LBM-DSMC hybrid method for complex out-of-equilibrium flows

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Motivation

Coupling Methodology

Hybrid DSMC-LB approach

Numerical results and speed-up

Extension to complex flow geometries

Conclusions and perspectives
The presence of both \textit{rarefied} and \textit{continuum} domains is a typical feature of many complex gas flows (high altitude flights, NEMS/MEMS, next-generation lithography tools).

Extent of the departure of a flow from equilibrium state measured in terms of the \textit{Knudsen number}:

\[
Kn = \frac{\lambda}{\ell} \approx \frac{\lambda}{Q} \left| \frac{dQ}{d\ell} \right|
\]

- Direct Simulation Monte Carlo (\textbf{DSMC}): $Kn \sim \mathcal{O}(1)$
- Lattice Boltzmann Method (\textbf{LBM}): $Kn \sim \mathcal{O}(0.1)$, \textit{Toschi and Succi} (2005)$^1$

Hybrid DSMC-LBM scheme useful for intermediate \textit{Kn} number and for flows with changing rarefaction

\textbf{Key point:} LBM and DSMC, sharing a common kinetic heritage, operate at \textit{closer length-} and \textit{time-scales} than other hybrid models

Direct Simulation Monte Carlo

- Deterministic ballistic move
- Stochastic binary collisions
Lattice Boltzmann Method

Streaming to neighboring nodes

Relaxation towards equilibrium
Lattice Boltzmann Method at finite Kn
How to increase the range of applicability of LBM to finite Kn (slip-)flows?

- **Kinetic boundary conditions** (Ansumali and Karlin (2002)\(^1\)): diffuse reflection

- **Regularization procedure** (Zhang et al. (2006)\(^2\), Niu et al. (2007)\(^3\), Montessori et al. (2014)\(^4\)): filter on high-order moments not supported by the used lattice

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Comparison between DSMC and LBM solutions at $Kn=0.10$

- Velocity profiles for Couette flow at $Kn=0.10$
- DSMC vs LB-D3Q19

\[ u(y/H) \]

\[ \frac{H}{Kn} \approx \lambda \]

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Comparison between DSMC and LBM solutions at Kn=0.10

- Error for velocity profiles for Couette flow at Kn=0.10
- DSMC vs LB-D3Q19

Largest error for LB-D3Q19 within Knudsen layer (stronger non-equilibrium effects)
DSMC-LBM Hybrid scheme
Hybrid scheme

Flow domain decomposition:

Use DSMC where non-equilibrium effects are strong (e.g. Knudsen layer) and LBM in the rest of the domain.

- Two steps required for coupling DSMC and LBM: \( \text{LBM} \rightarrow \text{DSMC} \) and \( \text{DSMC} \rightarrow \text{LBM} \).

- Coupling recipes based on Grad’s moments expansion of the \( f(x, \xi, t) \) and Gauss-Hermite quadratures:

\[
f(x, \xi, t) \approx f^N(x, \xi, t) = \omega(\xi) \sum_{n=0}^{N} \frac{1}{n!} a^{(n)}(x, t) \mathcal{H}^{(n)}(\xi)
\]

\[
a^{(n)} \equiv \int f^N(x, \xi, t) \mathcal{H}^{(n)}(\xi) d\xi = \sum_{a=1}^{q} \frac{W_a}{\omega(\xi)} f^N(x, \xi_a, t) \mathcal{H}^{(n)}(\xi)
\]

- Coupling occurs where both methods provide accurate solution.

How to pass information between the two methods?
Non-equilibrium LBM discrete distributions obtained projecting DSMC moments onto the LBM lattice\textsuperscript{1}

\textsuperscript{1}Di Staso et al. (2016a), Journal of Computational Science, 17, 357-369.
Coupling scheme: LBM $\rightarrow$ DSMC

**Reconstruction** LBM $\rightarrow$ DSMC step

- DSMC particles velocities are sampled from a distribution reconstructed from the discrete LBM distributions\(^1\)

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\(^1\)Di Staso et al. (2016a), Journal of Computational Science, 17, 357-369.
Coupling schemes

PDF \( f(\xi_x, \xi_y) \): example of sampling for a 2D case

- Entering the f
...isolating the $f_a$

Number of particles in correspondence of $c_i$ obtained from DSMC pdf
Coupling schemes

- Comparing the **pdf of the fluid velocity** along the forcing realized by the sampling of $f^N$ and by an independent DSMC simulation
- Node in proximity of the wall and for force-driven Poiseuille flow: $Kn = 0.15$, $Ma = 0.10$

Sampling from $f^N$ guarantees accordance both at molecular and fluid level
Hybrid DSMC-LBM model

- DSMC particles
- DSMC cell
- Particle sampled from $f^N$
- Buffer layer cell
- LB cell
Hybrid model results

- Hybrid approach is applied to the Couette flow\(^1\)
- DSMC extends in proximity of the walls (\(\alpha\) part of the domain) and D3Q19 LBM is used

\(^1\text{Di Staso et al. (2016b) Phil. Trans. R. Soc. A 374:20160226.}\)
• **Mass conservation** requirement fulfilled

• Number of DSMC particles within the DSMC area is on average constant

![Graph showing mass conservation](image-url)
- As particles cross the border between the DSMC and LBM, they are removed.

- **Fluxes (mass, momentum)** towards LBM region evaluated and correction is applied to $f_a$:

$$f_a = f^*_a(x, t) + \Delta f_a(x, t), \quad \Delta f_a(x, t) = w_a \sum_{n=1}^{N} \frac{1}{n!} a^{(n)}(x, t) H^{(n)}(\xi_a)$$
Hybrid model results: velocity profiles

- Comparison of the velocity profiles ($Ma_{\text{wall}}=0.1$ and $Kn=\lambda/H=0.1$)
- $\alpha=0.2$, buffer layer: 1 cell wide

Good agreement with reference DSMC: error <2% within the Knudsen layer
Comparison of times needed to reach a 3% error on the velocity and shear profiles

- Computational times as a function of $\alpha$ ($Ma_{\text{wall}}=0.1$ and $Kn=\lambda/H=0.1$)
- Speed-up $T_{\text{DSMC}}/T_{\text{LBM+DSMC}}$ vs $T_{\text{DSMC}}/T_{\text{Hybrid}}$
Extension to complex flow geometries
New implementation of the DSMC solver to simulate flows in complex geometries

Requirements:

✓ Fully compatible with the implementation of complex geometries in LBM
✓ Fully compatible with the developed DSMC-LBM coupling scheme
Conclusions

- LBM for slip flow regime: largest difference w.r.t. DSMC in the Knudsen layer

- A flow **domain decomposition approach** implemented: DSMC is confined in areas of large non-equilibrium effects and LBM everywhere else

- The required coupling recipes based on Grad’s formalism and Gauss-Hermite quadratures

- Good agreement is found between reference DSMC and hybrid simulations (error <2% in the Knudsen layer)

- **Large computational gain** obtained and $T_{\text{hybrid}} < T_{\text{LB+DSMC}}$

- LB in accordance with DSMC up to about $Kn=0.1$ also for more complex flows
Continuous description and need for a particle description

\[
\frac{\partial f}{\partial t} + \xi \cdot \nabla_x f + F \cdot \nabla_\xi f = Q(f, f)
\]

**Boltzmann Equation**

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0 ⇔ Kn 0.1 1 10 100 Kn ⇒ ∞

**Continuous eq. models:**
- Chapman-Enskog exp.\(^1\)
- Euler eqs.
- Navier-Stokes eqs.
- Burnett & S.-B. eqs.

\[ f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \ldots \]

**Continuous eq. models:**
- Euler eqs.
- moments method\(^2\)

5-M 13-M, 26-M, 45-M, \ldots

**Discrete particles or molecular models**

**Lattice Boltzmann**\(^3\)

**Direct Simulation Monte Carlo**\(^4\)

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\(^1\)S. Chapman and T.G. Cowling, 1970 \(^2\)H. Grad, 1949 \(^3\)S. Succi, 2001 \(^4\)G.A. Bird, 1994