



UNIVERSITÀ degli STUDI di ROMA  
TOR VERGATA



**HPG-LEAP**  
EUROPEAN JOINT DOCTORATES



**BERGISCHE  
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WUPPERTAL**



European Research Council  
Established by the European Commission

# Entropic Lattice Boltzmann Method

## An implicit Large-Eddy Simulation?

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Erlangen - July 13, 2017



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No' 642069

# Outline

- 1 Introduction to Entropic LBM (ELBM)
- 2 Motivation: An implicit Sub-Grid Scale (SGS) model?
- 3 Analysis tool for hydrodynamic check
- 4 Statistical analysis
  - Validation: LBGK vs. Pseudo-spectral - 2D decaying flows
  - Benchmark: LBGK - Forced 2D turbulent flows
  - Benchmark: ELBM - Forced 2D turbulent flows
- 5 Conclusion

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# ELBM: A search for LBGK stabilization

## **Can we use LBGK to study turbulent flows?**

Instabilities arise when  $\tau \rightarrow 0.5$  ( $\nu \rightarrow 0$ ) making standard LBGK unadapted to the study of turbulent flows

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**ELBM principle is to equip LBGK with an in-built H-theorem**



## ELBM: A LBGK with an in-built H-theorem

- ▶  $\mathbf{f}^{eq}$  is defined as the maxima of a convex H-function under the constraints of mass and momentum conservation:

$$H(\mathbf{f}) = \sum_0^{q-1} f_i \log \left( \frac{f_i}{\omega_i} \right), \quad \rho = \sum_i f_i^{eq}, \quad \rho \vec{u} = \sum_i \vec{c}_i f_i^{eq}$$

### LBGK Equation

$$f_i(\vec{X} + \vec{c}_i, t + 1) - f_i(\vec{X}, t) = -\frac{1}{\tau} [f_i(\vec{X}, t) - f_i^{eq}(\vec{X}, t)]$$

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$$f_i(\mathbf{x} + \mathbf{c}_i, t + 1) = f_i(\mathbf{x}, t) + \alpha\beta [f_i^{eq}(\mathbf{x}, t) - f_i(\mathbf{x}, t)]$$

where  $\beta = \frac{1}{2\tau}$  and LBGK is recovered if  $\alpha \equiv 2$

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ELBM Equation

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

where  $\beta = \frac{1}{2\tau}$ , with  $0 < \beta < 1$  as we have  $0.5 < \tau < +\infty$

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- ▶  $\alpha$  is calculated at each node and each time step as the solution of the following equation:

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

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## Is ELBM a LBGK with an implicit SGS?

- ▶ The viscosity  $\nu$  is allowed to fluctuate locally:

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$$\nu(\alpha) = c_s^2 \left( \frac{1}{\alpha\beta} - 0.5 \right)$$

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- ▶ Chapman-Enskog expansion was performed for  $\alpha \approx 2$  and an additional term of the form  $\nu_r S_{ij}$  appeared with:

$$\nu_r = - \frac{c_s^2 \Delta t}{3(2\beta)^2} \frac{S_{\theta\kappa} S_{\kappa\gamma} S_{\gamma\theta}}{S_{\lambda\mu} S_{\lambda\mu}}$$

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**Objective: Numerically check the existence of an implied SGS**

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$$\begin{aligned} \partial_t \frac{\rho \vec{u}^2}{2} = & -c_s^2 u_i \partial_i \rho - \nu \rho (\partial_j u_i + \partial_i u_j) \partial_j u_i + u_i F_i \\ & + \partial_j \left[ -\frac{\rho \vec{u}^2}{2} u_j + \nu \rho u_i (\partial_j u_i + \partial_i u_j) \right] \end{aligned}$$

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- ▶ Enstrophy  $\Omega = \frac{\vec{\omega}^2}{2}$  balance equation:

$$\begin{aligned} \partial_t \frac{\vec{\omega}^2}{2} = & -\frac{\vec{\omega}^2}{2} \partial_j u_j + \omega_i \omega_j \partial_j u_i + \nu \vec{H} \cdot (\vec{\nabla} \times \vec{\omega}) + \vec{\omega} \cdot \left( \vec{\nabla} \times \frac{1}{\rho} \vec{F} \right) \\ & + \partial_j \left[ -\frac{\vec{\omega}^2}{2} u_j + \nu \epsilon_{ijk} \omega_i H_k \right], \text{ where } \vec{H} = \frac{1}{\rho} \vec{\nabla} \cdot \left[ \rho \left( \vec{\nabla} \vec{u} + (\vec{\nabla} \vec{u})^T \right) \right] \end{aligned}$$

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We will focus on 2D flows and 2D sub-volumes in this presentation

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where  $\langle \dots \rangle$  denotes average over a sub-volume  $V$

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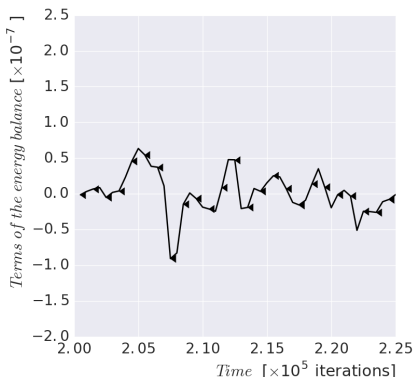
$$\begin{aligned} \partial_t \left\langle \frac{\omega^2}{2} \right\rangle &= - \left\langle \frac{\omega^2}{2} \partial_j u_j \right\rangle + \nu \langle H_x \partial_y \omega - H_y \partial_x \omega \rangle + \left\langle \omega \left( \partial_x \frac{F_y}{\rho} - \partial_y \frac{F_x}{\rho} \right) \right\rangle \\ &\quad - \left\langle \partial_j \frac{\vec{\omega}^2}{2} u_j \right\rangle + \nu \langle \epsilon_{ijk} \omega_i H_k \rangle, \text{ where } \vec{H} = \frac{1}{\rho} \partial_j [\rho (\partial_j u_i + \partial_i u_j)] \end{aligned}$$

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# Example of a term by term balance of $E$ and $\Omega$

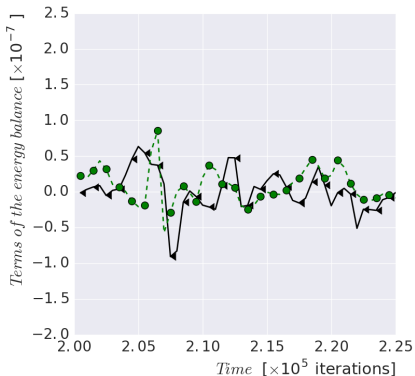
- ← LHS:  $\partial_t \langle \frac{\rho \bar{u}^2}{2} \rangle$ 
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→ RHS
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From energy balance

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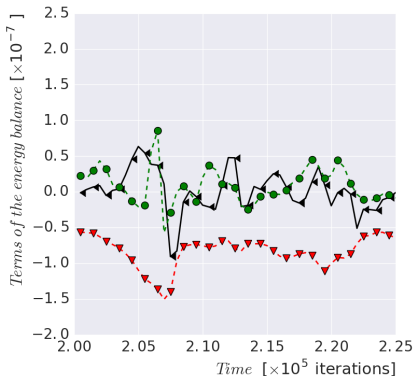
- - 
  - 
  -
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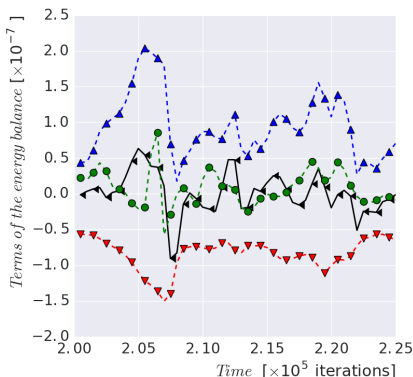
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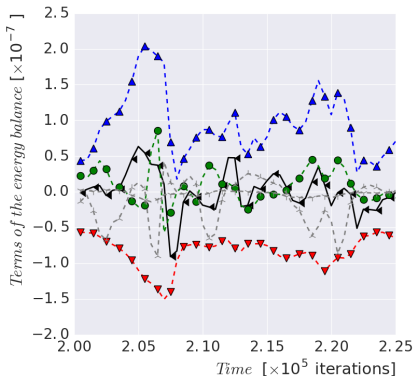
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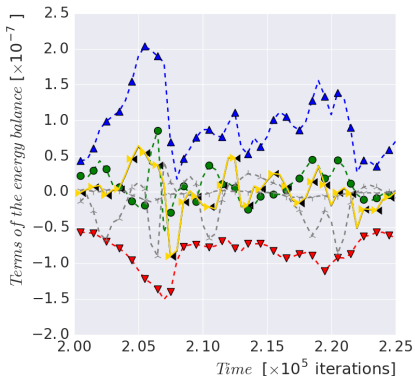
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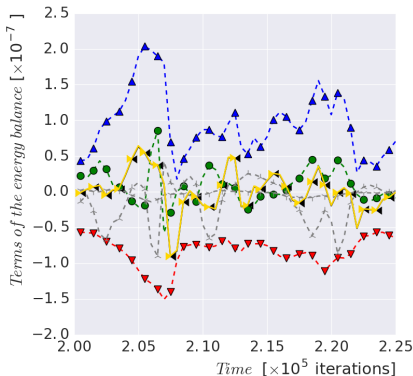
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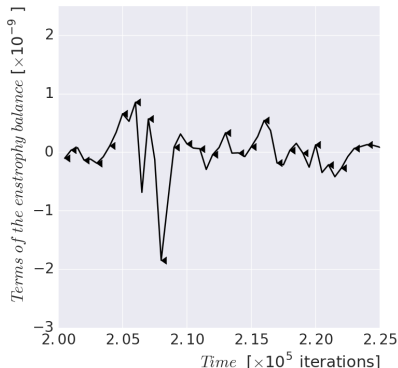
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|---|--|---|--|
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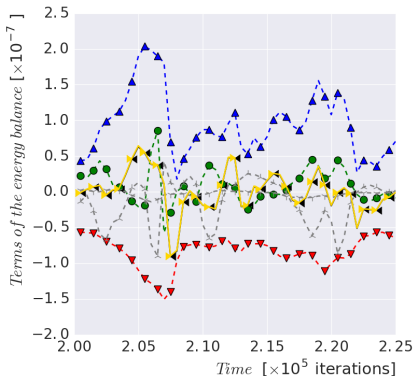
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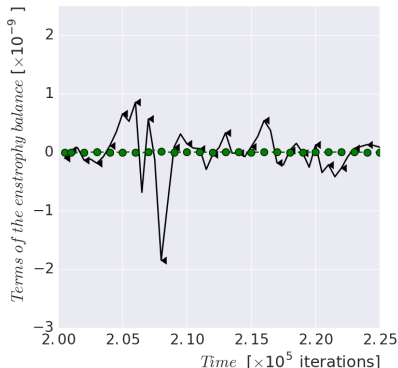
From enstrophy balance

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| - - - $-c_s^2 \langle u_i \partial_i \rho \rangle$                                 | - - - $-\langle \partial_j \frac{\omega^2}{2} u_j \rangle$                    | - - - $-\langle \frac{\omega^2}{2} \partial_j u_j \rangle$                                 | - - - $-\langle \partial_j \frac{\omega^2}{2} u_j \rangle$      |
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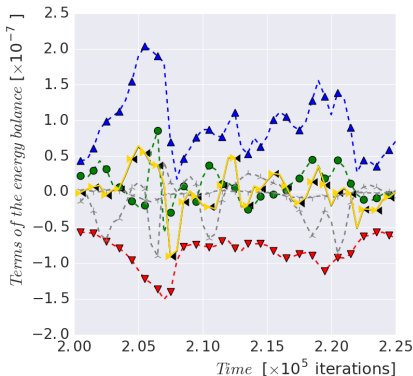
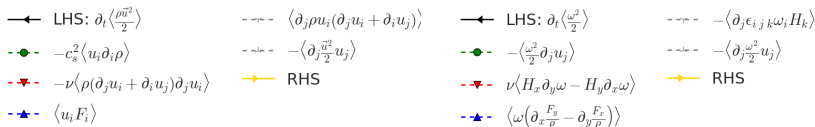
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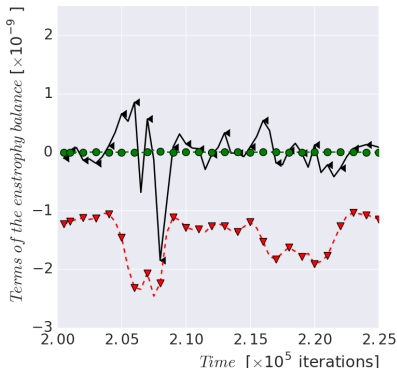
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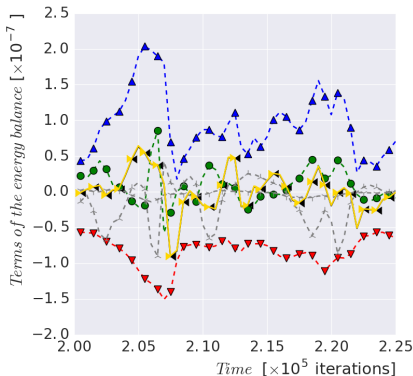
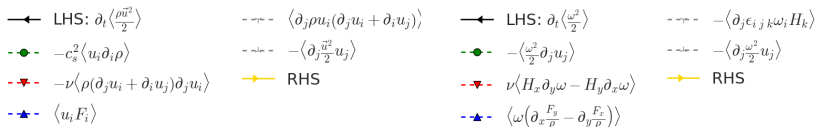


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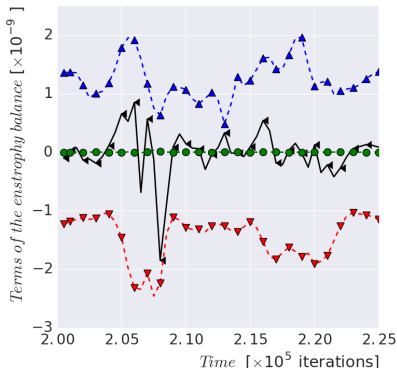


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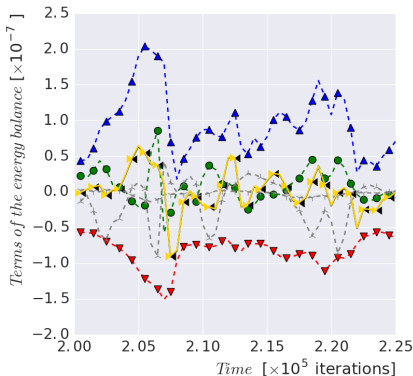
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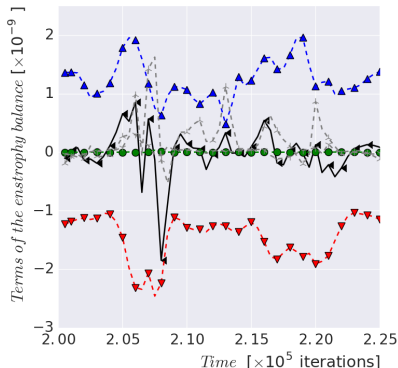
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# Example of a term by term balance of $E$ and $\Omega$

- |   |  |   |  |
|---|--|---|--|
| <ul style="list-style-type: none"> <li>—●— LHS: <math>\partial_t \langle \frac{\rho u^2}{2} \rangle</math></li> <li>—●— <math>-c_s^2 \langle u_i \partial_i \rho \rangle</math></li> <li>—▲— <math>-\nu \langle \rho (\partial_j u_i + \partial_i u_j) \partial_j u_i \rangle</math></li> <li>—▲— <math>\langle u_i F_i \rangle</math></li> </ul> | <ul style="list-style-type: none"> <li>--- <math>\langle \partial_j \rho u_i (\partial_j u_i + \partial_i u_j) \rangle</math></li> <li>--- <math>-\langle \partial_j \frac{\omega^2}{2} u_j \rangle</math></li> <li>→ RHS</li> </ul> | <ul style="list-style-type: none"> <li>—●— LHS: <math>\partial_t \langle \frac{\omega^2}{2} \rangle</math></li> <li>—●— <math>-\langle \frac{\omega^2}{2} \partial_j u_j \rangle</math></li> <li>—▲— <math>\nu \langle H_x \partial_x \omega - H_y \partial_x \omega \rangle</math></li> <li>—▲— <math>\langle \omega (\partial_x \frac{F_y}{\rho} - \partial_y \frac{F_x}{\rho}) \rangle</math></li> </ul> | <ul style="list-style-type: none"> <li>--- <math>-\langle \partial_j \epsilon_{i j k} \omega_i H_k \rangle</math></li> <li>--- <math>-\langle \partial_j \frac{\omega^2}{2} u_j \rangle</math></li> <li>→ RHS</li> </ul> |
|---|--|---|--|



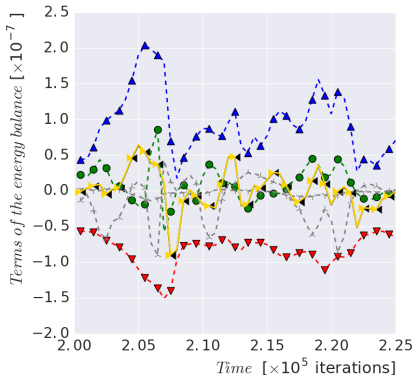
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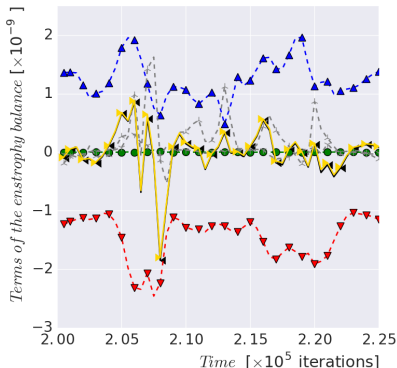
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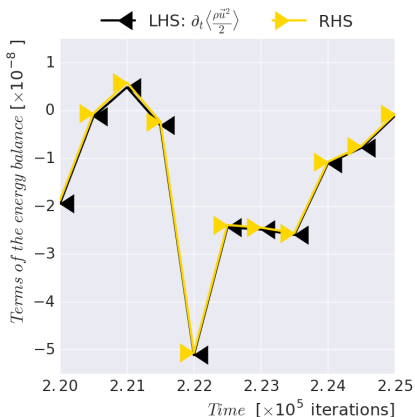


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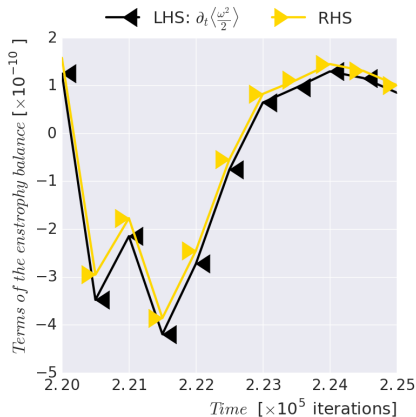


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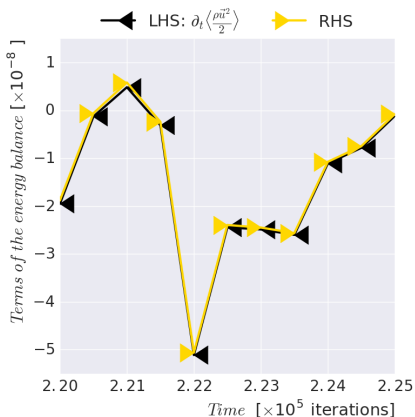


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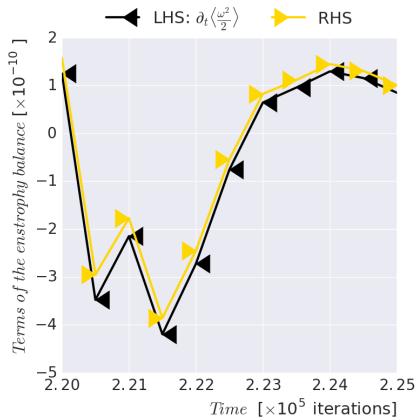


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## Example of a term by term balance of $E$ and $\Omega$



From energy balance



From enstrophy balance

**What is the accuracy with which LBGK/ELBM can recover the hydrodynamic balance equations?**

## Measurement of the relative effective viscosity

In order to evaluate the inaccuracy of the recovery of the balance equation averaged over a sub-volume, we can define an effective viscosity:

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## Relative effective viscosity

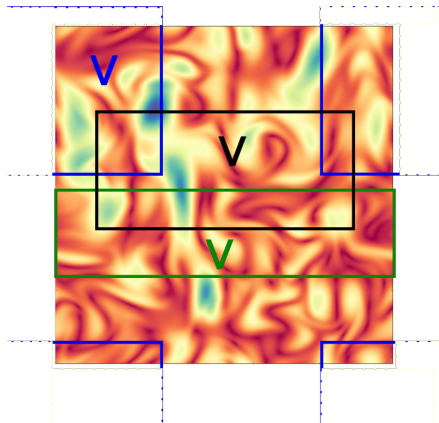
$$\frac{\nu_{\text{eff}}^{E, \Omega}}{\nu} = \frac{\nu_{\text{eff}}^{E, \Omega}}{c_s^2 \left( \tau - \frac{1}{2} \right)} \approx 1$$

# Outline

- 1 Introduction to Entropic LBM (ELBM)
- 2 Motivation: An implicit Sub-Grid Scale (SGS) model?
- 3 Analysis tool for hydrodynamic check
- 4 Statistical analysis**
  - Validation: LBGK vs. Pseudo-spectral - 2D decaying flows
  - Benchmark: LBGK - Forced 2D turbulent flows
  - Benchmark: ELBM - Forced 2D turbulent flows
- 5 Conclusion

# Statistical analysis of $\frac{\nu_{eff}}{\nu}$

- ▶ Calculation on random sub-volumes of  $\frac{\nu_{eff}}{\nu}$  for both kinetic energy and enstrophy balance equations.
- ▶ Sorting the results based on  $L$ , characteristic length of the sub-volume  $V$  defined as the square root of its volume  $V$ .

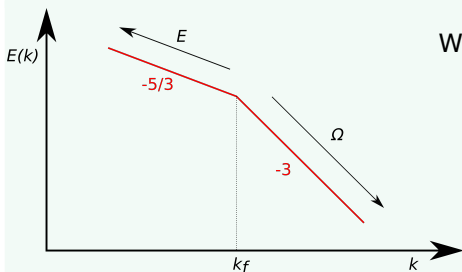


# Numerical apparatus: 2D homogeneous turbulence

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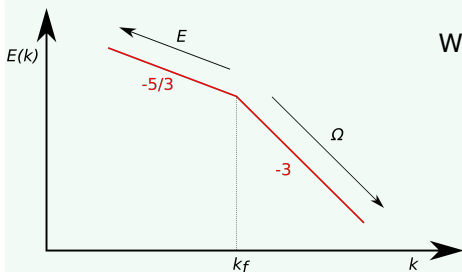


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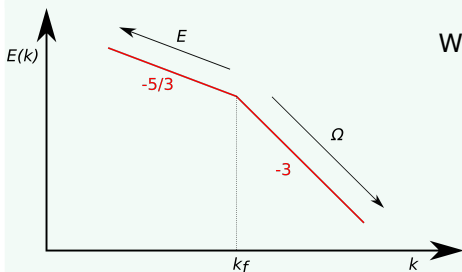
Forcing on a shell of wavenumber

$$F_{\Psi}^T = F_0^T \sum_{\|\vec{k}\|=5}^7 \cos\left(\frac{2\pi}{L} \vec{k} \cdot \vec{x} + \phi\right)$$

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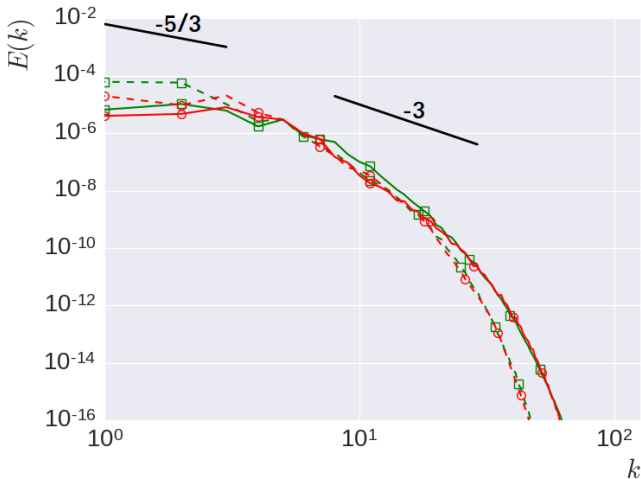
Energy removal at large scale

$$\vec{F}^E(\vec{x}, t) = -F_0^E \sum_{\|\vec{k}\|=1}^2 \vec{u}(\vec{k}, t) e^{\frac{2\pi}{L} \vec{k} \cdot \vec{x}}$$



## Validation: LBGK vs. Pseudo-spectral - Decaying spectrum

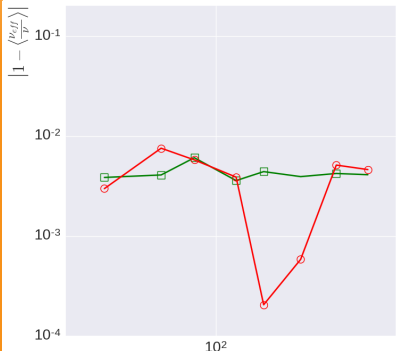
- PS,  $\nu=0.0045$  – *First conf.*      —○— LBGK,  $\tau=0.54$  – *First conf.*  
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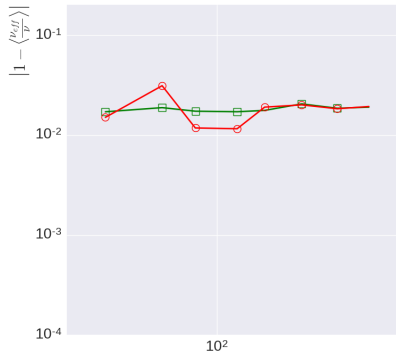
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$|1 - \langle \frac{\nu_{eff}}{\nu} \rangle|$  against sub-volume characteristic length  $L$

—□— *PS*,  $\nu = 0.0045$       —○— *LBGK*,  $\tau = 0.54$



From energy balance

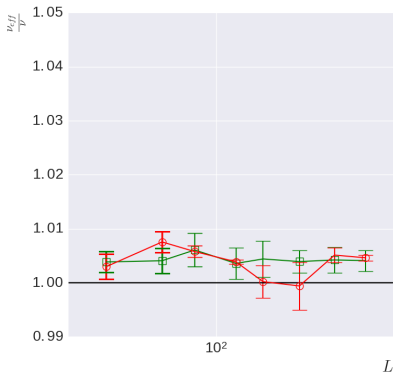


From enstrophy balance

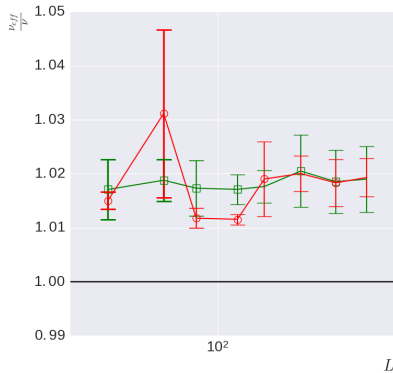
# Validation: LBGK vs. Pseudo-spectral - Variation of $\frac{\nu_{eff}}{\nu}$

$\frac{\nu_{eff}}{\nu}$  against sub-volume characteristic length  $L$

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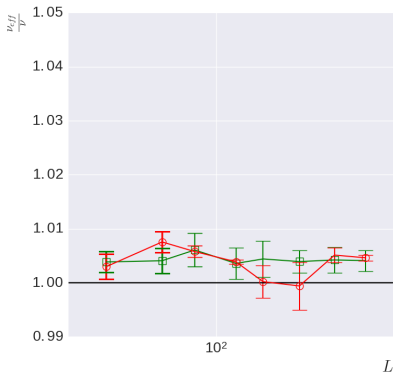


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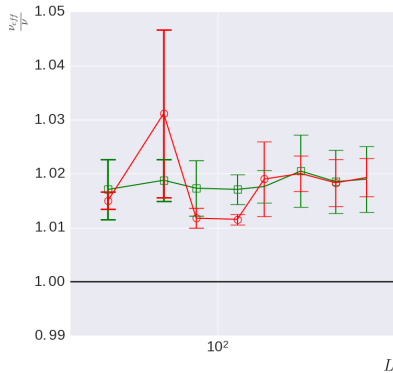
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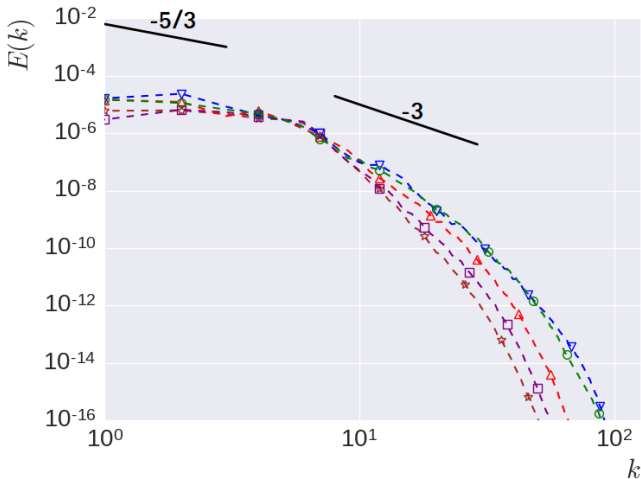


From enstrophy balance

**Good agreement for both Pseudo-Spectral and LBGK**

## Benchmark: Forced LBGK - Superposed spectrum

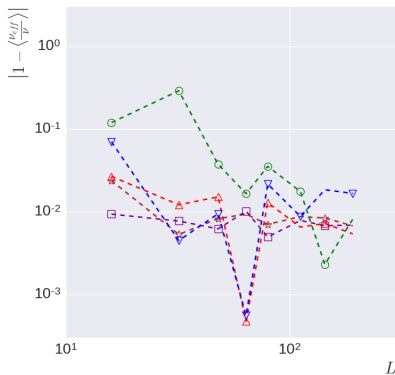
- ★- LBGK,  $\tau=0.55$
- △- LBGK,  $\tau=0.53$
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- ▽- LBGK,  $\tau=0.52$



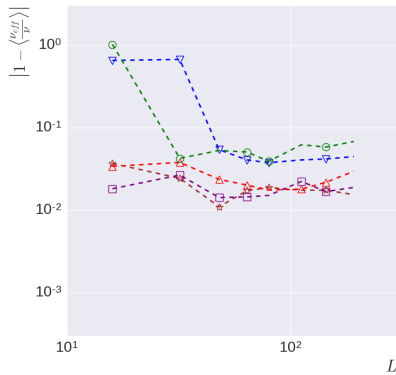
# Benchmark: Forced LBGK - Error in $\langle \frac{\nu_{eff}}{\nu} \rangle$

$|1 - \langle \frac{\nu_{eff}}{\nu} \rangle|$  against sub-volume characteristic length  $L$

- \* - LBGK,  $\tau = 0.55$       - ▲ - LBGK,  $\tau = 0.53$       - ⊖ - LBGK,  $\tau = 0.515$
- □ - LBGK,  $\tau = 0.54$       - ▼ - LBGK,  $\tau = 0.52$



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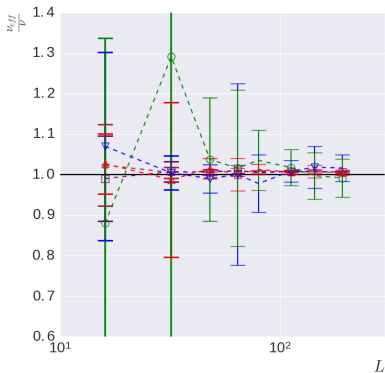


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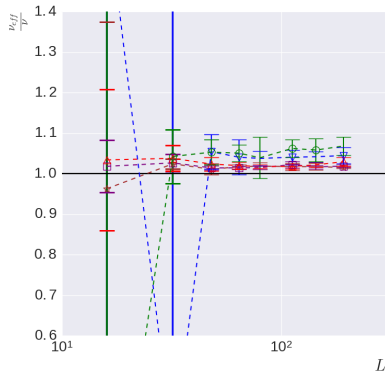
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- \* - LBGK,  $\tau = 0.55$
- $\Delta$  - LBGK,  $\tau = 0.53$
- $\ominus$  - LBGK,  $\tau = 0.515$
- $\boxminus$  - LBGK,  $\tau = 0.54$
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From energy balance

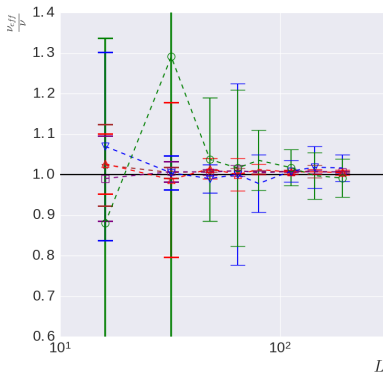


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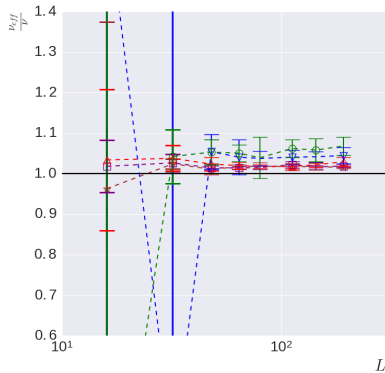
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- ★- LBGK,  $\tau = 0.55$
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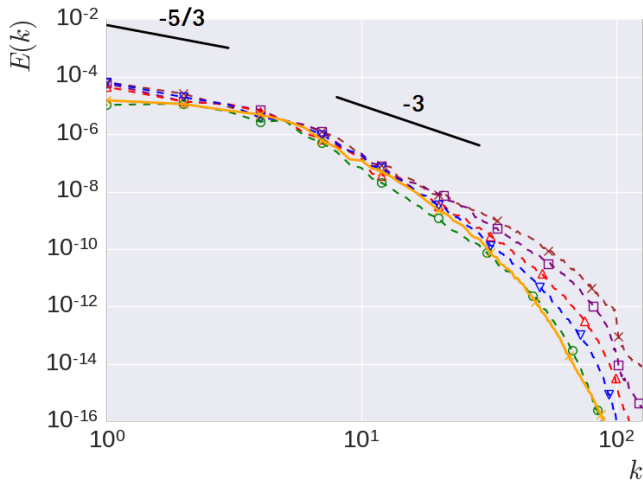
From entrophy balance

**Reynolds number effect + proximity to  $\tau_{critical}$  ?**



## Benchmark: Forced ELBM - Superposed spectrum

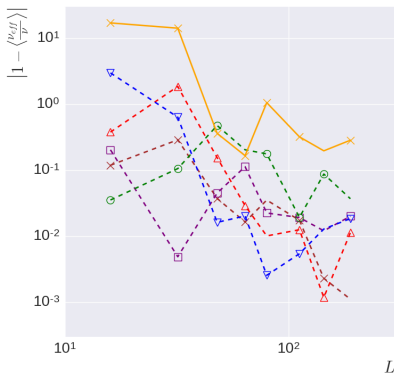
- x- ELBM,  $\tau = 0.5025$     -△- ELBM,  $\tau = 0.5075$     -○- ELBM,  $\tau = 0.515$   
-□- ELBM,  $\tau = 0.505$     -▽- ELBM,  $\tau = 0.51$     -×- LBGK,  $\tau = 0.515$



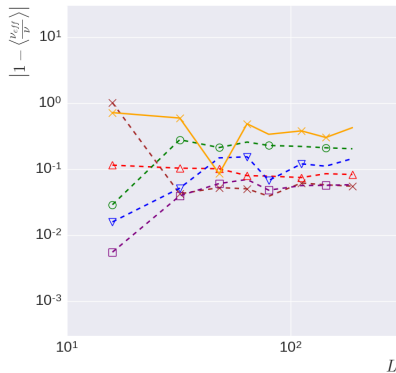
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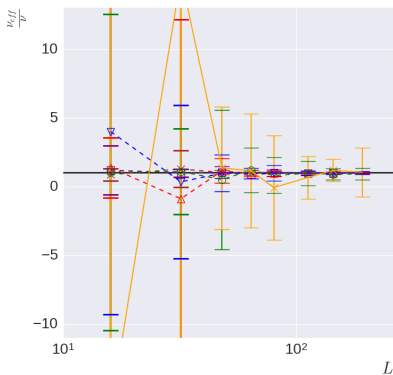


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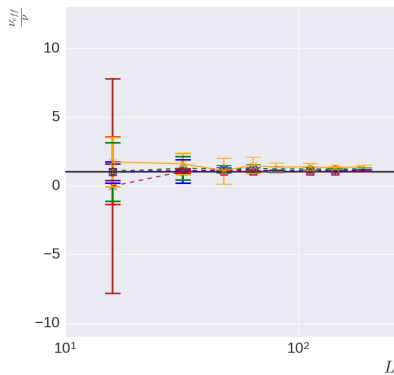
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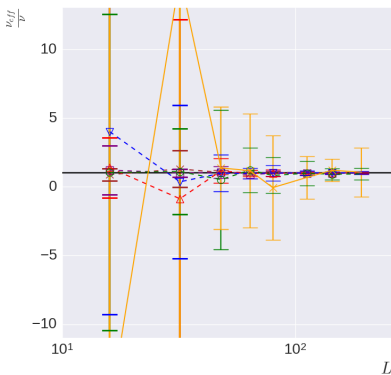


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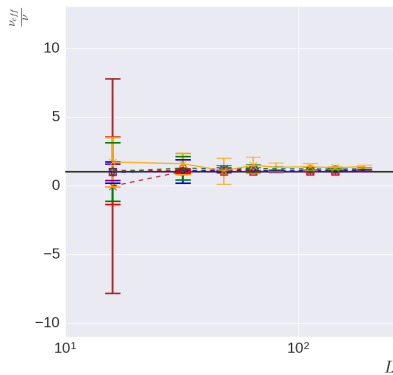
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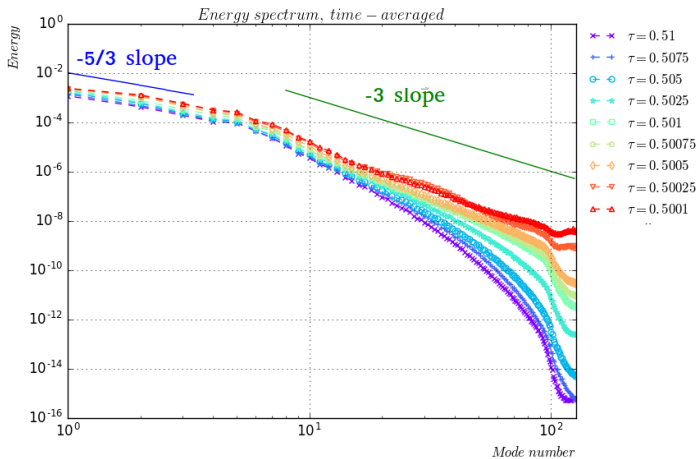


From enstrophy balance

**No agreement expected for ELBM: An extra term in the balance eqs?**

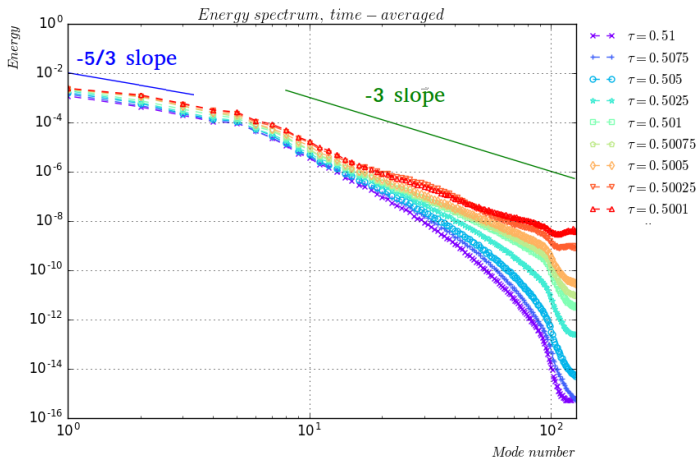
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Going further to  $\tau \rightarrow 0.5$ , we observe an extension of the inertial range



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**ELBM has the dissipative properties expected from a LES**

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# Conclusion & Outlook

## Conclusions:

- ▶ Developed a tool to check the balance equations and validated it on configurations obtained from a Pseudo-Spectral code.
- ▶ LBGK's recovery of hydrodynamics gets broken as the critically stable  $\tau$  is approached.
- ▶ ELBM's effective visosity  $\nu_{eff}$  as  $\tau \rightarrow 0.5$  cannot be represented by a simple renormalization of the input viscosity  $\nu$ :  
Presence of an extra SGS to be taken into account in the balance equations?
- ▶ ELBM dissipative properties as  $\tau \rightarrow 0.5$  are as expected for a LES.



# Conclusion & Outlook

## Conclusions:

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- ▶ ELBM dissipative properties as  $\tau \rightarrow 0.5$  are as expected for a LES.

## Outlook:

- ▶ Validate Malaspinas' suggested implicit SGS to the balance equations on ELBM simulations
- ▶ Switch to 3D turbulent simulations.

# References

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Thank you for your attention!

Any questions?



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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

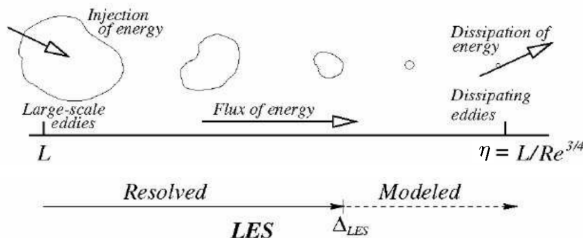
# What is Large Eddy Simulation (LES)?

- ▶ Reduces the number of degrees of freedom by resolving scales only up to a cutoff scale and modeling the remaining smaller scales
- ▶ Enables cost-effective high Reynolds turbulent flow simulations

LES equation: Filtered Navier-Stokes + SGS model

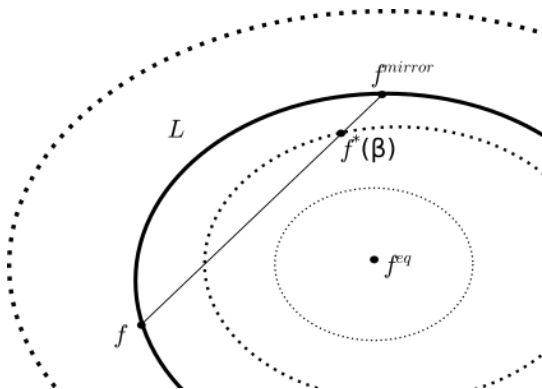
$$\partial_t \bar{u}_i + \partial_j (\bar{u}_i \bar{u}_j) = -\frac{1}{\rho} \partial_i \bar{p} + \nu \partial_j \bar{S}_{ij} - \partial_j \tau_{ij}, \text{ where } \bar{S}_{ij} = (\partial_j \bar{u}_i + \partial_i \bar{u}_j)$$

$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$  must be modeled using a Sub-Grid Scale (SGS) Model



# ELBM: Perspective from H-functional hypersurface

Calculation of  $\alpha$  and convexity of H insure monotonic decreases of H



# Solving the Entropic step equation

## Entropic step Equation

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

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

- ▶ Nont-trivial: typically solved using Newton-Raphson in 6-8 iterations for a tolerance of  $10^{-5}$
- ▶ When Newton-Raphson does not converge, 2, the LBGK's value of  $\alpha$  is used