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Applications of the Molecular Dynamics lattice gas analysis tool

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DSFD Workshop
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Acknowledgments

Introduction

- Fluid dynamics is relevant for a wide range of applications.
- Only few analytical solutions exist (limiting cases).
- We need numerical methods to solve them

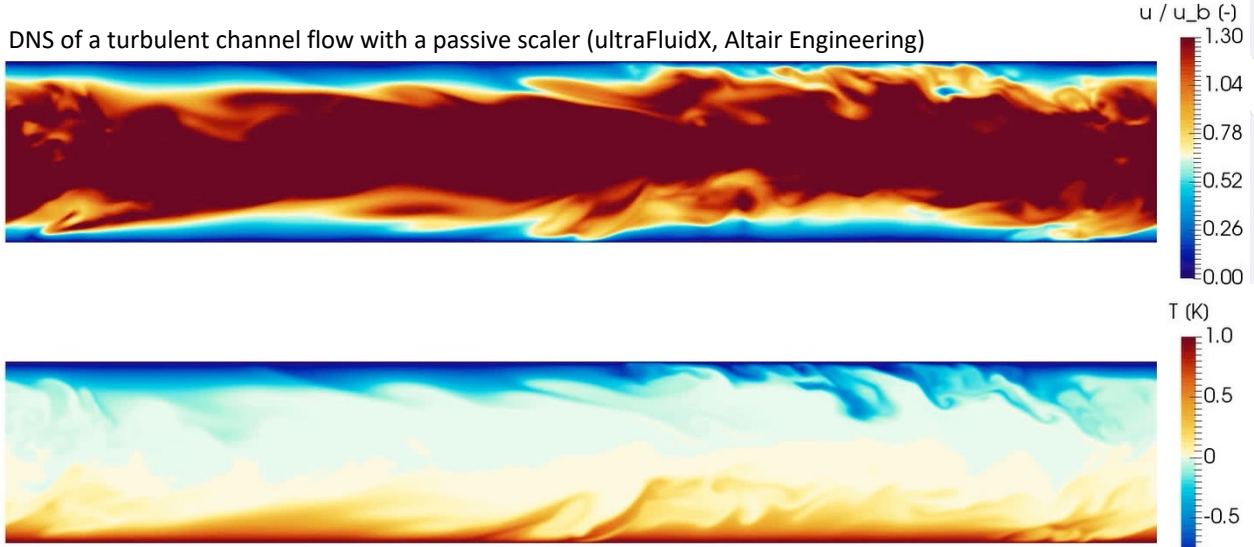
  Molecular Dynamics Simulations

  Lattice Boltzmann Methods (LBM)

  Discretization of the Navier-Stokes Equation

Heated cylinder (OpenLB, KIT)

DNS of a turbulent channel flow with a passive scaler (ultraFluidX, Altair Engineering)



Motivation

- There is a “Zoo” of LBM collision operators…

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A Model fo
Processes
P. L. Bhatnagar, E.
Phys. Rev. **94**, 511

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Physics Lette
Volume 374, Issue 34, 26 July 201

Research article

Entropic lattice Boltzmann methods

Bruce M Boghosian, Jeffrey Yepez, Peter V Coveney and Alexander Wager
Published: **08 March 2001** https://doi.org/10.1098/rspa.2000.0689

Double MRT thermal lattice Boltzmann method
for simulating conv
Ahmed Mezrhab [a], Mohammed Amine

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Computers & Mathematics with Applications
Volume 70, Issue 4, August 2015, Pages 507-547

Cascaded digital lattice Boltzmann automata for high Reynold
number flow
Martin Geier, Andreas Greiner, and Jan G. Korvink
Phys. Rev. E **73**, 066705 – Published 20 June 2006

The cumulant lattice Boltzmann equation in three dimensions: Theory and validation
Martin Geier, Martin Schönherr, Andrea Pasquali, Manfred Krafczyk

… and there is no established method to derive these collision operators from first principles.

We develop an analysis tool which derives the LBM from Molecular Dynamics simulations.

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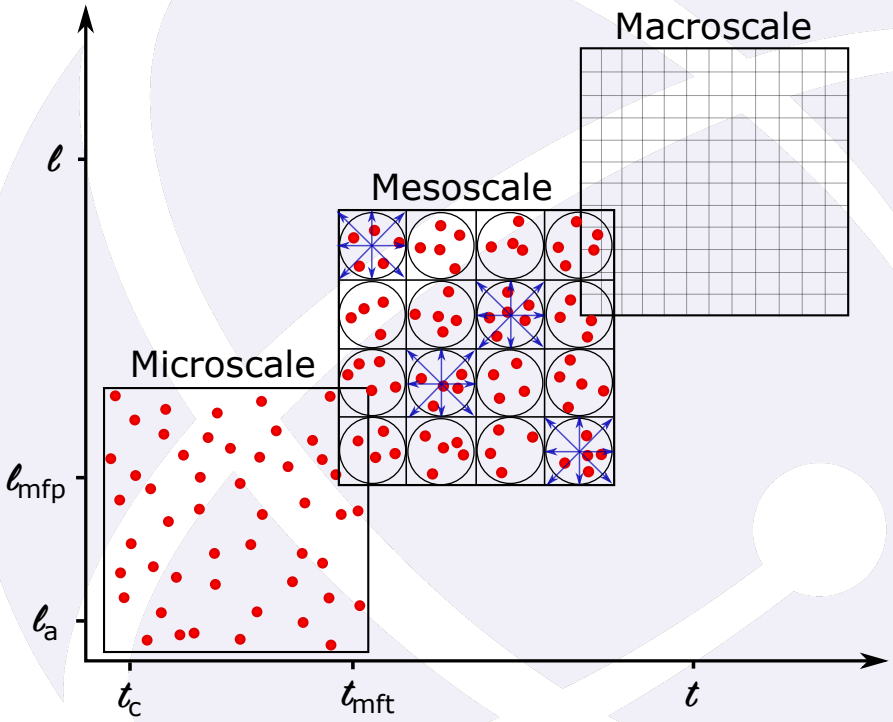
Fluid Dynamics Length and Time Scales

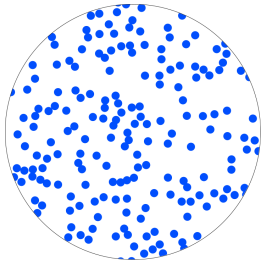
- ***Microscale*** – tracks the evolution of individual particles (Newtonain dynamics, Molecular Dynamics Simulation)
- ***Mesoscale*** – tracks the evolution of a distribution of particles (Boltzmann equation, LGCA, LBM,…)
- ***Macroscale*** – observables are quantities such as velocity and density (Navier Stokes Equation)

How can we bring some of the microscale properties to the mesoscale/macroscale?

What happens if we coarse-grain a Molecular Dynamics simulation?



Molecular Dynamics



"***Molecular Dynamics approximates a real physical system***"

– Statistical Mechanics: Theory and Molecular Simulation by M. Tuckerman

We can describe individually the fluid molecules using their positions $x_i(t)$ and velocities $v_i(t)$. The interaction between atoms is described through appropriate forces $f_i(t)$. The evolution of atoms is given by the Newton's second law:

$$\frac{d^2x_i}{dt^2} = \frac{f_i}{m_i} = \frac{1}{m_i}\sum_{j\neq i} f_{ij}$$

with velocity Verlet integrator:

$$x_i(t+\Delta t) = x_i(t) + v_i(t)\Delta t + \frac{1}{2}\frac{f_i(t)}{m_i}\Delta t^2$$

$$v_i(t+\Delta t) = v_i(t) + \frac{1}{2}\left(\frac{f_i(t)}{m_i} + \frac{f_i(t+\Delta t)}{m_i}\right)$$

Even though this approach is very successful, it is not typically used because of it's too expensive even with the current HPC technologies.

Boltzmann Equation

The kinetic theory of gases is considered a brigde between the microscale (motion of individual particles) and the macroscale (quantities such as density and velocity).

The Boltzmann Equation is given by

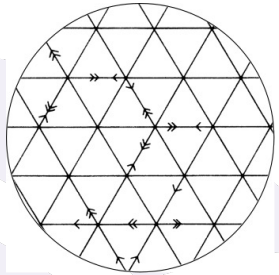
$$\underbrace{\frac{\partial f}{\partial t} + \xi_\beta \frac{\partial f}{\partial x_\beta}}_{\textit{advection}} + \underbrace{\frac{F_\beta}{\rho}\frac{\partial f}{\partial \xi_\beta}}_{\textit{forcing}} = \underbrace{\Omega(f)}_{\textit{collision rule}}$$

f – probability density function
ξ – particle velocity
Ω – collision rule (redistributes f)

The LBM is considered a numerical solver for the Boltzmann equation. However, for regimes where a good solution for the Boltzmann equation is needed, the LBM is not applicable due to the small number of discrete velocities.

This link to kinetic theory enables LBM to simulate phenomena beyond the hydrodynamic limit.

Lattice-Gas Cellular Automata (LGCA)



Lattice-Gas Cellular Automata are much cheaper than MD simulations. In LG the atoms are restricted to lattice nodes x and can move only to neighboring lattice sites $x + \delta x_i$. The local density and momentum are given by

$$\rho(x,t) = \frac{m}{v_0}\sum_i n_i(x,t); \qquad \rho(x,t)u(x,t) = \frac{m}{v_0}\sum_i c_i n_i(x,t)$$

The LGCA evolution equation reads

$$n_i(x + \delta x_i, t + \delta t) = n_i(x,t) + \Xi_i(x,t),$$

with Ξ_i being the collision operator and obeys conservation of mass and momentum.

The main characteristics of the LG are

- fully fluctuating model
- statistical noise
- many collisions to consider in higher dimensions

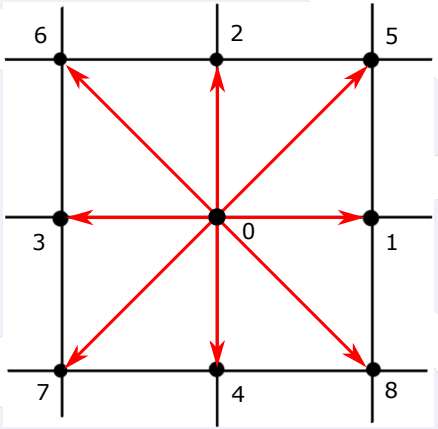
Lattice Boltzmann Method

The BGK-LBM evolution equation is given by

$$f_i(x + c_i\Delta t, t + \Delta t) = f_i(x, t) + \Omega_i(x, t)$$

which can be divided into two simple steps:

$$f_i^*(x, t) = f_i(x, t) + \Omega_i(x, t)$$
$$f_i(x + c_i\Delta t, t + \Delta t) = f_i^*(x, t)$$



The collision rule relaxes the populations towards equilibrium at some relaxation rate:

Single-Relaxation Time, Multi-Relaxation Time, Entropic, Cumulant, ...

The equilibrium distribution function is given by the second-order truncation of the Maxwell-Boltzmann distribution function

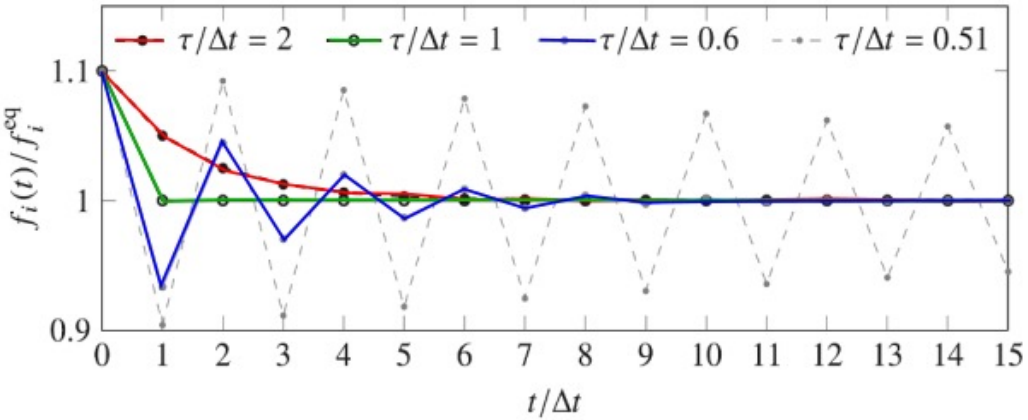
$$f_i^{eq}(x, t) = \rho w_i \left(1 + \frac{u \cdot c_i}{c_s^2} + \frac{(u \cdot c_i)^2}{2c_s^4} - \frac{u \cdot u}{2c_s^2}\right)$$

Lattice Boltzmann Method

In LBM, the BGK evolution equation can evolve in f_i immediately or even past f_i^{eq} .
Depending on the value of $\tau/\Delta t$, we define three regimes of the collision operator:

$$f_i(x + c_i\Delta t, t + \Delta t)$$

$$= \left(1 + \frac{\Delta t}{\tau}\right) f_i(x,t) + \frac{\Delta t}{\tau} f_i^{eq}(x,t)$$



Source: T. Krüger et al., *The Lattice Boltzmann Method* (2018)

Under-relaxation $\left(\frac{\tau}{\Delta t} > 1\right)$: f_i decays exponentially towards f_i^{eq};

Full relaxation $\left(\frac{\tau}{\Delta t} = 1\right)$: f_i decays directly towards f_i^{eq};

Over-relaxation $\left(\frac{1}{2} < \frac{\tau}{\Delta t} < 1\right)$: f_i oscillates around f_i^{eq} with an exponentially decreasing amplitude.

Molecular Dynamics Lattice Gas

Algorithm:

1. Impose a lattice with spacing Δx onto the MD simulation.
2. Track the current position and the position displaced by c_i after a time step Δt.

The occupation number $n_i(x,t)$ is given by

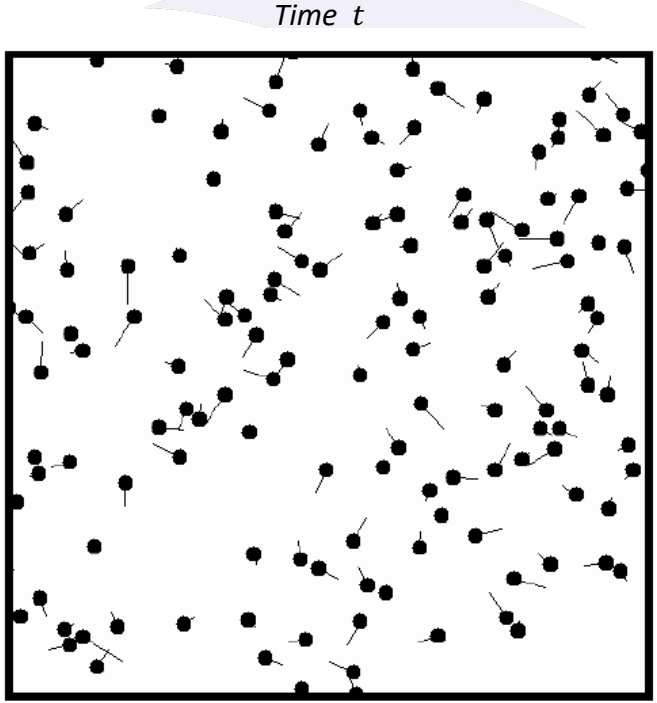
$$n_i(x,t) = \sum_j \Delta_x\left[x_j(t)\right]\Delta_{x-c_i}\left[\mathrm{x_j(t-\Delta t)}\right],$$

then the MDLG evolution equation is

$$n_i(x + c_i, t + \Delta t) = n_i(x,t) + \Xi_i,$$

and the collision term is then defined as

$$\Xi_i = n_i(x + c_i, t + \Delta t) - n_i(x,t)$$



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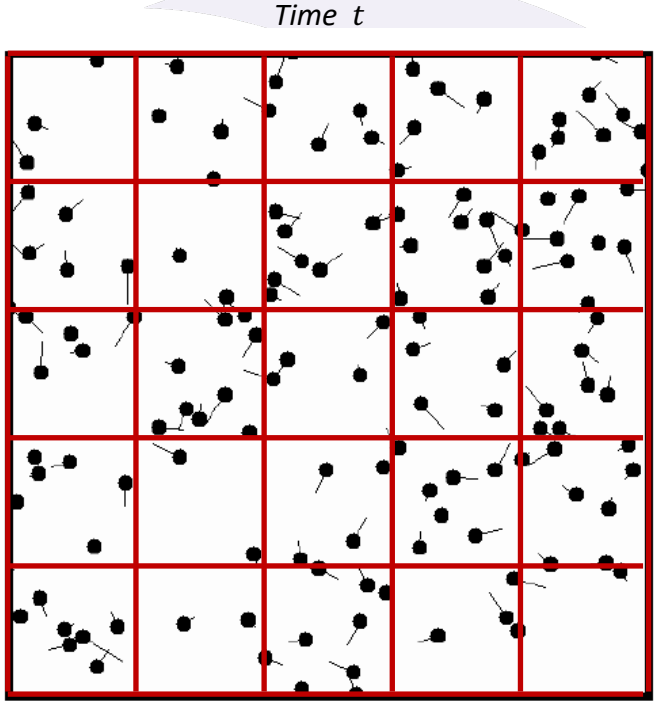

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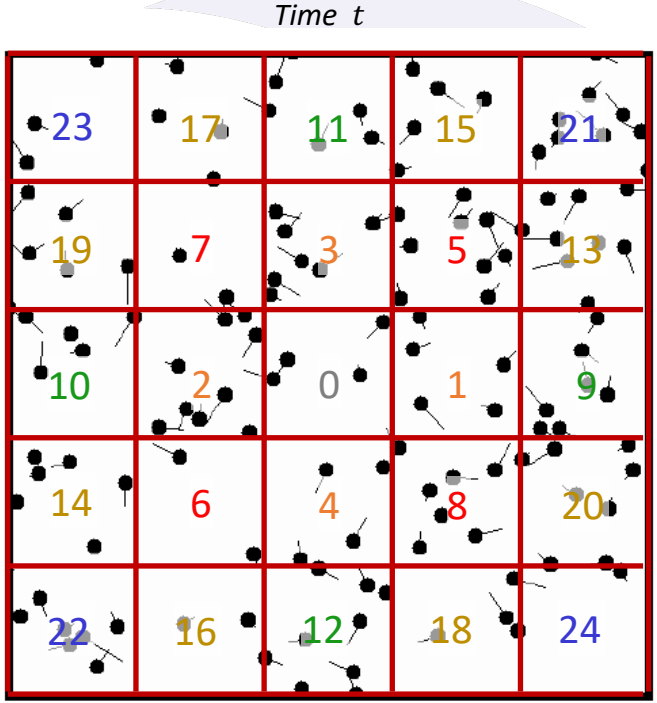

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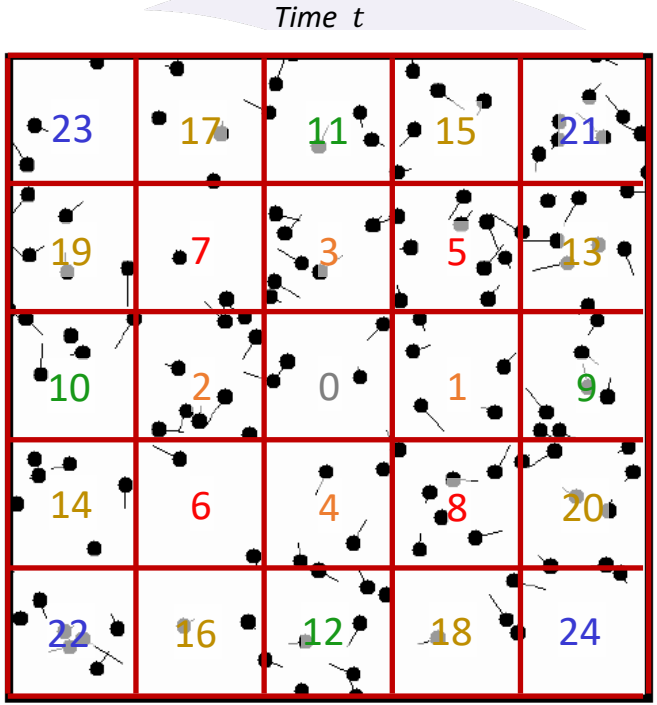

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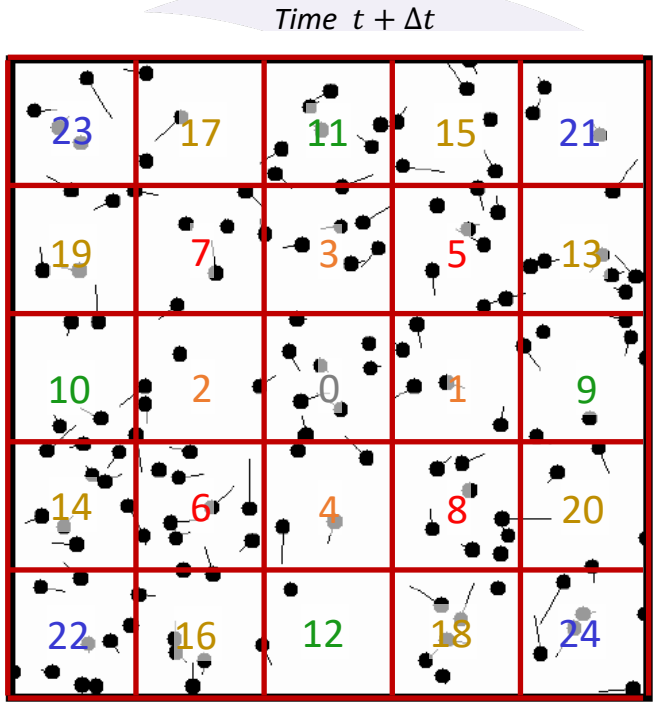

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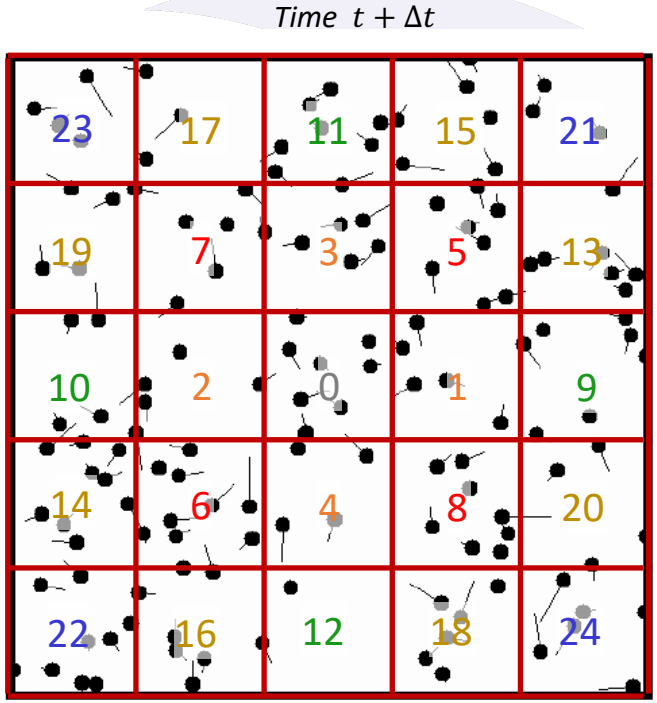

This is an Integer Lattice Gas description that measures exactly the coarse-grained properties of the underlying physical system.

Molecular Dynamics Lattice Boltzmann

If we average over an ensample of MD simulations in the same macroscopic state, we obtain a description which resembles the LBM

probability distribution function: $f_i(x,t) = \langle n_i \rangle_{neq},$

evolution equation: $f_i(x + c_i, t + \Delta t) = f_i(x,t) + \Omega_i(x,t),$

collision rule: $\Omega_i(x,t) = \langle \Xi_i \rangle_{neq}.$

We use these measurements as a ground-truth to compare to our theoretical description of the MDLG/MDLB models.

The theoretical description of the MDLB-$f_i(x,t)$ is defined as a double integral over a one-particle displacement probability distribution function, given by

$$f_i\,(x,t) = \langle n_i \rangle_{neq} = \left\langle \sum_j \Delta_x[x_j(t)]\Delta_{\mathrm{x-v_i}}[\mathrm{x_j(t-\Delta t)}] \right\rangle_{neq} = N \int dx_1 \int d\delta x_1 P^{(1)}(x_1, \delta x_1, t, \Delta t)\Delta_x[x_1]\Delta_{x-c_i}[x_1 - \delta x_1]$$

Molecular Dynamics Lattice Boltzmann

- The simplest system we can analyze is one in equilibrium:
- The probability distribution function is stationary in time
- The collision rule is equal to zero

We measure f_i^{eq} from an underlying MD simulation

1. Running MD simulations (using LAMMPS)
2. Postprocessing the MD simulations using the MDLB tool
3. Varying the discretization in time and space (Δt and Δx) to obtain results from a ballistic to diffusive description
4. Measuring the equilibrium probability distribution function (f_i^{eq}) and compare it to theory from the moments ($\langle(\delta x)^2\rangle, \langle(\delta y)^2\rangle, \langle \delta x \delta y\rangle$).

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We obtain a theory based on the probability of displacements in equilibrium

1. Since $P^{(1)}(x_1, \delta x_1, t, \Delta t)$ is Gaussian distributed for very short and very long times, originally, it was assumed that it is Gaussian throughout
2. Thus, the MDLB equilibrium distribution function is described by

$$P_\alpha^G(\delta x) = \frac{1}{[2\pi\langle(\delta x_\alpha)^2\rangle]^{1/d}} \exp\left[-\frac{(\delta x_\alpha - u_\alpha \Delta t)^2}{2\langle(\delta x_\alpha)^2\rangle}\right]$$

3. The solution factorizes for higher dimensions
4. We need to integrate over the position and the displacements in each dimension

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We obtain a theory based on the probability of displacements in equilibrium

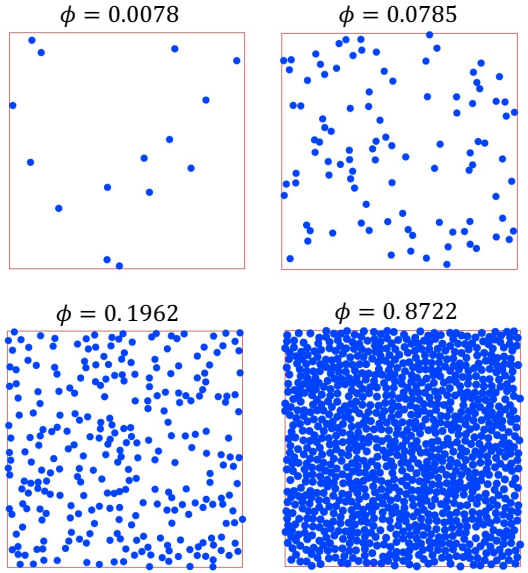
Parsa et al. found this theoretical description matches the measured equilibrium distribution function from MD.

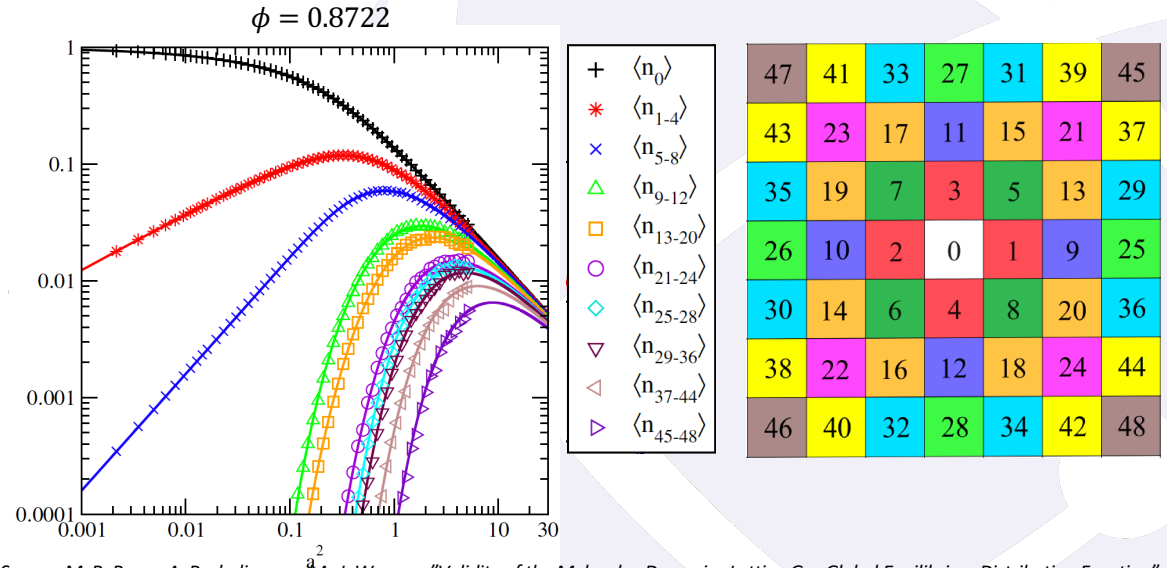
But a question remains…

To what extend is this theoretical description valid?

Validity of the MDLB equilibrium distribution function

- We vary the volume fraction ϕ of the system and compare f^{eq} measured from MD and estimated from theory using the measured $\langle(\delta x)^2\rangle$ from MD





Source: M. R. Parsa, A. Pachalieva and A. J. Wagner, "Validity of the Molecular-Dynamics-Lattice-Gas Global Equilibrium Distribution Function", International Journal of Modern Physics C, Vol. 30, No. 10, 1941007 (2019)"

The single Gaussian distirbution function is a good description for the measured f^{eq} from MD

Towards non-equilibrium dynamics

When trying to estimate the collision rule from coarse-graining of MD simulation, we observed that the collision operator does not relax towards the $f_i^{eq}(x,t)$ obtained from a single Gaussian.

$$\left|f_i(x,t) - f_i^{eq}(x,t)\right| > \left|f_i(x,t) + \Omega_i(x,t) - f_i^{eq}(x,t)\right|$$

This is concerning because in hydrodynamics, the system of interest is not too far from equilibrium, thus even small deviations in the equilibrium distribution function play a crucial role.

The only assumption for the derivation of $f_i^{eq}(x,t)$ is that $P^{(1)}(x_1, \delta x_1, t, \Delta t)$ is Gaussian distributed which must be flawed.

A key interest of having a good approximation of the equilibrium distribution function is to analyze non-equilibrium predictions of the MDLB mapping, which would be nearly impossible without an in-depth understanding of its equilibrium behavior.

Non-Gaussian MDLB equilibrium distribution function

How to measure the discrepancies between probability distribution functions?

Kullback-Leibler divergence

$$D_{KL}(R||Q) = \sum_i R(X_i)\log\left[\frac{R(X_i)}{Q(X_i)}\right]$$

Do collisions change the probability of certain displacements to occur?

Use an alternative displacement probability distribution function which considers the average number of collisions (λ) a particle has experienced.

Poisson Weighted Sum of Gaussians

$$P^{WSG}(\delta x) = \sum_{c=0}^{\infty} e^{-\lambda}\frac{\lambda^c}{c!}\frac{\sqrt{(\lambda+1)}}{\sqrt{2\pi(c+1)\langle(\delta x)^2\rangle}}\exp\left[-\frac{(\lambda+1)(\delta x - u\Delta t)^2}{2(c+1)\langle(\delta x)^2\rangle}\right]$$

The only assumptions we make is that the collisions are evenly spread instead of the more physical random collisions

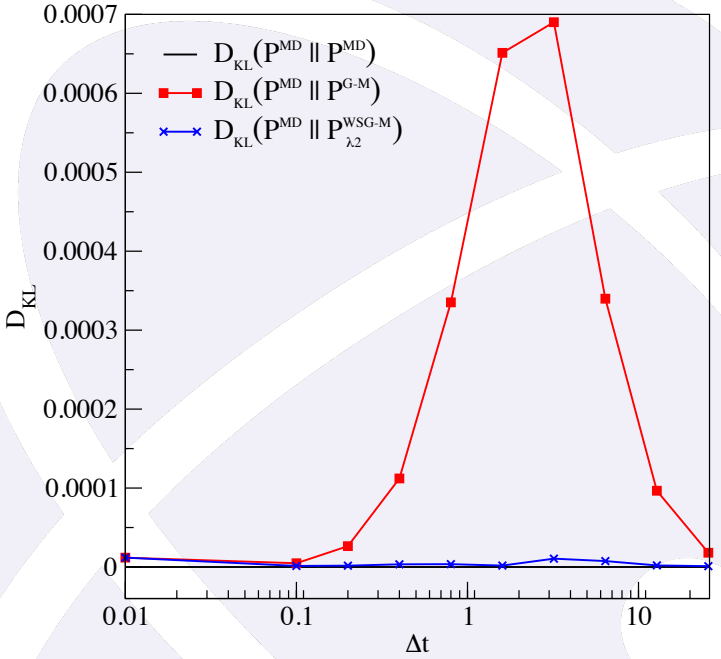
We consider the distribution function to be a *mixture of Gaussian distribution functions* that have *undergone a number of collisions given by a Poisson distribution*.

Non-Gaussian MDLB equilibrium distribution function

This is more complex $P^{(1)}(\delta x)$ and to close to system we need a good approximation of the average number of collisions λ using the second- and fourth-order moments ($\langle(\delta x)^2\rangle$ and $\langle(\delta x)^4\rangle$).

In extreme regimes (purely ballistic or purely diffusive) this description reduces again to a single Gaussian distribution function.

Follows much closely the measured probability distribution function of displacements.



The Poisson Weighted Sum of Gaussians shows a better agreement with the probability distribution function of displacements measured from MD simulations.

Source: A. Pachalieva and A. J. Wagner, "Non-Gaussian distribution of displacements for Lennard-Jones particles in equilibrium", Physical Review E, 102(5), 053310 (2020) [83]

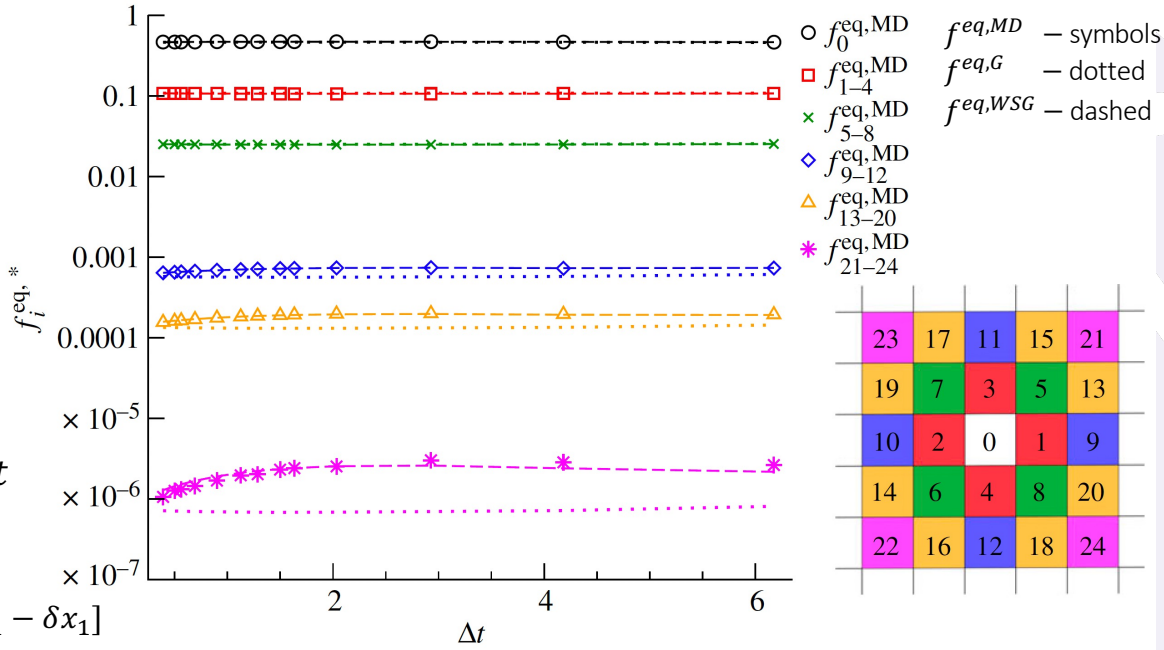
Non-Gaussian MDLB equilibrium distribution function

We apply the $P^{WSG}(\delta x)$ to obtain a new equilibrium distribution function f_i^{eq}

1. The solution factorizes for higher dimensions
2. We need to integrate over the position and the displacements in each dimension
3. We keep $a^2 = \langle(\delta x)^2\rangle/\Delta x^2 = const$

$$f_i = \langle n_i \rangle_{neq}$$

$$= N \int dx_1 \int d\delta x_1 P^{(1)}(x_1, \delta x_1, t, \Delta t)\Delta_x[x_1]\Delta_{x-v_i}[x_1 - \delta x_1]$$



The WSG equilibrium distribution function captures much better the measured equilibrium distribution function from MD simulations.

Source: A. Pachalieva and A. J. Wagner, "Molecular dynamics lattice gas equilibrium distribution function for Lennard-Jones particles", Philosophical Transactions of the Royal Society A, (2021)

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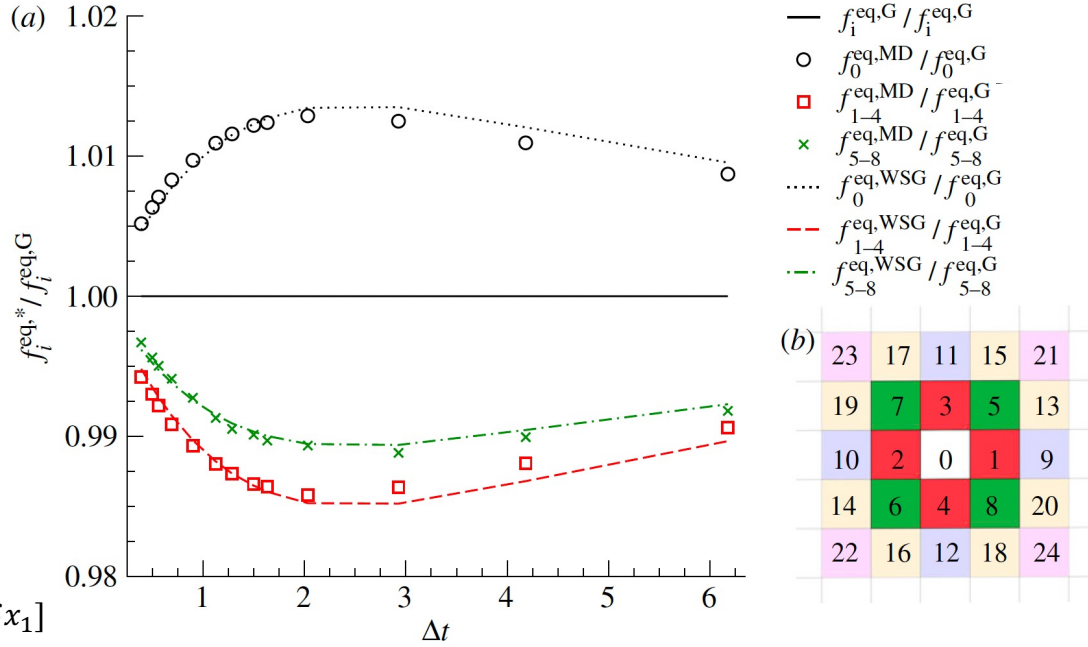

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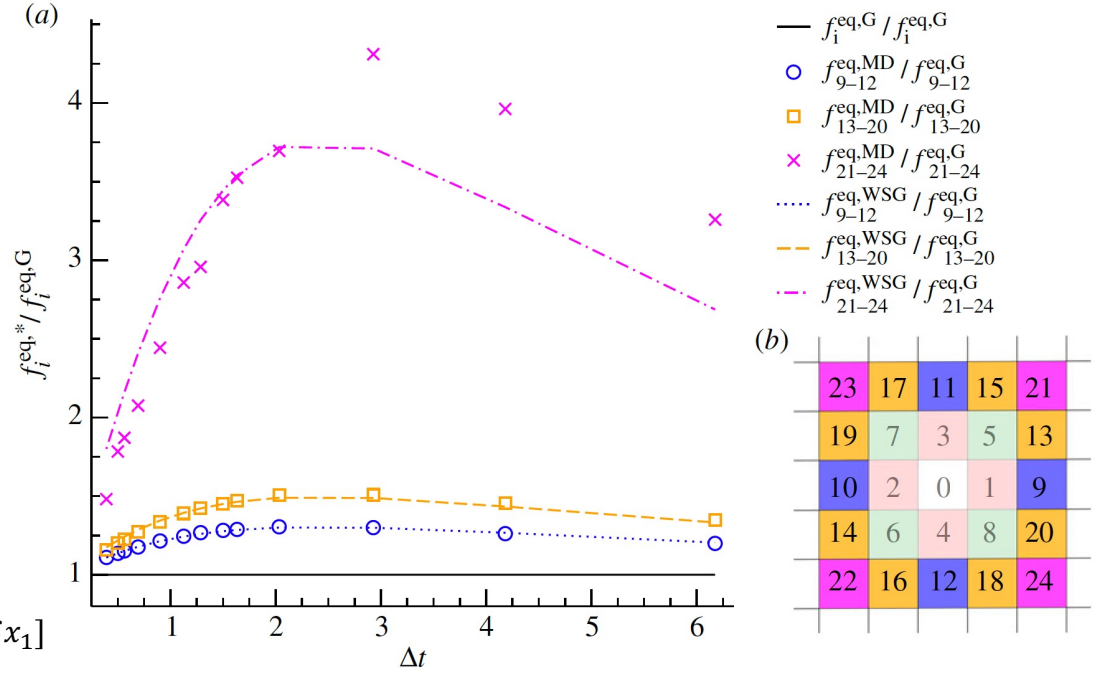

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Source: A. Pachalieva and A. J. Wagner, "Molecular dynamics lattice gas equilibrium distribution function for Lennard-Jones particles", Philosophical Transactions of the Royal Society A, (2021)

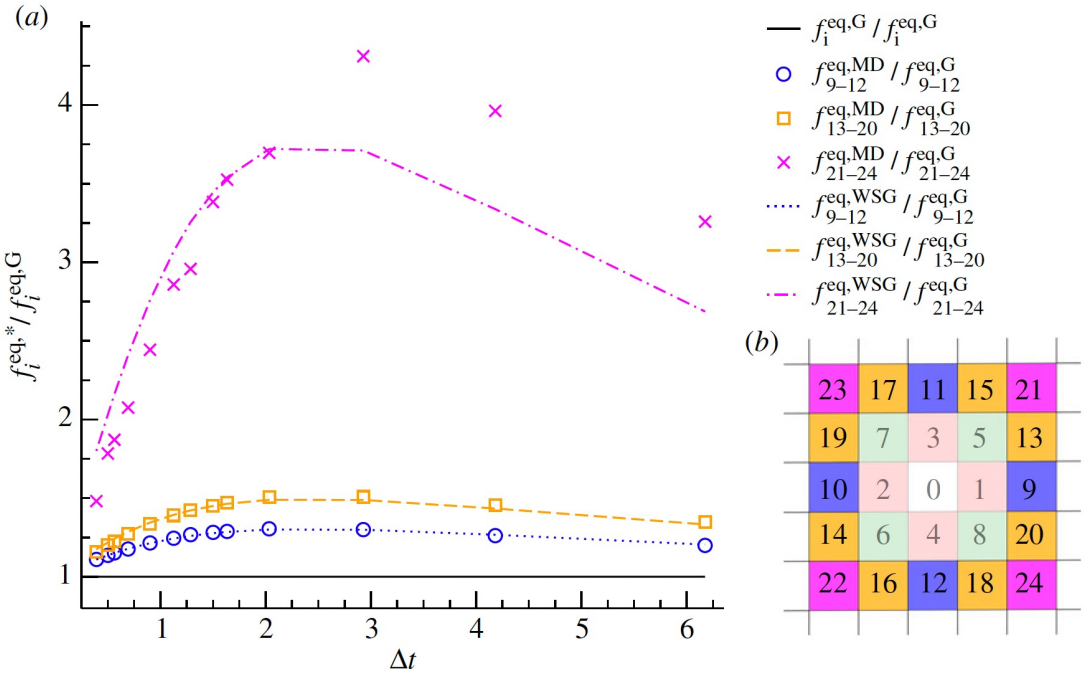
Non-Gaussian MDLB equilibrium distribution function

We apply the $P^{WSG}(\delta x)$ to obtain a new equilibrium distribution function f_i^{eq}

1. The solution factorizes for higher dimensions
2. We need to integrate over the position and the displacements in each dimension
3. We keep $a^2 = \langle(\delta x)^2\rangle/\Delta x^2 = const$

$$f_i = \langle n_i \rangle_{neq}$$

$$= N \int dx_1 \int d\delta x_1 P^{(1)}(x_1, \delta x_1, t, \Delta t)\Delta_x[x_1]\Delta_{x-v_i}[x_1 - \delta x_1]$$



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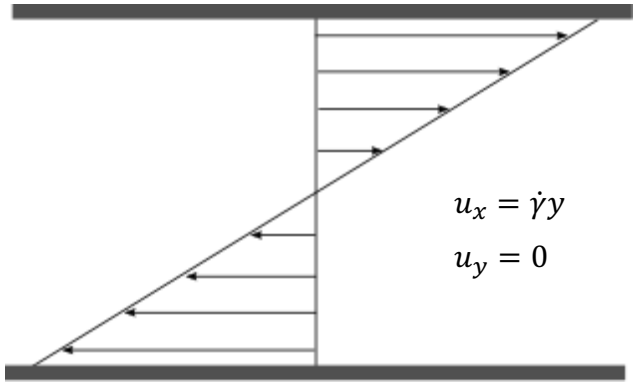
Non-equilibrium system

Simple shear flow



- symmetric system;
- averaging in space (Galilean transformation);
- averaging in time (steady state);
- linear velocity profile given by the shear rate.

LAMMPS:

- The MD simulations are performed by LAMMPS using the Lees-Edwards boundary conditions
- We use LAMMPS `nvt/sllod` thermostat to generate the desired non-equilibrium dynamics

Collecting and postprocessing sufficient data from MD was not trivial:

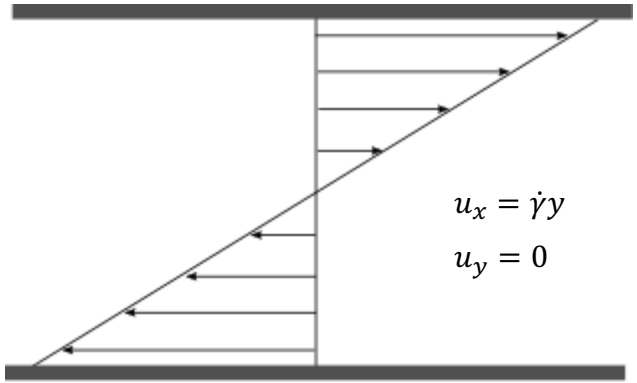
- To ensure sufficient averaging in space we use Galilean transformation
- We allow for the system to fully develop before we start collecting data to ensure that it has reached steady state and we can average in time

The MDLG Tool can be found at:

https://gitlab.lrz.de/ga35pak/MDLG_GUI

MDLB collision operator

Simple shear flow



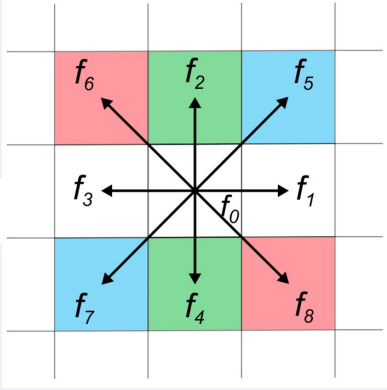
- symmetric system;
- averaging in space (Galilean transformation);
- averaging in time (steady state);
- linear velocity profile given by the shear rate.

How to measure the collision operator from MD?

$$\Omega_i = f_i(x + c_i, t + \Delta t) - f_i(x, t)$$

$$\Omega^{\alpha} = \Omega_6 - \Omega_5 + \Omega_8 - \Omega_7$$

$$\Omega^{\beta} = \Omega_2 + \Omega_4$$



Pre-collision: $M^{\alpha} = f_6 - f_5 + f_8 - f_7$

Post-collision: $M^{\alpha,*} = M^{\alpha} + \Omega^{\alpha}$

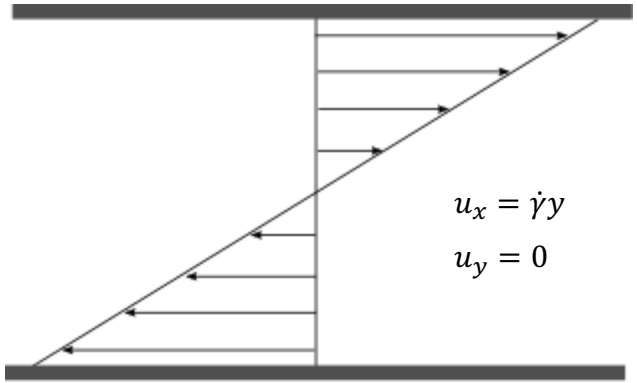
$$M^{\alpha,*} = M^{\alpha} + \frac{1}{\tau}(\overset{=0}{M^{\alpha,eq}} - M^{\alpha})$$

The relaxation time is equal to $\tau = \dfrac{M^{\alpha}}{M^{\alpha} - M^{\alpha,*}}$

Source: A. Pachalieva and A. J. Wagner, " Connecting lattice Boltzmann methods to physical reality by coarse-graining Molecular Dynamics simulations*",* arXiv:2109.05009, (2021)

MDLB collision operator

Simple shear flow



Now we need a theory for the MDLB collision operator.

- f_i can be expressed in terms of one-particle probability distribution function.
- In the diffusive limit an analytical solution exists, and it is given by a multivariate Gaussian probability distribution:

$$P(x, y, \delta x, \delta y) = \frac{\sqrt{-\frac{\langle(\delta x)^2\rangle}{\langle \delta x \delta y\rangle^2} + \frac{4}{\langle(\delta y)^2\rangle}}}{2\pi\sqrt{\langle(\delta x)^2\rangle}} exp\left(-\frac{(\delta x - y\dot{\gamma}\Delta t)^2}{\langle(\delta x)^2\rangle} - \frac{(\delta x - y\dot{\gamma}\Delta t)\delta y}{\langle \delta x \delta y\rangle} - \frac{(\delta y)^2}{\langle(\delta y)^2\rangle}\right)$$

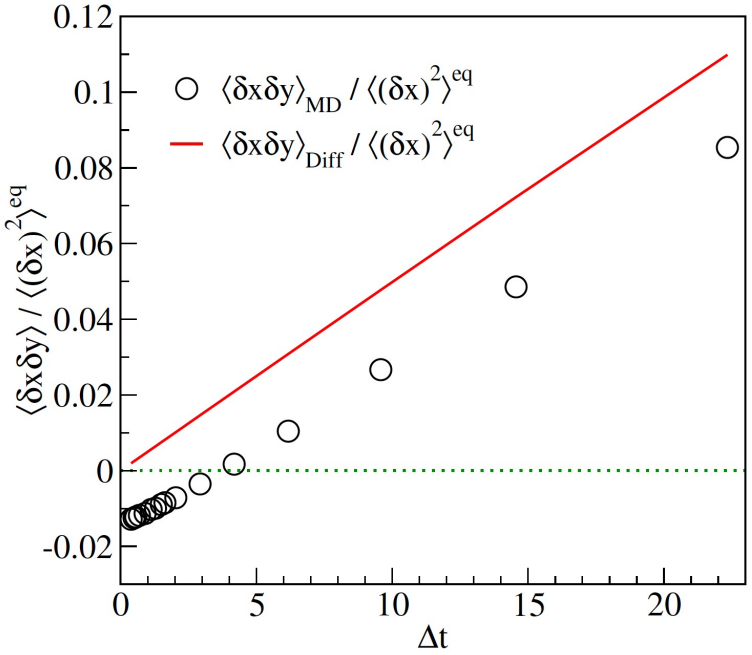
Again, to obtain the probability distribution function $f_i(x, t)$ we need to integrate over the positions (x, y) and displacements $(\delta x, \delta y)$

MDLB collision operator

For the modest shear considered here ($(\dot{\gamma}\Delta t)^2 \ll 3$),
The measured moments are

$$\langle(\delta x)^2\rangle \approx \langle(\delta y)^2\rangle \approx \langle(\delta x)^2\rangle^{eq}$$

Thus, the key change is in the off-diagonal moment $\langle\delta x\delta y\rangle$.



Ballistic behavior

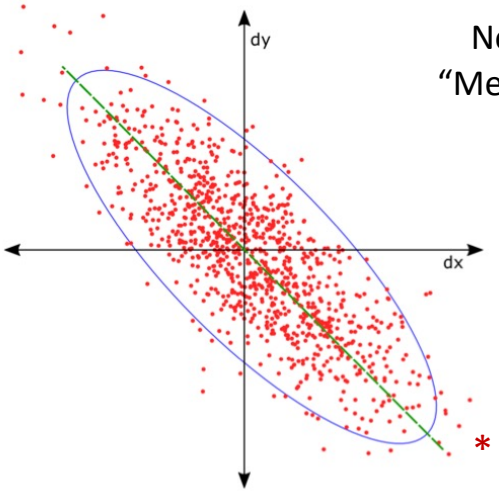
→ collisions are rare, and particles carry memory of their history over larger distances

Diffusive behavior

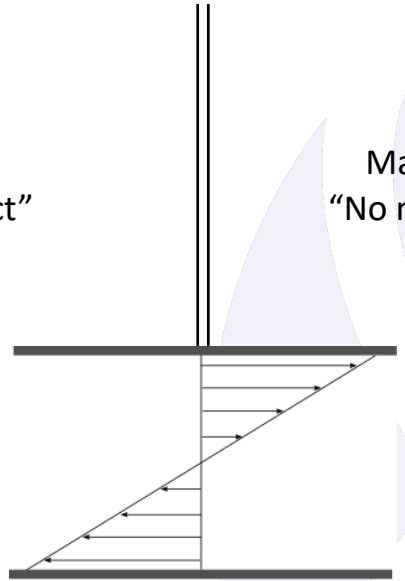
→ memory is quickly lost in frequent collisions

MDLB collision operator

DDF in Ballistic Regime
UR

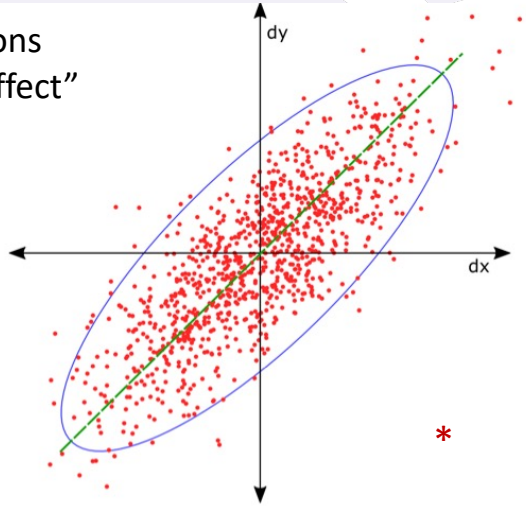


No collisions
“Memory effect”



Many collisions
“No memory effect”

DDF in Diffusive Regime
OR



In diffusive case any memory is quickly lost in frequent collisions, while in ballistic case, collisions are rare, and particles carry a memory of their history over larger distances.

** exaggerated sketch*

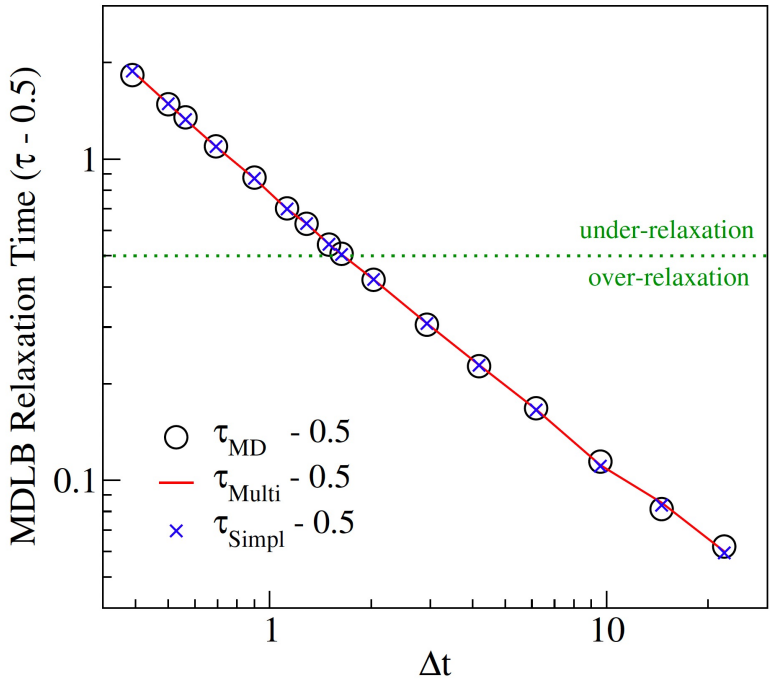
MDLB collision operator

Over-relaxation is considered to be a *numerical trick* to simulate low viscosity flows.

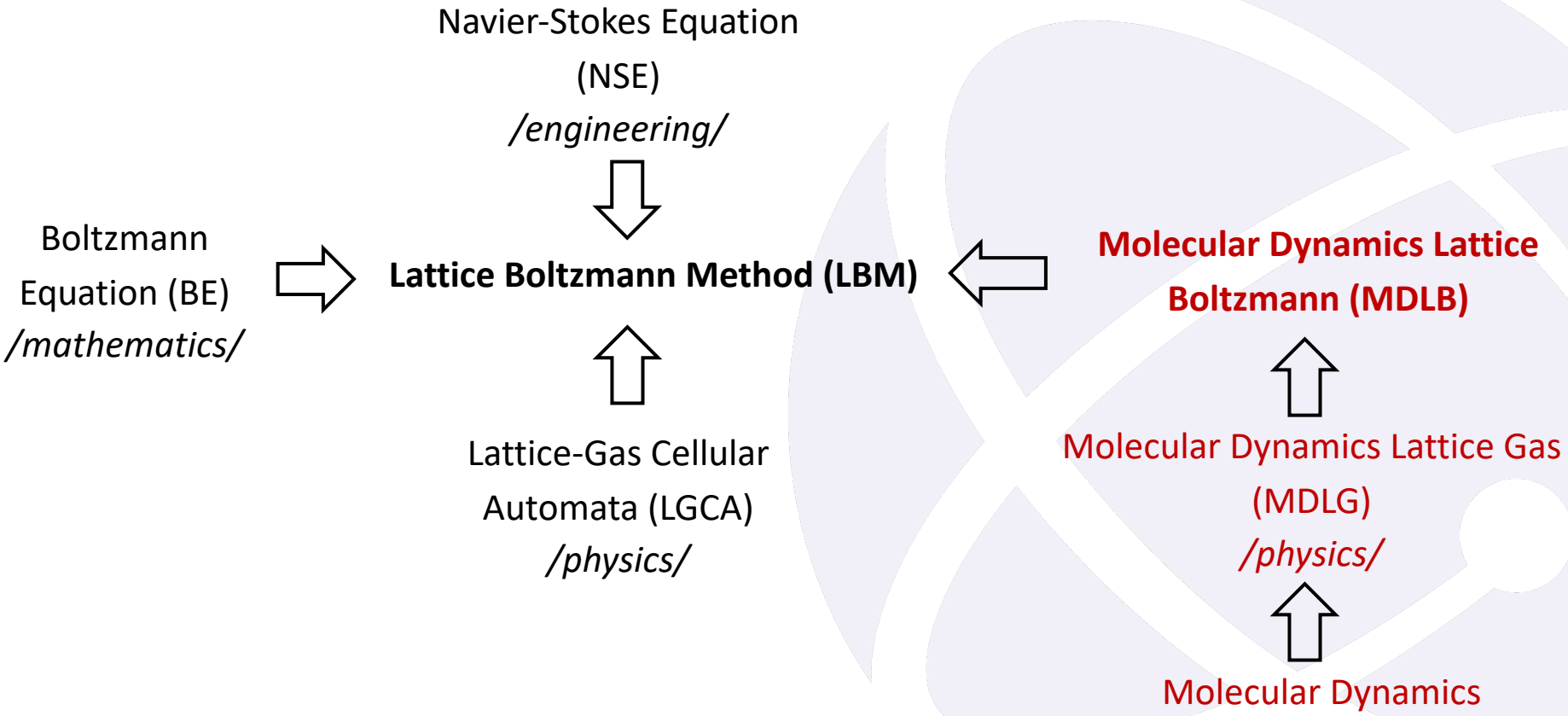
1. In general, LGCG do not show over-relaxation.
2. In [F. Bösch et al., PRL 111(9), 090601] the authors prove that over-relaxation cannot be achieved from kinetic theory.

The MDLB collision operator
naturly transitions from under- to over-relaxation.

Thus, LBM‘s over-relaxation can be derived from first principles and it is a cosequence of the coarse-grained representation of the LBM.

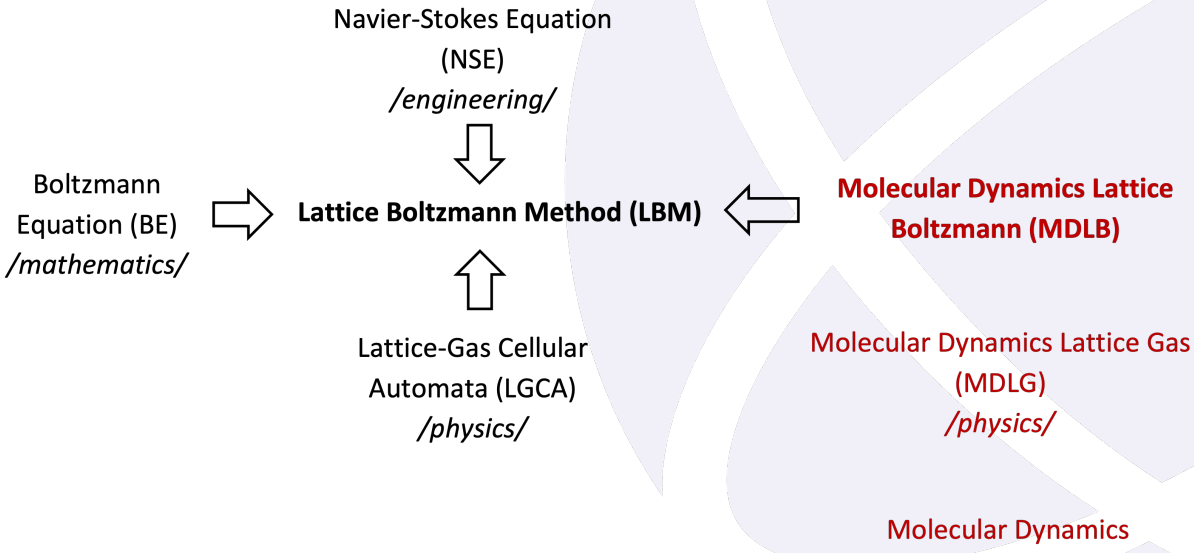


MDLB in the context of LBM



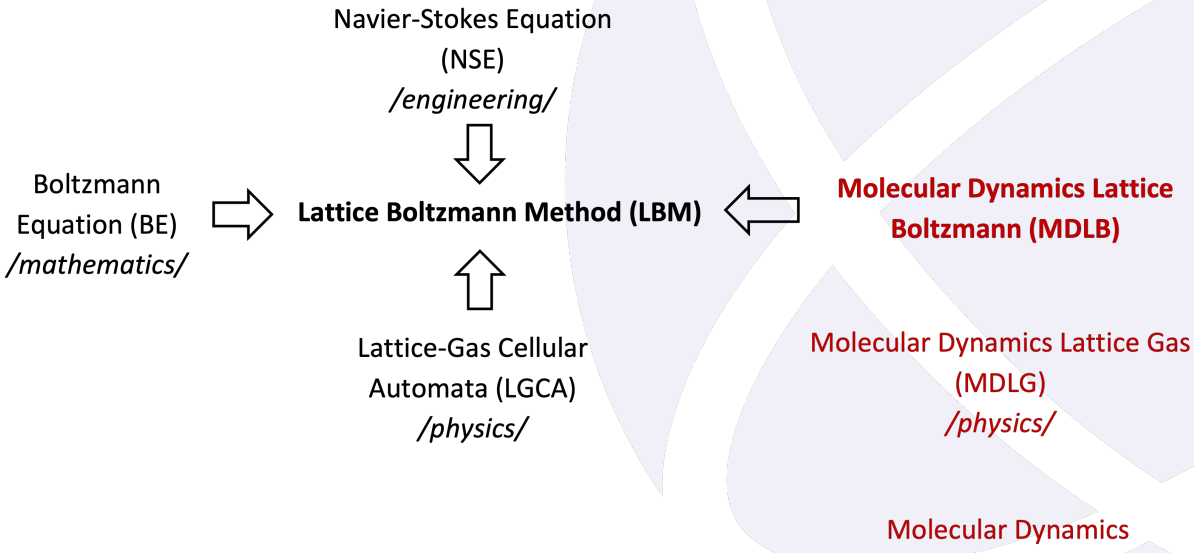
Conclusions

- Novel derivation method for the LBM from an underlying MD simulation
- To achieve this we only track the migration of particles between coarse-grained time steps, which is sufficient to derive the LBM
- MDLB restores the broken link between LBM and it‘s microscopic nature



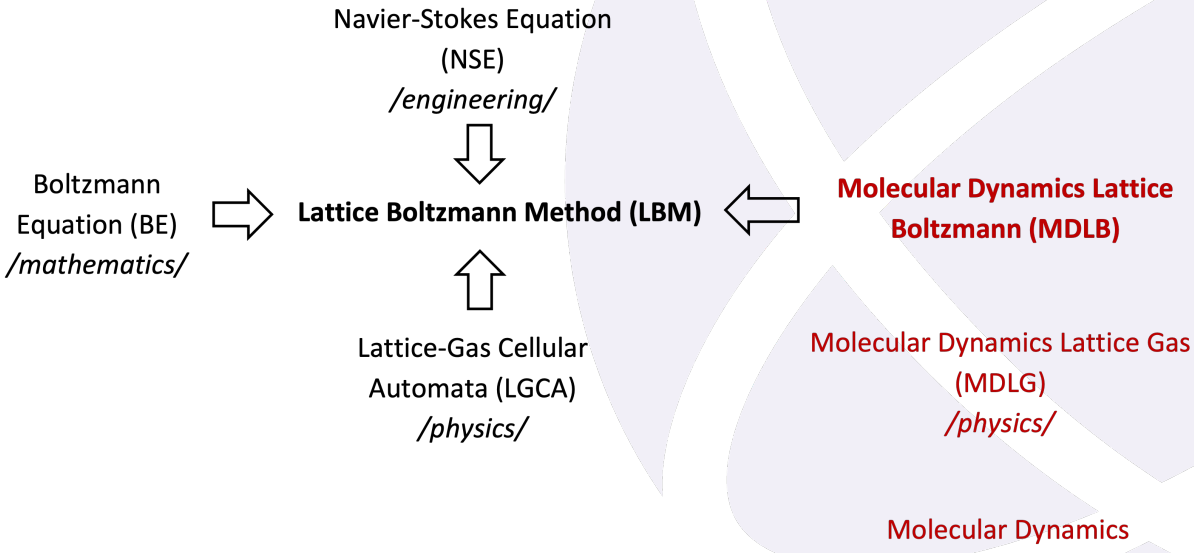
Conclusions

- MDLB has proven useful for understanding key elements of the LBM such as the equilibrium distribution function and collision operator
- We could show that the most frquently used property of the LBM – over-relaxation, arises naturally from physical lattice gases



Outlook

- True form of the collision operator: how does it relate to known collision operators?
- Apply MDLG to more complex flows such as looking at fluctuations, forcing terms, boundary conditions, multi-phase and multi-component systems, thermal models



Publications

[1] A. Pachalieva and A.J. Wagner, ”Over-relaxation as a physical effect”, *arXiv:2109.05009* (2021, submitted to *Physical Review Letters*).

[2] A. Pachalieva and A. J. Wagner, ”Molecular dynamics lattice gas equilibrium distribution function for Lennard-Jones particles”, *Philosophical Transactions of the Royal Society A*, (2021).

[3] A. Pachalieva and A.J. Wagner, ”Non-Gaussian distribution of displacements for Lennard-Jones particles in equilibrium”, *Physical Review E*, 102(5), 053310, (2020).

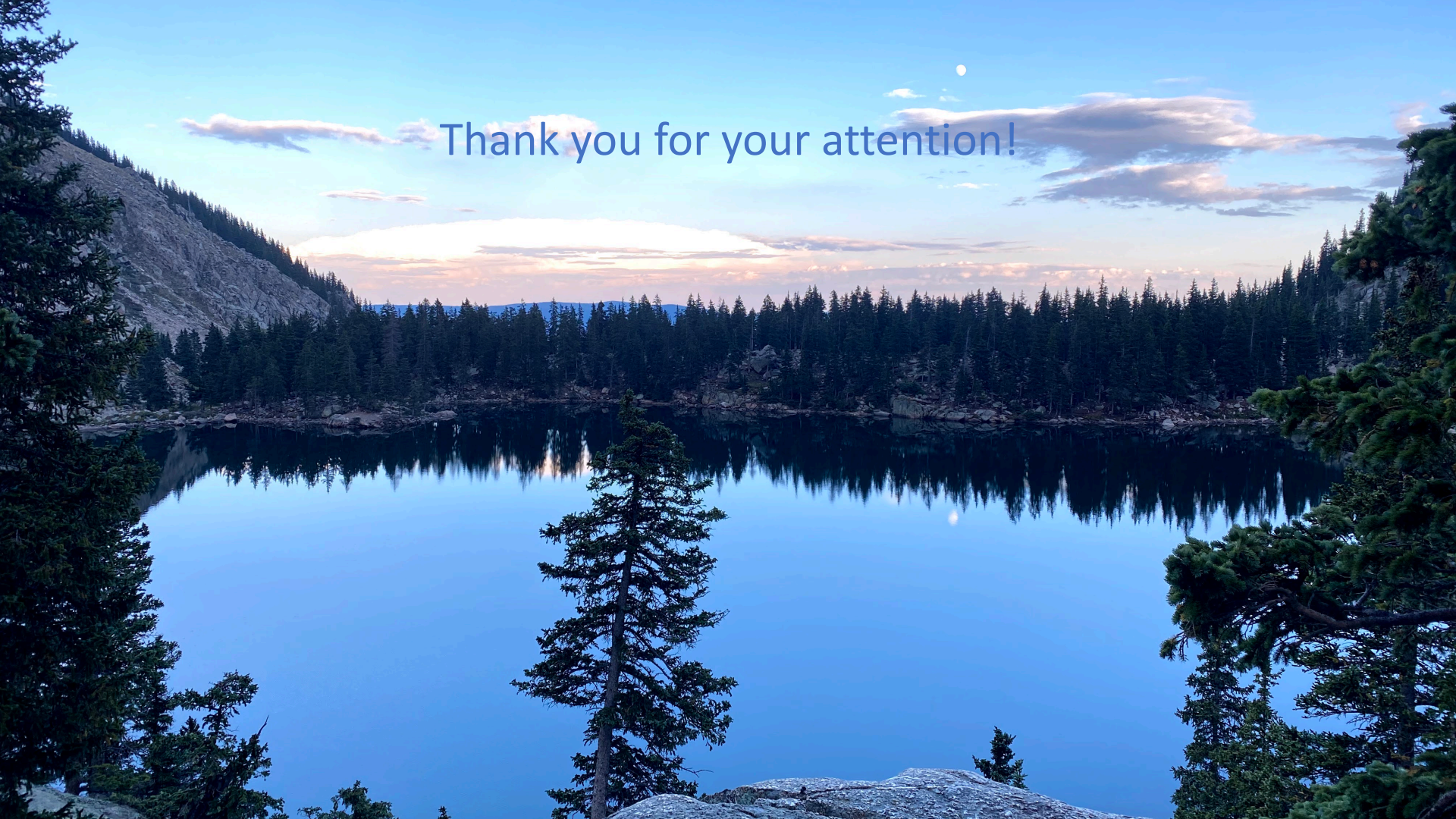
[4] M.R. Parsa, A. Pachalieva and A.J.Wagner, ”Validity of the Molecular-Dynamics-Lattice-Gas global equilibrium distribution function”, *International Journal of Modern Physics C*, Vol. 30, No. 10, 1941007, (2019).

Related publications:

[1] K. Strand and A. J. Wagner. Over-relaxation in diffusive integer lattice gas, *arXiv:2203.01380*, (2022).

[2] M.R. Parsa and A. J. Wagner. Large fluctuations in nonideal coarse-grained systems. *Physical Review Letters*, 124:234501, (2020).

[3] M.R. Parsa and A. J. Wagner. Lattice gas with molecular dynamics collision operator. *Physical Review E*, 96(1):013314, (2017).


Thank you for your attention!