Monte Carlo Integer Lattice Gas in Diffusive and Hydrodynamic Systems

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Overview

1. Lattice Gas History

2. The Monte Carlo Lattice Gas in the Diffusive Case

3. Testing the Method

4. Timing Results for the diffusive case

5. Extending to the Hydrodynamic Regime

Boolean Lattice Gases[1]

$$n_i(x + v_i, t + 1) = n_i(x, t) + \Xi_i$$

n_i boolean occupation number;
v_i lattice velocity;
Ξ_i collision operator.

- Popular in the 1980s and 1990s - Allowed for the simulation of the Navier-Stokes equations, something revolurionary for their time.

- Equilibrium is Fermi-Dirac: leads to velocity dependence of viscosity and other artifacts.

- Lookup methods had difficulty scaling to three dimensions.

- EXA company developed the Digital Physics approach which solved some issues, but results are proprietary.

- Eventually replaced by lattice Boltzmann due to these issues

[1]Uriel Frisch, Brosl Hasslacher, and Yves Pomeau, "Lattice-gas automata for the navier-stokes equation," Physical Review Letters 56, 1505 (1986)

Lattice Boltzmann[2]

$$f_i(x + v_i, t + 1) = f_i(x, t) + \Omega_i$$

f_i non-equilibrium ensemble average of n_i;
v_i lattice velocity;
Ω_i collision operator.

- Originally created by taking the Boltzmann average of the lattice gas equation.
- Used as a tool for testing lattice gas simulations before being introduced in its own right.
- Equilibrium is Maxwell-Boltzmann by default, however for entropic lattice Boltzmann equilibrium is Poisson distributed.
- Does not include fluctuations by default.

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[2]G. McNamara and G. Zanetti, Phys. Rev. Lett. 61, 2332 1988!.

Integer Lattice Gases[3456]

- n_i become integers
- Equilibrium distribution becomes Poisson Distributed
- Fixes nearly all of the issues with the Boolean lattice gases except for efficiency and over-relaxation.
- Goal: find an efficient form of Ξ_i (Previous approach based on binary particle collisions)

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[3]B. Chopard, A. Masselor and M. Droz. Phys. Rev.Lett. 81:9, 1998.

[4]Thomas Blommel and Alexander J Wagner, Physical Review E 97, 023310 (2018).

[5]H. Chen, C. Teixeira, and K. Molvig, Digital physics approach to computational fluid dynamics: Some basic theoretical features, Int. J. Mod. Phys. C 8, 675 (1997).
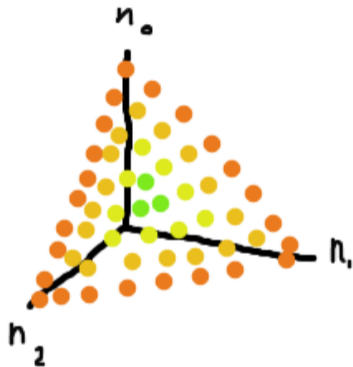
[6]B. M. Boghosian, J. Yepez, F. J. Alexander, and N. H. Margolus,Integer lattice gases, Phys. Rev. E 55, 4137 (1997).

Why Integer Lattice Gases?

- The discrete nature of the integer lattice gas allows for several types of previously difficult simulations to become simple.
- Chemical reactions within fluids and extremely low-density systems are just a few examples of what these discrete methods can do better than the LBM, which struggles with them due to its nondiscrete and deterministic nature.

Developing a Monte Carlo collision operator[7]

- **Idea:** the effect of the collision operator is to bring the n_i closer to equilibrium.
- Define the new n_i by sampling from equilibrium distribution with probability $P(n_1, \cdots, n_V)$
- Ordinarily sampling requires picking points off of a $V - C$ dimensional hypersurface where C are the number of conserved quantities.
- In practice, we've found that this can be simplified due to decoupled axes.

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[7]B. M. Boghosian, J. Yepez, F. J. Alexander, and N. H. Margolus, Integer lattice gases, Phys. Rev. E 55, 4137 (1997).

Simplest case: diffusive lattice gas[10]

Only mass is conserved. We want to impose a local equilibrium distribution

$$f_i^{eq} = \langle n_i \rangle_N^{eq} = N w_i \tag{1}$$

with $\sum_i w_i = 1$. We do this by demanding detailed balance

$$f_i^{eq} P_{i \rightarrow j} = f_j^{eq} P_{j \rightarrow i}$$

Where $P_{i \rightarrow j}$ is the probability of a particle with velocity i, if selected, becoming a particle with velocity j. This can be achieved in a very simple manner:

$$P_{i \rightarrow j} = w_j$$

(We demand detailed balance first instead of imposing a local equilibrium distribution. This leads to different results in the hydrodynamic case where only $f_i^{eq}(\rho, u \equiv 0)$ can be imposed[8],[9])

[8]B. Chopard, A. Masselor and M. Droz. Phys. Rev.Lett. 81:9, 1998.

[9]Thomas Blommel and Alexander J Wagner, Physical Review E 97, 023310 (2018).

[10]B. Chopard and M. Droz, Cambridge University Press, 1998, section 5.7 and 7.3

Determining the Local Equilibrium Distribution

As the diffusive system does not conserve momentum, we represent all collisions as being with a probability matrix.

Thus, the probability of finding n particles in a specific velocity i after a collision, when the lattice site has N total particles, is:

$$P_i(n) = \frac{N!}{n!(N-n)!} w_i^n (1-w_i)^{N-n}.$$

Due to there being more than one velocity, and each having its own w_i, we must sample this distribution successively, so that for a second velocity j sampled after velocity i is found to have n_i particles:

$$P_j(n) = \frac{(N-n_i)!}{n!(N-n_i-n)!} w_j^n (1-w_j)^{N-n_i-n}.$$

Local equilibrium distribution: The Multinomial Distribution

$$P(n_1, \cdots, n_V) = \begin{cases} \frac{N!}{n_1! \cdots n_V!} w_1^{n_1} \cdots w_V^{n_V} & \text{for } n_1 + \cdots + n_V = N \\ 0 & \text{otherwise} \end{cases}$$

- For our diffusive lattice gas with weights w_i, we find that the equilibrium distribution of occupation numbers n_i is given by a multinomial distribution.
- In practice we sample from the multinomial distribution by sampling from successive binomial distributions.
- We use the GNU Scientific Library[11] for higher densities, and we created our own algorithm, which is actually more efficient for lower densities

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[11] Galassi et al, GNU Scientific Library Reference Manual (2nd Ed.), ISBN 0954161734

Sampling

- As it is the core of our method, it is important to discuss sampling as a concept.
- In general, sampling functions by comparing a uniformly distributed random number r to the cumulative probability distribution:

$$C(n) = \sum_{m=0}^{n} P(m)$$

- Since we are dealing with discrete values of n, each n will have a range of values of r that correspond to it.
- Thus, if $C(n) = 0.6$ and $C(n+1) = 0.7$, any value of r from 0.6 to 0.7 would correspond to n.

Sampling Visualized
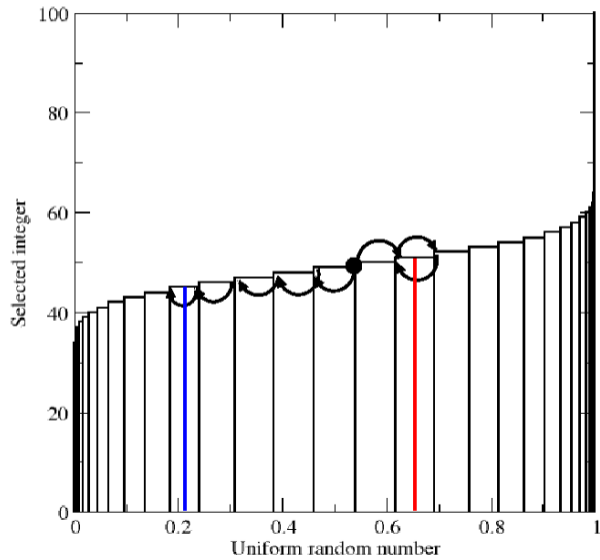
Our Sampling Method

- Sampling for a distribution with an unknown cumulative distribution function (as is the case for the binomial distribution) requires the cumulative distribution function to be calculated on each call.

- We save time by precalculating and saving key points (in the case of the visualized example, $C(n)$ 0.5) in order to make the process easier.

- This works for any distribution with a known recursive relation, whereas many libraries may not have a sampling method for uncommon or unique distributions (such as the one we will be discussing with regards to hydrodynamic systems).

Partial Collisions

- Partial collisions are useful to alter the viscosity of a simulated fluid.
- Due to the integer nature of lattice gases, partial collisions must be sampled for in addition to the velocity set sampling.
- In order to undertake partial collisions, we define the fraction of collided particles in a given timestep as ω.
- Utilizing ω as a probability for collision, we are able to sample the particles to be collided in each velocity utilizing a binomial distribution, thus the probability of n particles being collided in a velocity with N particles becomes:

$$P(n) = \binom{N}{n} \omega^n (1 - \omega)^{(N-n)}$$

Hydrodynamic limit

In order to prove that this method is viable, one of the important steps is ensuring that the hydrodynamic limit returns the proper form, in this case, the diffusion equation.
We first take an ensemble average to obtain a lattice Boltzmann equation

$$f_i(x + v_i, t + 1) = f_i(x, t) + \omega[\rho(x, t)w_i - f_i(x, t)]$$

where $\rho = \sum_i f_i$. We also demand

$$\sum_i v_i w_i = 0 \quad \sum_i v_i^2 w_i = d\theta$$

Where d is the number of spatial dimensions, and θ is a constant.
We are able to Taylor expand the averaged equation to find:

$$f_i(x, t) = \rho(x, t)w_i - \frac{1}{\omega}(\partial_t + v_i\nabla) + O(\partial^2)$$

Hydrodynamic Limit

Reinserting our Taylor expansion into the averaged equation, we get:

$$\partial_t \rho(x,t) w_i + v_i \nabla f_i^{eq} - (\frac{1}{\omega} - \frac{1}{2})(\partial_t + v_i \nabla)^2 \rho(x,t) w_i = \omega(\rho(x,t) w_i - f_i) + O(\partial^2)$$

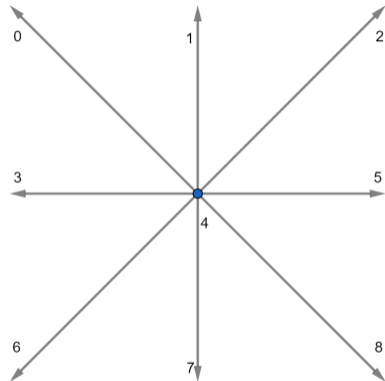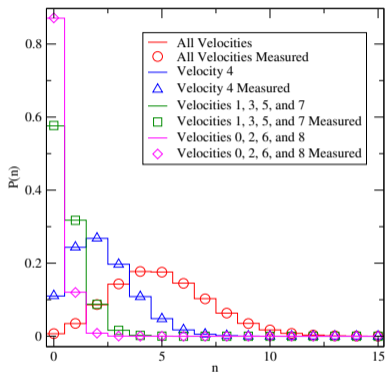which, if we then sum over i, allows us to utilize the restrictions we posed earlier.

$$\partial_t \rho + (\frac{1}{\omega} - \frac{1}{2})(\partial_t^2 \rho + \nabla^2(\rho\theta)) = 0 + O(\partial^3)$$

and finally, simplifying this gives us

$$\partial_t \rho(x,t) = \left(\frac{1}{\omega} - \frac{1}{2}\right) \theta \nabla^2 \rho$$

which is the diffusion equation with $D = (\frac{1}{\omega} - \frac{1}{2})\theta$ and $\theta = \frac{1}{3}$ by convention.

- We recover the Poisson distribution in equilibrium
- Fluctuating lattice Boltzmann methods fail to do this for low densities.
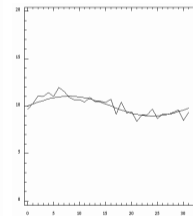
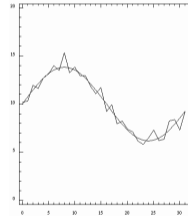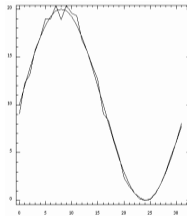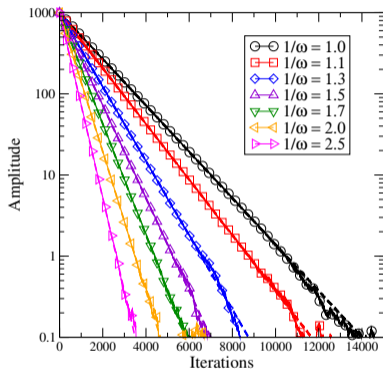# Solution to the Diffusion Equation

In order to look at the evolution of the system in a controlled manner, we set up a sinusoidal profile utilizing a Poisson distribution. This allows us to utilize the following solution to the diffusion equation to compare to our results:

$$\rho(x, t) = N^{av} \left[1 + \sin\left(\frac{2\pi x}{L_x}\right) \right] \exp\left(-\frac{4\pi^2 D t}{L_x^2}\right)$$

Where

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

- Decay of sine wave is well recovered for different relaxation times (i.e. diffusivities)
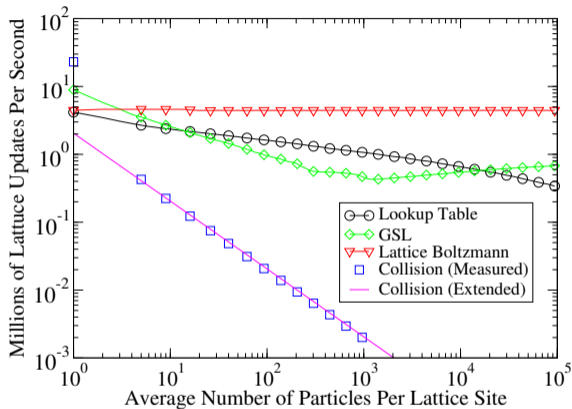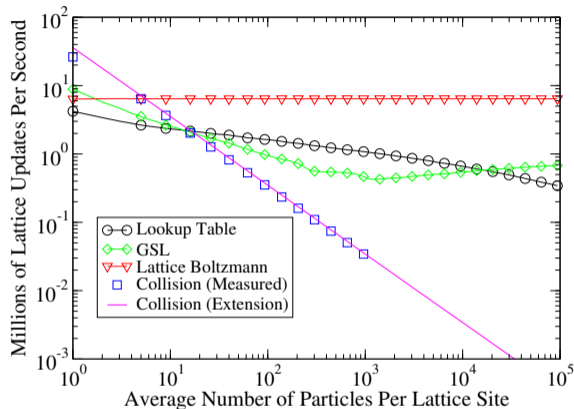
# Timing Results[12]

Figure: $1/\omega = 1$

Figure: $1/\omega = 2$

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[12]Alexander J Wagner and Kyle Strand, "Fluctuating lattice Boltzmann method for the diffusion equation," Physical Review E 94, 033302 (2016).

Hydrodynamic Systems

- Momentum is conserved.
- Returns the Navier-Stokes Equations in the Hydrodynamic limit
- This allows for most standard forms of flow to be observed, where the diffusion equation is more limiting.
- The simulations of wind tunnels, airfoils, engine exhaust pipes, and... cows... used in manufacturing and research all utilize a hydrodynamic flow in their calculations.
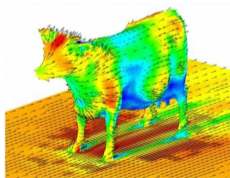
Challenges for Hydrodynamic Systems

- Due to the requirement of Momentum conservation the basic algorithm requires (at least) binary collisions.

- We still require detailed balance which applies to binary collisions thusly:

$$w_i w_j P_{ij \to kl} = w_k w_l P_{kl \to ij}$$

- The resulting equilibrium distribution is not as common as the Multinomial Distribution, meaning that there are no pre-analyzed packages to increase the efficiency.

Sampling from the Moments: D1Q3 example

Instead of sampling from the equilibrium distribution of the particles, we instead move to moment space to sample. The moments are defined as follows (or, the first three that we use for sampling):

$$N = \sum_i n_i = n_{-1} + n_0 + n_1$$

$$J = \sum_i n_i v_i = n_1 - n_{-1}$$

$$\pi = \sum_i n_i v_i^2 = n_1 + n_{-1}.$$

$$n_{-1} = \frac{\pi - J}{2}$$

$$n_0 = N - \pi$$

$$n_1 = \frac{\pi + J}{2}.$$

We can utilize these moments, and their relations with each other, to find an equilibrium distribution over π to sample by defining the n_i values in terms of the local moments.

Which moment to sample?

- The velocities $v + i$ are sampled in the diffusive case directly via the weights for individual velocities, however this leads to improper momentum handling for two particle collisions.

- J is a representation of momentum in the system, thus is conserved over the collision step.

- This just leaves π as the only moment that is able to be sampled.

π is non-trivial to sample, as its local equilibrium distribution is nonstandard. Thus, we must derive the local equilibrium distribution for π in order to sample it.

Proper π distribution

- In order to find the local equilibrium distribution, the detailed balance

$$P(\pi + 2) = \frac{w_1 w_{-1}}{w_0^2} * \frac{2(N - \pi)^2 - (N - \pi)}{\pi^2 - J^2} * P(\pi).$$

  relation:

$$P(\pi)t_{\pi \to \pi+2} = P(\pi + 2)t_{\pi+2 \to \pi}$$

  must be satisfied.

- In this relation, $P(\pi)$ is the probability of the π moment taking a specific value, and $t_{\pi \to \pi+2}$ and $t_{\pi+2 \to \pi}$ are the transition probabilities.

- The transition moves from π to $\pi + 2$ and not to $\pi + 1$ since J must be conserved, and thus the velocities of particles can only be changed in positive and negative pairs.

Transition Probabilities

- To find the transition probabilities, we look at the probability of having a pair of moving particles go to rest particles ($t_{\pi+2\to\pi}$) and vice versa ($t_{\pi\to\pi+2}$).
- The probability of picking a rest particle is given by n_0/N, and the probability of picking a second rest particle is $(n_0 - 1)/(N - 1)$.
- Thus, the transition probability $t_{\pi\to\pi+2}$ is given by:

$$t_{\pi\to\pi+2} = p_{\pi\to\pi+2} * \frac{n_0^2 - n_0}{N^2 - N}$$

where n_0 is the number of rest particles, N is the total number of particles, and $p\pi \to \pi + 2$ is a normalization factor which by convention we pick as $1/16$.

Transition Probabilities

- There are two ways to pick a pair of moving particles: either pick one moving in the positive direction and then one in the negative direction, or vice versa.
- The probability of the first option is given by n_1/N for the positive particle, and $n_{-1}/(N-1)$ for the negative.
- The probability of the second option is given by n_{-1}/N for the negative particle, and $n_1/(N-1)$ for the positive.
- Thus, the transition probability $t_{\pi \to \pi+2}$ is given by:

$$t_{\pi+2 \to \pi} = p_{\pi+2 \to \pi} * \frac{2n_1 n_{-1}}{N^2 - N}$$

where n_1 is the number of particles moving in the positive direction, n_{-1} is the number of particles moving in the negative direction, and $p_{\pi \to \pi+2}$ is a normalization factor which by convention we pick as 1.

Proper π distribution

These transition probabilities can then be rewritten in terms of the known moments: N, J, and π, giving us:

$$t_{\pi \to \pi+2} = p_{\pi \to \pi+2} * \frac{(N-\pi)^2 - (N-\pi)}{N^2 - N}$$

$$t_{\pi+2 \to \pi} = p_{\pi+2 \to \pi} * \frac{\pi^2 - J^2}{2(N^2 - N)}$$

Which leads the recursive probability distribution to be:

$$P(\pi + 2) = \frac{p_{\pi \to \pi+2}}{p_{\pi+2 \to \pi}} * \frac{2(N-\pi)^2 - (N-\pi)}{\pi^2 - J^2} * P(\pi)$$

Weighted Probabilities

- The values of $p_{\pi \to \pi+2}$ and $p_{\pi+2 \to \pi}$ are the probabilities of having two rest particles become moving particles and vice versa.

- This means that although two rest particles are selected, they will not always become moving particles.

- The chance of this happening is given by the weights of the system:
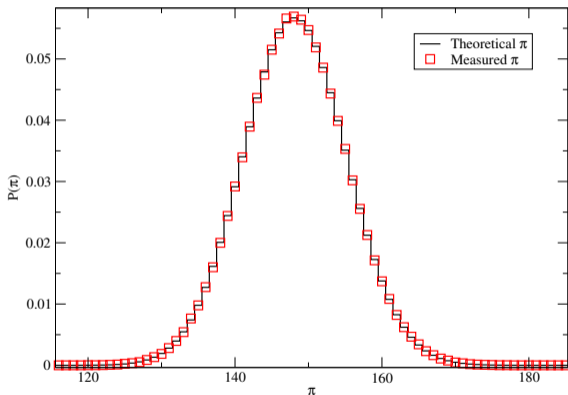
$$p_{\pi \to \pi+2} = w_1 w_{-1}$$

$$p_{\pi+2 \to \pi} = w_0^2$$

- Thus, the π distribution becomes

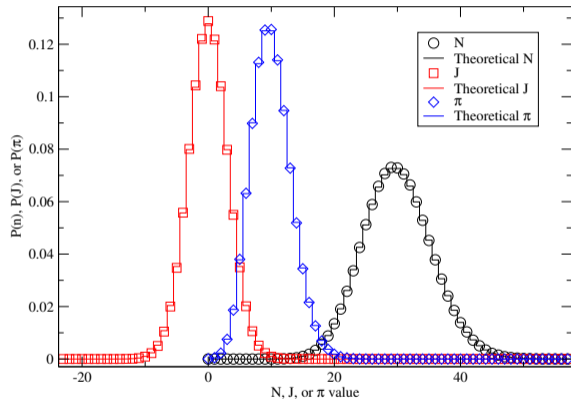$$P(\pi + 2) = \frac{w_1 w_{-1}}{w_0^2} * \frac{2(N - \pi)^2 - (N - \pi)}{\pi^2 - J^2} * P(\pi).$$

- We have, by utilizing a similar algorithm to that used by Blommel *et al.*, been able to show that our equilibrium distribution is accurate.
- As is shown on the left, given no streaming, a system will fall into equilibrium in this way for both the x and y axis in terms of π.
- As this distribution is not simple, utilizing a library like the GSL may not be an option.

- Globally, the N, J, and π values have different equilibrium distributions than they do locally.
- N and π are Poisson distributed.
- J is Skellam distributed.

Testing the method in full

- In order to ensure the proper functioning of the method, it is necessary to utilize several test cases. The 1D test cases we have decided to utilize are the SOD shock tube and potentially a decaying sound wave.
- Neither of these examples is fully implemented, as we are working on finding applicable analytical solutions for how these develop to influence the setup and testing of the systems.

More dimensions
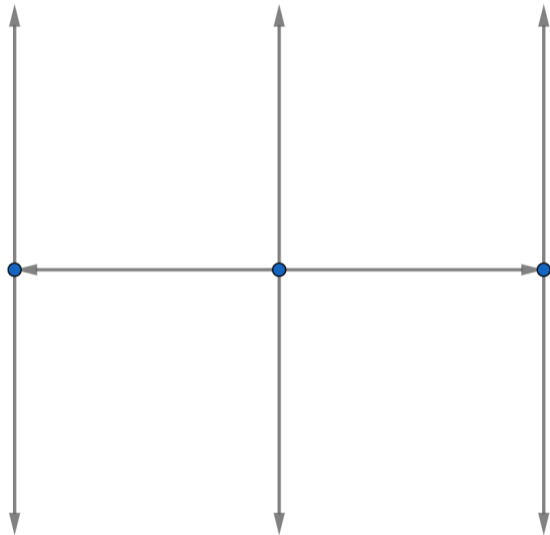
- Increasing from 1D to more dimensions is a nontrivial process for the Hydrodynamic system (as opposed to the diffusive system where it is as simple as increasing the dimension of the particle array and the number of velocities).

- This complexity results from the fact that J must be conserved locally, and thus, the total J value across several axes must be conserved in order for the axis-decoupling strategy to remain valid.

More dimensions cont.
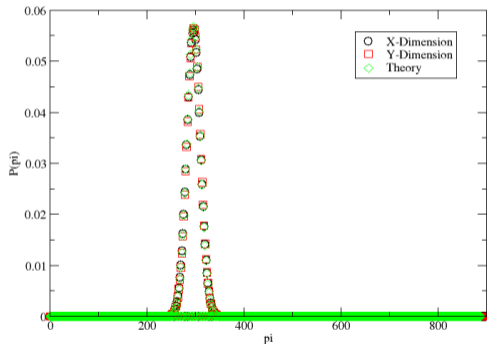
- The process of increasing the number of dimensions is slightly easier due to the fact that the x and y dimension π distributions for a 2D system are identical to the 1D π distribution found earlier.
- This leaves the most difficult part as figuring out how to properly split the momentum among the axes.

Outlook

- Our paper on the diffusive Monte Carlo lattice gas has been officially published[13].

- We have a functioning prototype for a 1D Hydrodynamic Monte Carlo lattice gas, and intend to write a paper on that as well, including additional proof for the functionality of the method and 1D Hydrodynamic MCLG Overrelaxation, in part thanks to the work of Kyle Strand *et. al.*[14].

- We have some ideas on how to move the system to 2D (and 3D), however they remain untested thusfar, and this is intended to be included in a follow-up paper to the 1D version.

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[13]Noah Seekins and Alexander J. Wagner, Integer lattice gas with a sampling collision operator for the fluctuating diffusion equation, Phys. Rev. E **105** (2022), 035303.

[14]Kyle Strand and Alexander J. Wagner, Overrelaxation in a diffusive integer lattice gas, Phys. Rev. E **105** (2022), L063301

Questions