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MODELLING DYNAMICAL GEOMETRY WITH LATTICE GAS AUTOMATA

Brosl Hasslacher[*] and David A. Meyer[†]

Institute for Physical Sciences

[*] *Theoretical Division, MS B213, Los Alamos National Laboratory*
Los Alamos, NM 87545
bhass@raptor.lanl.gov

[†] *Project in Geometry and Physics, Department of Mathematics*
University of California/San Diego, La Jolla, CA 92093-0112
dmeyer@chonji.ucsd.edu

ABSTRACT

Conventional lattice gas automata consist of particles moving discretely on a fixed lattice. While such models have been quite successful for a variety of fluid flow problems, there are other systems, *e.g.*, flow in a flexible membrane or chemical self-assembly, in which the geometry is dynamical and coupled to the particle flow. Systems of this type seem to call for lattice gas models with dynamical geometry. We construct such a model on one dimensional (periodic) lattices and describe some simulations illustrating its nonequilibrium dynamics.

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1. Introduction

Lattice gas automata (LGA) [1,2] have successfully modelled a variety of fluid mechanics systems: low Reynolds number flow in complicated geometry [3], multiphase flow [4], micellular assembly [5] and even, transformed into discrete quantum systems, the Dirac [6] and Schrödinger [7] equations. All of these systems, however, consist of flow in a *fixed* background geometry which is represented in the LGA models by a fixed lattice (and boundary conditions). In contrast, there are many natural systems with *dynamical* geometry. These range from the biological (flow in cell membranes [8] and gels [9]) to the chemical (self-assembling lipid bilayers [10] and CO oxidation on Pt monocrystal surfaces [11]) to the physical (spatial hypersurfaces in general relativity [12]).

The question we address in this talk is how to model such systems using LGA. We are interested in modelling geometry *intrinsically*, *e.g.*, a membrane as a two dimensional manifold with dynamical geometry, not as a fluctuating surface embedded in a fixed three dimensional manifold. Since it is the lattices in LGA which define the geometry, this means that we want to construct models in which the *lattice* is dynamical.

There has been only limited investigation of such models. Two notable exceptions are the work of Ilachinski [13] and Hillman [14], but their models have undergone little further development. The two research programs face complementary difficulties: Ilachinski's family of structurally dynamic cellular automata (CA) is so loosely constrained that the rule space is too large to explore usefully [13]. Hillman constrains his models to be reversible [14] but then faces the familiar difficulty of finding reversible CA rules without partitioning [15] or going to second order in time [16].

Lattice gas models may be expected to resolve both of these difficulties. Not only do they constitute a physically natural class of models, but particle number and momentum conservation impose tight constraints on the rule space. To construct fundamental models we should also require reversibility.* But the separation of each LGA timestep into advection and scattering phases makes reversibility straightforward to implement: as we will discuss further in Section 3, making the scattering matrix invertible suffices. Nevertheless, the simultaneous requirements of particle number and momentum conservation, an exclusion principle, and reversibility, tightly constrain the set of local deterministic LGA with dynamical geometry. After discussing the general problem of dynamical lattices in one dimension in the next section, however, we demonstrate by construction in Section 3 that this set is not empty. In Section 4 we describe the results of simulations and conclude in Section 5 with a discussion and some directions for further investigation.

2. Lattice dynamics in one dimension

The simplest situation is one dimensional. This is not terribly realistic—although it does provide the intrinsic description of interfaces in multiphase flow restricted to two dimen-

* By which we will always mean *local* reversibility.

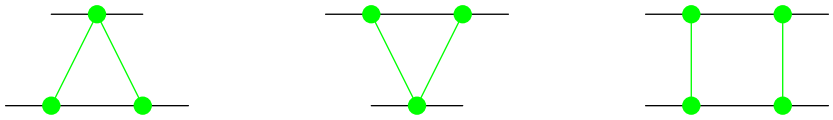

Figure 1. There are two local changes for a one dimensional lattice: The leftmost diagram shows the deletion of an edge while the middle diagram shows the creation of an edge. The rightmost diagram illustrates the absence of any change, locally. In each diagram the spatial lattice is horizontal and time runs upward.

sions [5]. Furthermore, the classical (*i.e.*, local, deterministic, single species) LGA in one dimension is completely trivial as it can be interpreted as consisting of particles which simply move to the left or right without change even upon scattering. Nevertheless, the one dimensional LGA with dynamical geometry we will consider in Sections 3 and 4 is significantly more interesting, illustrating some of the difficulties encountered in constructing such models, how to resolve them, and also some of their novel properties.

So let us develop a toy model on the periodic integer lattices $\mathbb{Z}_N$. These one dimensional lattices can change locally in two ways: two adjacent vertices can be identified, deleting the edge connecting them, or a vertex can split into two vertices, creating a new edge connecting them. And, of course, a lattice may locally undergo no change at all. Figure 1 illustrates these three possibilities. Implicit in the diagrams of Figure 1 is a feature our models for dynamical geometry have in common with standard lattice gas models: time advances globally, in discrete steps. While this seems likely to be the wrong way to begin constructing a discrete model for general relativity [12], it is perfectly natural for classical (nonrelativistic) problems involving biological membranes [8] or chemical self-assembly [17,10], for example.

The one dimensional lattices $\mathbb{Z}_N$, however, are *homogeneous*: there is no local (spatial) geometry, only the global volume (length) N. Without additional structure any local evolution rule must be the same everywhere on the lattice. The edge deleting rule is not reversible since every $\mathbb{Z}_N$ for $N > 1$ collapses to $\mathbb{Z}_1$ in one timestep as illustrated in Figure 2. Similarly, the edge creating rule shown in Figure 3 does not have a locally defined inverse; once the lattice evolves backwards to an odd size some global information is required for any further evolution. So the only evolution rule which is local, deterministic and reversible on $\mathbb{Z}_N$ alone is just the identity map—which does not lead to a very dynamical lattice!

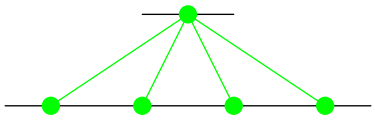

Figure 2. Applying the edge deleting rule homogeneously collapses any one dimensional lattice to a single point.

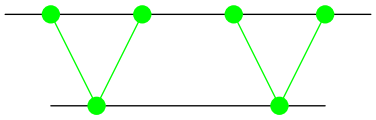

Figure 3. The edge creating rule also fails to be locally reversible; for odd size lattices, additional (global) information is required.

The difficulty is that there are not enough local degrees of freedom in $\mathbb{Z}_N$—none—to record sufficient information about the state at the previous timestep to allow nontrivial evolution to be reversed locally. There are two ways to generalize to interesting models: allow the evolution rule to be second (or higher) order in time or introduce additional (matter) degrees of freedom on the lattice. Because this is a lattice gas meeting, and because we are interested in chemical self-assembly [17,10], for example, we will investigate the latter alternative, while remarking that the former might be appropriate were we constructing a discrete model for pure general relativity [12].

3. Constructing the model

Particles in standard LGA have both position and momentum, where the momentum is constrained to be in some subset of lattice (difference) vectors. The evolution rule has two phases: first each particle *advects* to the lattice point obtained by adding its momentum to its current position; second, the particles at each lattice point *scatter* according to some deterministic [1], probabilistic [2], or quantum mechanical [6,7] rule. The advection phase is trivially reversible and the scattering phase will be also, provided it is described by a permutation, a doubly stochastic, or a unitary matrix, respectively.

We remark, however, that *physical* time reversibility is not achieved exactly by (parity) inverting all particle momenta and then running the forward evolution rule. Consider the (two dimensional, triangular lattice) FHP evolution rule [2], for example: The scattering of three particles with zero total momentum is illustrated in Figure 4. The evolution is successfully reversed from $t = 2$ to $t = 0$ by inverting the momenta of the particles, evolving for two timesteps, and inverting the momenta again. But the same procedure applied for a single timestep fails to reverse the evolution from $t = 1$ to $t = 0$: Inverting the momenta in the final $t = 1$ configuration and then advecting the particles doesn't even take them to the same lattice points as at $t = 0$. The difficulty is, of course, that even though both advection and scattering are reversible, they do not commute. So exact time reversibility is achieved by backward evolution with advection *preceded* by scattering, or more precisely, the inverse scattering rule conjugated with parity (momentum inversion), which may or may not be the same as the forward scattering rule. This is all quite straightforward, but is worth clarifying in the standard LGA setting to avoid confusion about the meaning of reversibility in the dynamical geometry LGA which we are about to construct.

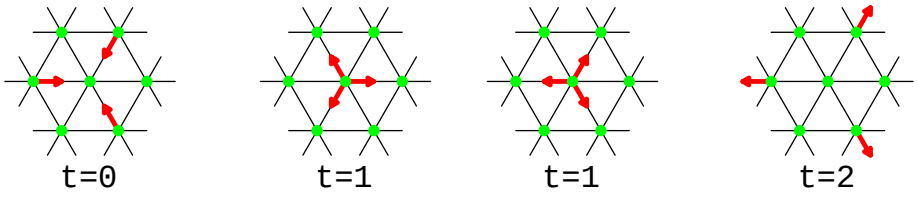

Figure 4. The zero momentum three particle scattering rule in the FHP model. Advection takes the $t = 0$ configuration to the the first $t = 1$ configuration shown; then the scattering rule changes that to the second $t = 1$ configuration; advecting again (followed by scattering, which has no effect) produces the $t = 2$ configuration.

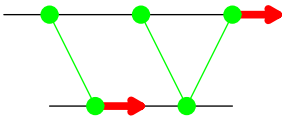

Figure 5. A possible scattering rule which creates an edge behind the lattice point to which a single particle has just advected. The spatial lattice is horizontal and time runs upward.

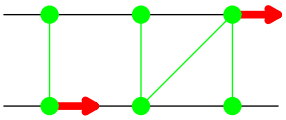

Figure 6. The pair of possible scattering rules which create an edge behind and delete the edge in front of a lattice point to which a single particle has just advected.

In our one dimensional dynamical geometry model we want to maintain the same advect/scatter formalism for particle evolution, but to modify the rules to allow for the local changes of the lattice shown in Figure 1. That is, after advection some local particle configurations should catalyze local edge deletions or creations. Since an edge is created when a vertex splits into two vertices, the most local rule would depend only on the particle configuration at a single vertex. The exclusion principle restricts these configurations to consist of no particles, one particle, or two particles with opposite momenta:

(0) We found already in Section 2 that reversibility fails if the evolution rule splits vertices at which there are no particles.

(1) Suppose a vertex occupied by a single particle splits, with the new edge created behind the particle as shown in Figure 5. If this is the only edge creation/deletion rule for vertices occupied after advection by a single particle, the forward evolution will continually expand the lattice—and the backward evolution will collapse it to a stage at which the evolution is no longer defined, not unlike the situation illustrated in Figure 3. This is unsatisfactory, so suppose we also include an edge deletion rule, for the edge in front of the particle (in as much as deleting the edge *behind* the particle could be defined—the problem is that the domains of application of the two rules would overlap—it would simply cancel the effect of the edge creation rule). The effect of this pair of rules is illustrated in Figure 6. The two rules work together to double* the velocity of each particle, when it does not scatter off another particle. Notice that if these are the only edge creation/deletion rules then the total number of vertices is constant. Since our interest is in dynamical *spatial* geometry† let us keep our model simple by not splitting the vertex when it is occupied by a single particle.

(2) This leaves only the possibility of splitting a vertex which is occupied by two particles, as shown in Figure 7. Reversibility implies the dual edge deletion rule also shown in Figure 7. These rules are well defined as they cannot have overlapping

* The opposite choice, namely that the new edge is created in front of the particle and an edge is deleted behind it, makes the velocity of isolated particles zero, destroying the reversibility of the advection phase—and almost all the dynamics in the model.

† This rule does affect the *spacetime* geometry and so might be reconsidered in the context of relativistic models [12].

domains of application. They do not leave the total number of vertices invariant and thus they define the simplest lattice gas model with dynamical geometry.

The reversible scattering rule shown in Figure 7 ensures nontrivial dynamical geometry for our LGA. In doing so it breaks the $\mathbb{Z}_2$ symmetry of the standard one dimensional LGA with its associated 'spurious' conservation of the number of particles on even (odd) lattice points [18]. To examine further properties of this dynamical geometry LGA we turn next to simulations.

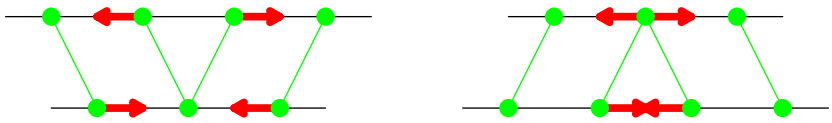

Figure 7. The scattering rules for our dynamical geometry LGA: An edge is created when two particles advect to the same lattice point and an edge is deleted if after advection each endpoint is occupied by a single particle with outward momentum.

4. Simulations

Simulation of one dimensional LGA is straightforward, even with dynamical geometry. The lattice points, with their local particle configurations, form a list of pairs of bits (the left/right bit being 0 (1) indicates the absence (presence) of a particle moving left/right). At each timestep advection shifts the left/right bit of each pair to the left/right bit of the adjacent pair to the left/right. After advection, the scattering phase replaces each 11 pair of bits with two pairs $10, 01$ and *vice versa*. Since the numbers of left/right moving particles are separately conserved, the exclusion principle constrains the lattice size to be no less than the larger of these numbers. There is, however, no *a priori* upper bound to the possible size of the lattice. Thus, in contrast to standard reversible LGA in which every orbit must be periodic, it is in principle possible for some initial configuration of our dynamical geometry LGA to cause the lattice to grow without bound, and thus to lie on an infinite orbit.

In order for the geometry to be dynamical there must be both left and right moving particles on the lattice. Figure 8 shows the results of 10^4 timestep simulations starting on a lattice of size 10 with randomly distributed particles. The graphs plot the size of the lattice at each timestep; as always, time runs upward. The graph with smaller lattice sizes is for 4 left moving and 6 right moving particles, while the one with larger sizes is for 7 left moving and 10 right moving particles.

We can make a few heuristic remarks immediately: In each case the initial configuration appears to lie on an infinite orbit: the trend in the lattice size is to increase. The increase is not constant, however; there are irregular fluctuations in the lattice size. Furthermore, these fluctuations develop intermittent structure: Figure 9 shows the 17 particle

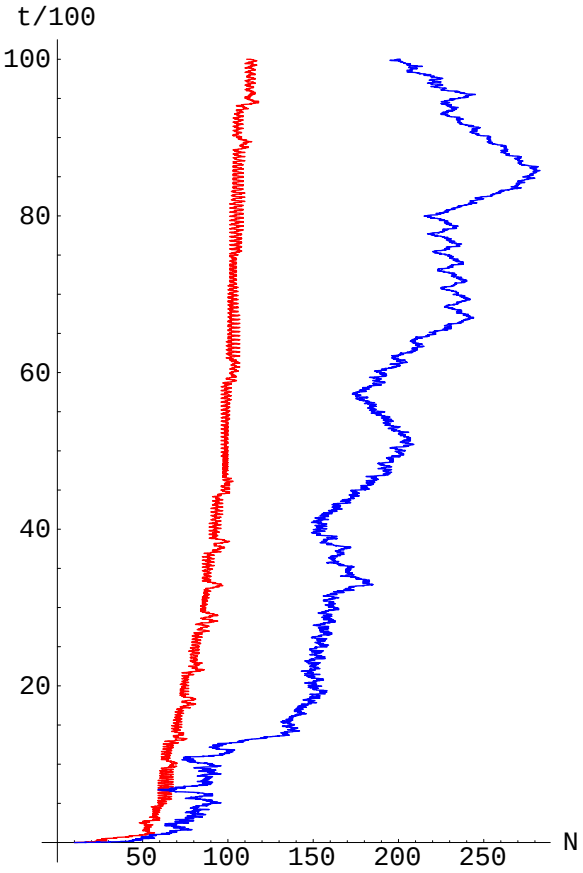

Figure 8. Lattice sizes for simulations of 10000 timesteps from initial configurations of 10 and 17 particles on a lattice of size 10. Time runs upward and the graph of (mostly) smaller sizes is the 10 particle simulation.

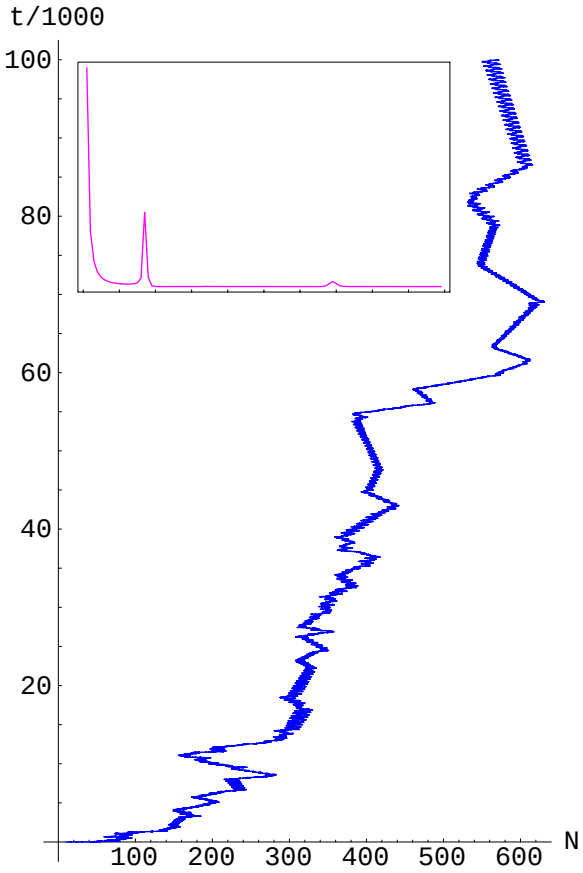

Figure 9. The 17 particle simulation extended to 100000 timesteps. The insert shows the norm squared of the first 100 Fourier coefficients (the ticks are at multiples of 20) calculated for the last 10000 sizes in the time series.

simulation continued for 10^5 timesteps, while the inset graphs the norm squared of the first 100 Fourier coefficients calculated for the last series of 10^4 lattice sizes. Notice the spikes at about 18 and 69. The *emergence* of structure at multiple scales is one of the most interesting features of this simple reversible model.

5. Discussion

We have taken advantage of the natural physical interpretation of, and ease with which reversibility can be implemented in, the lattice gas formalism to construct the unique one dimensional reversible model with dynamical geometry satisfying our simplifying assumptions. One may imagine many variations which might tailor this basic model to particular applications: multiple particle species, additional labels on the lattice points, *etc.* We expect, however, that some features of the simulations described in Section 4 are universal and appropriate for modelling the biological and chemical systems of interest. Specifically,

these are reversible systems far from equilibrium which 'explore' more and more of their phase space as they evolve. The simulations indicate that almost any initial condition on a finite lattice is out of equilibrium, in the sense that the lattice size will tend to increase.

This model poses a multitude of questions, however: Can we analyze *exactly* which initial configurations lie on open orbits? Are there useful conserved quantities—beyond the numbers of left and right moving particles—which would help identify orbits? (Any initial configuration itself is, of course, an invariant of its orbit, but not a particularly useful one.) Is there a macroscopic/continuum limit of this model and if so, what is it? Finally, how do we generalize to higher dimensional models with dynamical geometry? There is *local* geometry in higher dimensions so one may investigate local changes to the lattice which preserve the total lattice size, or change it as in our one dimensional model. The Pachner moves provide a complete set of local changes to simplicial lattices in any dimension [19]; we are currently using them to develop dynamical geometry LGA in two dimensions.

Acknowledgements

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