A Flux-Based Approach to Hybrid Molecular Dynamics–Lattice Boltzmann Simulations

ICMMES 2011

Philipp Neumann, Calin Dan and Jens Harting

05.07.2011
Contents

Motivation & Review

Computational Methods: LB and MD

Coupling Lattice Boltzmann and Molecular Dynamics
  Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann
  Coupling: Lattice Boltzmann $\rightarrow$ Molecular Dynamics

Results

Conclusion & Outlook
Motivation

• Study the impact of surface interactions in micro-/nanofluidic devices
  → wettability, wall slip, structured/charged surfaces
• Molecular model may exist, coarse-grained wall-model shall be developed/improved
• Idea: Model surface region by (expensive) MD and bulk domain by (cheaper) LB
Motivation

- Study the impact of surface interactions in micro-/nanofluidic devices
  - wettability, wall slip, structured/charged surfaces
- Molecular model may exist, coarse-grained wall-model shall be developed/improved
- Idea: Model surface region by (expensive) MD and bulk domain by (cheaper) LB

- If surface effects matter, overlap regions may represent a huge part of the flow domain! → Try to avoid overlap domain
Motivation

- Study the impact of surface interactions in micro-/nanofluidic devices
  → wettability, wall slip, structured/charged surfaces
  - Molecular model may exist, coarse-grained wall-model shall be developed/improved
  - Idea: Model surface region by (expensive) MD and bulk domain by (cheaper) LB

- If surface effects matter, overlap regions may represent a huge part of the flow domain! → **Try to avoid overlap domain**

→ New coupling algorithm on the following slides
Review: What has been done before...

- Establishment of MD interface within LB3D
- Parallel USHER [1] implementation within LB3D
- MD–LB coupling (with overlap regions)
- Generalized Zou-He condition to allow for velocity/ density conditions in arbitrary directions [4]
Review: What has been done before...

- Establishment of MD interface within LB3D
- Parallel USHER [1] implementation within LB3D
- MD–LB coupling (with overlap regions)
- Generalized Zou-He condition to allow for velocity/ density conditions in arbitrary directions [4]

Open Points:
- How to map both velocity and density between MD and LB
- Further reduction of overlap
The Methods, Pt I: Molecular Dynamics

- Störmer-Verlet method for time integration of laws of motion
- Intermolecular interactions: (Truncated shifted) Lennard-Jones potential
- Linked-Cell method
  \[\rightarrow \text{MD cell} \leftrightarrow \text{LB cell}\]
- Periodic boundaries
The Methods, Pt II: Lattice Boltzmann

- Standard D2Q9 model with BGK approximation

\[ f_i(x + c_i dt, t + dt) = f_i(x, t) - \frac{1}{\tau} (f_i - f_i^{eq}) \]

- Periodic boundaries

- Incorporation of (external) force terms via Guo-formulation [3]
Coupling Lattice Boltzmann and Molecular Dynamics

General approach:

- Direct mapping of fluxes exchanged over the (sharp) MD–LB interface
- LB → MD: Transfer mass/ momentum from outgoing distribution functions to MD
- MD → LB: If molecules cross the MD–LB interface, translate their mass and momentum into LB distributions

One coupled step:

```
DoOneLatticeBoltzmannStep() <- LB simulation
for t=0; t < numberMDsteps; t++
    DoOneMolecularDynamicsTimestep() <- MD simulation
end
CoupleLBandMD() <- exchange fluxes
```
Algorithmic steps:

- Collect mass and momentum of particles leaving the MD domain

\[ \rho \vec{u} = \sum_{\text{known}} f_{\text{known}} \vec{c}_{\text{known}} + C_{\text{mass}} \sum_{p} m_{p} \vec{v}_{p} \]

\[ \rho \vec{u} = \sum_{\text{known}} f_{\text{known}} \vec{c}_{\text{known}} + C_{\text{momentum}} \sum_{p} m_{p} \vec{v}_{p} \]

\( \sum_{\text{known}} \) refers to the known particles in the molecular dynamics (MD) domain. \( C_{\text{mass}} \) and \( C_{\text{momentum}} \) are constants determined via periodic MD simulation.

- Reconstruct missing particle densities by Zou-He condition
Coupling: Molecular Dynamics → Lattice Boltzmann - Algorithmic steps

Algorithmic steps:

- Collect mass and momentum of particles leaving the MD domain
- Compute density and momentum in LB unit cells near MD interface:

\[
\begin{align*}
\rho &= \sum_{\text{known}} f_{\text{known}} + C_{\text{mass}} \sum_p m_p \\
\rho \vec{u} &= \sum_{\text{known}} f_{\text{known}} \vec{c}_{\text{known}} + C_{\text{momentum}} \sum_p m_p \vec{v}_p 
\end{align*}
\]

with particle mass \( m_p \), particle velocity \( \vec{v}_p \), (LB) density \( \rho \), (LB) velocity \( \vec{u} \) and constants \( C_{\text{mass}}, C_{\text{momentum}} \)
Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann - Algorithmic steps

Algorithmic steps:

- Collect mass and momentum of particles leaving the MD domain
- Compute density and momentum in LB unit cells near MD interface:

$$\rho = \sum_{\text{known}} f_{\text{known}} + C_{\text{mass}} \sum_p m_p$$

$$\rho \vec{u} = \sum_{\text{known}} f_{\text{known}} \vec{c}_{\text{known}} + C_{\text{momentum}} \sum_p m_p \vec{v}_p$$

with particle mass $m_p$, particle velocity $\vec{v}_p$, (LB) density $\rho$, (LB) velocity $\vec{u}$ and constants $C_{\text{mass}}$, $C_{\text{momentum}}$

- $C_{\text{mass}}$, $C_{\text{momentum}}$: Determined via periodic MD simulation

P. Neumann, C. Dan and J. Harting: A Flux-Based Approach to Hybrid Molecular Dynamics–Lattice Boltzmann Simulations
ICMMES 2011, 05.07.2011
Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann - Algorithmic steps

Algorithmic steps:

- Collect mass and momentum of particles leaving the MD domain
- Compute density and momentum in LB unit cells near MD interface:

$$\rho = \sum_{\text{known}} f_{\text{known}} + C_{\text{mass}} \sum_p m_p$$

$$\rho \vec{u} = \sum_{\text{known}} f_{\text{known}} \vec{c}_{\text{known}} + C_{\text{momentum}} \sum_p m_p \vec{v}_p$$

with particle mass $m_p$, particle velocity $\vec{v}_p$, (LB) density $\rho$, (LB) velocity $\vec{u}$ and constants $C_{\text{mass}}, C_{\text{momentum}}$

- $C_{\text{mass}}, C_{\text{momentum}}$: Determined via periodic MD simulation
- Reconstruct missing particle densities by Zou-He condition
**Coupling: Molecular Dynamics → Lattice Boltzmann - Algorithmic steps**

**Algorithmic steps:**

- Collect mass and momentum of particles leaving the MD domain
- Compute density and momentum in LB unit cells near MD interface:
  \[
  \rho = \sum \text{known}\ f_{\text{known}} + C_{\text{mass}} \sum p_m \rho \vec{u} = \sum \text{known}\ f_{\text{known}} \vec{c}_{\text{known}} + C_{\text{momentum}} \sum p_m \vec{v}_p
  \]
  with particle mass \( m_p \), particle velocity \( \vec{v}_p \), (LB) density \( \rho \), (LB) velocity \( \vec{u} \) and constants \( C_{\text{mass}}, C_{\text{momentum}} \):
  - Determined via periodic MD simulation
- Reconstruct missing particle densities by Zou-He condition
Zou-He:

- Problem: If \( d \) macroscopic quantities are given, the \((d + 1)\)-th quantity is automatically determined.
- However: All \( d + 1 \) quantities are dictated by the flux exchange between LB and MD.
Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann: Zou-He (1)

Zou-He:

- Problem: If $d$ macroscopic quantities are given, the $(d + 1)$-th quantity is automatically determined.
- However: All $d + 1$ quantities are dictated by the flux exchange between LB and MD.

$\rightarrow$ One more degree of freedom required!
New Zou-He-like condition:

- Compute $\rho$ and $\rho \mathbf{u}$ from black distributions and incoming (MD) fluxes
New Zou-He-like condition:

- Compute $\rho$ and $\rho \tilde{u}$ from black distributions and incoming (MD) fluxes
- Reconstruct distributions $(0,3,4,6)$
Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann: Zou-He (2)

New Zou-He-like condition:

- Compute $\rho$ and $\rho \vec{u}$ from black distributions and incoming (MD) fluxes
- Reconstruct distributions $(0, 3, 4, 6)$
Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann: Zou-He (3)

\[
\sum_{in} f_{in}^{neq} + f_{rest}^{neq} = \rho - \sum_{t} f_{t}^{eq} - \sum_{out} f_{out}^{eq} - \sum_{in} f_{in}^{eq} - f_{rest}^{eq} \tag{2}
\]

\[
\sum_{in} f_{in}^{neq} c_{in} = \rho \vec{u} - \sum_{t} f_{t} c_{t} - \sum_{out} f_{out} c_{out} - \sum_{in} f_{in}^{eq} c_{in} \tag{3}
\]
Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann: Zou-He (3)

\[
\sum_{\text{in}} f_{\text{in}}^{\text{neq}} + f_{\text{rest}}^{\text{neq}} = \rho - \sum_{\text{t}} f_{\text{t}} - \sum_{\text{out}} f_{\text{out}} - \sum_{\text{in}} f_{\text{in}}^{\text{eq}} - f_{\text{rest}}^{\text{eq}} \quad (2)
\]

\[
\sum_{\text{in}} f_{\text{in}}^{\text{neq}} c_{\text{in}} = \rho \mathbf{u} - \sum_{\text{t}} f_{\text{t}} c_{\text{t}} - \sum_{\text{out}} f_{\text{out}} c_{\text{out}} - \sum_{\text{in}} f_{\text{in}}^{\text{eq}} c_{\text{in}} \quad (3)
\]

Eq.(2) $- \mathbf{n} \cdot $ Eq.(3) yields expression for $f_{\text{rest}}^{\text{neq}}$:

\[
f_{\text{rest}}^{\text{neq}} = \rho \left(1 - \mathbf{u} \cdot \mathbf{n}\right) - \sum_{\text{t}} f_{\text{t}} - 2 \sum_{\text{out}} f_{\text{out}} - f_{\text{rest}}^{\text{eq}}
\]


\[ \sum_{in} f_{in}^{\text{neq}} + f_{\text{rest}}^{\text{neq}} = \rho - \sum_{t} f_{t} - \sum_{out} f_{\text{out}} - \sum_{in} f_{\text{in}}^{\text{eq}} - f_{\text{rest}}^{\text{eq}} \]  

(2)

\[ \sum_{in} f_{in}^{\text{neq}} c_{in} = \rho \hat{\mathbf{u}} - \sum_{t} f_{t} c_{t} - \sum_{out} f_{\text{out}} c_{\text{out}} - \sum_{in} f_{\text{in}}^{\text{eq}} c_{in} \]  

(3)

Eq.(2)–\( \vec{n} \cdot \text{Eq.}(3) \) yields expression for \( f_{\text{rest}}^{\text{neq}} \):

\[ f_{\text{rest}}^{\text{neq}} = \rho \left(1 - \hat{\mathbf{u}} \cdot \vec{n}\right) - \sum_{t} f_{t} - 2 \sum_{out} f_{\text{out}} - f_{\text{rest}}^{\text{eq}} \]

Computation of \( f_{in}^{\text{neq}} \) analogous to general Zou-He procedure
**Coupling: Lattice Boltzmann → Molecular Dynamics - Algorithmic steps**

Algorithmic steps:

- Transfer mass, momentum from outgoing pdfs to MD
- Mass insertion → USHER [1]
- Momentum transfer: Add momentum to particles over subsequent time intervals
- Apply thermostat after each momentum/mass exchange step
Coupling: Lattice Boltzmann → Molecular Dynamics - Pressure boundary condition

MD boundary:

- Exert pressure-force $f_{p\text{pressure}}$ on all particles $p$ near boundary

- Current state [2]:

$$f_{p\text{pressure}} = w_p \cdot P_{LB} \cdot C_{\text{pressure}}$$
Results: Empty Box (1)
Results: Empty Box (2)

- Use LB and MD parameter settings from Horbach and Succi [5]
  \[ k_B = 1, \nu = 0.5, \sigma = 1.0, \epsilon = 1.0, n = 0.8\sigma^{-2}, r_{\text{cutoff}} = 2^{1/6}\sigma \ldots \]

- For facilitated testing: Consider 2D scenarios

- Domain: 4 \times 4 LB cells, 4 \times 4 MD cells with 12^2 molecules/ cell

- Characteristic scales: \( dx_{LB}, dt_{LB}, m_{LB} \)
  \[ \rightarrow \text{Scale } \tau, c_s \text{ on LB side} \]
  \[ \rightarrow \text{Scale LJ-parameters on MD side, respectively} \]

- Equilibrate MD simulation first (\( \approx 10,000 \) timesteps), using periodic boundaries
Results: Empty Box (3)
Conclusion & Outlook

- New flux-based approach for spatial coupling of MD and LB:
  - No overlap region required
  - Mapping of mass and momentum fluxes by Zou-He-like boundary conditions on LB side
Conclusion & Outlook

- New flux-based approach for spatial coupling of MD and LB:
  - No overlap region required
  - Mapping of mass and momentum fluxes by Zou-He-like boundary conditions on LB side

- Future challenges:
  - Improve stability
  - Consider scenarios with (shear) velocity gradients
  - Long term: Coupling of (in-house) MD solver MarDyn and adaptive LB solver
Conclusion & Outlook: MarDyn & Peano
References

Usher: an algorithm for particle insertion in dense fluids.  
2003.

Hybrid model for combined particle and continuum dynamics.  

Discrete lattice effects on the forcing term in the lattice boltzmann method.  

Implementation of on-site velocity boundary conditions for d3q19 lattice boltzmann simulations.  

Lattice boltzmann versus molecular dynamics simulation of nanoscale hydrodynamic flows.  
Cheers...

Thank you for your attention!