CSE 599D Physics of Computation, Autumn 2013
Theory and Simulation of Thermodynamic Quantities in LGA Model

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1 Abstract

Proposed to simulate fluid flows for years, lattice gas automata (LGA) has shed lights on studying a range of macroscopic aspects in thermodynamics due to the fact that in theory, their dynamics are based on the same model as fluid flows. Specifically, interests in LGA methods have led to formal expression of entropy as a thermodynamic quantity using the Boltzman distribution, yet no work has exhibited that in practise, how the theoretical model and actual entropy by definition in the LGA simulator can be compared. In this report, by implementing the formal expression and the actual entropy in a two-chamber scenario in the LGA framwork, we show that the theoretical model can precisely describe the actual entropy of the system. Furthermore, we show systematically how other macroscopic quantities can be simulated in the LGA model in order to study complex behaviors that could happen for a Billiard-ball computer we could build using the LGA model.

2 Introduction

LGA is a type of cellular automaton used to sumulate fluid flows. From LGA, it is possible to derive the macroscopic Navier-Stokes equations, forming a relatively new and promising methods for the numerical solution of (nonlinear) partial differential equations. The fact that different microscopic interactions can lead to the same form of macroscopic equations is the starting point for the development of the LGA framework. In addition to real gases or real liquids one may consider artificial micro-worlds of particles that live on lattices with interactions that conserve mass and momentum. In our 2-D LGA model, we consider a hexagonal lattice with six cells at each site such that one site is associated with each link to the next neighbor node. These sites may be empty or occupied by at most one particle with unit mass. Thus each cell has only two possible states; volocity and thereby also momentum can be assigned to each particle by the vector connecting the site to its next neighbor node along the link where the particle is located. The microscopic interation is strictly local in that it involves only particles at a single site. The particles exchange momentum while conserving the mass and momentum summed up over each node. After this collision each particle propagates along its associated link to its next neighbor site. The micro-dynamics consists on a repetition of collision and propagation. Microscopic values of mass and momentum density are calculated by calculating the mean values over large

spatial regions with hundreds to thousands of sites. Theories have shown that values do not necessarily obey the Naview-Stokes equations if the third essential condition in addition to mass and momentum conservation is absent. The third condition is that in 2-D, for example, 4-fold rotational symmetry (square lattice) is not enough whereas hexagonal symmetry (triangular lattice) is sufficient. A further condition should be mentioned here, which is the microdynamics must not possess more invariants than required by the desired macroscopic equations becuase such so-called spurious invariants can alter the macroscopic behavior by unphysical constraints.
With the complete logical basis we have introduced above, it is time for the comparison between a theoretical derivation of the entropy from a thermodynamic perspective with specification to hexagonal 2-D LGA and the actual instantaneous entropy by deifinition in the hexagonal 2-D LGA. In the following sections, we sequentially introduce how we derive the entropy formula in 2-D hexagonal LGA, and how we compute the actual entropy in the same model without any additional assumptions to the model we have been considering.

3 Theoretical Model

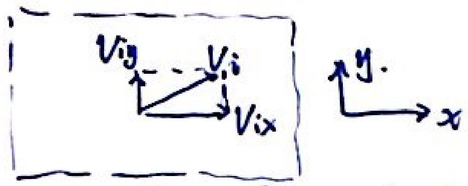
3.1 The entropy formula

From a microscopic view, we try to express the entropy with only the pressure, heat capacity and volumn which can be strictly defined in the 2-D hexagonal LGA model.

Initial Results: Angli Liu.

1. Defining Pressure in LGA.

Chamber:



pressure: $P = \frac{\Delta F}{\Delta S} = \frac{\sum_i I_i}{\Delta S\, \Delta t}$ (impulse)

$$= \frac{1}{2} \sum_i (m \cdot n_i\, V_{ix}\, \Delta t \cdot \Delta S) \cdot 2V_{ix} / (\Delta S \cdot \Delta t)$$

where $m \cdot (n_i V_{ix}\, \Delta t\, \Delta S)$ is the mass of particles that hit the wall of the chamber within time Δt.

$\frac{1}{2}$ means the probability of V_{ix} heading $\pm x$ are equal.

As particles hitting the right-hand side wall is the scenario we are interested in, we have

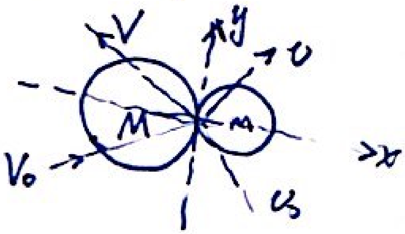
$$P = nm \frac{\sum_i V_{ix}^2 n_i}{n}.$$

Because. $\overline{V_x^2} = \frac{\sum_i V_{ix}^2 n_i}{n} = \frac{1}{3} \overline{V^2}$ (3 ~~ratio~~ orthogonal directions)

We have $P = \frac{1}{3} n m \overline{V^2} = \frac{2}{3} n \left(\frac{1}{2} m \overline{V^2}\right) = \frac{2}{3} n \cdot$ kinetic energy.

2. Temperature.

Though in LGA all particles have same mass, we are starting with the assumption that particles can have differences in mass and velocity for convenience of getting the mathematical expression of the temperature.



After the collision, particle M loses kinetic energy

$$\Delta E = \tfrac{1}{2}M\left(V_0^2 - V^2\right) = \tfrac{1}{2}M\left(V_{0x}^2 - V_x^2\right) \quad (\text{since } V_{0y} = V_y)$$

$$= \tfrac{1}{2}M\,(V_{0x} - V_x)(V_{0x} + V_x)$$

Due to the conservation of momentum, by solving the equation:

$$V_x = \frac{M V_{0x} + m v_{0x}}{M+m} - \frac{m(V_{0x} - v_{0x})}{M+m} = \frac{(M-m)V_{0x} + 2m v_{0x}}{M+m}$$

Therefore $\quad V_{0x} - V_x = \dfrac{2m(V_{0x} - v_{0x})}{M+m}, \quad V_{0x} + V_x = \dfrac{2(M V_{0x} + m v_{0x})}{M+m}$

So $$\Delta E = \frac{2mM}{(M+m)^2}\left[M V_{0x}^2 - m v_{0x}^2 - (M-m)\, v_{0x} V_{0x}\right]$$

Averaging over the huge number of particles, we have

$$\overline{\Delta E} = \frac{2mM}{(M+m)^2}\left[M \overline{V_{0x}^2} - m\overline{v_{0x}^2} - (M-m)\,\overline{v_{0x}V_{0x}}\right]$$

Because $\overline{V_{0x}} = \overline{v_{0x}} = 0$ and V_{0x} is independent from v_{0x}

We have $\quad \overline{v_{0x}V_{0x}} = 0.$

Therefore

$$\overline{\Delta \varepsilon} = \frac{2mM}{3(M+m)^2}\left(M\overline{V_0^2} - m\overline{v_0^2}\right) \qquad \left(\overline{v_x^2} = \frac{1}{3}\overline{v^2}\right)$$

$$\propto \frac{1}{2}M\overline{V_0^2} - \frac{1}{2}m\overline{v_0^2}$$

From a microscopic perspective, the temperature is rooted from the kinetic energy of particles, so we assume

$$\frac{1}{2}m\overline{v^2} = B\cdot T.$$

3. Particles equation in LGA

According to 1 and 2. We have

$$P = \frac{2}{3} n \left(\frac{1}{2} m \bar{v}^2\right)$$

and $\frac{1}{2} m \bar{v}^2 = B \cdot T$

Therefore $P = \frac{2}{3} n B T = \frac{2}{3} \frac{N}{V} B T$

as n is the number of particles in a unit volumn

Then we have

$$PV = \frac{2}{3} N \cdot B T$$

where B is a coeffecent we define in 2.

For the equation above. we have

$$\frac{PV}{T} = \frac{2}{3} N \cdot B = Const$$

Which means in LGA, for same type of particle(mass, velocity, directions of movement).

$$\frac{P_i V_i}{T_i} = \frac{P_j V_j}{T_j}$$

And for different types of particles

$$\frac{P_{all} V_{all}}{T_{all}} = \frac{2}{3} B \sum_i N_i = \sum_i \frac{P_i V_i}{T_i}$$

We will be considering the conservation of energy. while ignoring all the sinks and sources in LGA, as well as considering entropy all the way to Maxwell's daemon. then.

4. Macro quantities:

statistical average of micro quantities.

We want to derive macro quantities from a model of the micro quantities. In LGA, the Bolzmann distribution looks like a good model for describing the properties of the particles.

① ε_i : particle energy on energy level i.

②. g_i : the degeneracy of energy level i.

③. n_i : the number of particles on energy level i.

$\{n_i\}$: distribution of # of particles v.s energy level.

$W\{n_i\} = \prod_i W_i$ # of micro states corresponding to distribution $\{n_i\}$

④ constraits: $\sum_i n_i = N$, $\sum_i \varepsilon_i n_i = E$.

$\uparrow$ # of particles $\uparrow$ total energy.

equal propability assumption: $P\{n_i\} = \dfrac{W(\{n_i\}, N, V, E)}{\sum_{\{n_i\}} W(\{n_i\}, N, V, E)}$

In LGA, assuming there are more than one energy levels, particles follow Bolzmann distribution:

$$W_{Bol}\{n_i\} = N! \prod_i \frac{g_i^{n_i}}{n_i!} = \prod_i C_{N-\sum_{0}^{i-1} n_i}^{n_i} g_i^{n_i}$$

$\because \dfrac{\partial}{\partial n_i} \ln W_{Bol}\{n_i\} = 0$

$\therefore \quad n_i = g_i e^{-\alpha - \beta \varepsilon_i}$

partition function: $z(\beta, y) = \sum_i e^{-\beta \varepsilon_i} g_i$..

See last equation in space coordinate.

(definition).

\# of particles: $N = \sum_i g_i e^{-\alpha-\beta\varepsilon_i} = e^{-\alpha} z$, $\alpha = \ln \frac{z}{N}$.

inner energy: $E = \sum_i \varepsilon_i g_i e^{-\alpha-\beta\varepsilon_i} = -N \frac{\partial \ln z}{\partial \beta}$.

Regarding ~~imagine~~ sinks and sources in LGA as exchange of energy. according to the 2nd law of thermaldynamics.

$$dE = \sum_i n_i d\varepsilon_i + \sum_i \varepsilon_i dn_i = dW + dQ$$

Because

$$dW = \sum_k Y_k dy_k = \sum_i n_i \sum_k \frac{\partial \varepsilon_i}{\partial y_k} dy_k = \sum_k \Big(\sum_i n_i \frac{\partial \varepsilon_i}{\partial y_k}\Big) dy_k$$

where

$$Y_k \triangleq \sum_i n_i \frac{\partial \varepsilon_i}{\partial y_k} = -\frac{N}{\beta} \frac{\partial \ln z}{\partial y_k}$$ representing one macro quantity.

for example $P = \frac{N}{\beta} \frac{\partial \ln z}{\partial V}$.

We have

$$dQ = dE - \sum_k Y_k dy_k = \frac{N}{\beta} d\Big(\ln z - \beta \frac{\partial}{\partial \beta} \ln z\Big) \overset{\text{also}}{=} T dS$$

therefore $S = \int \frac{dQ}{T} = Nk\Big(\ln z - \beta \frac{\partial \ln z}{\partial \beta}\Big) + S'$ where $\beta = \frac{1}{kT}$

Our LGA is a 2-D simulator, therefore

$$z(\beta, y) = \sum_i e^{-\beta \varepsilon_i} g_i \propto \int_0^\infty e^{-\beta \varepsilon} g(\varepsilon) d\varepsilon$$ (continuous degeneracy).

In 2γ-dimensional phase space.

$$\varepsilon = \varepsilon(q_1, q_2 \cdots q_\gamma, p_1, p_2 \cdots p_\gamma, y)$$

$$\Omega(\varepsilon) = \int \cdots \int_{(0,\varepsilon)} dq_1 \cdots dq_\gamma \, dp_1 \cdots dp_\gamma$$

$$g(\varepsilon) d\varepsilon = \frac{d\,\Omega(\varepsilon)}{h^\gamma}$$

Therefore, in LGA, assuming multi-energy level exists,

$$Z = \int_0^\infty e^{-\beta\varepsilon} g(\varepsilon) d\varepsilon$$

$$= \int_0^\infty e^{-\beta\varepsilon} \frac{d\Omega(\varepsilon)}{h^\gamma}$$

$$= \int_0^\infty e^{-\beta\varepsilon} \frac{2\pi A J m}{h^2} d\varepsilon$$

$$= \frac{2\pi A J m}{\beta h^2}$$

Finally. $E = -N \frac{\partial \ln Z}{\partial \beta} = NkT$

$P = \frac{N}{\beta} \frac{\partial \ln Z}{\partial A} = \frac{NkT}{A} = \frac{E}{A}$ where A is the area.

also $S = Nk\left(\ln Z - \beta \frac{\partial \ln Z}{\partial \beta}\right) = Nk(1 - \ln N)$.

$F = E - TS = -NkT \ln \frac{\partial Z}{N}$. (enthalpy).

$\vdots$

3.2 The estimate of the actual entropy

Operationally, we may define local states of the LGA model at time step t, and we can evaluate the occurrence probability of a configuration s by measuring the occurrence frequency over the whole lattice at each time step. A second measure of the occurrence probability is the occurrence frequency at a given location of the LGA, over a large number of realizations. At each run the LGA is initialized independently with a giben set of macroscopic constraints. Therefore, we obtain a local estimate of entropy that changes with time. Moreover, in order to make the result comparible with the theoretical result, we will need to obtain a global estimate of the entropy. In fact, we know that particles in the LGA model consist of two actions: propagation and collision, and if the propagation does not produce correlations between the sites, then the global entropy H is entirely determined by the local entropy h:

$$H = \sum_x h(x) \tag{1}$$

where

$$h(x) = -\sum p(x) \ln p(x) \approx -\sum_t f(x,t) \ln f(x,t) \tag{2}$$

The summation holds for equation 1 because the uncertainty is in fact summable over the entire 2-D hexagonal LGA space. And the estimate of local entropy would be more accurate if the time window within which we average over the instantaneous entropy is small enough. In the following sections, we will introduce the implementation of the comparison of the entropy, and the evaluation of the result.

4 Implementation

In this secition, we use the 2-D hexagonal LGA simulator to implement the two proposed expression of the entropy of a closed particle system. We adopt a reflecting wall scenario where two chambers connect to each other by a tunnel. The system is closed without any sink or source, therefore, there is no energy or mass exchange with outside. However, the momentum is consistantly changing as particles will exchange momentum with the wall under the assumption that the wall has an infinite mass. The initial state of the simulator is shown below.

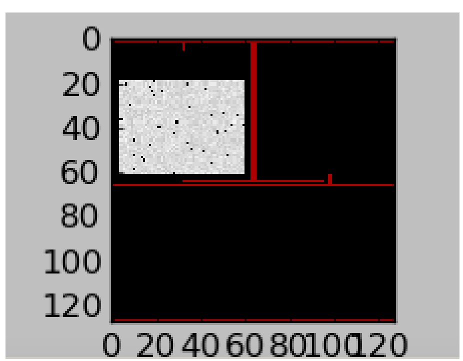


Figure 1: The initial state of the LGA

At time step 500, we terminate the simulation, and the state of the simulator at this time is shown below.

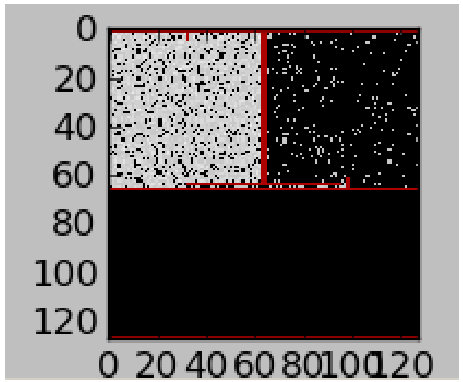


Figure 2: The final state of the LGA

We choose 5 as the number of time steps within which we average the occurrence times to estimate the occurrence probability. We will look at the entropy of the right region.

5 Evaluation

We denote log(u) as the theoretical entropy of the particle system in the 2-D hexagonal LGA model, and H as the global estimate of the entropy using an averaging scheme. The result is shown below.

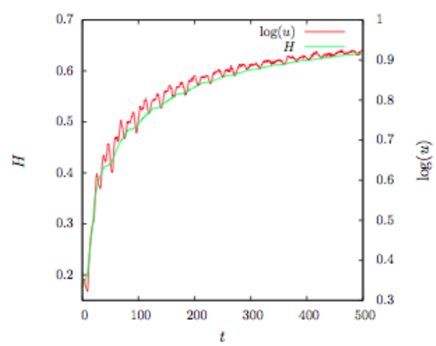


Figure 3: The comparison of the entropy estimated using two approaches, one based on thermodynamic theories taking specifications in the 2-D hexagonal LGA into consideration and the other based on the definition of entropy using information theory

6 Discussion

So far, we have introduced how the comparison of the entropy is done under a logical LGA framework, which also has successfully proved that the physical definition of entropy can

be enbodied by particles in a closed space as the two estimate curves are reasonably close with some fluctuations associated with the theoretical estimate. The reason for that is the theoretical model is an instantaneous one, which leads to unstable states when the number of particles is small. In comparison, the estimate of the actual entropy with averaging manifests significant stability, and proximity to the theoretical estimate as well.
This overall result reveals the potential on the simulation of other macroscopic quantities that are essential in thermodynamic, if a certain logical estimate of that quantity can be come up with like the one we use for estimating entropy, an estimation idea borrowed from information theory.

7 Related Work

An arcicle about entropy estimation under the LGA model ("Entropy and Correlations in Lattice Gas Automata without Detailed Balance") uses a different approach where the notion of locality is introduced to define quantities accessible to measurements by treating the coupling between nonlocal bits as perturbation. It takes into account inhomogeneous systems, while also considering homogeneous sites in the LGA model. Our work is a simplification version with respect to the entropy estimator in that we don't have to make assumptions for the particles and states as it does, while our work achieves a bettwe estimation. The result shown in that work is as follows.

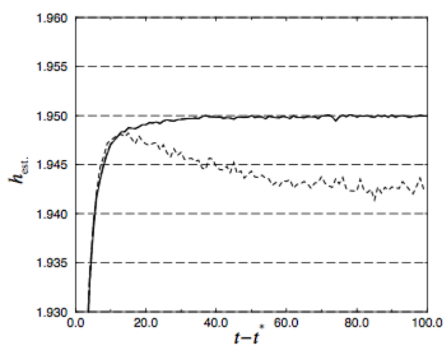


Figure 4: The initial state of the LGA

The solid line corresponds to the exact theoretical model we have used, with strictly local collision rules, and the dashed line denotes the estimation of entropy the paper uses with a set of assumptions about locality. The comparison of the two plots, the one in our evalution and the one the referred paper shown, reveals that our approach has the advantage while retaining the simplicity.

8 Conclusion

In this paper we have shown that the estimation of entropy can be achieved by two different approaches. The theoretical approach is derived from fundamental thermodynamic while adapting to the specific conditions in the 2-D hexagonal LGA model, and the approach using averaging has more smoothness and is based on the definition of entropy in information theory. We also compare our approach with another estimator which involves assumptions about particles in LGA and the states they define that are associated with the sites. The experiment result shows that our approach has a better coherence regarding two different algorithms without any assumptions in addition to the LGA model we base all our work on. In the future, it would also be desirable to explore ways of estimating other thermodynamic quantities in the 2-D hexagonal LGA model, such that more interesting thermodynamic simulations could be legitimized within this framework without solving complex partial differential equations.

9 Acknoledgements

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