CITS4403, Computational Modelling

The Hardy–de Pazzis–Pomeau (HPP) lattice gas model"

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Task

Implement the 'HPP' cellular automaton rule, which model a gas of colliding particles. The HPP lattice gas automata is defined on a 2D square lattice. Particles can move along the orthogonal directions of the lattice. Particles are associated with both a position on the lattice (lattice site), and a discrete velocity (four cardinal directions), i.e. the velocity with which the particle is assumed to have *entered* the site (see Figure). An exclusion principle is assumed, which prevents more than one particle to be at a same position with the same velocity. However, more than one particle can be found at a lattice site if the particles have different velocities.

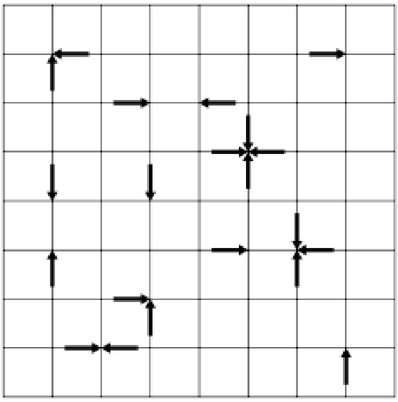
Four bits of information in each site are enough to describe the system during its evolution. For instance, if at time t the lattice site at $\boldsymbol{r}$ has the following state $s(t, \boldsymbol{r}) = [1011]$, it means that three particles are entering the site along directions 1, 3, and 4, respectively.

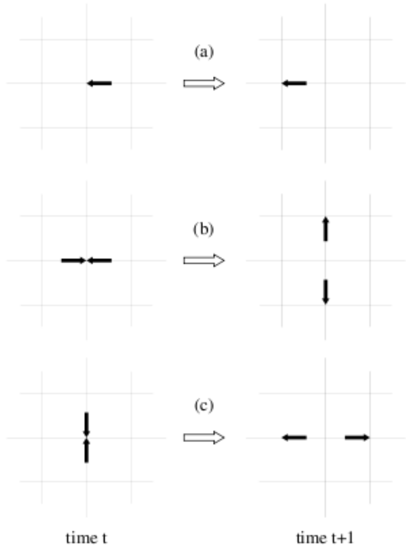
The CA rule describing the evolution of $s(t, \boldsymbol{r})$ is usually split into two steps: collision and motion. The collision phase specifies how particles entering the same site will interact and change their trajectories. During the motion phase, or propagation, the particles are actually moved to the nearest neighbor site they were traveling to.

The figure (right) illustrates the HPP rules:

(a) a single particle has a ballistic motion until it experiences a collision

(b) and (c) the two nontrivial collisions of the model: two particles experiencing a head-on collision are deflected in the perpendicular direction. In the other situations, the motion is ballistic, that is the particles are transparent to each other when they cross the same site.





According to the boolean representation of the particles at each site, the collision part for a two-particle head-on collision is expressed as:

$$[1010] \rightarrow [0101], \qquad [0101] \rightarrow [1010]$$

all the other configuration being unchanged. During the propagation phase, the first bit of the state is shifted to the east neighbor cell, the second bit to the north, and so on.

Be sure to start from an initial condition in which the exclusion principle is satisfied.

- Write a rule for a collision with a hard wall, at which the particle 'bounces back'
- Implement the HPP CA model
- Start with periodic boundary conditions and a concentrated density of cells around the middle of the lattice. Does the gas spread to a homogeneous distribution?
- Modify the periodic boundary conditions into hard walls. Measure the pressure on one wall (i.e. the number of particles colliding with the wall during a time increment divided by the length of the wall) and make a plot of how pressure varies with the initial density of particles (i.e. number of particles divided by the area of the lattice).
- Add a wall separating the left hand side from the right hand side. Include a small opening in the wall. Show the evolution of pressure on the wall on the right hand side and the wall on the left hand side.

- Do you observe the phenomenon of “relaxation”? Does the system evolve to a state that is uniform in a certain sense? Discuss this in light of the microscopic reversibility of the system and the 2nd law of thermodynamics.
- Imagine new situations that could be modelled with the HPP CA model and implement them (e.g. obstacles, flow collisions etc.) Exemplify and discuss your results.

Background

The purpose of the HPP rule is to model a gas of colliding particles. The essential features that are borrowed from the real microscopic interactions are the conservation laws, namely local conservation of momentum and of particle number.

References

[1] Hardy J, de Pazzis O and Pomeau Y, Molecular dynamics of a classical lattice gas: transport properties and time correlation functions, *Phys. Rev. A*, **13**, 1949–1961