Overrelaxation for Diffusive Integer Lattice Gases

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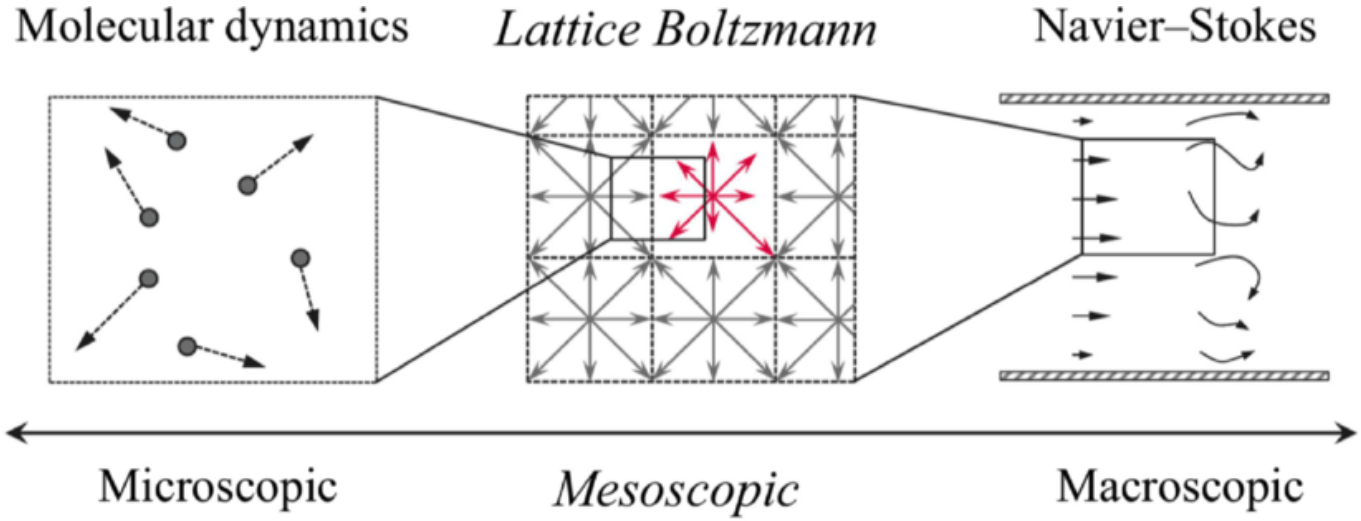
Outline

The plan for this talk is a brief introduction to integer lattice gases and overrelaxation.

1. Lattice gas and lattice Boltzmann methods
2. Integer lattice gases
3. General overview of overrelaxation
4. Overrelaxation for an integer lattice gas

Background of Lattice Boltzmann and Lattice Gas

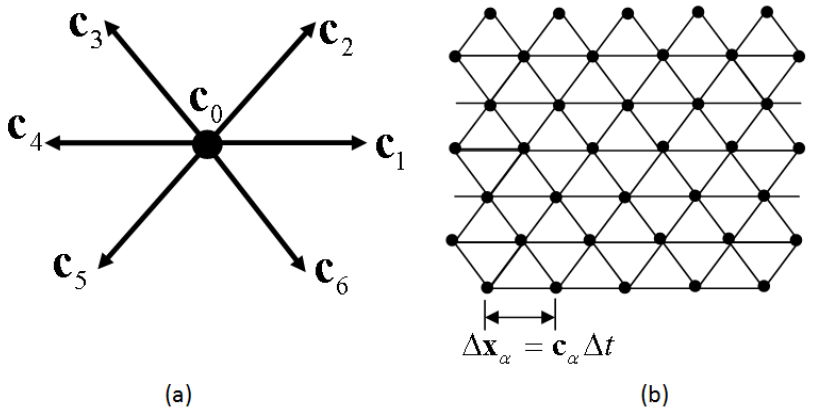
- The lattice Boltzmann method (LBM) is a computational algorithm which is commonly used for hydrodynamics.
- LBM models the dynamics of both the microscopic and macroscopic regimes by simulating discretized mesoscopic kinetic equations.
- LBM uses probability distributions of particles with explicit moments of conserved quantities to model the equations of motion.



Microscopic, mesoscopic, and macroscopic representations.
Shimpei Saito, Yutaka Abe, and Kazuya Koyama. "Lattice Boltzmann modeling and simulation of liquid jet breakup". In: *Phys. Rev. E* 96 (1 July 2017), p. 013317

How It All Got Started

- LBM was developed through its predecessor, lattice gas cellular automata (LGCA). LBM was developed to improve upon the shortcomings of LGCA methods.
- LGCA methods simulate hydrodynamics by placing discrete particles as Boolean valued occupation numbers on nodes of a hexagonal lattice. The particles are allowed to move to neighboring nodes at discrete time steps through a prescribed set of lattice velocities. If there are two or more particles which occupy a specific lattice point, the particles will undergo a collision which is designed to conserve mass and momentum.



LGCA velocity set and hexagonal lattice.

How It All Got Started

- The discrete nature of LGCA inherently includes fluctuations in the form of statistical noise.
- Although LGCA could simulate fluid systems, problems arose which seemed to limit its functionality.
  - The Boolean nature of the occupation numbers led to a Fermi-Dirac distribution rather than the expected Boltzmann distribution.
  - This Boolean nature was the reason for the exclusion principle allowing only a single particle of a given velocity at a lattice node.
  - The exclusion principle led to Galilean invariance violations.

Lattice Boltzmann Methods

Lattice Boltzmann methods (LBM) was first derived from LGCA as a Boltzmann average of the discrete model. Rather than discrete occupation numbers, lattice Boltzmann utilizes continuous particle distribution functions, $f_i(\boldsymbol{x}, t)$. The general evolution equation for LBM is written

$$f_i(\boldsymbol{x} + v_i, t + 1) = f_i(\boldsymbol{x}, t) + \Omega_i(\{f_i\}) \tag{1}$$

where $\{v_i\}$ is the set of discrete velocities at which the particle distribution functions propagate and $\Omega_i(\{f_i\})$ is a collision operator which model particle collisions and modify the distribution functions

- This version of LBM was useful for systems which a limited range of transport coefficients and in which fluctuations are not relevant.
- However, in systems with wider range of transport coefficients, this method fails and a different approach to LBM was required to expand its versatility.

Lattice Boltzmann Methods

A change in the collision by relaxing the distribution functions towards a local equilibrium allowed for higher range of transport coefficients and higher computational efficiency.

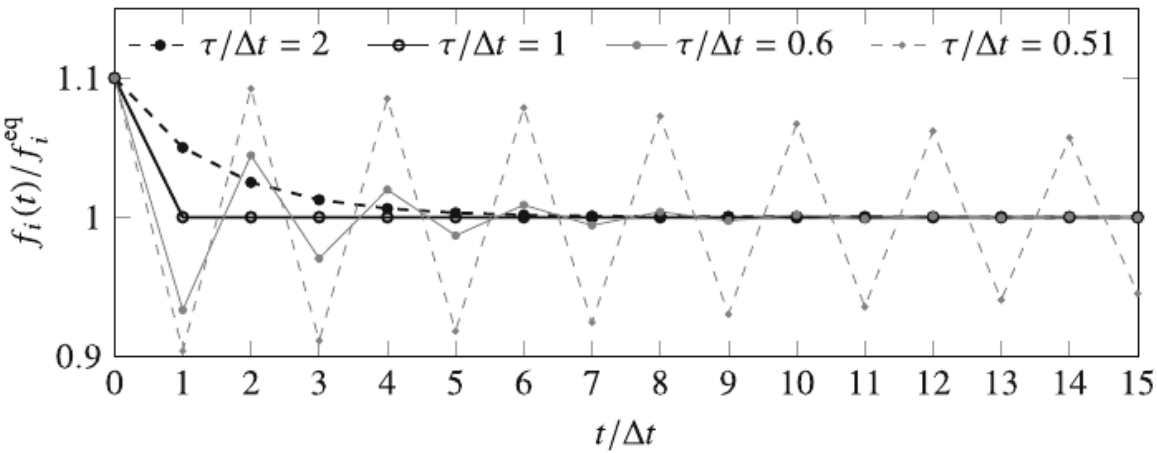
- BGK collision operator

$$\Omega_{i,BGK} = \frac{1}{\tau}(f_i^0 - f_i) \tag{2}$$

  where f_i^0 is the local equilibrium distribution.
- Occupation numbers are no longer Fermi-Dirac distributed, but follow a Maxwell-Boltzmann distribution.
  - Allowed for easier removal of Galilean invariance violations.
  - Can be overrelaxed to give a higher range of transport coefficients (low viscosity).
- This method is not derivable from LGCA.
- This can be derived from kinetic theory.

Lattice Boltzmann Methods

- The BGK collision operator in Eqn. (2) gives rise to the concept of overrelaxation.
  - Overrelaxation is a technique used in fluid dynamics in which local collisions over-shoot local equilibrium leading to an oscillating like convergence to local equilibrium.
  - Overrelaxation can be used to help to establish convergence in a diverging iterative process.
  - Overrelaxation allows to achieve lower transport coefficients (low viscosity) than could normally be achieved.
  - Utilizing a BGK collision operator will allow LBM to overrelax and explore systems not possible in the Boltzmann averaged version.



Kruger *et al.*, 2018

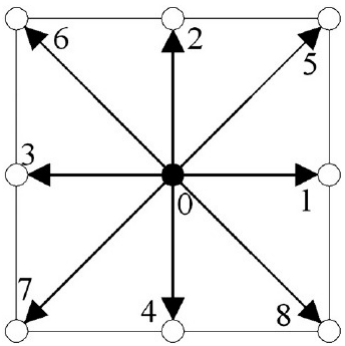
Lattice Boltzmann Methods

The distribution functions can be used to find the macroscopic quantities of a system through weighted sums known as velocity moments. For particle density, the moment is

$$\rho(\boldsymbol{x}, t) = \sum_i f_i(\boldsymbol{x}, t). \tag{3}$$

LBM models are imposed on spatial lattice of dimension, d with the number of velocities in the discrete velocity set, $\{v_i\}$, q. The LBM model is determined by the naming. convention, DdQq.

- The correct set of weights $\{w_i\}$ depends on the spatial dimensions and the choice of the velocity set and lattice temperature, θ.



Graphical representation of D2Q9 model.

Lattice Boltzmann Methods

- The LBM algorithm can be separated into two distinct steps:
  1. Collision - The local redistribution of distribution functions according to the specified rules of the collision operator.
  2. Streaming - The movement of the distribution functions on the lattice according to the velocity set.
- The collision operator $\Omega_i(\{f_j\})$ is designed to model particle collision within a system. These collisions must not modify the conserved quantities of the system.
- For diffusive systems, the collision operator must simply fulfill the following:

$$\sum_i \Omega_i(\{f_j\}) = 0. \tag{4}$$

- For diffusion, we choose an equilibrium distribution with a mean zero macroscopic velocity in the form

$$f_i^0 = \rho w_i. \tag{5}$$

Integer Lattice Gases

- Although the original Boolean LGCA methods had the ability to model Navier-Stokes equations, due to issues such as Galilean invariance violations, lattice Boltzmann methods overtook LGCA in popularity.
- It is desirable to find an LGCA from which we can derive recent versions of LBM.
- Recently, Blommel *et al.* presented a discrete lattice gas method using integer valued occupation numbers rather than the Boolean valued occupation numbers in classic LGCA.[1]
- This integer lattice gas (ILG) fully models hydrodynamic behavior and the discrete nature automatically includes fluctuations and is evolved by the equation

$$n_i(\boldsymbol{x}_i + v_i\Delta t, t + \Delta t) = n_i(\boldsymbol{x}, t) + \Xi_i(\{n_i\}) \tag{6}$$

where Ξ_i is a collision operator which uses the Monte Carlo method to determine collision rules.

[1] Thomas Blommel and Alexander J Wagner. "Integer Lattice Gas with Monte Carlo Collision Operator Recovers the Lattice Boltzmann Method with Poisson-Distributed Fluctuations". In: *Phys. Rev. E* 97.2 (2018), p. 023310.

Overrelaxation for Diffusive Integer Lattice Gas

- ILG is evolved by the equation

$$n_i(\boldsymbol{x} + v_i \Delta t, t + \Delta t) = n_i(\boldsymbol{x}, t) + \Xi_i(\{n_i\}) \tag{7}$$

  where n_i are integer valued occupation numbers and Ξ_i is the collision operator.
- By taking an ensemble average of the occupation numbers to acquire distribution functions

$$f_i = \langle n_i \rangle \tag{8}$$

- The lattice Boltzmann collision operator can also be found through an ensemble average

$$\Omega_i = \langle \Xi_i \rangle = \omega(f_i^0 - f_i). \tag{9}$$

- The ILG algorithm is relaxed by a collision probability ω.
  - For deterministic LBM collisions, $\omega \in \{0, 2\}$.
  - Since ILG collisions are probabilistic, it is only allowed that $\omega \in \{0, 1\}$.

Overrelaxation for Diffusive Integer Lattice Gas

- To successfully overrelax ILG, we must have extend the allowed range of collision probabilities to $\omega \in \{1, 2\}$.
- To remedy this mathematical impossibility, a modification to the collision process is introduced which flips the occupation numbers such that

$$F_i(n_i) = n_{-i} \tag{10}$$

where negative indices are interpreted as $v_{-i} = -v_i$, which modifies Eqn. (7),

$$n_i(\boldsymbol{x} + v_i \Delta t, t + \Delta t) = F_i(n_i) + \Xi_i(\{F_i(n_i)\}). \tag{11}$$

- This flip will send the particles back to where they were initially.
- In this form, this leads to full overrelaxation ($\omega = 2$), which fully suppresses diffusion.

Overrelaxation for Diffusive Integer Lattice Gas

- To remedy the full overrelaxation of the flip, we introduce an additional collision step to the full collision.
- This additional collision is then taken with probability $\omega^* \in \{0, 1\}$ which then determines the chance which a particle will be chosen to be flipped, thus only permuting a fraction of the particles which should be equivalent to overrelaxation seen in LBM.
  - The limiting case of $\omega^* = 1$ will redistribute all particles in the same manner as full relaxation.
- With this augmented collision, we can show that this overrelaxed ILG is equivalent to a diffusive multi-relaxation time (MRT) LBM.

Moment Space Representation

- Moment space is an eigenvector basis which will allow us to decouple each mode.
- The distribution functions are transformed from velocity space into moment space. Each moment will contain a degree of freedom.
- The forward transformation into moment space is written

$$M^a = \sum_i m_i^a f_i. \tag{12}$$

- The back transform is

$$f_i = \sum_a n_i^a M^a \tag{13}$$

- m_i^a and n_i^a are transformation matrices which have the orthogonality relations

$$\sum_i n_i^a m_i^b = \delta^{ab} \qquad \sum_a n_i^a m_j^a = \delta_{ij}. \tag{14}$$

Moment Space Representation

- To properly transform f_i to moment space, the transformation matrix must be defined.
- If we define the zeroth moment as the mass, we have $M^0 = \rho$ which is equivalent to

$$m_i^0 = (1, \ldots, 1) \tag{15}$$

  for any set of n velocities.
- The remaining elements of the transformation matrix can be derived through a Gram-Schmidt orthonormalization.
- Since moment space gives access to individual moments, we can assume that the moment space representation of the collision matrix is diagnoal such that

$$\Lambda^{ab} = \frac{1}{\tau^a}\delta^{ab} \tag{16}$$

  where τ^a is the relaxation time which corresponds to a given moment a.

Moment Space Representation

- The construction of this transformation matrix is dependent on the number of desired modes in the model.
- For a D1Q3 model:

$$m_i^a = \begin{pmatrix} 1 & 1 & 1 \\ 0 & \sqrt{\frac{1}{\theta}} & -\sqrt{\frac{1}{\theta}} \\ -\sqrt{\frac{\theta}{1-\theta}} & \sqrt{\frac{1-\theta}{\theta}} & \sqrt{\frac{1-\theta}{\theta}} \end{pmatrix} \tag{17}$$

- For a D2Q5 model:

$$m_i^a = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & \sqrt{\frac{1}{\theta}} & -\sqrt{\frac{1}{\theta}} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{\frac{1}{\theta}} & -\sqrt{\frac{1}{\theta}} \\ 0 & \sqrt{\frac{1}{2\theta}} & \sqrt{\frac{1}{2\theta}} & -\sqrt{\frac{1}{2\theta}} & -\sqrt{\frac{1}{2\theta}} \\ -\sqrt{\frac{2\theta}{1-2\theta}} & \sqrt{\frac{1-2\theta}{2\theta}} & \sqrt{\frac{1-2\theta}{2\theta}} & \sqrt{\frac{1-2\theta}{2\theta}} & \sqrt{\frac{1-2\theta}{2\theta}} \end{pmatrix} \tag{18}$$

Overrelaxation for Diffusive Integer Lattice Gas

- In the Boltzmann limit, Eqn. (11) becomes

$$f_i(\boldsymbol{x}+v_i\Delta t, t+\Delta t) = F_i\left[f_i(\boldsymbol{x},t)\right]+\omega\{f_i^0(\boldsymbol{x},t)-F_i\left[f_i(\boldsymbol{x},t)\right]\} \tag{19}$$

- If we invoke a moment space transformation, we can gain access to the individual moments of the physical quantities

$$M^a = \begin{pmatrix} \sum_i f_i \\ \sum_i v_i f_i \\ \sum_i v_i^2 f_i \end{pmatrix} = \begin{pmatrix} \rho \\ j \\ \Pi \end{pmatrix}. \tag{20}$$

- Applying our flipping operation gives

$$F(M^a) = \begin{pmatrix} \rho \\ -j \\ \Pi \end{pmatrix}. \tag{21}$$

- In general, all even velocity moments are unaffected by the flipping operation and all odd moments acquire a negative sign.

Overrelaxation for Diffusive Integer Lattice Gas

- The effect of the collision is similarly simple such that conserved quantities are unaffected and non-conserved quantities are multiplied by the probability ω.
- This gives the full effect of the collision operator as

$$M^a + \Omega^a = \begin{pmatrix} \rho \\ (1-\omega^j)j \\ (1-\omega)\Pi \end{pmatrix} \tag{22}$$

  where we have introduced $\omega^j = 2 - \omega$.
- With this, the corresponding lattice Boltzmann equation becomes

$$f_i(x + v_i\Delta t, t + \Delta t) = \sum_a w_i m_i^a (1-\omega^a) m_j^a (f_j^0 - f^j), \tag{23}$$

  where m_i^a are moment space transformation matrices.

Overrelaxation for Diffusive Integer Lattice Gas

- Taking the Boltzmann limit of Eqn. (23), we obtain the diffusion equation

$$\partial_t \rho = -D\nabla^2 \rho \tag{24}$$

with a diffusion constant of

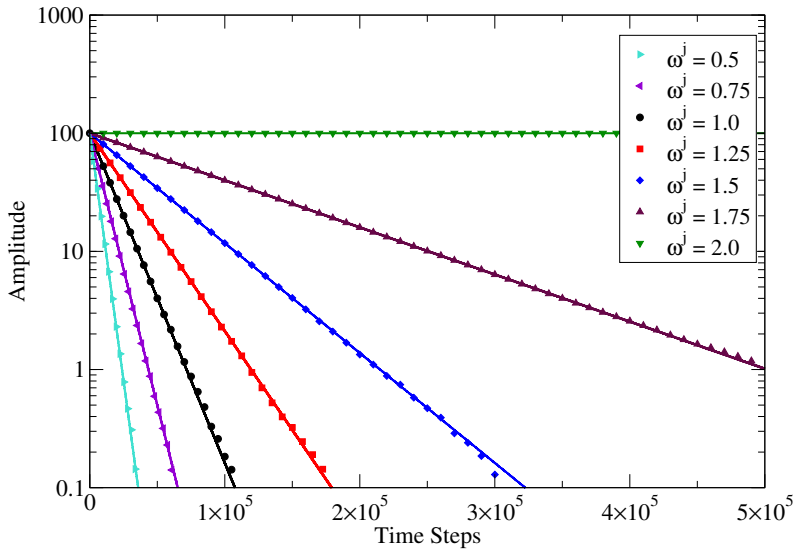
$$D = \theta \left(\frac{1}{\omega^j} - \frac{1}{2} \right). \tag{25}$$

- This is equivalent to a diffusive MRT LBM where overrelaxation can be achieved in the range $\omega^j \in [1, 2]$.

Overrelaxation for Diffusive Integer Lattice Gas

To verify that this flipping operation does give overrelaxation, we can examine the amplitude of a decaying of a sine wave:

$$A^{LG}(t) = \frac{\sum_x \sin\left(\frac{2\pi x}{L}\right) N(x,t)}{\sum_x \sin^2\left(\frac{2\pi x}{L}\right)}. \tag{26}$$



We see good agreement between the measured simulation data (symbols) and the theoretical prediction (solid lines) from Eqn. (26) both inside and outside the over-relaxation regime. This data was a result of the average of 500 individual simulations on a D1Q3 lattice with size $L = 320$ and $N^{ave} = 100$.

Conclusions and Outlook

- We have presented a method for implementing overrelaxation into integer lattice gases.
  - We achieve this by introducing a flipping operation to the occupation numbers which will send send the particles back to where they came from.
  - We introduce a second augmentation to the collision process which then will choose a fraction of particles to actually flip with probability ω^*.
  - This method allows us to mimic probabilities greater than 1 which was why overrelaxation was conventionally thought to be impossible for lattice gas methods.
- We hope to generalize this overrelaxation method to the hydrodynamic case.
- Develop a formalism for ILG collisions?