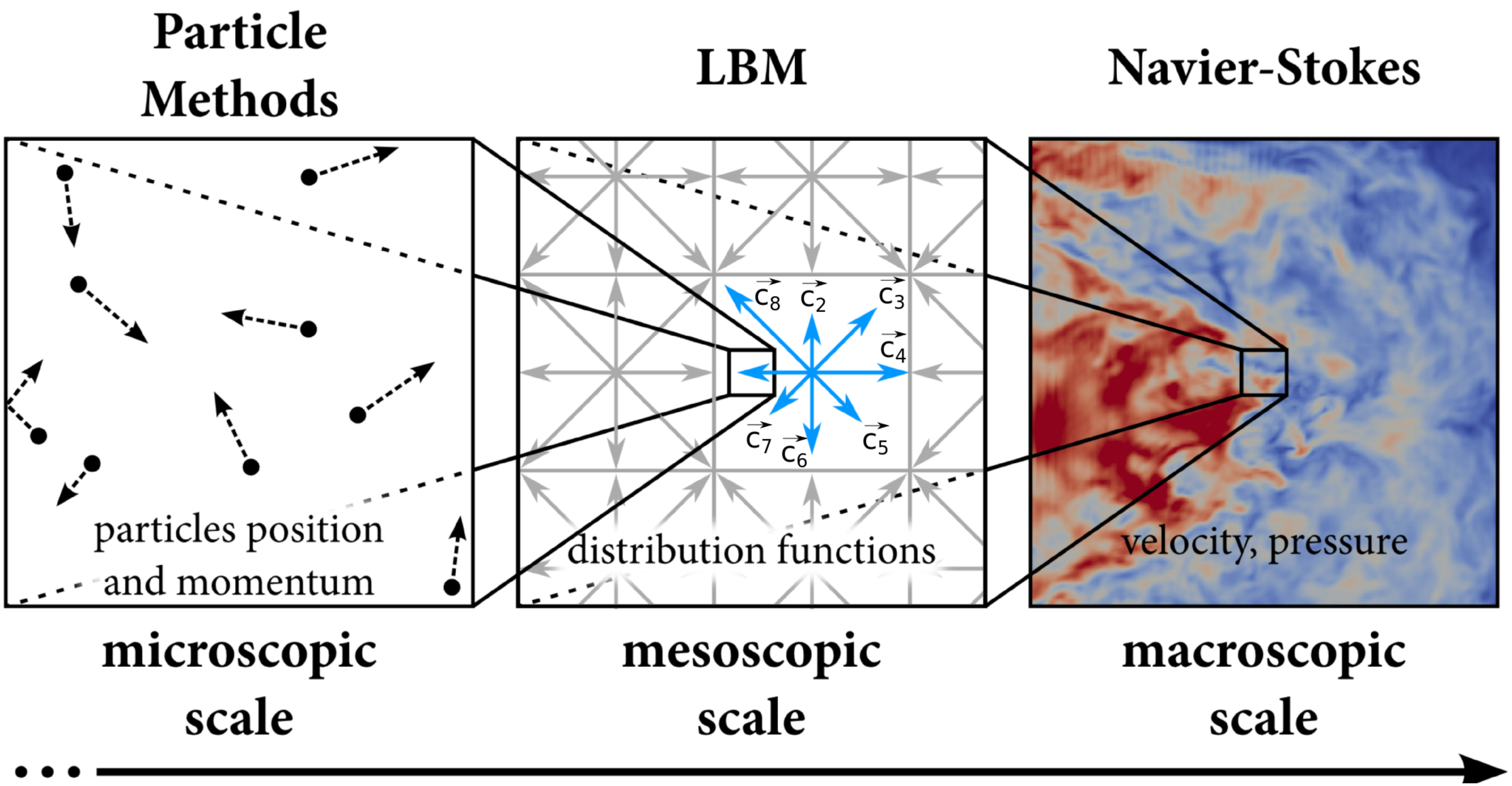
DEFINITE-POSITIVE ⇒ **PURELY DISSIPATIVE**

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 $\rho\vec{u} = \sum_i f_i \vec{c}_i$



Introduction to LBM

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Chapman-Enskog expansion $Ma = \frac{u_{RMS}}{c_s^2}$

$\nu = c_s^2(\tau - 0.5)\Delta t$ $Kn = \frac{\lambda}{L}$

Weakly compressible Navier-Stokes with viscosity $\nu \equiv \nu_0$ fixed

$$\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) = -\partial_i p + \partial_j \rho\nu\left(\partial_j u_i + \partial_i u_j\right) + \mathcal{O}(M_a^3) + \mathcal{O}(K_n^2)$$

We want to use LBM to simulate highly turbulent flows

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?

[Karlin et. al., 1999]

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

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

- Calculating α locally by solving the entropic step eq.

$$H\,(\mathbf{f}) = H\,(\mathbf{f} - \alpha\,(\mathbf{f} - \mathbf{f}^{eq}))$$

- Unconditionally stable (apparently)
- $\alpha \to 2$, $i.e.$ $\tau_{\text{eff}} \to \tau_0$ whenever the simulation is resolved

ELBM: implicit eddy viscosity SGS model

$$\nu_{\text{eff}} = c_s^2(\tau_{\text{eff}} - 0.5)\Delta t \qquad \tau_{\text{eff}} = \frac{1}{\alpha\beta}$$

- ELBM recovers N-S with

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

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

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

[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**

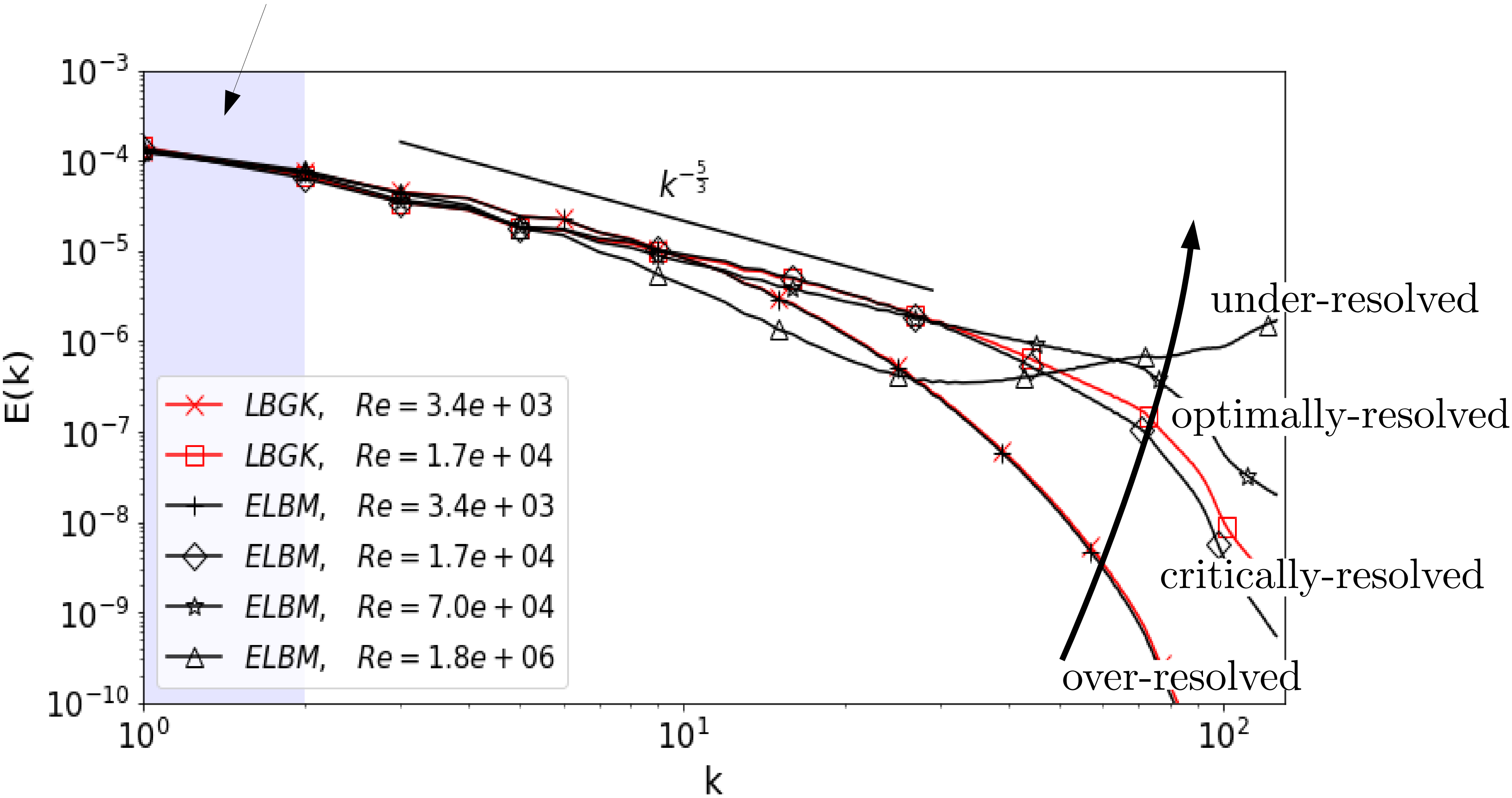
Objectives

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

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

Superposed energy spectra of the simulations

Forcing at k = 1 to 2 D3Q27 Periodic 256^3 Ma ≈ 0.05



1) Physical relevance of the implicit SGS

Energy balance

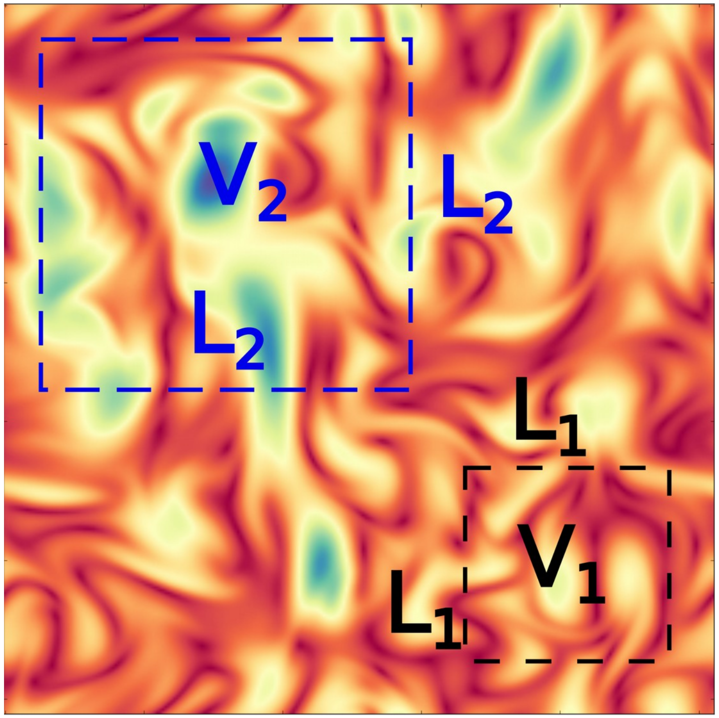
$$
\begin{aligned}
LHS_V^E &= \partial_t \langle \frac{\rho u_i u_i}{2} \rangle_V \\
&= - \left\langle \partial_j \left(\frac{\rho u_i u_i}{2} u_j \right) \right\rangle_V - \left\langle u_i \partial_i p \right\rangle_V + \left\langle u_i F_i \right\rangle_V \\
&\quad - \left\langle \nu_0\, \rho \left(\partial_j u_i + \partial_i u_j \right) \partial_j u_i \right\rangle_V + \left\langle \partial_j \left(\nu_0\, \rho u_i \left(\partial_j u_i + \partial_i u_j \right) \right) \right\rangle_V \\
&\quad - \left\langle \delta\nu_e\, \rho \left(\partial_j u_i + \partial_i u_j \right) \partial_j u_i \right\rangle_V + \left\langle \partial_j \left(\delta\nu_e\, \rho u_i \left(\partial_j u_i + \partial_i u_j \right) \right) \right\rangle_V \\
&= RHS_V^E
\end{aligned}
$$

Balancing error

$$
\mathrm{V}_L = L \times L \times L
$$

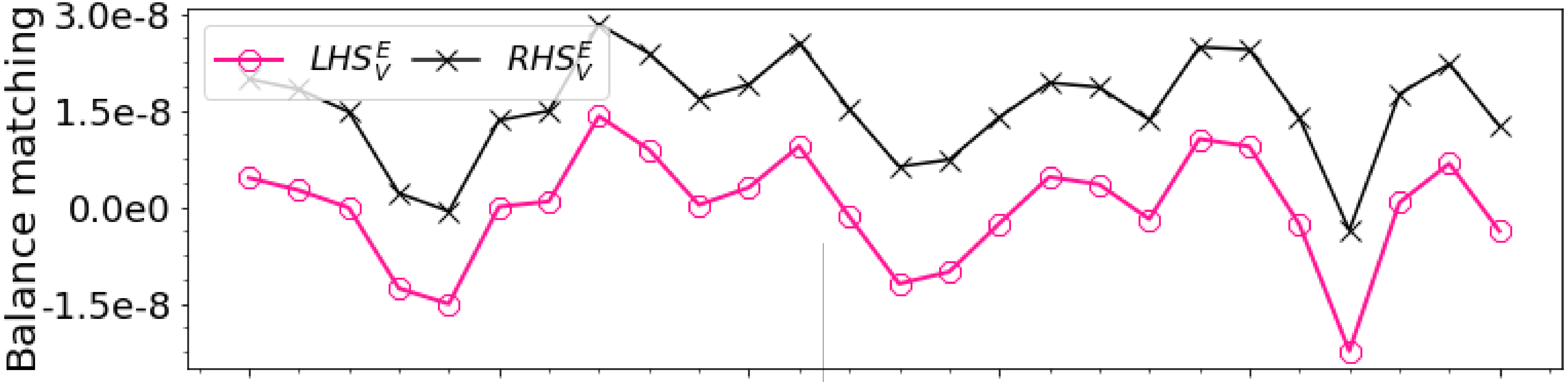
$$
\delta_{V_L}^E(t) = \frac{\left| RHS_{V_L}^E(t) - LHS_{V_L}^E(t) \right|}{L_0^{-1} \left(\max_t \left\langle E(t) \right\rangle \right)^{\frac{3}{2}}}
$$

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

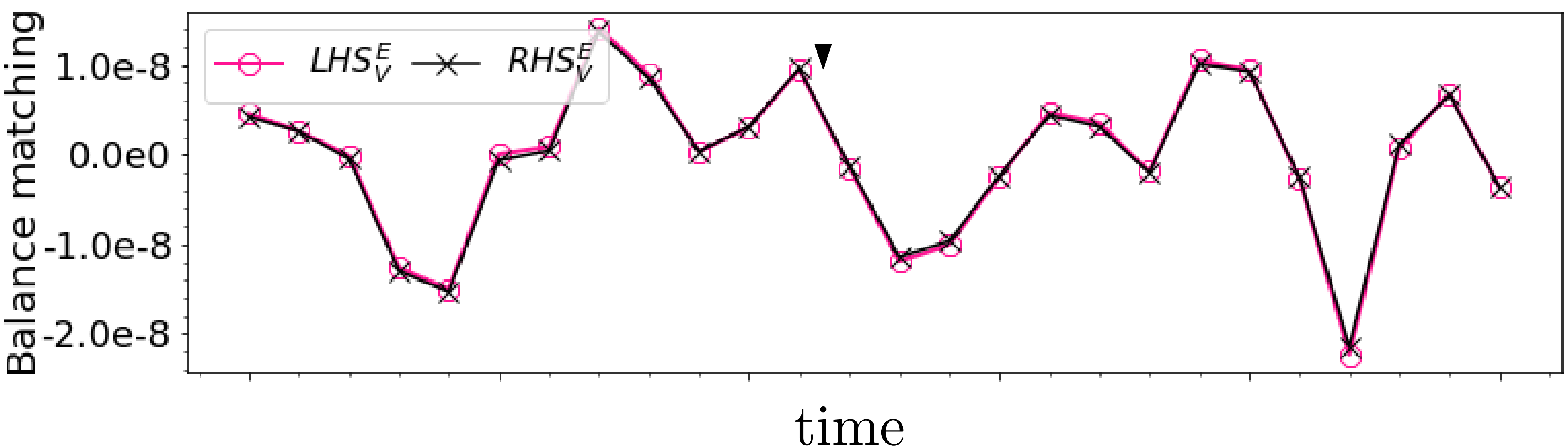


Evolution of the balance over a sub-volume

critically-resolved LBGK simulaion L=128

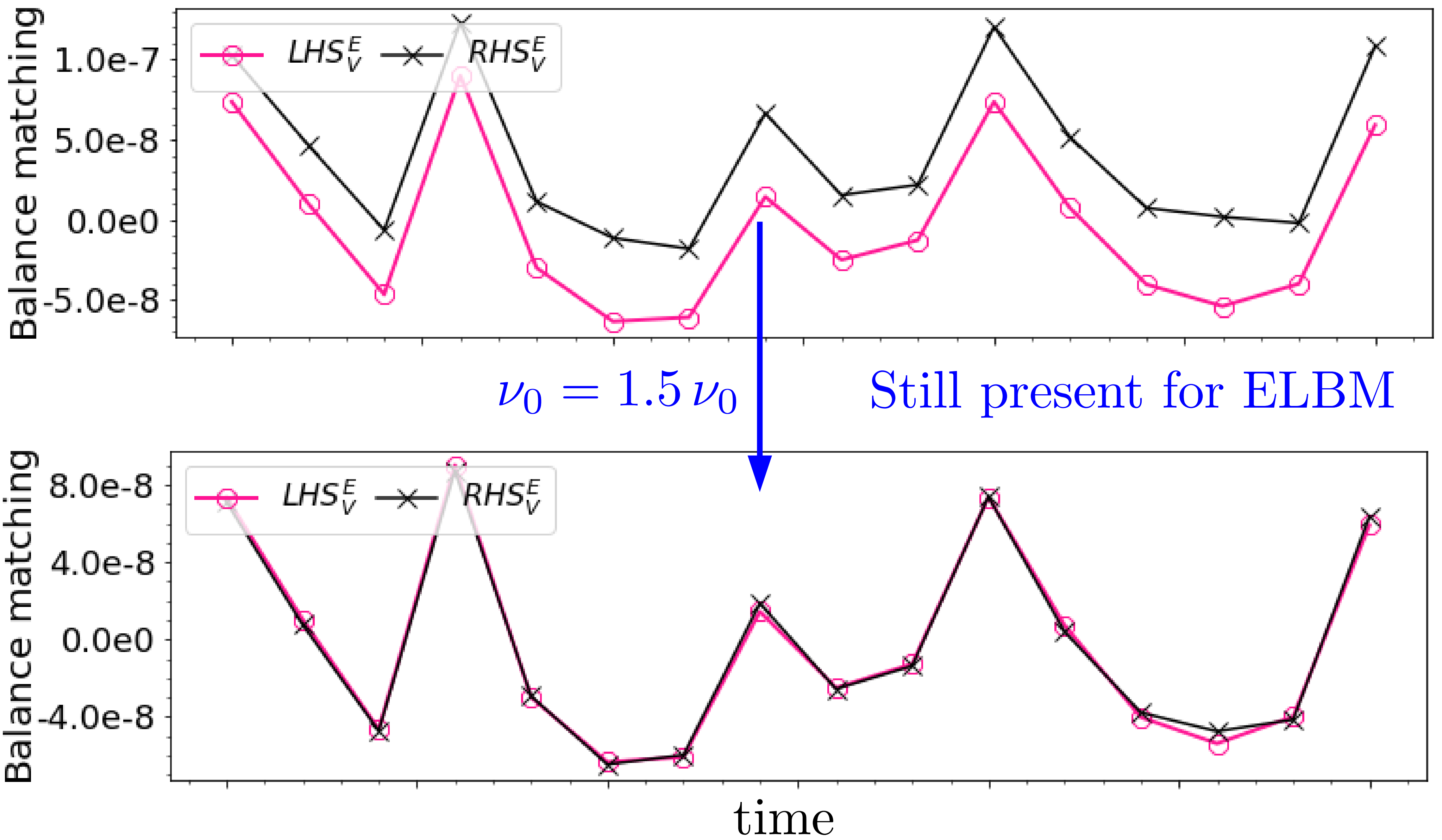


$\nu_0 = 1.2\,\nu_0$ Numerical dissipation?



Evolution of the balance over a sub-volume

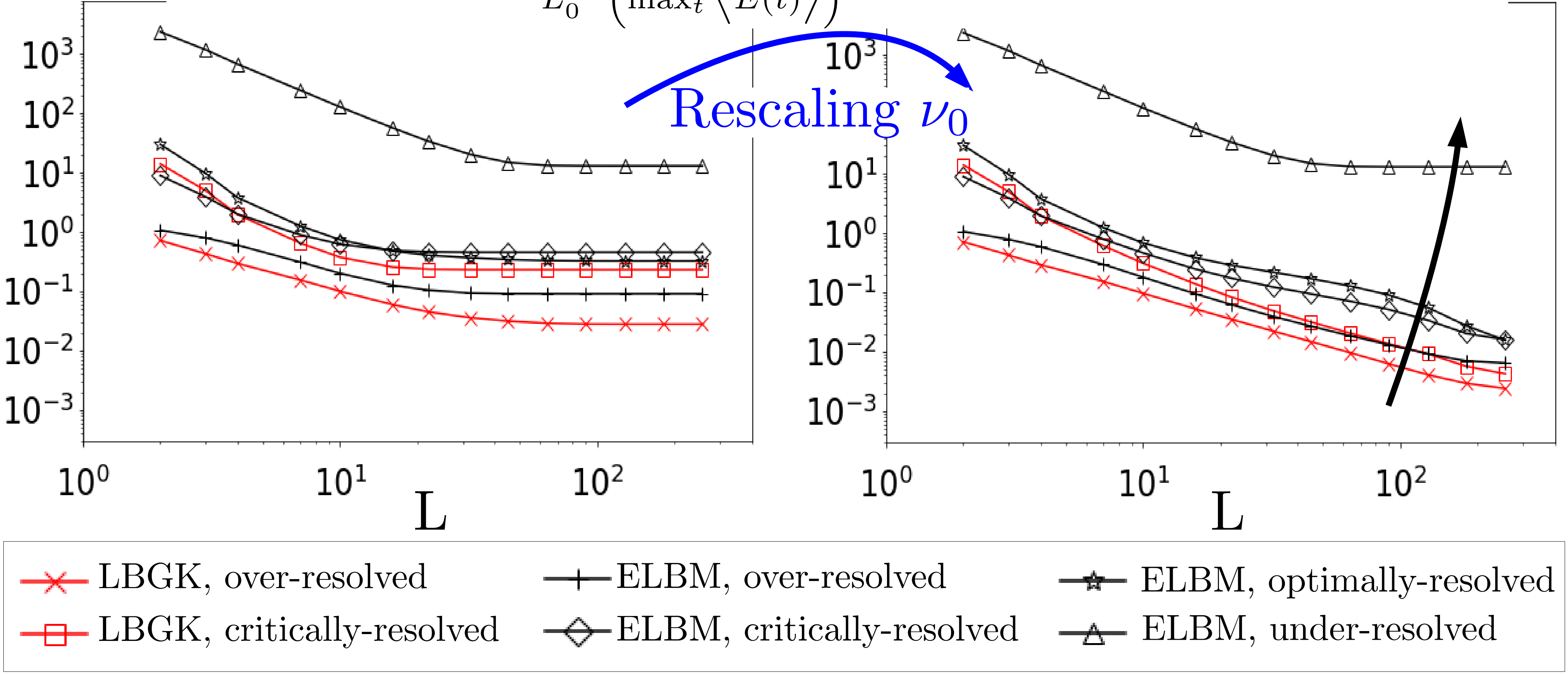
critically-resolved ELBM simulaion L=128



Statistical analysis of the energy balancing error

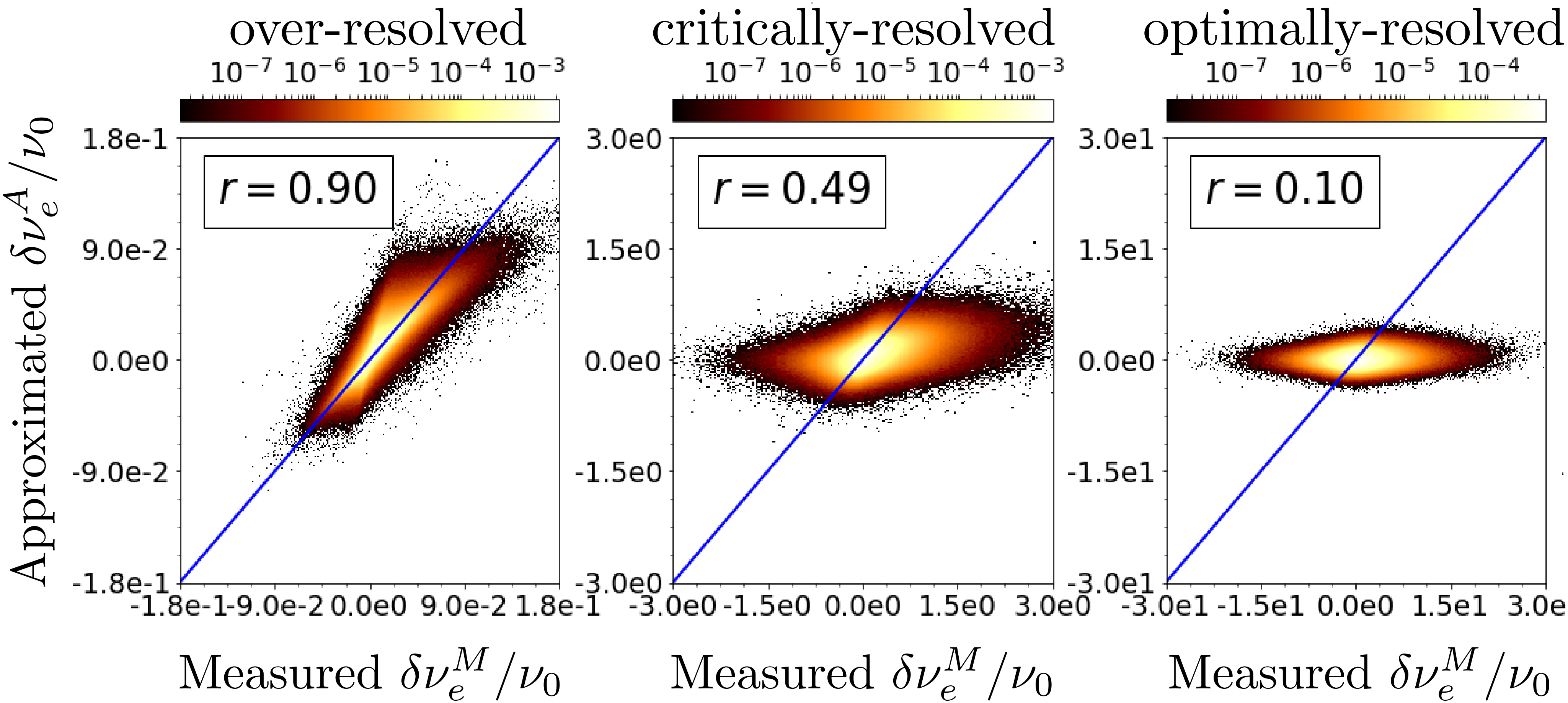
For a sub-volume size L, we calculate the balancing error for 10,000 random sub-volumes of size $V_L = L \times L \times L$

Mean of $\delta^E_{V_L}(t) = \frac{\left|RHS^E_{V_L}(t) - LHS^E_{V_L}(t)\right|}{L_0^{-1}\left(\max_t \left\langle E(t) \right\rangle\right)^{\frac{3}{2}}}$ for all subvolume V_L against L



[Tauzin et al., In preparation]

2) Numerical check of Approximated viscosity

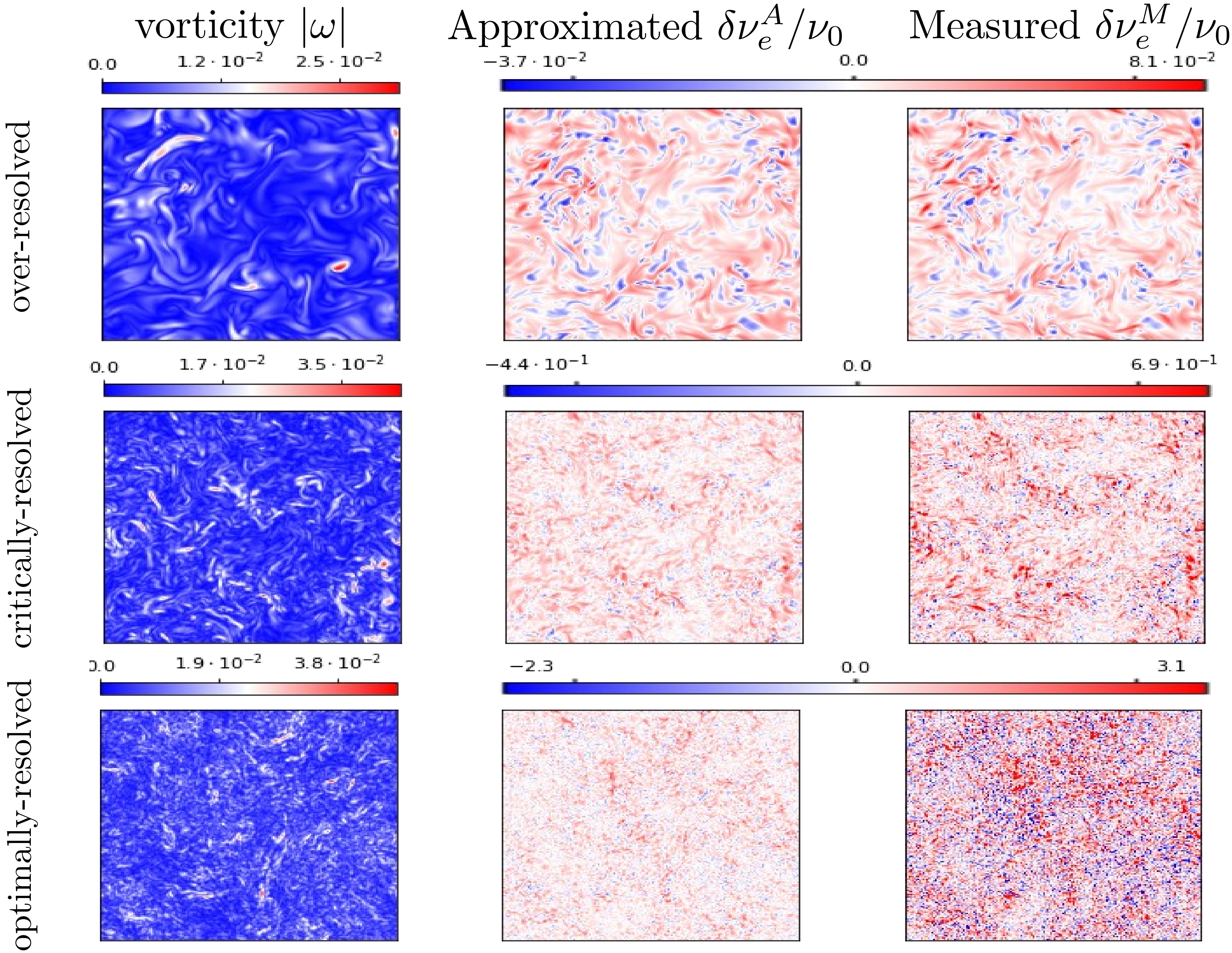


Measured eddy viscosity

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

Approximated eddy viscosity

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


vorticity $|\omega|$
Approximated $\delta\nu_e^A/\nu_0$
Measured $\delta\nu_e^M/\nu_0$
over-resolved
critically-resolved
optimally-resolved
0.0
$1.2 \cdot 10^{-2}$
$2.5 \cdot 10^{-2}$
$-3.7 \cdot 10^{-2}$
0.0
$8.1 \cdot 10^{-2}$
0.0
$1.7 \cdot 10^{-2}$
$3.5 \cdot 10^{-2}$
$-4.4 \cdot 10^{-1}$
0.0
$6.9 \cdot 10^{-1}$
$1.9 \cdot 10^{-2}$
$3.8 \cdot 10^{-2}$
-2.3
0.0
3.1

Conclusions

- 3D Homogeneous Isotropic Turbulence simulations at increasing Re
- ELBM implicit SGS enables an extension of the inertial range
- The implicit turbulence models is inactive when the simulations is fully-resolved and gets increasingly active with Re
- Numerical check of the balance of kinetic energy and enstrophy on sub-volumes of the computational domain reveals numerical dissipation

  ELBM was shown to maintain accuracy up to Reynolds 20 times larger than the one of the critical LBGK
- Approximated viscosity model is in fair agreement only when the simulations is still well resolved
- Need to check higher order hydrodynamic correlations of ELBM simulations and Pseudo-Spectral LES with approximated SGS

$\langle \partial_r \mathbf{v}^2 \rangle \approx E(k)$ LOCAL $\langle \partial_r \mathbf{v}^4 \rangle$ NON-LOCAL [Tauzin et al., In prep.]

Thank you for your attention

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