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

ICMMES 2011

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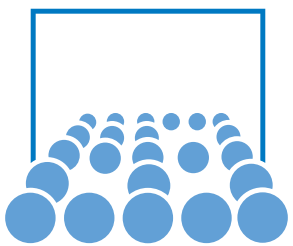

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Motivation

- Study the impact of surface interactions in micro-/ nanofluidic devices
  - $\rightarrow$ 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

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$\rightarrow$ 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]

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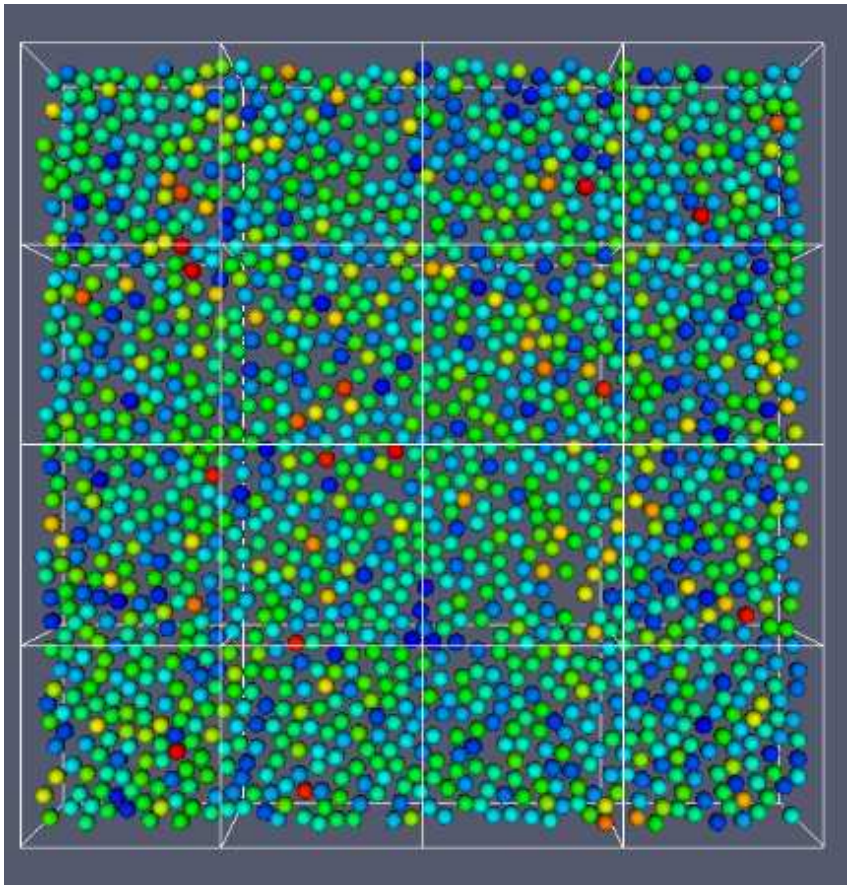
Open Points:

- 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

  $\rightarrow$ $\boxed{\text{MD cell} \Leftrightarrow \text{LB cell}}$
- Periodic boundaries

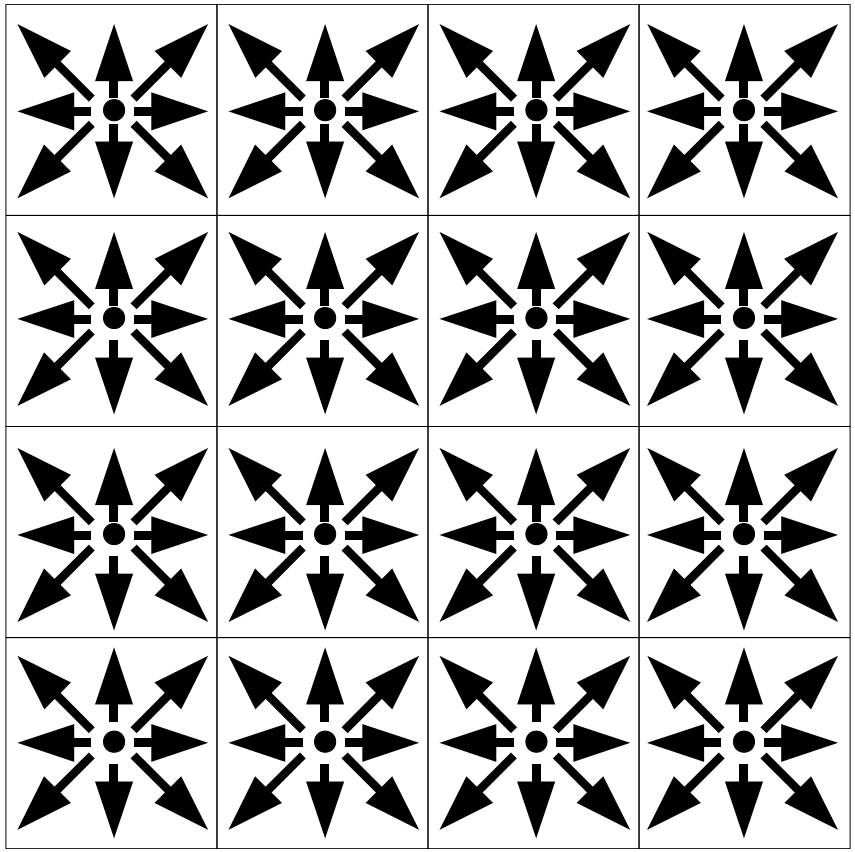


The Methods, Pt II: Lattice Boltzmann

- Standard D2Q9 model with BGK approximation

$$f_i(\mathbf{x}+\mathbf{c_i}dt, t+dt) = f_i(\mathbf{x}, t) - \frac{1}{\tau}\left(f_i - f_i^{eq}\right)$$

- 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$\rightarrow$MD: Transfer mass/ momentum from outgoing distribution functions to MD
- MD$\rightarrow$LB: If molecules cross the MD–LB interface, translate their mass and momentum into LB distributions

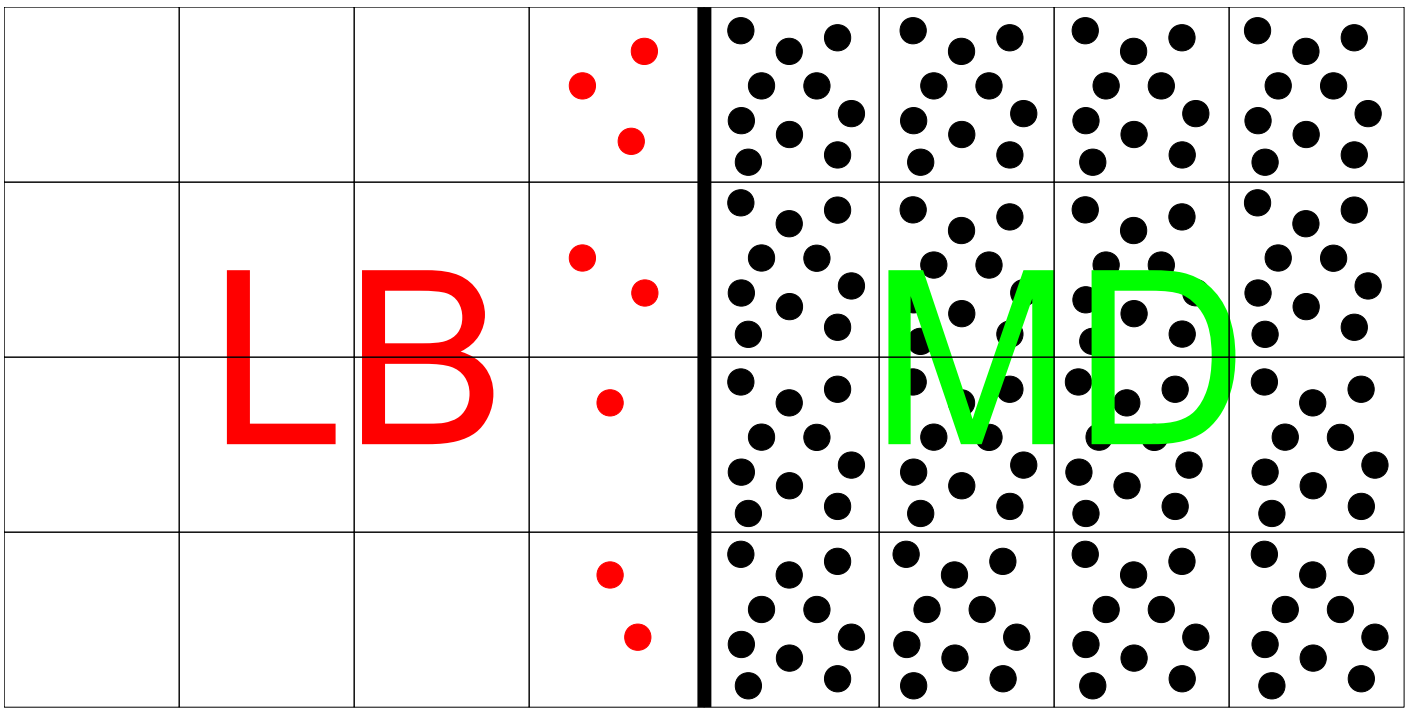
One coupled step:

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

Coupling: Molecular Dynamics → Lattice Boltzmann - Algorithmic steps

Algorithmic steps:

- Collect mass and momentum of particles leaving the MD domain



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 :

$$\begin{aligned} \rho &= \sum_{known} f_{known} + C_{mass} \sum_{p} m_p \\ \rho\vec{u} &= \sum_{known} f_{known}\vec{c}_{known} + C_{momentum} \sum_{p} m_p \vec{v}_p \end{aligned} \tag{1}$$

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

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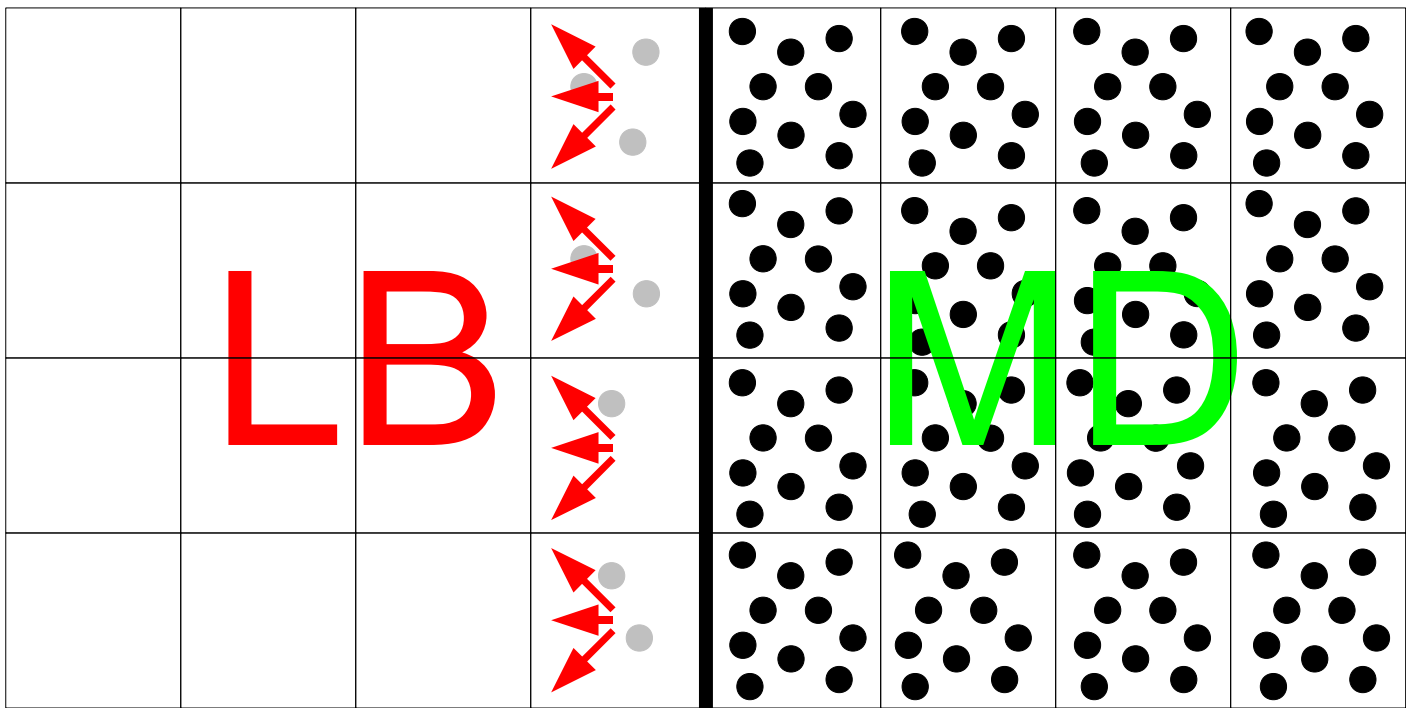
Coupling: Molecular Dynamics → Lattice Boltzmann - Algorithmic steps

Algorithmic steps:



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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

Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann: Zou-He (1)

Zou-He:

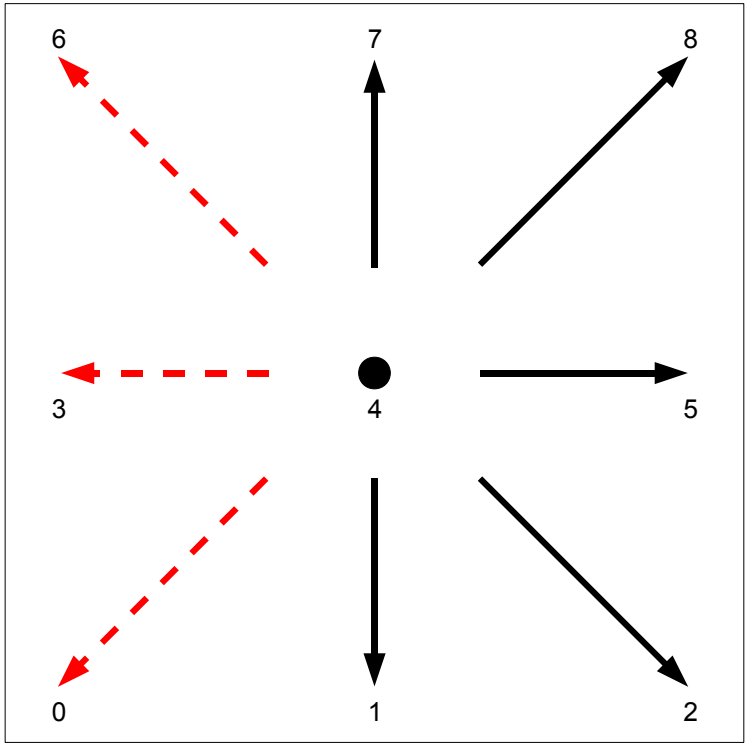
- Problem: If d macroscopic quantities are given, the $(d+1)$-th quantity is automatically determined
- However: All $d+1$ quantities are dictated by the flux exchange between LB and MD

$\rightarrow$ One more degree of freedom required!

Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann: Zou-He (2)

New Zou-He-like condition:

- Compute ρ and $\rho\vec{u}$ from black distributions and incoming (MD) fluxes



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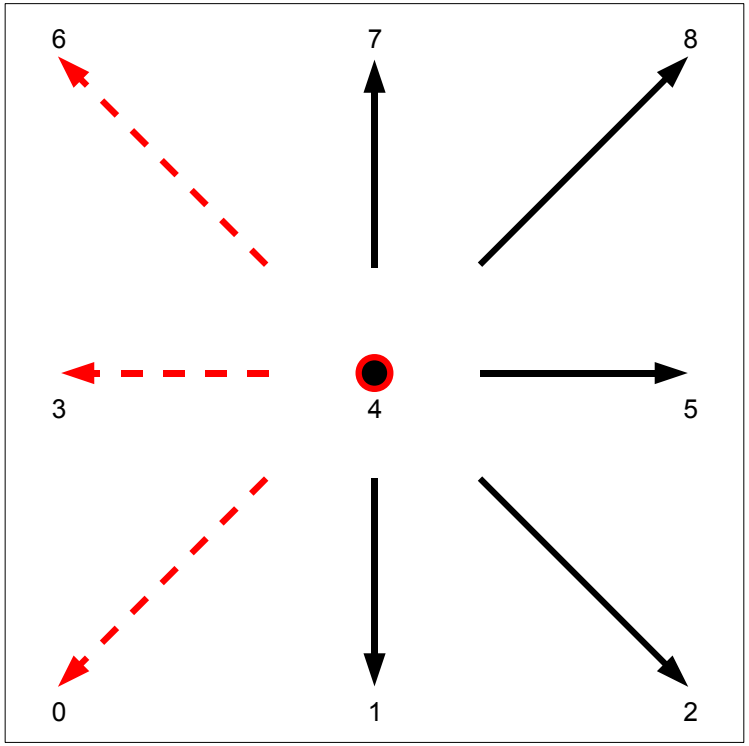

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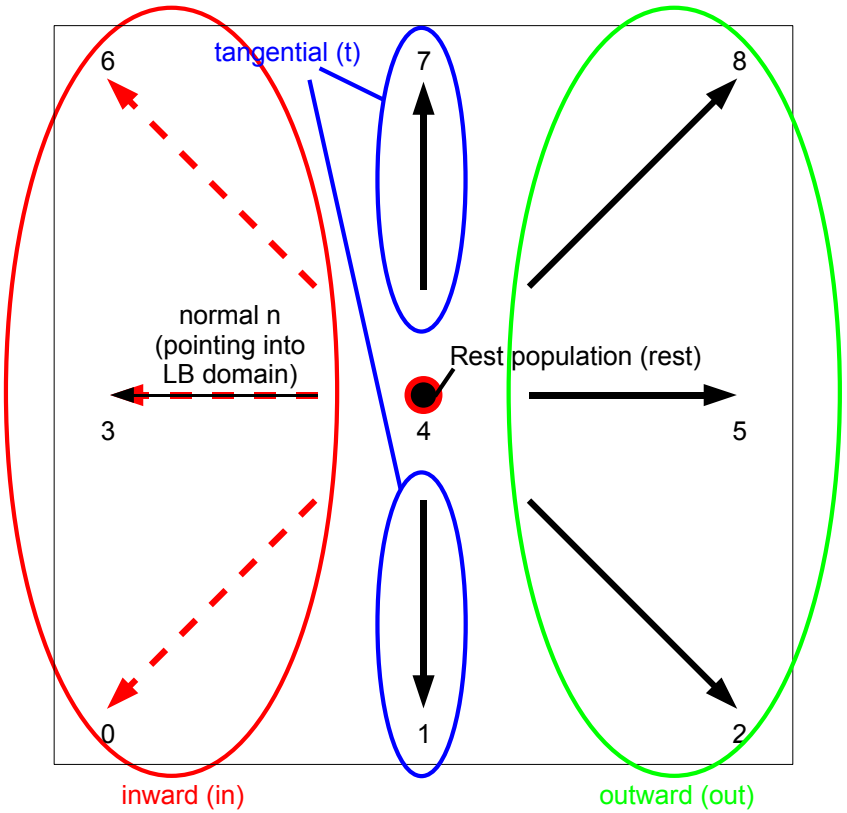

Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann: Zou-He (3)

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

$$\sum_{in} f_{in}^{neq} c_{in} = \rho \vec{u} - \sum_{t} f_t c_t - \sum_{out} f_{out} c_{out} - \sum_{in} f_{in}^{eq} c_{in} \quad (3)$$

Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann: Zou-He (3)

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

$$f_{rest}^{neq} = \rho \left(1 - \vec{u} \cdot \vec{n}\right) - \sum_{t} f_t - 2 \sum_{out} f_{out} - f_{rest}^{eq}$$

Coupling: Molecular Dynamics $\rightarrow$ Lattice Boltzmann: Zou-He (3)

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

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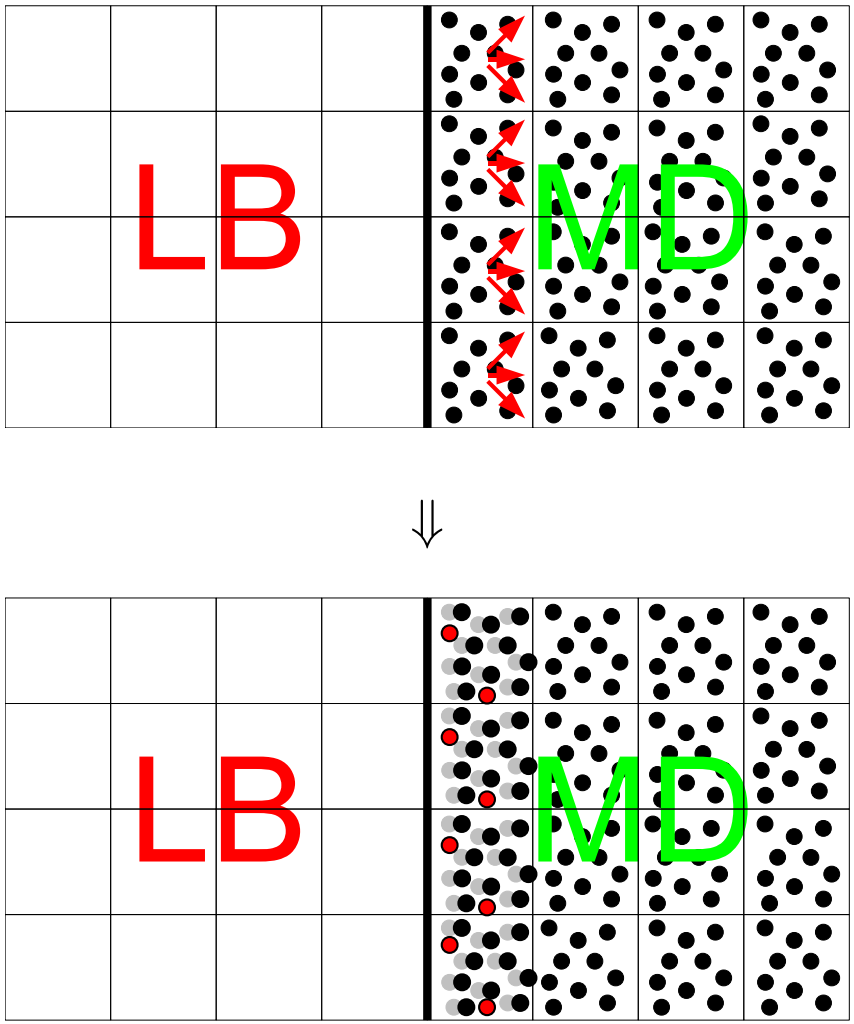
Computation of f_{in}^{neq} analogous to general Zou-He procedure

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



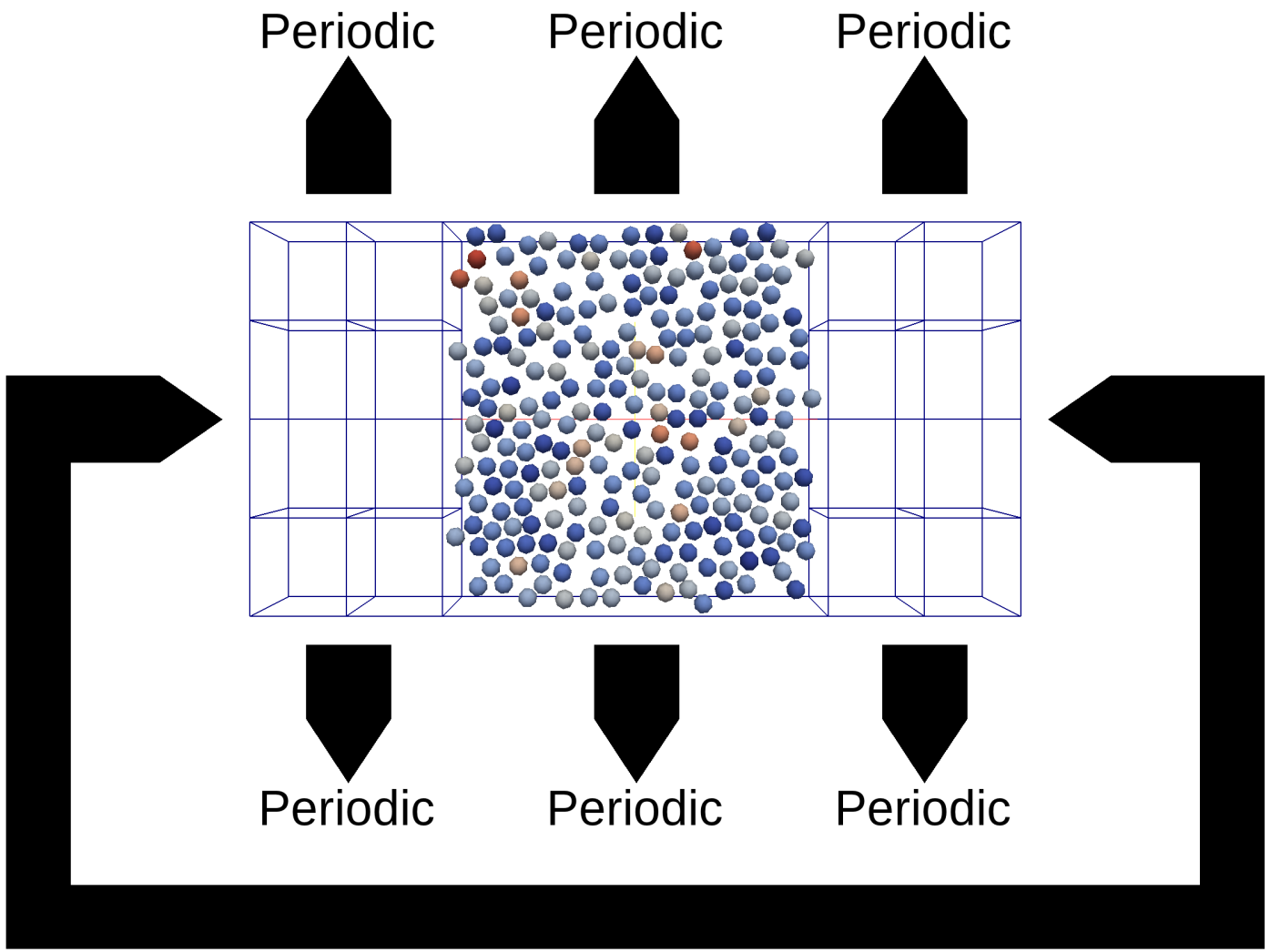
Coupling: Lattice Boltzmann $\rightarrow$ Molecular Dynamics - Pressure boundary condition

MD boundary:

- Exert pressure-force $f_{p_{pressure}}$ on all particles p near boundary
- Current state [2]:

$$f_{p_{pressure}} = w_p \cdot P_{LB} \cdot C_{pressure}$$

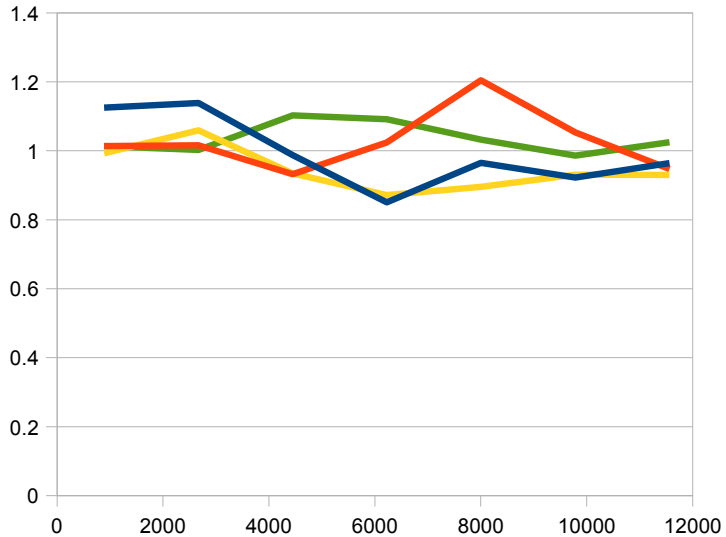
Results: Empty Box (1)

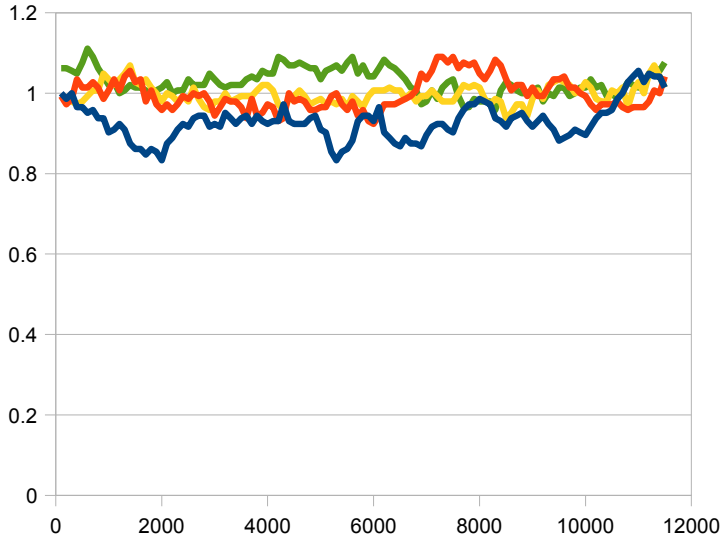


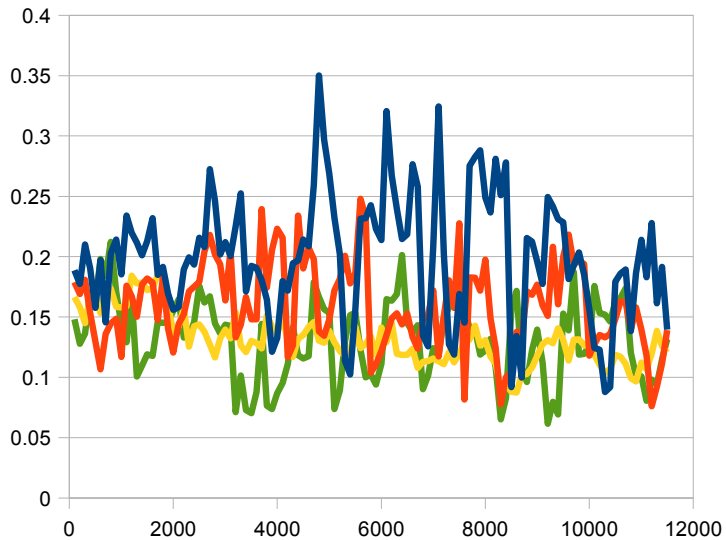
Results: Empty Box (2)

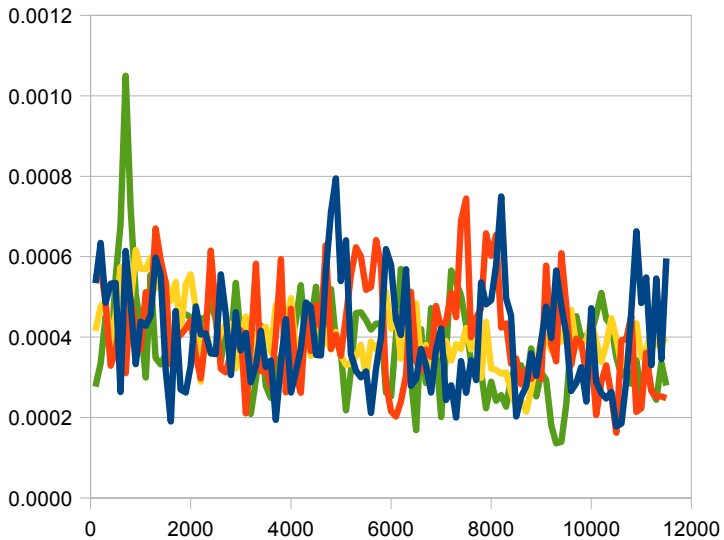
- Use LB and MD parameter settings from Horbach and Succi [5]
  $\rightarrow k_B = 1$, $\nu = 0.5$, $\sigma = 1.0$, $\epsilon = 1.0$, $n = 0.8\sigma^{-2}$, $r_{cutoff} = 2^{1/6}\sigma$ ...
- For facilitated testing: Consider 2D scenarios
- Domain: 4×4 LB cells, 4×4 MD cells with 12^2 molecules/ cell
- Characteristic scales: dx_{LB}, dt_{LB}, m_{LB}
  $\rightarrow$ Scale τ, c_s on LB side
  $\rightarrow$ Scale LJ-parameters on MD side,respectively
- Equilibrate MD simulation first ($\approx$ 10 000 timesteps), using periodic boundaries

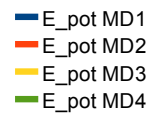
Results: Empty Box (3)











Conclusion & Outlook

- New flux-based approach for spatial coupling of MD and LB:
  - No overlap region required
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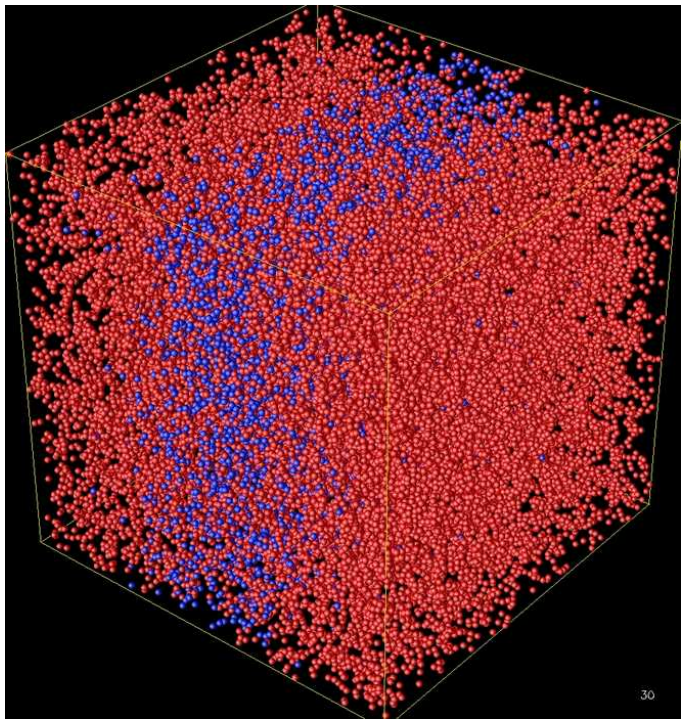
Conclusion & Outlook

- 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



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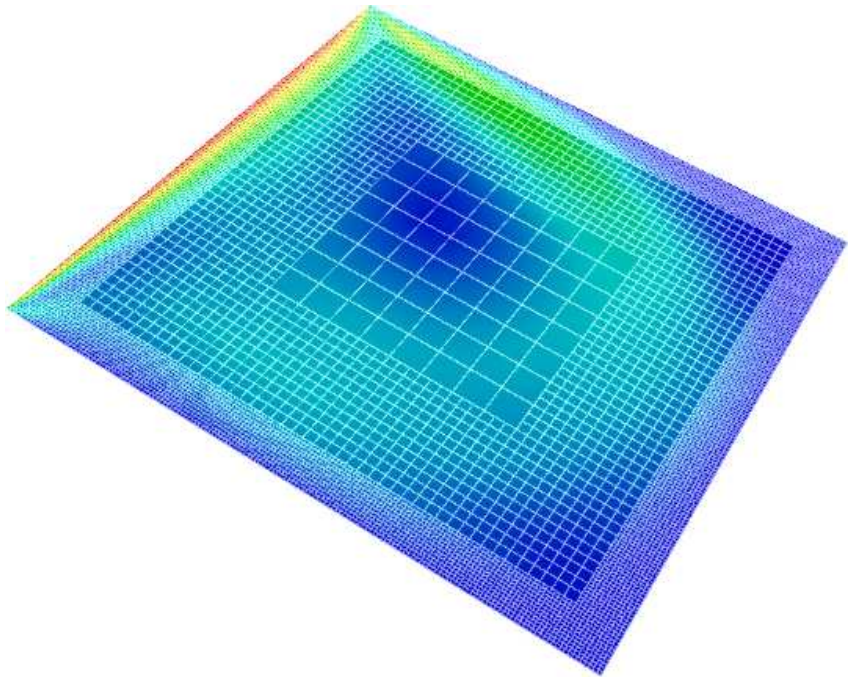

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Cheers...

Thank you for your attention!