Entropic Lattice Boltzmann Method:
An implicit Large-Eddy Simulation ?

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HPC-LEAP EUROPEAN JOINT DOCTORATES

Motivations

Lattice Boltzmann Method:

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

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Current direction: Study of Entropic Lattice Boltzmann Method as an implicit LBM-LES

Lattice Boltzmann Equation

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[Succi, 2001]

LBGK Equation

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

which is a relaxation of typical time τ to the local equilibirum distribution:

$$f_i^{eq}(\vec{x}, t) = w_i\,\rho(\vec{x}, t)\left[1 + \frac{\vec{c}_i \cdot \vec{u}(\vec{x}, t)}{c_s^2} + \frac{\left(\vec{c}_i \cdot \vec{u}(\vec{x}, t)\right)^2}{2\,c_s^4} - \frac{|\vec{u}(\vec{x}, t)|^2}{2\,c_s^2}\right]$$

a 2^{nd} order expansion in $\frac{\vec{u}}{c_s}$ of the Maxwell-Boltzmann distribution

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- Chapman-Enskog expansion shows the relation between viscosity ν and the relaxation time τ

$$\nu = c_s^2 \left(\frac{1}{\tau} - 0.5 \right)$$ where c_s is the speed of sound in the lattice

ELBM: A search for LBM stabilization

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Can we use LBM to study turbulent flows?
Instabilities arise when $\tau \to 0.5$ ($\nu \to 0$) making standard LBGK irrelevant to the study of turbulent flows

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

ELBM: A LBM with an in-built H-theorem

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ELBM Equation

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

where $\beta = \frac{1}{2\tau}$. If $\alpha = 2$, the ELBM eq. becomes the LBGK eq.

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- $\mathbf{f^{eq}}$ is defined as the maxima of a convex H-function under the constraints of mass and momentum conservation: **[Karlin *et al.*, 1999]**

$$H(\mathbf{f}) = \sum_{0}^{q-1} f_i \log\left(\frac{f_i}{\omega_i}\right), \qquad \rho = \sum_i f_i^{eq}, \quad \rho\vec{u} = \sum_i \vec{c}_i f_i^{eq}$$

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- For $DdQ3^d$ lattices:

$$f_i^{eq} = \rho\, w_i \prod_{a=1}^{d}\left(2-\sqrt{1+3\,u_a^2}\right)\left(\frac{2\,u_a+\sqrt{1+3\,u_a^2}}{1-u_a}\right)^{c_{i,\,a}}$$

ELBM: Entropic step

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- ELBM adds a single extra step to the LBM algorithm. At each time step, at each node, the value of α is calculated to insure the monotonic decrease of H.

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

with $0 < \beta < 1$ as we have $0.5 < \tau < +\infty$

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- α is calculated at each node and each time step as the solution of the following equation:

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

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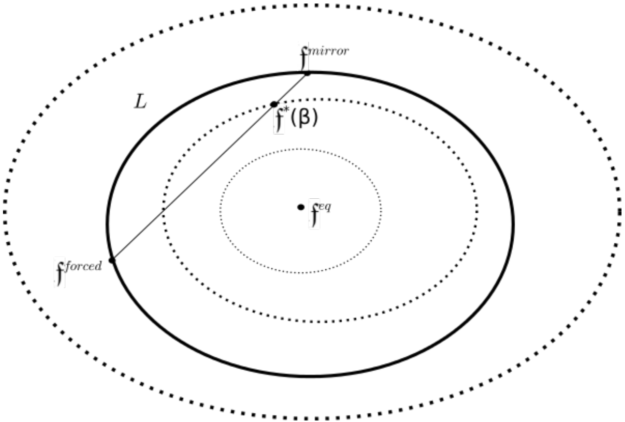
Calculation of α and the convexity of H insure monotonic decreases of H



Solving the Entropic step equation

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... but we need to understand if the right physics is represented

Is ELBM a LBM with an implicit LES?

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[Karlin *et al.*, 1999]

- The viscosity ν is allowed to fluctuate locally:

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[Malaspinas *et al.*, 2008]

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

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

Very similar to a Smagorinsky subgrid scale model

Brief introduction to KBC ELBM

KBC: Multi-relaxation time variation of ELBM **[Bosch *et al.*, 2015]**

$$f_i = k_i + s_i + h_i$$
$$f_i^{mirror} = k_i + [2s_i^{eq} - s_i] + [\gamma h_i^{eq} + (1-\gamma)h_i]$$

where k_i is the contribution of locally conserved fields
s_i are stresses
h_i are the remaining high order moments

γ is calculated to minimize the entropy of the post-collision distribution:

$$\frac{\mathrm{d}H\left[\mathbf{f}'\right]}{\mathrm{d}\gamma} = \frac{\mathrm{d}H\left[(1-\beta)\mathbf{f} + \beta f^{mirror}\right]}{\mathrm{d}\gamma} = 0$$

Research question

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Is the subgrid model nothing else than an artifact of the ELBM, or is it a realistic representation of the unresolved physics? [Malaspinas *et al.*, 2008]

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Objective:

- Numerically check the existence of an implicit Sub-Grid Scale model and its impact on the physics for both 2D and 3D turbulence

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Collaborations:

- Abhineet Gupta and Federico Toschi from TU/e
- Ilya Karlin from ETH Zurich

Thank you for your attention!

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Appendix - ELBM algorithm

for each time step **do**
    for each node **do**
        Calculate density $\rho = \sum_{i=0}^{q-1} f_i$
        Calculate velocity for equilibirum calculation $u^{\vec{eq}} = \frac{1}{\rho} \sum_{i=0}^{q-1} f_i \vec{c_i} + \frac{\vec{F}}{2\rho}$
        Calculate the non-equilibrium part of the distribution $f_i^{neq} = f_i - f_i^{eq}\left(\rho,\ u^{\vec{eq}}\right)$
        Apply the forcing's collision contribution to the distribution
        Check the deviation $\Delta\left(\mathbf{f^F}, \mathbf{f^{neq}}\right) = \max_{0<i<q-1} \left|\frac{f_i^{neq}}{f_i^F}\right|$
        if $\Delta\left(\mathbf{f^F}, \mathbf{f^{neq}}\right) \leq 10^{-3}$ **then**
            Set $\alpha = 2$
        else
            Calculate α_{max} corresponding to $\min_{0<i<q-1; f_i^{neq}>0} \left|\frac{f_i^F}{f_i^{neq}}\right|$
            if $\alpha_{max} < 2$ **then**
                Set $\alpha = 0.9 \times \alpha_{max}$
            else
                Use Newton-Raphson method to solve $H\left(\mathbf{f^F}\right) = H\left(\mathbf{f^F} - \alpha\mathbf{f^{neq}}\right)$ with $\alpha_{guess} = 2$, $\alpha_{min} = 1$ and previously calculated α_{max}
            end if
        end if
        Collide with a relaxation time of $\alpha \times \beta$
        Propagate
        Store density
        Calculate and store hydrodynamic velocity $u^{\vec{hydro}} = \frac{1}{\rho} \sum_{i=0}^{q-1} f_i \vec{c_i} + \frac{\vec{F}}{2\rho}$
    end for
end for