Novel perspectives on lattice Boltzmann and their underlying lattice gases

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What we are looking at

We see a moving substances that has multiple phases (water, ice, air/gas)
We would like to “understand” how the substances that make up our environment evolve.
But how can one understand something complex like this?

Physics of Fluids

At first glance the fluid looks like a continuous matter, and it makes sense to describe it in terms of continuous fields describing the density, momentum and energy of the matter.

But how do these fields evolve?

The answer to this is not obvious. There are three conservation principles:

1. mass $\int \rho(x,t)dx =$ const
2. momentum $\int j_\alpha(x,t)dx =$ const
3. energy $\int e(x,t)dx =$ const

Why are those the conserved quantities? We don't know, and those are not entirely fundamental either, since mass can be transformed into energy and back according to $E = mc^2$. In principle there could be more or fewer, but these conservations are experimental facts in the regime we are interested in.

Basic evolution principles for fields

We can re-state the conservation principles in terms of partial differential equations (related to Gauss' Theorem)

$$\partial_t \rho + \nabla_\alpha j_\alpha = 0 \tag{1}$$

$$\partial_t j_\alpha + \nabla_\alpha \Pi_{\alpha\beta} = 0 \tag{2}$$

$$\partial_t e + \nabla_\alpha q_\alpha = 0 \tag{3}$$

where the mass-current j_α is equal to the momentum current, making the first equation, the continuity equation, fully defined.

The momentum flux tensor $\Pi_{\alpha\beta}$ is a new quantity, for which we will require a constitutive equation.

The energy flux q_α is also a new vector field for which we need a constitutive equation.

This is exact, but only useful when we have expressions for $\Pi_{\alpha\beta}$ and q_α in terms of ρ, j_α and e.

Constitutive laws

In certain well-behaved situations the dynamics will be purely described in terms of the conserved quantities (and their derivatives). This is because local relaxation to equilibrium is much faster, but the conserved quantities have to move to establish equilibrium.

In those situations where the evolution is completely dominated by the slow relaxation of the conserved quantities, one can take a hydrodynamic limit and express the evolution purely in terms of the conserved quantities.

Constitutive laws (cont)

The momentum flux tensor consists of the advection of momentum as well as the diffusion of momentum. We can define a fluid velocity as $u_\alpha = j_\alpha/\rho$. This gives

$$\Pi_{\alpha\beta} = j_\alpha u_\beta + \nu\rho(\nabla_\alpha u_\beta + \nabla_\beta u_\alpha - \frac{d}{2}\nabla_\gamma u_\gamma \delta_{\alpha\beta}) + \zeta \nabla_\gamma u_\gamma \delta_{\alpha\beta} \tag{4}$$

and ν is called the shear viscosity and ζ is called the bulk viscosity. This simple constitutive equation corresponds to Newtonian viscosity and is not fundamental. Many fluids have more complex momentum flux, and viscoelastic fluids have additional memory, leading not just to a different constitutive law, but actually a separate evolution equation for the stress.

The simplest constitutive law for the energy is

$$q_\alpha = e u_\alpha + \nabla_\beta \sigma_{\alpha\beta} + \kappa \nabla_\alpha k_B T \tag{5}$$

where $\sigma_{\alpha\beta}$ is the second part of the momentum transport tensor above and the temperature is the kinetic energy that is not part of the advection velocity. We have a new transport coefficient, the heat conductivity κ.

Hydrodynamics

We have now described the evolution of a continuous fluid in terms of partial differential equations entirely in terms of the fields of conserved quantities.

While this is not exact, for most practical applications this is an entirely satisfactory description. Examples of exceptions would be very non-equilibrium situations where the spatial and local relaxation occur on similar time-scales.

Nature is discrete

It had long been suspected (Democritus and the Epicureans that followed his ideas like Lucretius) that matter is actually made up of discrete building blocks, which Democritus called Atoms.

This idea was only universally accepted after Einstein explained Browninan motion in terms of atomic collisions of discrete water molecules with larger (visible under a microscope) suspended particles.

This means that our continuous description is actually incorrect. A more correct description of the motion of our fluid should be molecular.

Molecular nature of matter

We have discrete molecules that interact with each other. A fundamental description would allow for a quantum mechanical description of those fundamental components of nature.

For this we would take into account the internal structure of atoms and would have to describe the evolution of nuclei and electron clouds in terms of a quantum mechanical evolution equation (say a Schrödinger equation for non-relativistic particles:

$$i\hbar\partial_t\psi(\{x_i\},t) = H\psi(\{x_i\},t) \tag{6}$$

where the Hamiltonian H is an operator that gives the energy of a particular configuration. The many-particle wavefunction ψ is related to finding particles in a particular configuration $\{x_i\}$ when a measurement takes place with a probability of $\int \psi\psi^* dx$. A more correct relativistic description would also include creation and anihilation of particles as well as the interactions of photons with matter.

We now describe the evolution of our fluid with the help of a complex partial differential equation that gives us the probability of finding a certain configuration.

A classical description

Sometimes a quantum mechanical description is essential, as is the case for liquid helium at very low temperatures where it can experience a fascinating phenomenon called superfluidity. [see https://physicstoday.scitation.org/doi/10.1063/PT.3.4067]

Often, as in the example of our flowing water, it is sufficient to describe the discrete components classically as particles with some two-particle interaction potentials that only depend on the distance of the particles (and possibly their orientation).

Their evolution is then given by Newton's second equation:

$$\partial_t^2 x_i(t) = \frac{F_i(\{x_i\}}{m} \tag{7}$$

Because this is a second order ordinary differential equation you need both the positions and the first time derivative of the positions (i.e. the velocities) to fully describe an initial configuration that you can evolve using this equation.

Models in Physics

We have now seen that we can derive very different models for our fluid, and these models don't seem very similar. But if they are models of the same real systems, they will have to make the same predictions at the level where they are supposed to be applicable to the same system. But clearly these models are not equivalent, since some make more detailed predictions than others, and at some scales they clearly disagree. We would still consider them valid if those disagreements occur in regions where we don't expect them to be valid.

Regions of applicability

1. Quantum description: gives the probability of finding particles at positions, but the evolution of the wave-function is deterministic, but measurement is a non-continuous process. In principle holds for all length and time-scales, but even numerically can only be solved for very small systems of a few particles (≈ 10) for short times.

2. Classical particle description: allows for many particles ($\approx 10^6$) and longer times. But still only hundereds of nanometers and picoseconds.

3. Classical hydrodynamical field description: allows for examination of macroscopically large systems.

Equivalence of descriptions

This only makes sense, if we can show that these very different descriptions are actually consistent. We won't talk about deriving Newton's equations from the Schrödinger equation (something where Ehrenfest's theorem comes to play) but only the second part of deriving the hydrodynamic equations from the classical molecular description.

The basic plan is:

- Newtons equation to Liouville equation
- Liouville equation over BBGKY hirarchy to Boltzmann description
- Boltzmann equation to Navier-Stokes equation

Newton to Liouville

Measurements have only finite accuracy. So we can't know the initial conditions to solve Newton's equation. But we can define a probability density of initial conditions $\rho(\{x_i(0), v_i(0)\})$ consistent with our measurement. and examine how this ensemble of initial conditions will evolve:

$$\partial_t \rho(\{x_i, v_i\}) + \sum_i \left[v_i \partial_{x_i} \rho(\{x_i, v_i\}) + \frac{F_i}{m} \nabla_{v_i} \rho(\{x_i, v_i\}) \right] = 0 \tag{8}$$

which is essentially a continuity equation for the evolution of the ensemble of configurations in phase-space and we have used the fact that

$$\frac{dx_i}{dt} = v_i \tag{9}$$

$$\frac{dv_i}{dt} = \frac{F_i}{m_i} \tag{10}$$

.

Liouville to BGKYY

From the phase-space density for N particles we can obtain distribution functions for a smaller numbers of particles. For simplicity we assume that there is only one kind of identical particle here. The extension to multiple species is straightforward.

$$f^s(\{x_i, v_i\}) = \frac{N!}{(N-s)!} \int dx_{s+1} \cdots dx_N dv_{s+1} \cdots dv_N \rho(\{x_i, v_i\}) \tag{11}$$

For the evolution of these s particle distribution functions we get

$$\begin{aligned} \partial_t f^s(\{x_i, v_i\}) =& \frac{N!}{(N-s)!} \int dx_{s+1} \cdots dx_N dv_{s+1} \cdots dv_N \partial_t \rho(\{x_i, v_i\}) && (12) \\ =& -\frac{N!}{(N-s)!} \int dx_{s+1} \cdots dx_N dv_{s+1} \cdots dv_N \sum_i \left[v_i \partial_{x_i} \rho + \frac{F_i}{m} \partial_{v_i} \rho \right] && (13) \end{aligned}$$

From this we get

$$\partial_t f^s + v \nabla_x f^s + \frac{F}{m} \nabla_v = -\int v_{s+1} \nabla_{x_{s+1}} f^{s+1} + \frac{F^{s+1}}{m} \nabla_{v_{s+1}} f^{s+1} \tag{14}$$

which is known as the BBGKY hierarchy.

BBGKY to Boltzmann

If we look at the evolution of the one-particle distribution function we get:

$$\partial_t f(x,v,t) + v_i \nabla f(x,v,t) + \frac{F}{m} = \int dx_2 dv_2 \left[v_2 \nabla_{x_2} + \frac{F_2}{m} \nabla_{v_2} \right] f^2(x,v,x_1,v_1,t) \qquad (15)$$

The second part after the "=" sign is the effect of interactions (collisions) with other particles. Under certain circumstances (mostly for a dilute gas) the f^2 factorize and we have expressed this as an evolution equation just in terms of the one particle distribution functions.

It can be shown that this Boltzmann equation will rigorously minimize an $H(\{f\}$ functional given by

$$H(\{f\}) = \int dx dv f(x,v,t) \log(f(x,v,t)) \qquad (16)$$

This in turn allows you to show that this negative entropy is maximized for the Maxwell Boltzmann distribution

$$f^0(v;\rho,u,\theta) = \frac{1}{(2\pi\theta)^{d/2}} \exp\left(-\frac{(v-u)^2}{2\theta} \right) \qquad (17)$$

BGK approximation of the Boltzmann equation

The collisions will bring the distribution closer to the Maxwell Boltzmann approximation. This suggests the approximation

$$\partial_t f(x,v,t) + v\nabla f(x,v,t) + \frac{F}{m}\nabla_v f(x,v,t) = \frac{1}{\tau}[f^0(v;\rho,u,\theta) - f(x,v,t)] \tag{18}$$

for some density dependent relaxation time τ. The conserved fields are simply

$$\rho(x,t) = \int dv f(x,v,t) \tag{19}$$

$$u(x,t) = \frac{1}{\rho}\int dv v f(x,v,t) \tag{20}$$

$$\theta(x,t) = \frac{1}{\rho}\int dv (v-u)^2 f(x,v,t) \tag{21}$$

and those are the same fields that we talked about in the beginning for the hydrodynamic equations.

Boltzmann to Navier-Stokes

The key idea here is to express the distribution function f in terms of the macroscopic fields ρ, u and θ. We can do that by using the inverted Boltzmann equation

$$f(x,v,t) = f^0(x,v,t) - \tau[\partial_t f - v\nabla f - \frac{F}{m}\nabla_v f] \tag{22}$$

and we obtain an approximation for the Boltzmann evolution equation in terms of the equilibrium distribution and its derivatives:

$$(\partial_t + v\nabla + \frac{F}{m}\nabla_v)[f^0(\rho,u,\theta) + (\partial_t + v\nabla + \frac{F}{m}\nabla_v)f^0] = \frac{1}{\tau}[f^0(\rho,u,\theta) - f(x,v,t)] \tag{23}$$

Now f only appears in the collision term, and taking velocity moments corresponding to mass, momentum and energy conservation mean that these moments of the collision terms vanish.

The resulting conservation equations are partial differential equations for ρ, u and θ, exactly the same ones as the hydrodynamic equations we first derived with some specific transport coefficients that depend on τ.

Solutions

Now that we have written down the evolution equations we can express how the system will evolve. But except in some very special situations we can't find analytical solutions. (One example of this will be shown by Jordan Larson this afternoon).

This means we need to find computational approaches to solve these equations. This is where the methods we will talk about today come into play.

Molecular Dynamics

The key variables are the positions $x_n(t)$ and velocities $v_n(t)$ of all atoms. Interactions between atoms is represented through appropriate forces $F_n(t)$. The atoms evolve according to Newton's equations that are solved numerically (usually using velcoity Verlet second order algorithm):

$$\frac{dx_n(t)}{dt} = v_n(t) \tag{24}$$

$$\frac{dv_n(t)}{dt} = F_n(\{x_m(t), v_m(t)\}) \tag{25}$$

The simulations give the positions and velocities of all particles as a function of time. This contains all the information needed to investigate most macroscopic systems. (It misses quantum mechanical effects, interaction with radiation . . .)

Highly accurate, but much too expensive for macroscopic systems!

Lattice Gas

To model gas and fluid systems much more cheaply, lattice gas methods were developed. Here particles are restricted to reside on lattice nodes x and move to neighboring lattice sites $x + c_i \delta t$. Occupation numbers of particles that came from lattice site $x - c_i \delta t$ are denoted by $n_i(x, t)$. This allows us to define a local density and momentum as

$$\rho(x,t) = \sum_i n_i(x,t); \quad \rho(x,t)u(x,t) = \sum_i n_i(x,t)c_i \tag{26}$$

Original lattice gases had Boolean occupation numbers, but integer occupation numbers (more relevant for us) have also been developed*. These particles then undergo collisions that lead to a re-distribution of the occupation numbers. The full evolution can be written as

$$n_i(x + c_i \delta t, t + \delta t) = n_i(x, t) + \Xi_i \tag{27}$$

where the collision operator Ξ_i is typically probabilistic and obeys conservation of mass and momentum

$$\sum_i \Xi_i = 0; \quad \sum_i \Xi_i c_i = 0 \tag{28}$$

*Thomas Blommel and A.J.W., *Phys. Rev. E* **97**, 023310 (2018)

Lattice Boltzmann

Lattice gases are probabilistic, and (especially for Boolean lattice gases) have large fluctuations. To analyze the macroscopic behavior of these models a non-equilibrium Boltzmann average of the lattice gas is taken:

$$f_i(x,t) = \langle n_i(x,t) \rangle \tag{29}$$

$$f_i(x+\delta x_i, t+\delta t) = f_i(x,t) + \Omega_i \tag{30}$$

where the f_i are real numbers and the collision operator $\Omega_i = \langle \Xi_i \rangle$ is deterministic.

The kinetic theory approach allows to derive the macroscopic equations for mass and momentum conservation:

$$\partial_t \rho + \nabla \rho = 0 \qquad \text{Continuity eqn.} \tag{31}$$

$$\partial_t(\rho u) + \nabla(\rho u u) = -\nabla P + \nabla(\rho\nu(\nabla u + (\nabla u)^T - 2/3\nabla.u1)) \qquad \text{Navier-Stokes eqn.} \tag{32}$$

This then, is a much cheaper way of simulating a macroscopic system (compared to MD)

More about lattice Boltzmann

One can use different collision operators than $\langle \Xi_i \rangle$, and such collision operators allow for simpler collision operators as well as helpful features. The simplest such collision operator is

$$\Omega_i = \frac{1}{\tau}[f_i^0(\rho, u) - f_i] \tag{33}$$

and the viscosity is given by

$$\nu = \left(\tau - \frac{1}{2}\right)\theta \tag{34}$$

where for technical reasons $\theta = 1/3$. This is known as the BGK approximation where the collision operator brings the distribution closer to the local equilibrium distribution f_i^0.

A curious result is that over-relaxing (i.e. $1 > \tau > 1/2$) will lead to a lower viscosity than could be reached by any physics inspired lattice gas collision operator. All lattice Boltzmann simulations of high Re flows use this feature, but the lattice Boltzmann method in this regime seems disconnected from the mesoscopic ideas of the underlying lattice gas.

There is a small industry to develop "better" lattice Boltzmann collision operators, known as MRT, entropic, cascaded, cumulant to name but a few. Also extensions for fluctuating systems and multiphase, multicomponent systems.

1 of 12

PHYSICAL REVIEW E **96**, 013314 (2017)

Lattice gas with molecular dynamics collision operator

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We introduce a lattice gas implementation that is based on coarse-graining a molecular dynamics (MD) simulation. Such a lattice gas is similar to standard lattice gases, but its collision operator is informed by an underlying MD simulation. This can be considered an optimal lattice gas implementation because it allows for the representation of any system that can be simulated with MD. We show here that equilibrium behavior of the popular lattice Boltzmann algorithm is consistent with this optimal lattice gas. This comparison allows us to make a more accurate identification of the expressions for temperature and pressure in lattice Boltzmann simulations, which turn out to be related not only to the physical temperature and pressure but also to the lattice discretization. We show that for any spatial discretization, we need to choose a particular temporal discretization to recover the lattice Boltzmann equilibrium.

DOI: 10.1103/PhysRevE.96.013314

I. INTRODUCTION

Lattice Boltzmann methods are an important computational tool that is most commonly employed to simulate hydrodynamic systems [1], and it has been adapted to address many complex phenomena from turbulence [2,3] over multiphase and multicomponet flow [4–8] to pore-scale simulations of porous media [9,10] and simulations of immersed boundaries [11,12]. It derives its power from an underlying mesoscopic description that ensures exact mass and momentum conservation. The exact physical meaning of the lattice Boltzmann densities, however, remains poorly understood.

The lattice Boltzmann method was derived as a theoretical tool for the analysis of lattice gas methods [13]. Lattice gas methods consist of particles moving on a lattice with velocities

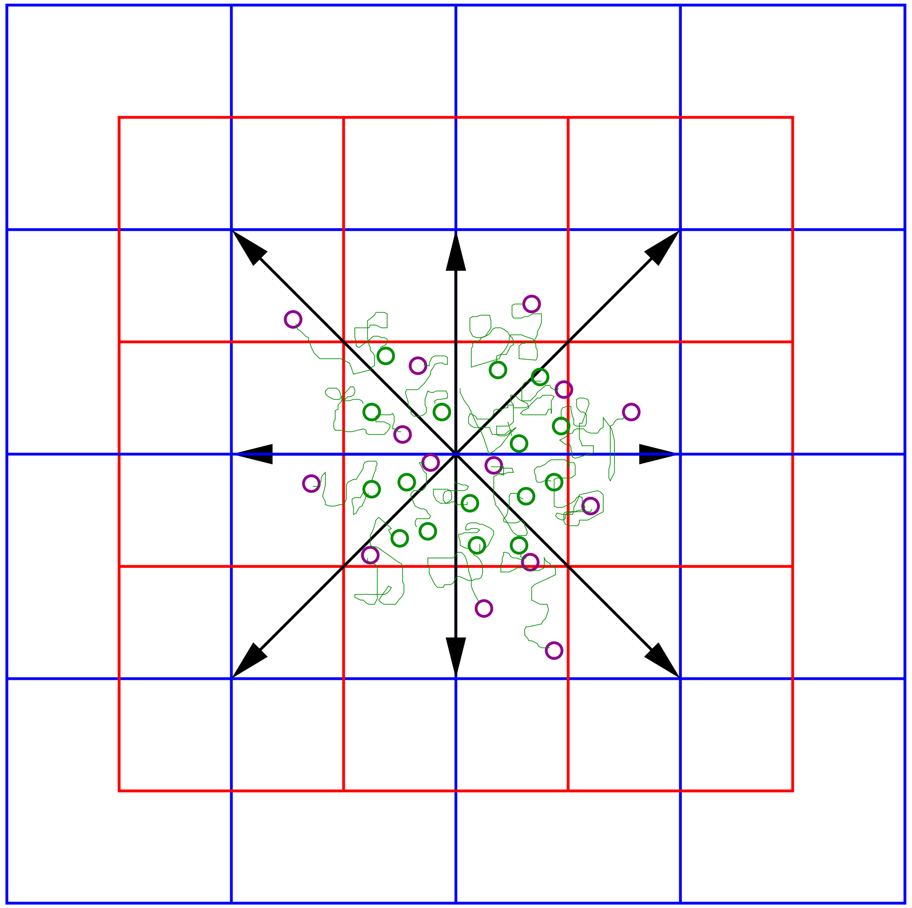
It was then realized that there existed much more freedom in the choice of the collision operator, and in particular the relaxation towards a local equilibrium function, often called the Bhatnagar-Gross-Krook (BGK) approach, allowed the full recovery of the Navier-Stokes equation to second order [17].

At this time a second approach to derive the lattice Boltzmann equation directly from the continuous Boltzmann equation with a BGK collision operator gained popularity [6]. Over the years several different local equilibrium distributions have been proposed, and currently the most popular method is a standard form of a second order expansion in terms of velocities.

Typically these lattice Boltzmann methods are validated by their ability to recover the Navier-Stokes equation. Here,

The connecting bridge: MDLG*

What is new here: we map Molecular Dynamics onto a lattice gas (or Boltzmann), ⇒ fundamental derivation of the "correct" lattice Boltzamann method.



- Impose a lattice with spacing Δx on the MD simulation.
- Observe the current lattice position of the particles.
- Particles moving to a lattice position displaced by v_i after a time-step Δt are called $n_i(x, t + \Delta t)$.
- Define a collision term as $\Xi_i = n_i(x + c_i\Delta t, t + \Delta t) - n_i(x, t)$

Then we have a lattice gas evolution equation:

$$n_i(x + c_i\Delta t, t + \Delta t) = n_i(x, t) + \Xi_i \qquad (35)$$

This MDLG gives an exact (coarse-grained) representation of the underlying real fluid system.

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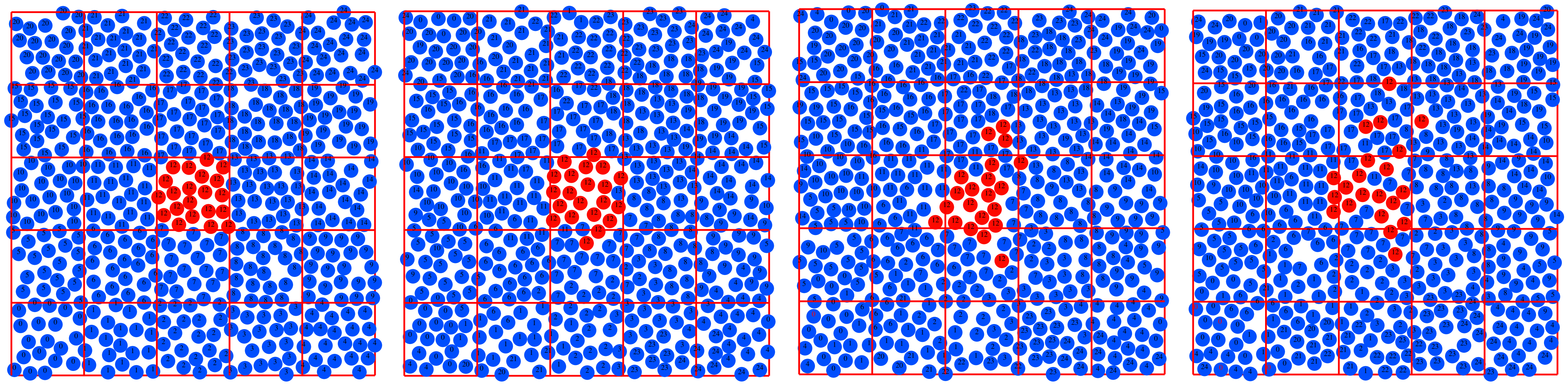
*M. R. Parsa and AJW Phys. Rev. E 96, 013314

An illustrative example



As time progresses particles in the central cell migrate to neighboring cells. The $n_i(x,t)$ are then the particles that moved into a new cell displaced by lattice vector v_i after a time-interval Δt.

Properties of MDLG

First important property of MDLG: what is the equilibrium?

We look at an equilibrium system and find the probability of a displacement for a particle is (approximately*) a Gaussian:

$$P^{(1)}(\delta x) = (2\pi\langle\delta x^2\rangle)^{-d/2} \exp\left(\frac{(\delta x)^2}{2\langle\delta x^2\rangle}\right) \tag{36}$$

With this we can calculate

$$\begin{aligned} f_i^{eq} &= \langle n_i \rangle \\ &= \left(\prod_m^N \int dx_m \int d\delta x_m\right) \; P^{(N)}(\{x_m, \delta x_m\}) \sum_n \Delta_0(x_n)\Delta_{v_i}(x_n - \delta x_n) \\ &= \frac{N}{V} \int dx \int d\delta x \; P^{(1)}(\delta x)\Delta_0(x)\Delta_{v_i}(x - \delta x) \end{aligned}$$

This has an analytical solution: (next slide)

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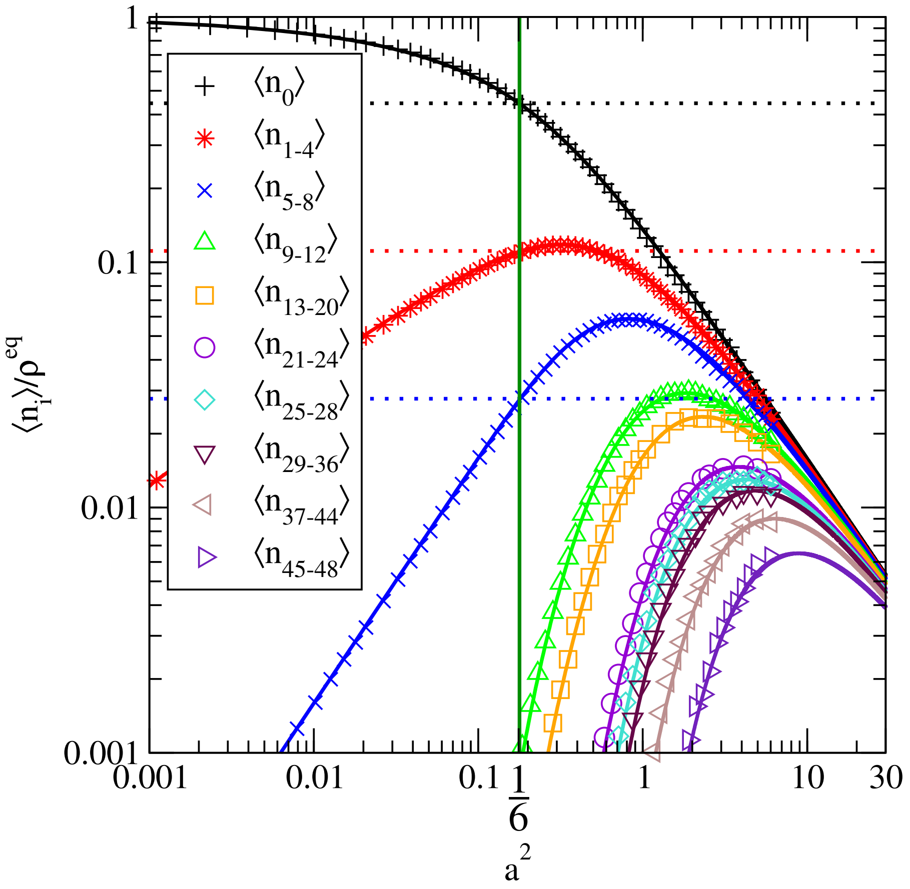
*This is exact in the ballistic and in the diffusive regime, but not inbetween: Aleksandra Pachalieva and AJW, arXiv:2006.05517

MDLG equilibrium distribution ($u = 0$)



Lattice Boltzmann equilibrium ($\theta = 1/3$):

$$f_i^{eq} = \rho w_i \left(1 + \frac{c_i.u}{\theta} + \frac{c_i.u}{2\theta^2} - \frac{u^2}{2\theta}\right) \tag{37}$$

Molecular Dynamics lattice gas*:

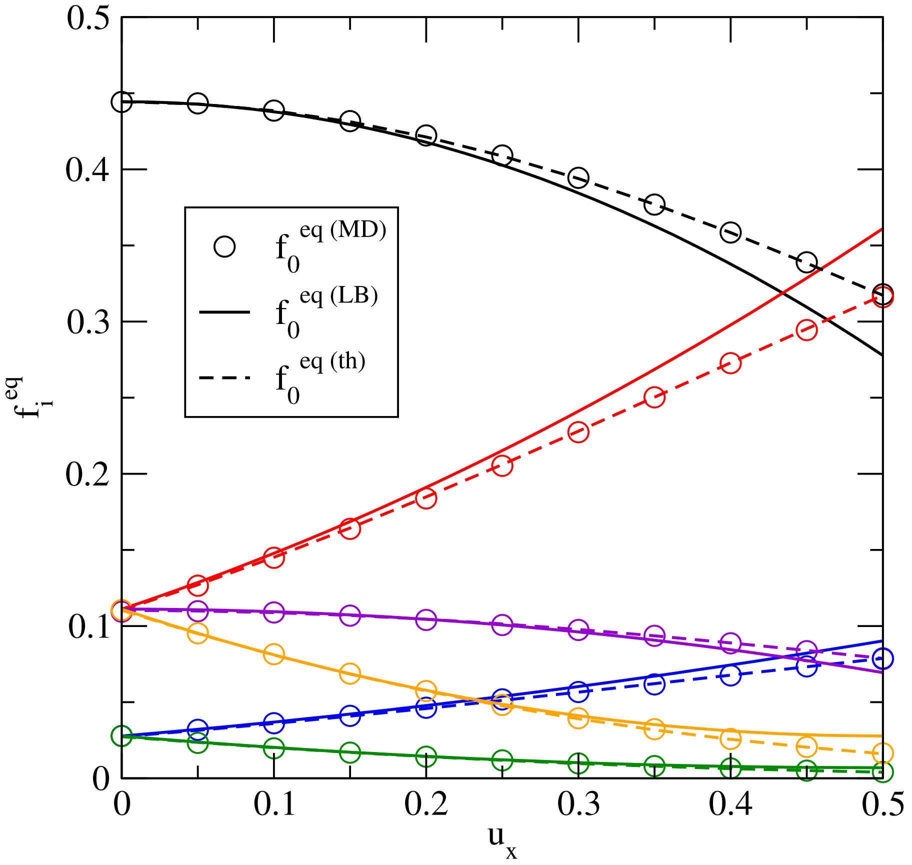
$$f_i^{eq} = \rho \prod_{\alpha=1}^{d} \left\{ N \left(e^{-\frac{(u_{i,\alpha}-1)^2}{2a^2}} - 2e^{-\frac{u_{i,\alpha}^2}{2a^2}} + e^{-\frac{(u_{i,\alpha}+1)^2}{2a^2}} \right) \right.$$
$$+ \frac{u_{i,\alpha}-1}{2} \left[\mathrm{erf}\left(\frac{u_{i,\alpha}-1}{\sqrt{2}a}\right) - \mathrm{erf}\left(\frac{u_{i,\alpha}}{\sqrt{2}a}\right) \right]$$
$$\left. + \frac{u_{i,\alpha}+1}{2} \left[\mathrm{erf}\left(\frac{u_{i,\alpha}+1}{\sqrt{2}a}\right) - \mathrm{erf}\left(\frac{u_{i,\alpha}}{\sqrt{2}a}\right) \right] \right\} \tag{38}$$

where

$$u_{i,\alpha} = c_{i\alpha} - u_\alpha; \quad a^2 = \langle \delta x^2 \rangle / (\Delta x)^2; \quad N = \frac{a}{\sqrt{2\pi}};$$

The graph on the left compares the equilibrium distribution for $u = 0$ between the lattice Boltzmann solution and the MDLG solution. There is a special point at $a^2 = 1/6$ where LB and MDLG equilibrium distributions (almost) agree.

Equilibrium distributions of the MDLG and LB (dependence on u)



Lattice Boltzmann equilibrium:

$$f_i^{eq} = \rho w_i \left(1 + \frac{v_i.u}{\theta} + \frac{v_i.u}{2\theta^2} - \frac{u^2}{2\theta}\right) \qquad (39)$$

Molecular Dynamics lattice gas:

$$\begin{aligned} f_i^{eq} = \rho \prod_{\alpha=1}^{d} \Bigg\{ & N \left(e^{-\frac{(u_{i,\alpha}-1)^2}{2a^2}} - 2e^{-\frac{u_{i,\alpha}^2}{2a^2}} + e^{-\frac{(u_{i,\alpha}+1)^2}{2a^2}} \right) \\ & + \frac{u_{i,\alpha}-1}{2} \left[\mathrm{erf}\left(\frac{u_{i,\alpha}-1}{\sqrt{2}a}\right) - \mathrm{erf}\left(\frac{u_{i,\alpha}}{\sqrt{2}a}\right) \right] \\ & + \frac{u_{i,\alpha}+1}{2} \left[\mathrm{erf}\left(\frac{u_{i,\alpha}+1}{\sqrt{2}a}\right) - \mathrm{erf}\left(\frac{u_{i,\alpha}}{\sqrt{2}a}\right) \right] \Bigg\} \end{aligned} \qquad (40)$$

While the two expressions are obviously different, they agree for $u < 0.1$ to good accuracy. Since LB is known to work, this is encouraging. Note that MDLG values overlap at $u = 0.5$, which is necessary for Galilean invariance symmetry (and unlike LB, the velocity set is not restricted).

Original motivation: fluctuations

We originally started this investigation because we wanted to understand what fluctuations in LB should look like, particularly for non-ideal gases.

For ideal gases we know from Pitaevskii & Lifshitz that the probability of finding n particles in a cell with average density of ρ^{eq} is given by a Poisson distribution:

$$P(\rho) = \exp\left(-\rho^{eq}\right) \frac{(\rho^{eq})^{\rho}}{\rho!} \tag{41}$$

This implies $\langle(\rho-\rho^{eq})^2\rangle = 1/\rho^{eq}$. This argument can be extended for occupation numbers:

$$P(n_i) = \exp(-f_i^{eq}) \frac{(f_i^{eq})^n}{n!} \tag{42}$$

You get this rigorously for ideal integer lattice gases*, and approximately for ideal fluctuating lattice Boltzmann†.

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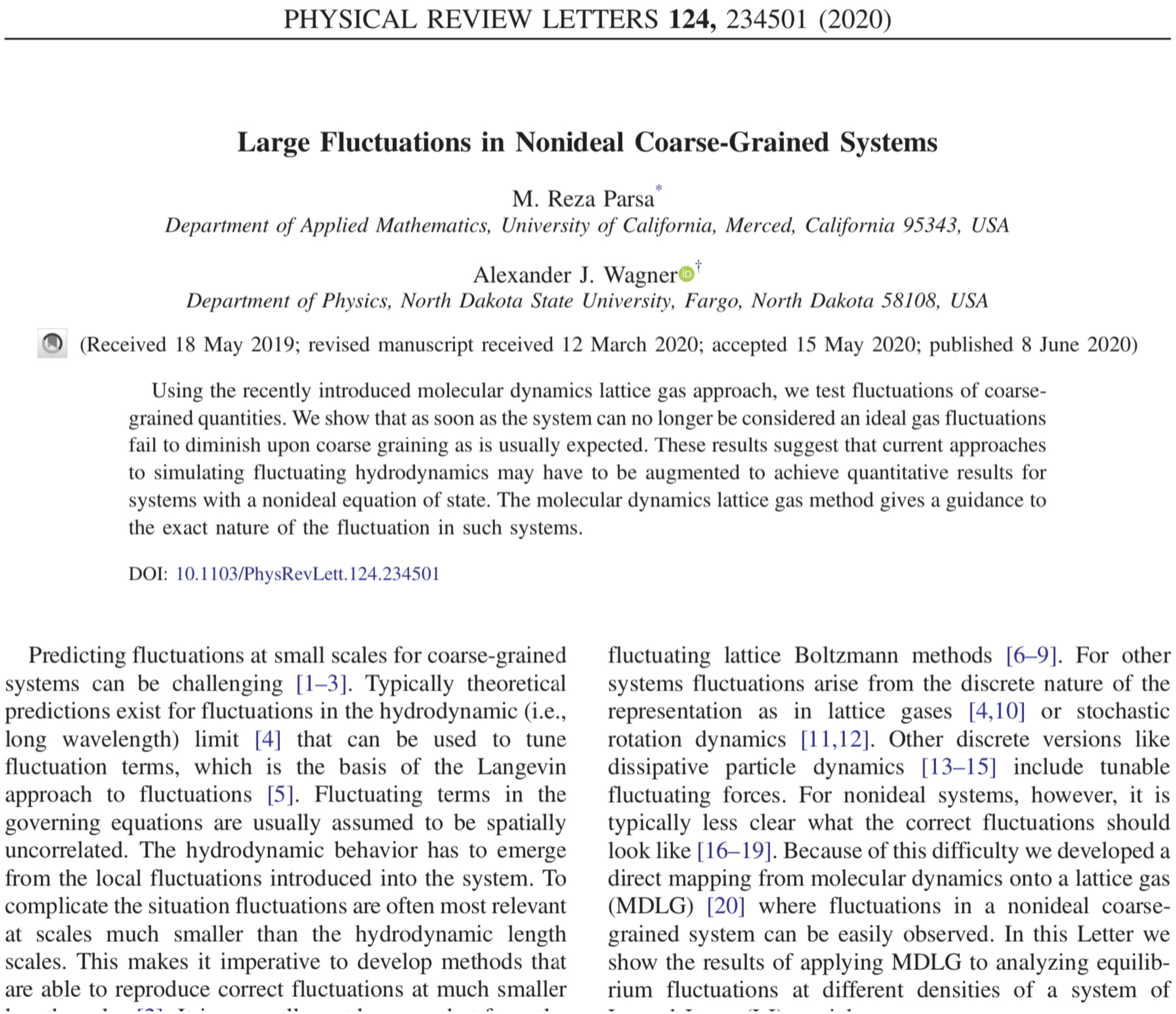
[*] T. Blommel and AJW Phys. Rev. E 97, 023310

[†] AJW and K. Strand Phys. Rev. E 94, 033302



PHYSICAL REVIEW LETTERS **124,** 234501 (2020)

Large Fluctuations in Nonideal Coarse-Grained Systems

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Using the recently introduced molecular dynamics lattice gas approach, we test fluctuations of coarse-grained quantities. We show that as soon as the system can no longer be considered an ideal gas fluctuations fail to diminish upon coarse graining as is usually expected. These results suggest that current approaches to simulating fluctuating hydrodynamics may have to be augmented to achieve quantitative results for systems with a nonideal equation of state. The molecular dynamics lattice gas method gives a guidance to the exact nature of the fluctuation in such systems.

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Predicting fluctuations at small scales for coarse-grained systems can be challenging [1–3]. Typically theoretical predictions exist for fluctuations in the hydrodynamic (i.e., long wavelength) limit [4] that can be used to tune fluctuation terms, which is the basis of the Langevin approach to fluctuations [5]. Fluctuating terms in the governing equations are usually assumed to be spatially uncorrelated. The hydrodynamic behavior has to emerge from the local fluctuations introduced into the system. To complicate the situation fluctuations are often most relevant at scales much smaller than the hydrodynamic length scales. This makes it imperative to develop methods that are able to reproduce correct fluctuations at much smaller

fluctuating lattice Boltzmann methods [6–9]. For other systems fluctuations arise from the discrete nature of the representation as in lattice gases [4,10] or stochastic rotation dynamics [11,12]. Other discrete versions like dissipative particle dynamics [13–15] include tunable fluctuating forces. For nonideal systems, however, it is typically less clear what the correct fluctuations should look like [16–19]. Because of this difficulty we developed a direct mapping from molecular dynamics onto a lattice gas (MDLG) [20] where fluctuations in a nonideal coarse-grained system can be easily observed. In this Letter we show the results of applying MDLG to analyzing equilibrium fluctuations at different densities of a system of

Scaling of fluctuations

For the Poisson distribution we have

$$\langle n_i \rangle = f_i^{eq} \tag{43}$$

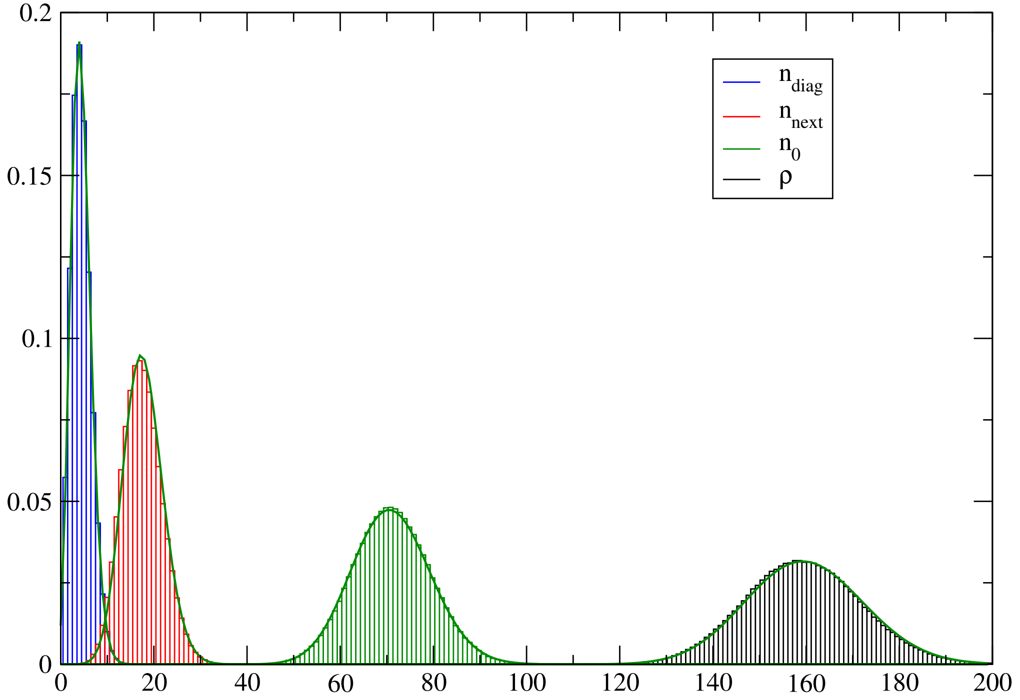
$$\langle n_i n_j \rangle = f_i^{eq} f_j^{eq} + f_i^{eq} \delta_{ij} \tag{44}$$

This means that the width of the distribution, compared to its mean, decreases as the mean increases:

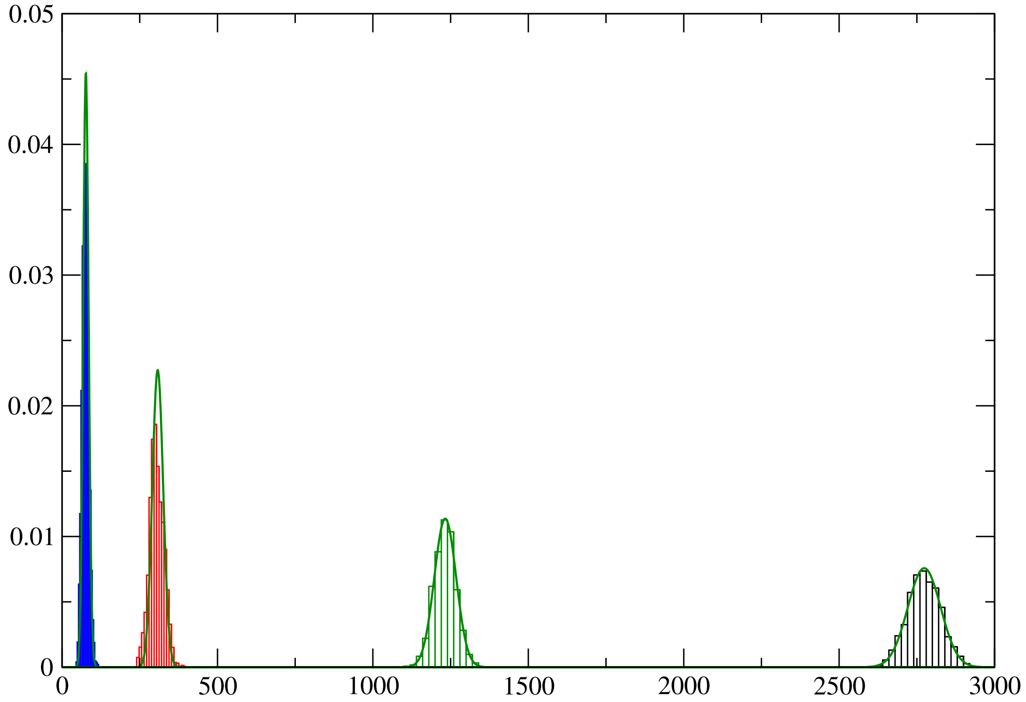
$$W_{ii} = \frac{\sqrt{\langle (n_i - f_i^{eq})^2 \rangle}}{\langle n_i \rangle} = \frac{1}{\sqrt{f_i^{eq}}} \tag{45}$$

This also predicts how the importance of fluctuations declines as we increase the lattice size, thereby increasing the average number of particles per lattice site.

Test of fluctuations for a dilute gas



A dilute gas with an average of 160 particles per lattice site. We observe excellent agreement between the theoretical Poisson distribution (green line) and the measured histograms.



The same system, but with a larger lattice size Δx, and an average number of particles per lattice side of 2700. Some minor deviations between Poisson and measurements are visible.

What to expect for fluctuations for particles at moderate densities?

If one includes a repulsive part to the particle potential, there is effective excluded volume. This reduces the available space for other particles, and this reduces the density fluctuations.

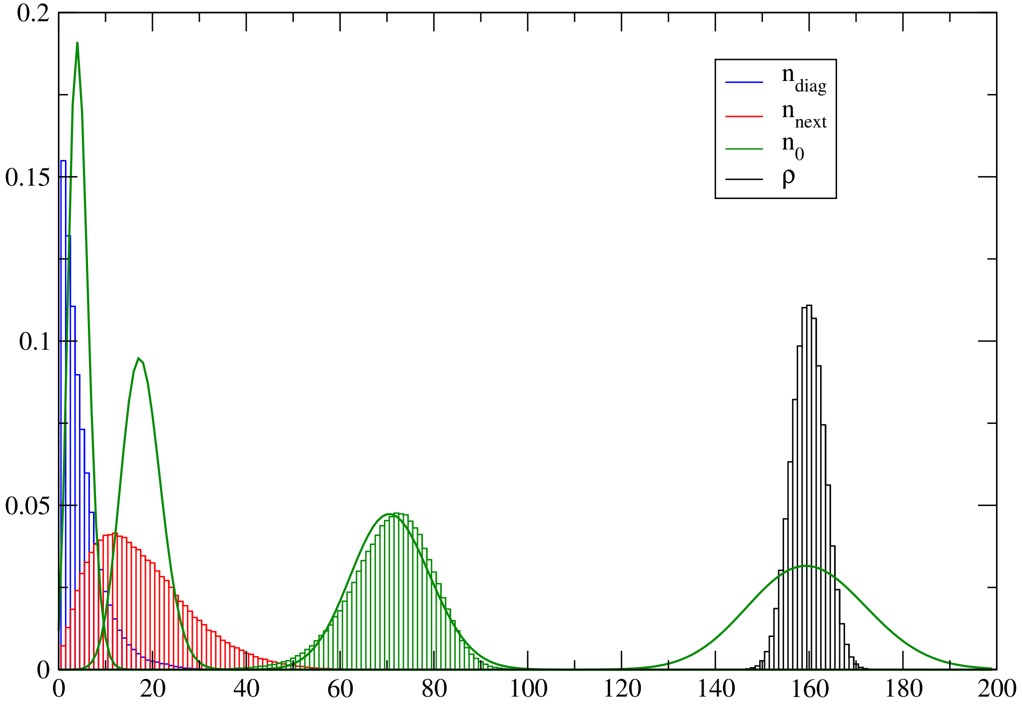
Under coarsegraining, the scaling is still

$$\frac{\langle\sqrt{(\rho-\rho^{eq})^2}\rangle}{\rho^{eq}} \propto 1/\sqrt{\rho^{eq}} \tag{46}$$

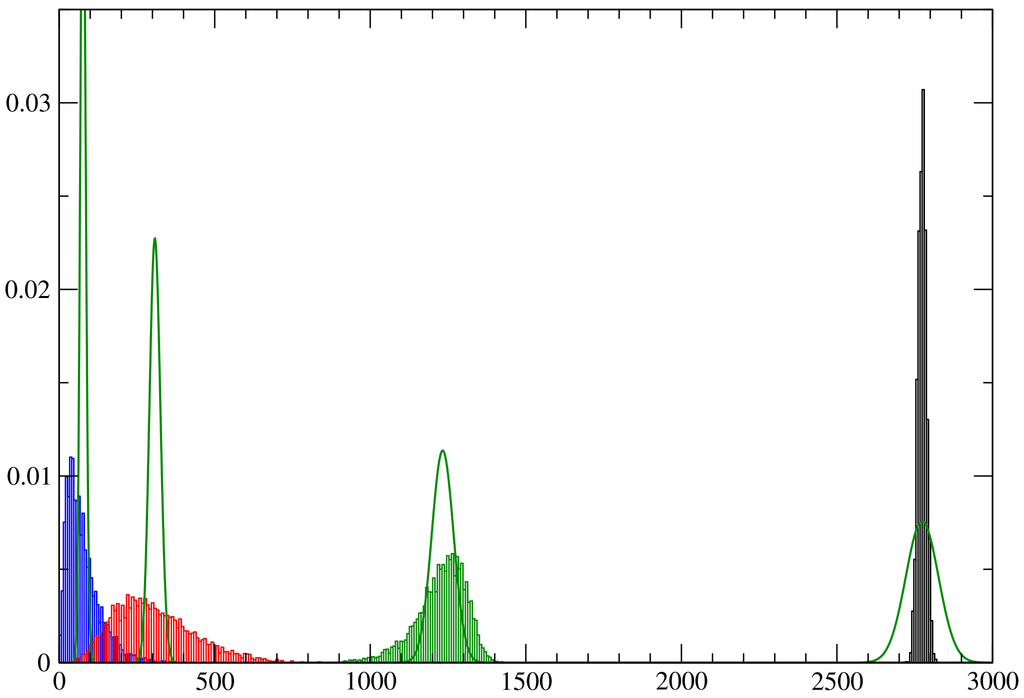
but with a smaller pre-factor. (This it true for any equal time quantity).

So what should we expect for the scaling of the n_i for larger lattice sizes?

The distributions for a dense system

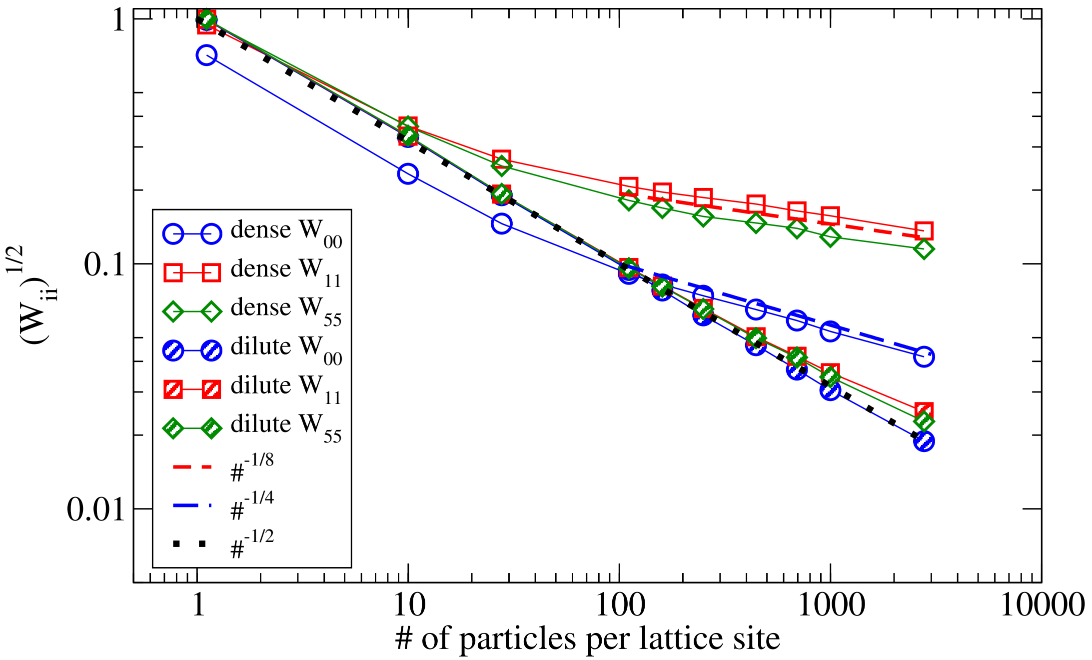


For a dense system distribution is not Poisson. More strikingly: while the density distribution is more narrow, the distribution for the n_i is wider! For wider distributions to combine to a narrow distribution, there must be significant negative correlations!



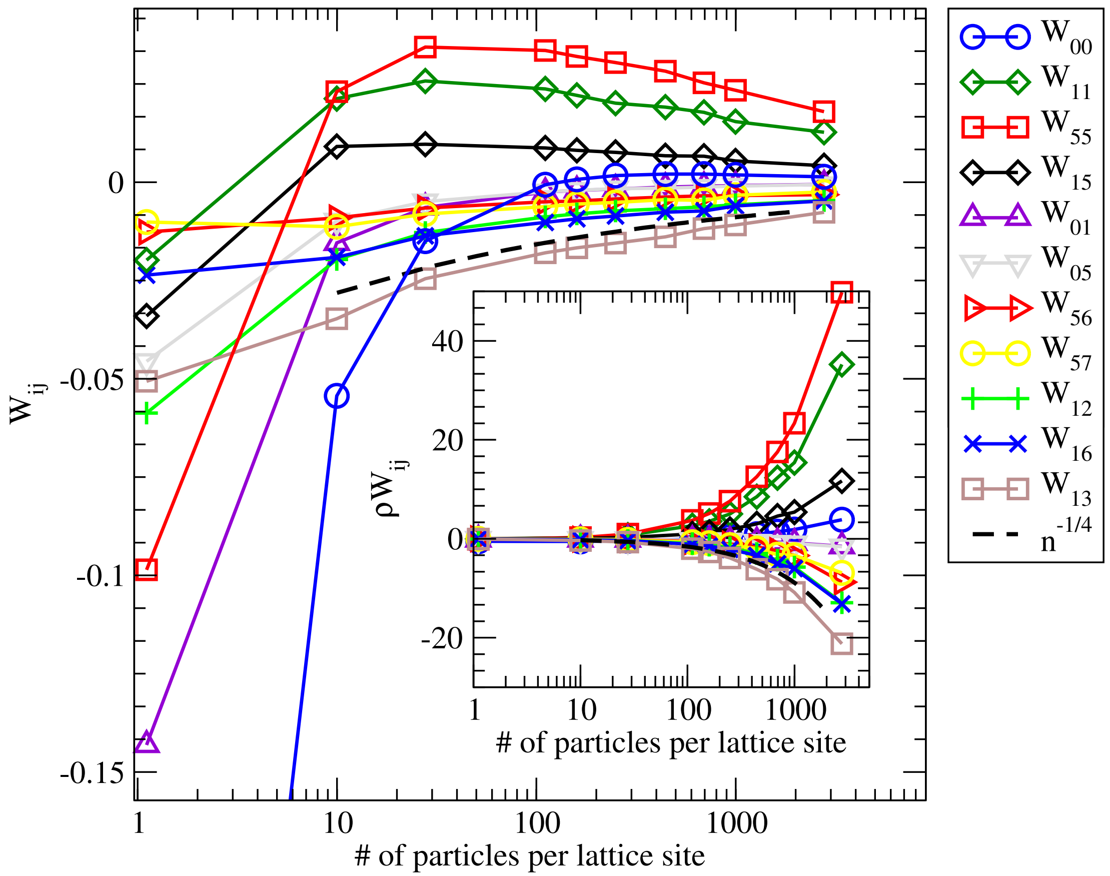
Upon coarse-graining the ρ-distribution narrows as expected. But the fluctuations of the n_i do not significantly more narrow, as we would expect!

If it did not narrow at all, the thermodynamic limit would no longer work.



Scaled width $\sqrt{W_{ii}}$ of the n_i distributions compared to that of a Poisson distribution.

$$W_{ij} = \frac{\langle (n_i - f_i^{eq})(n_j - f_j^{eq}) \rangle}{\rho^{eq} \sqrt{f_i^{eq} f_j^{eq}}} \qquad (47)$$



The cross correlators grow indeed big for large densities.

Theoretical model

Let us consider what we can predict analytically

$$\begin{aligned}
&\langle n_i(x)n_j(y)\rangle\\
=&\left\langle \sum_{k=1}^{M} \Delta_x(x_k)\Delta_{x-v_i}(x_k-\delta_k)\sum_{l=1}^{M}\Delta_y(x_l)\Delta_{y-v_j}(x_l-\delta_l)\right\rangle\\
=&\sum_{k,l}\int dx_1\int d\delta_1\cdots\int d\delta_M P^M(x_1,\delta_1,\cdots,x_M,\delta_M)\Delta_x(x_k)\Delta_{x-v_i}(x_k-\delta_k)\Delta_y(x_l)\Delta_{y-v_j}(x_l-\delta_l)\\
=&(M^2-M)\int dx_1\int d\delta_1\int dx_2\int d\delta_2 P^2(x_1,\delta_1,x_2,\delta_2)\Delta_x(x_1)\Delta_{x-v_i}(x_1-\delta_1)\Delta_y(x_2)\Delta_{y-v_j}(x_2-\delta_2)\\
&+M\int dx_1\int d\delta_1 P^1(x_1,\delta_1)\Delta_x(x_1)\Delta_{x-v_i}(x_1-\delta_1)\Delta_y(x_1)\Delta_{y-v_i}(x_1-\delta_1)\\
=&(M^2-M)\int dx_1\int d\delta_1\int dx_2\int d\delta_2 P^2(x_1,\delta_1,x_2,\delta_2)\Delta_x(x_1)\Delta_{x-v_i}(x_1-\delta_1)\Delta_y(x_2)\Delta_{y-v_j}(x_2-\delta_2)+f_i^{eq}\delta_{ij}\delta_{xy},
\end{aligned} \tag{48}$$

In principle, to predict any properties of the MDLG, all we need is contained in the (little studied) N-particle displacement probability:

$$P^N(\delta x_1,\delta x_2,\cdots,\delta x_N,t) \tag{49}$$

For a system in equilibrium there is no time-dependence. And here we only need P^2.

Two particle displacement probability distribution

While velocities are uncorreleated in equilibrium

$$\langle v_1(t) v_2(t)\rangle (x_1(t) - x_2(t)) = 0 \tag{50}$$

the same is not true for displacements:

$$\langle [x_1(t+\delta t) - x_1(t)][x_2(t+\delta t) - x_2(t)]\rangle (x_1(t) - x_2(t)) \neq 0 \tag{51}$$

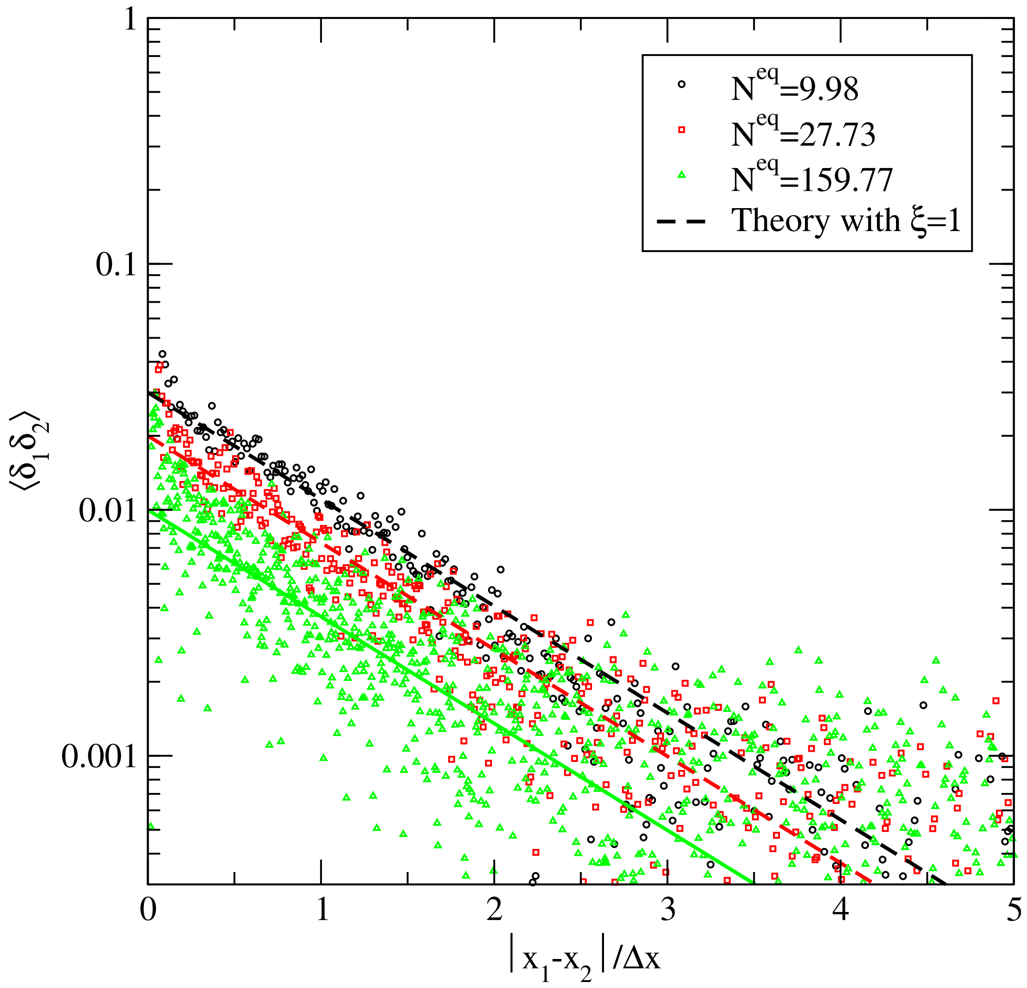
due to a build-up of correlations due to the interactions of particles. These correlations are responsible for the unexpectedly large fluctuations of the n_i.

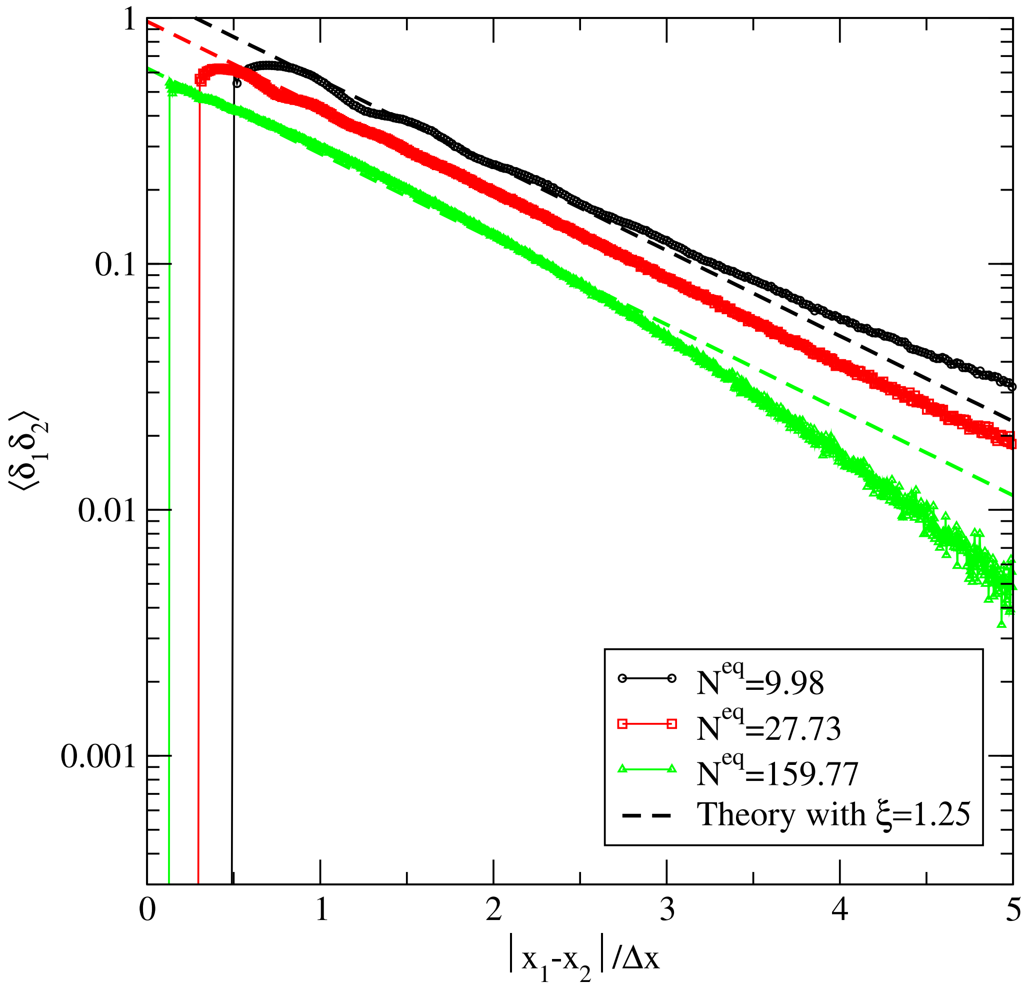
When one wants to build a realistic fluctuating lattice Boltzmann method for non-ideal systems, these correlations are likely important.

The correlations

What we find is

$$\langle [x_1(t+\delta t)-x_1(t)][x_2(t+\delta t)-x_2(t)]\rangle (x_1(t)-x_2(t)) \approx 2\,(\rho\Delta x)^{\frac{1}{2}} \exp\left(-\frac{|x_1-x_2|}{\xi\Delta x}\right) \quad (52)$$





Model for correlations

The simplest model that recovers the distance dependence of the correlations is

$$P(x_1, \delta_1, x_2, \delta_2) \propto g(r) \exp\left(-\frac{(\delta_1 + \delta_2)^2}{4\sigma_+^2(r)}\right) \exp\left(-\frac{(\delta_1 - \delta_2)^2}{4\sigma_-^2(r)}\right) \tag{53}$$

where $r = |x_1 - x_2|$ and

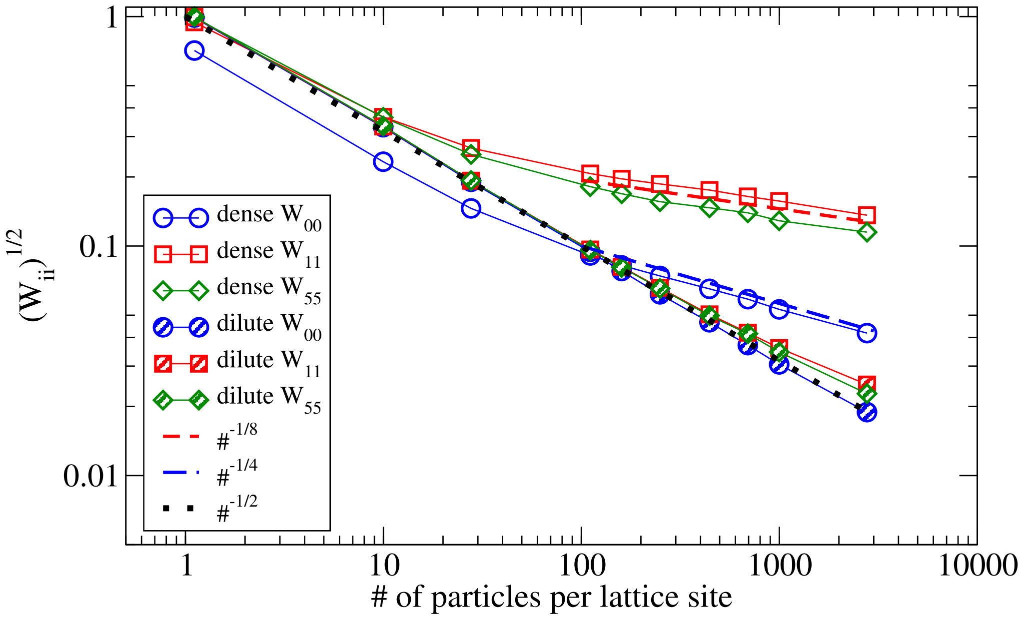
$$\sigma_\pm(r) = a\Delta x \sqrt{1 \pm \frac{\langle \delta_1 \delta_2 \rangle (r)}{\langle \delta_1 \delta_1 \rangle}}. \tag{54}$$

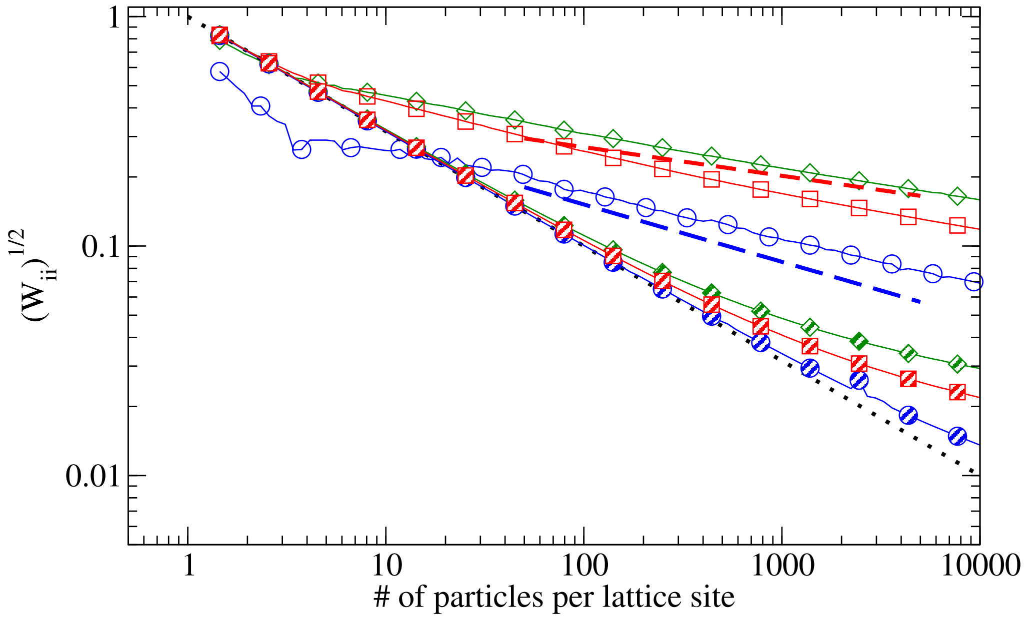
This is only expected to be a zeroth order approximation to the real two particle displacement distribution, but we can use this as a theoretical starting point to numerically evaluate $\langle n_i n_j \rangle$ and compare it to the MDLG results.

Comparison of theory and MDLG

Here we compare the width of the distribution

$$W_{ii} = \langle (n_i(x) - f_i^{eq})^2 \rangle / (N^{eq} f_i^{eq}). \tag{55}$$





Despite smaller differences in the details the overall scaling are recovered quite well, indicating that our displacement probability distribution captures the key effects here.

We have focused on the density ρ, but what about momentum?

The lattice gas/lattice Boltzmann definition of momentum

$$\rho u^{LG} = \sum_i n_i v_i \tag{56}$$

$$\rho u^{LB} = \sum_i f_i v_i = \langle \rho u^{LG} \tag{57}$$

The MD definition of momentum in a lattice site ξ

$$\rho u^{MD} = \sum_n v_n \Delta_\xi(x_n) \tag{58}$$

We had previously shown that

$$\rho u^{LB} = \langle \rho u^{MD} \rangle \tag{59}$$

as should be expected for any scheme that recovers correct hydrodynamics, but what about the fluctuating contributions?

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Nonuniqueness of fluctuating momentum in coarse-grained systems

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Coarse-grained descriptions of microscopic systems often require a mesoscopic definition of momentum. The question arises as to the uniqueness of such a momentum definition at a particular coarse-graining scale. We show here that particularly the fluctuating properties of common definitions of momentum in coarse-grained methods like lattice gas and lattice Boltzmann do not agree with a fundamental definition of momentum. In the case of lattice gases, the definition of momentum will even disagree in the limit of large wavelength. For short times we derive analytical representations for the distribution of different momentum measures and thereby give a full account of these differences.

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I. INTRODUCTION

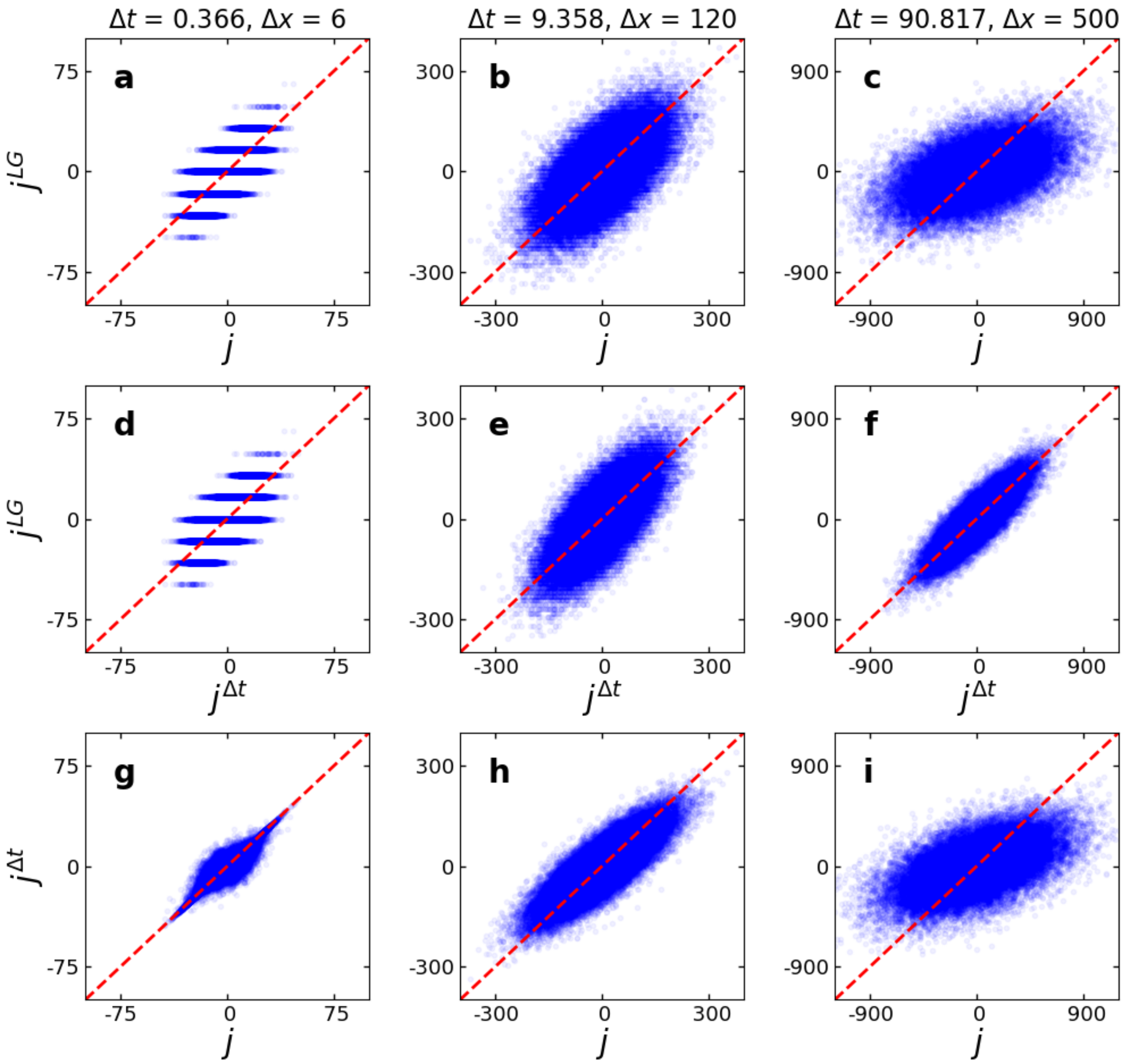
The definition of coarse-grained quantities for a mesoscopic simulation method can be subtle [1]. In this article we investigate the connection between the atomistic definition of momentum and the lattice gas (or lattice Boltzmann) definition of momentum [2], in particular, the definition of the fluctuating component of the momentum [3]. It is usually assumed that momentum is a uniquely defined quantity. For coarse-grained descriptions, however, this is not necessarily the case, since space and time averages impact the definition of fluctuating components of the momentum.

We show here that different definitions of microscopic momentum differ significantly. In particular the definition of the fluctuating momentum through a lattice gas deviates significantly from a molecular definition of momentum. We

II. LATTICE GAS AND MDLG

The key idea of the MDLG procedure is to map an MD simulation onto a discrete particle evolution on a lattice that has the same formal representation as a lattice gas. To explain this procedure we briefly introduce boolean as well as integer lattice gas models and explain in which key aspects they differ from the MDLG coarse-graining onto a lattice gas. Boolean lattice gases were originally developed as minimal models for statistical mechanics. To simulate hydrodynamic systems, the lattice collisions that conserved both particle number and lattice gas momentum were chosen. It was the key accomplishment by Frisch, Hasslacher and Pomeau [2] and Wolfram [13] to select a lattice with sufficient rotational symmetry to recover the Navier-Stokes equations, albeit with some constants that contain unwanted density and velocity

Scatter plot of momenta



$$j^{LG} = \sum_i n_i v_i \qquad (60)$$

$$j = \sum_n v_n \Delta_\xi(x_n) \qquad (61)$$

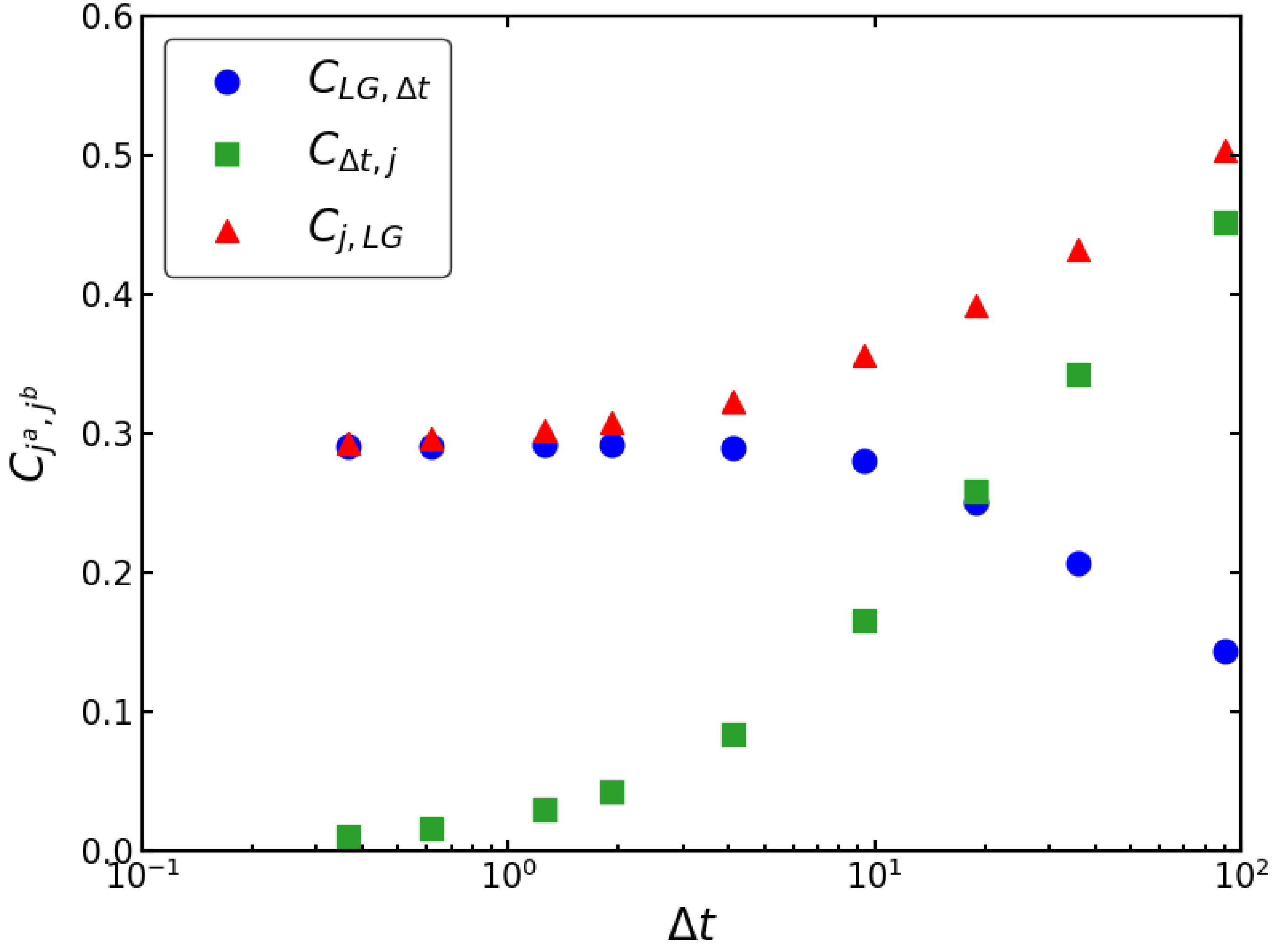
$$j^{\Delta t} = \frac{1}{\Delta t}\int_t^{t+\Delta t} dt j(t) \qquad (62)$$

j^{LG} is discrete lattice gas momentum.

j is standard MD momentum

$j^{\Delta t}$ is j averaged over one timestep.

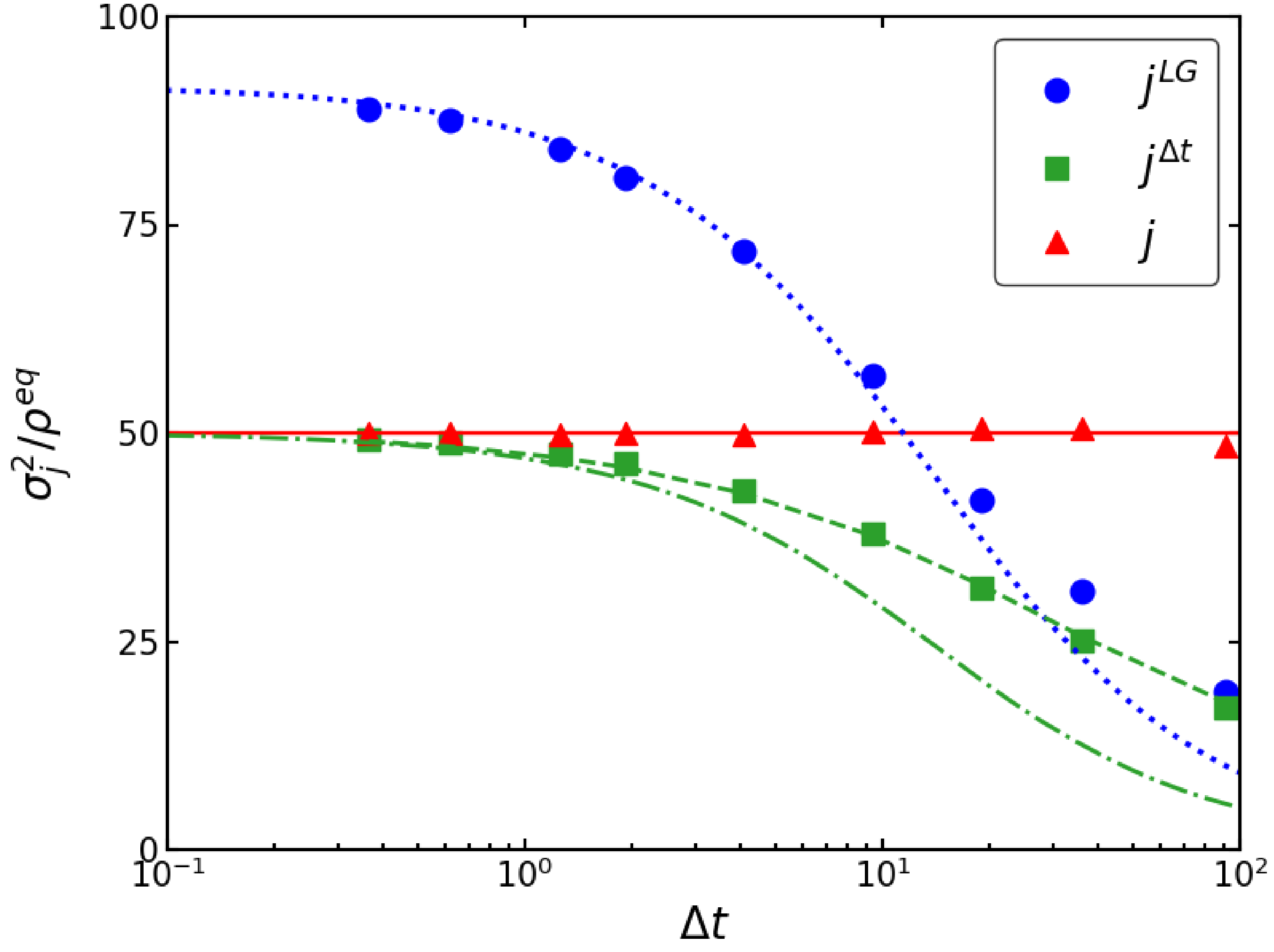
Correlations between momenta



$$C_{j^a,j^b} = \frac{1}{2XT} \sum_{\xi} \sum_{t} \left[\frac{j^a(\xi,t)}{\sigma_{j^a}} - \frac{j^b(\xi,t)}{\sigma_{j^b}} \right]^2 \tag{63}$$

For small Δt j and $j^{\Delta t}$ are highly correlated (as would be expected)
But j^{LG} and $j^{\Delta t}$ are getting more correlated as Δt increases.

What about the magnitude of the current fluctuations σ_j?



We all know

$$\sigma_j = \rho k_B T \qquad (64)$$

and we do get a straight line as expected.

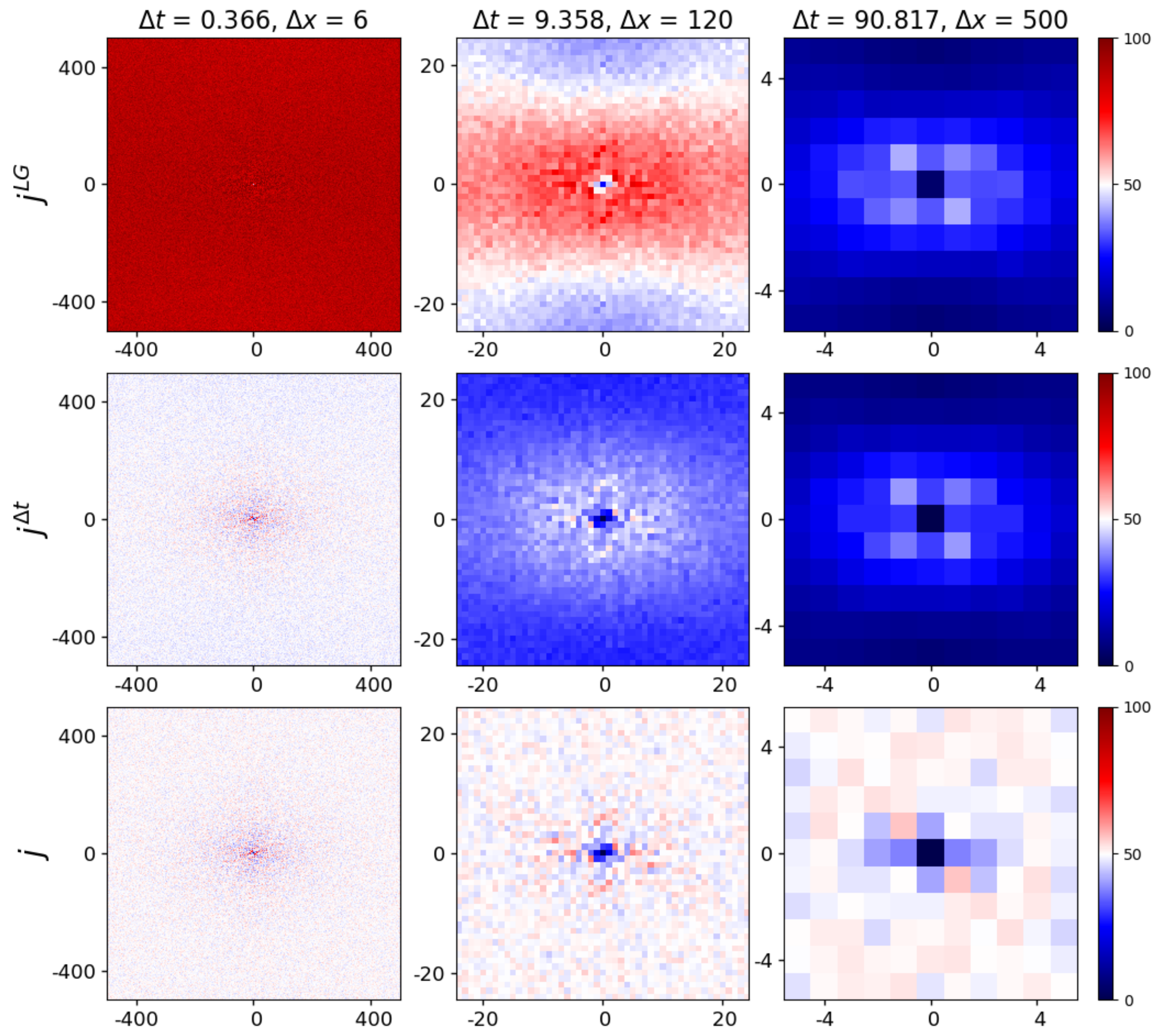
$\sigma_{j^{LG}}$ follows the ideal gas theory (i.e. Poisson distributed independent n_i) reasonably well.

$\sigma_{j^{\Delta t}}$ does not agree well with a theory that assumes independent displacements of particles (dash-dot line). But a theory that includes correlations of particles give good predictions (dashed line).

What about the small Δt limit?

Either lattice gas momentum does not agree with MD momentum in the small scale limit, or the ideal gas prediction of a flat momentum fluctuation spectrum fails.

Fourier transforms of the current fluctuations



For small Δt j^{LG} has a flat spectrum, which means the lattice gas current fluctuations are larger than the MD current fluctuations for all k.

The j^{MD} are initially flat, but then converge to something very similar to the j^{LG} fluctuations.

The j fluctuations remain flat for a all Δt, as expected from basic theory.

Non-equilibrium behavior

So far we have focused on equilibrium behavior:

- Local equilibrium distribution
- Equilibrium fluctuations in density
- Equilibrium fluctuations in momentum, and different definitions of momentum.

Now it is time to look at some non-equilibrium behavior, which after all is where lattice gas and lattice Boltzmann should be applied.

The collision operator

We defined the Boltzmann collision operator as a non-equilibrium ensemble average

$$\Omega_i = \langle \Xi_i \rangle = \langle n_i(x + \delta x_i, t + \delta t) - n_i(x, t) \rangle \tag{65}$$

To measure this collision operator we should average over all (or at least a sufficiently large representative sample of) possible microscopic configurations. To do this we set up a MD simulation with Lees-Edwards boundaries to simulate simple shear flow. The average of the flow will be stationary, and we can then sample over the whole system (using Galilean transformations to have the center of each cell at 0 velocity).

Rest of the workshop

Monday 1:30 Jordan Larson, Analytical solution to LBM

Tuesday 10am Hamed Vaseghnia, Deriving the LBM forcing term through MDLG

Tuesday 11am Adam Quintana, A new form of double phase separation in the Cahn Hiliard equation

Wednesday 10am Kyle Strand, Overrelaxation in Integer lattice gases

Wednesday 11am Aleksandra Pachalieva, Applications of the Molecular Dynamics lattice gas analysis tool

Rest of the workshop

Tuesday 10am Matteo Lulli, MDLG like analysis of an Ising model.

Tuesday 11am Adam Quintana, The He-Chen-Zhong method for multiphase systems

Friday 10am Noah Seekins, Monte Carlo integer lattice gas

Friday 11am Luiz Czelusniak, Phase change considerations.

In the afternoon we will have research meetings with me and with each other too facilitate research interactions. Lunch will be at noon in the MU and we will have coffee at 3pm at the same place (unless I get our kitchen to work).

Conclusions

- We have examined (very) different models for a real fluid and explained what goes into showing their equivalence.

- Molecular dynamics simulations can be used to define an exact version of lattice Boltzmann (MDLB). Really what is needed is just $P(x, \delta x, t)$ for the particular situation.

- The equilibrium distribution agrees with standard LBM for small mean velocities

- This allows us to predict fluctuating properties lattice gases for non-ideal systems, which are quite different than what has been previously expected. As usual, fluctuating methods require more information, in this case $P(x_1, \delta x_1, x_2, \delta x_2, t)$.

- It also provides a first-principles derivation of the lattice Boltzmann collision operator. All the properties of lattice Boltzmann have been reduced to finding the 1-particle displacement distribution function.