Lattice Gas

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- Presentation: The lattice gas Please do G&T Problem 5.23. Explain to us how a lattice gas is like or unlike an Ising model. Is there a critical temperature Tc? What happens to the gas when the temperature crosses this value? What happens when you lower the temperature very quickly, a “quench”? What happens when you turn on a gravitational field?

Lattice gas

- Is essentially an Ising model in 2D since in the fluid model s=+1 correlates to a particle at the grid point and s=-1 means no particle is present
  - The difference between the tw0 is a change of variable from s (spin) to n (occupancy)

$$n_i \equiv (s_i + 1)/2,$$

- Only one particle per site = hard core repulsion
  - Two things cannot occupy the same space at the same time

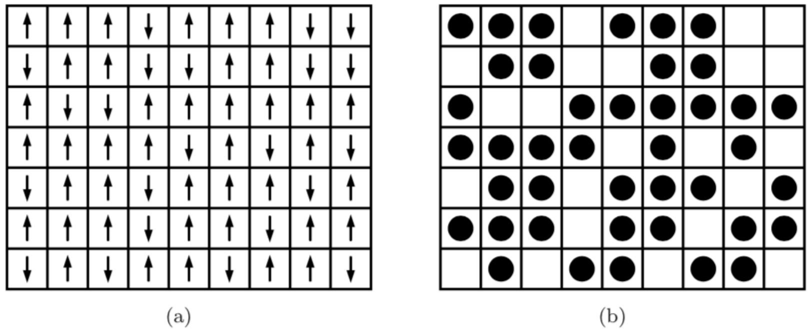


Figure 5.17: (a) A typical microstate of the Ising model. (b) The same microstate in the lattice gas picture with spin up replaced by a particle and spin down replaced by an empty cell.

(a) What is the value of the critical temperature T_c for the lattice gas in two dimensions (in units of u_0/k)?

- We can use the derivation the textbook uses for the Onsager solution since it was derived for a 2D Ising model

$$\frac{kT_c}{J} = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269.$$

- Except in this case

$$E = -u_0 \sum_{i,j=\mathrm{nn}(i)}^{N} n_i n_j - \mu \sum_{i=1}^{N} n_i + N(H - 2J).$$

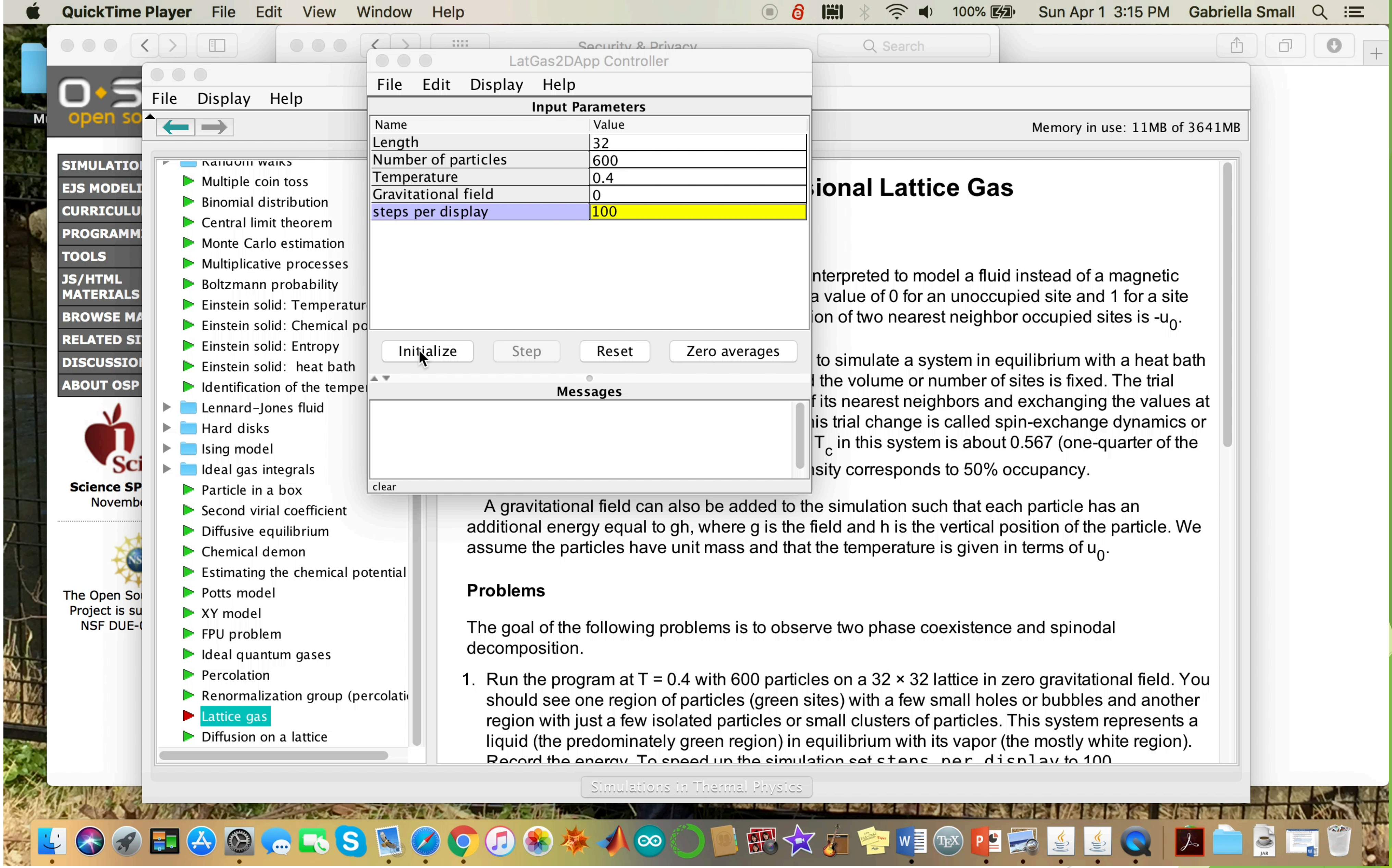
- and

$$u_0 \equiv 4J$$

- Replacing J by $u_0/4$ we get
    - $T_c = J/k * 2.269 = u_0/4k * 2.269 = 0.567 * u_0/k$

(b) Program `LatticeGas` simulates the lattice gas on a square lattice of linear dimension L. The initial state has all the particles at the bottom of the simulation cell. Choose $L = 32$ and set

the gravitational field equal to zero. Do a simulation at $T = 0.4$ with $N = 600$ particles. After a few Monte Carlo steps you should see the bottom region of particles (green sites) develop a few small holes or bubbles and the unoccupied region contain a few isolated particles or small clusters of particles. This system represents a liquid (the predominately green region) in equilibrium with its vapor (the mostly white region). Record the energy. To speed up the simulation set `steps per display` equal to 100.


QuickTime Player File Edit View Window Help
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Sun Apr 1 3:15 PM Gabriella Small
LatGas2DApp Controller
File Edit Display Help
Input Parameters
Name
Value
Length
32
Number of particles
600
Temperature
0.4
Gravitational field
0
steps per display
100
Initialize
Step
Reset
Zero averages
Messages
clear
File Display Help
Memory in use: 11MB of 3641MB
SIMULATIO
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Multiple coin toss
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Identification of the tempe
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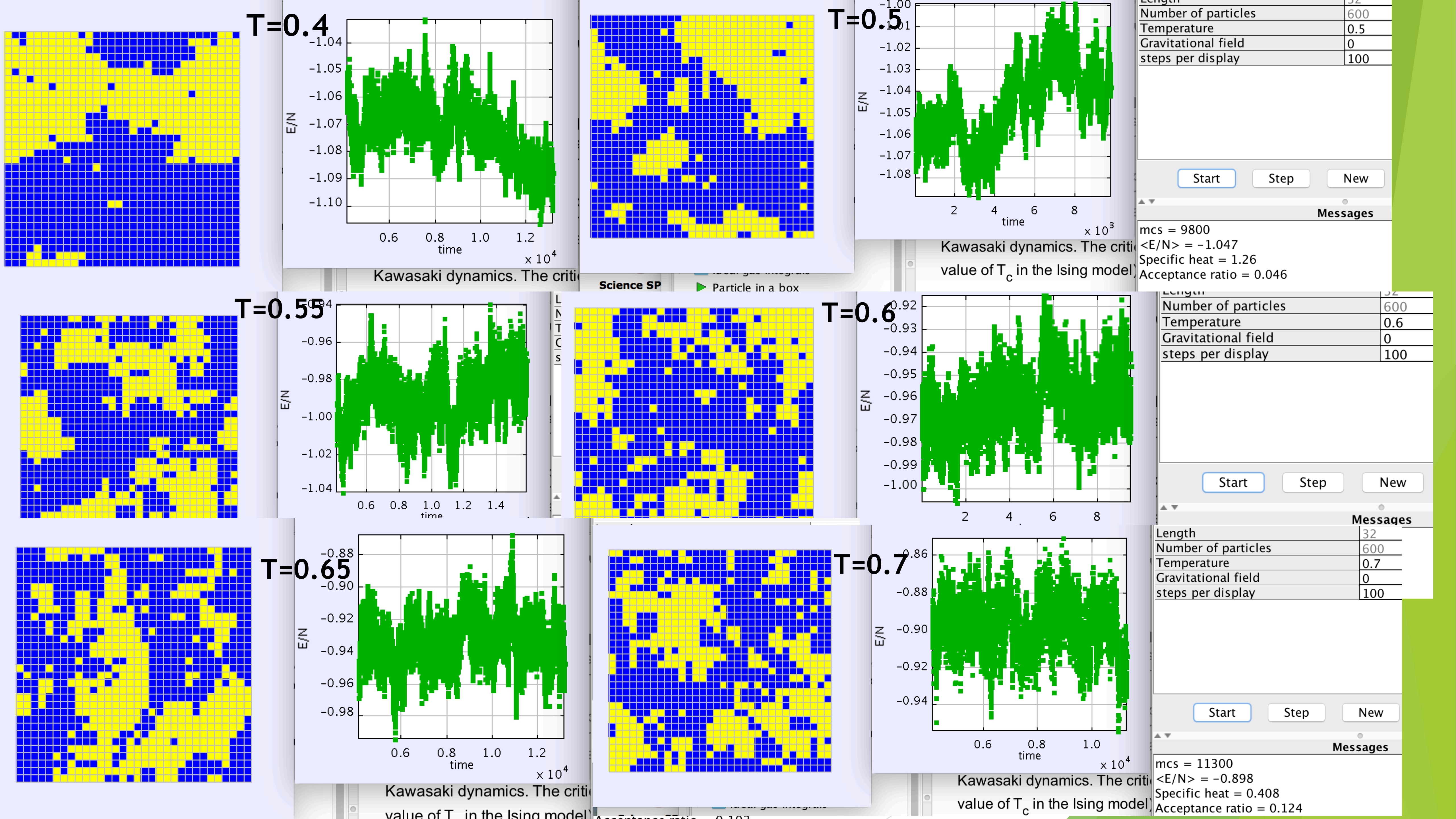
Hard disks
Ising model
Ideal gas integrals
Particle in a box
Second virial coefficient
Diffusive equilibrium
Chemical demon
Estimating the chemical potential
Potts model
XY model
FPU problem
Ideal quantum gases
Percolation
Renormalization group (percolati
Lattice gas
Diffusion on a lattice
ional Lattice Gas
nterpreted to model a fluid instead of a magnetic
a value of 0 for an unoccupied site and 1 for a site
ion of two nearest neighbor occupied sites is -u0.
to simulate a system in equilibrium with a heat bath
the volume or number of sites is fixed. The trial
f its nearest neighbors and exchanging the values at
is trial change is called spin-exchange dynamics or
Tc in this system is about 0.567 (one-quarter of the
sity corresponds to 50% occupancy.
A gravitational field can also be added to the simulation such that each particle has an additional energy equal to gh, where g is the field and h is the vertical position of the particle. We assume the particles have unit mass and that the temperature is given in terms of u0.
Problems
The goal of the following problems is to observe two phase coexistence and spinodal decomposition.
1. Run the program at T = 0.4 with 600 particles on a 32 × 32 lattice in zero gravitational field. You should see one region of particles (green sites) with a few small holes or bubbles and another region with just a few isolated particles or small clusters of particles. This system represents a liquid (the predominately green region) in equilibrium with its vapor (the mostly white region).
Simulations in Thermal Physics

(c) Increase the temperature in steps of 0.05 until $T = 0.7$. At each temperature run for at least 10,000 mcs to reach equilibrium and then press the `Zero Averages` button. Run for at least 20,000 mcs before recording your estimate of the energy. Describe the visual appearance of the positions of the particle and empty sites at each temperature. At what temperature does the one large liquid region break up into many pieces, such that there is no longer a sharp distinction between the liquid and vapor region? At this temperature there is a single fluid phase. Is there any evidence from your estimates of the energy that a transition from a two-phase to a one-phase system has occurred? Repeat your simulations with $N = 200$.

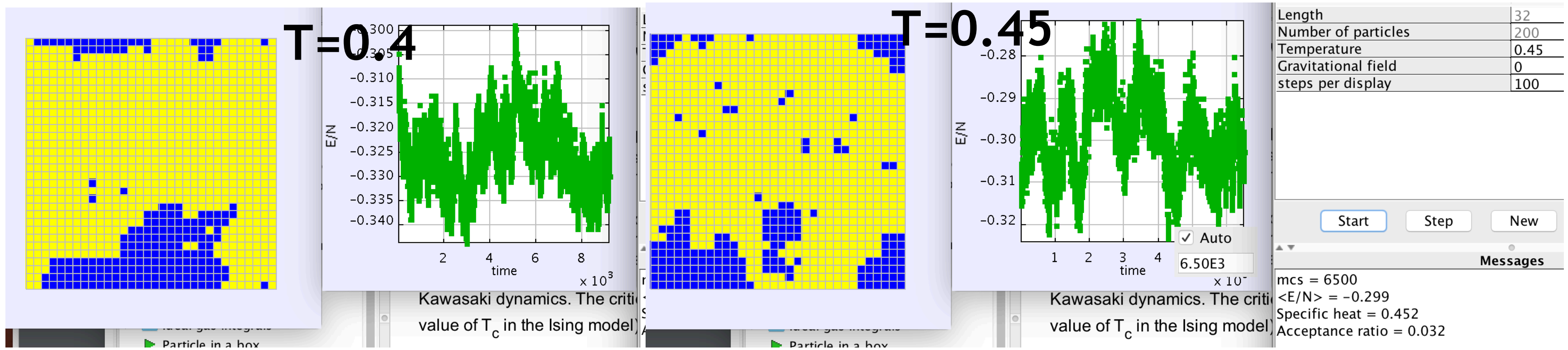
Temperature	<E/N>
0.4	-1.106
0.45	-1.074
0.5	-1.047
0.55	-0.996
0.6	-0.962
0.65	-0.934
0.7	-0.898



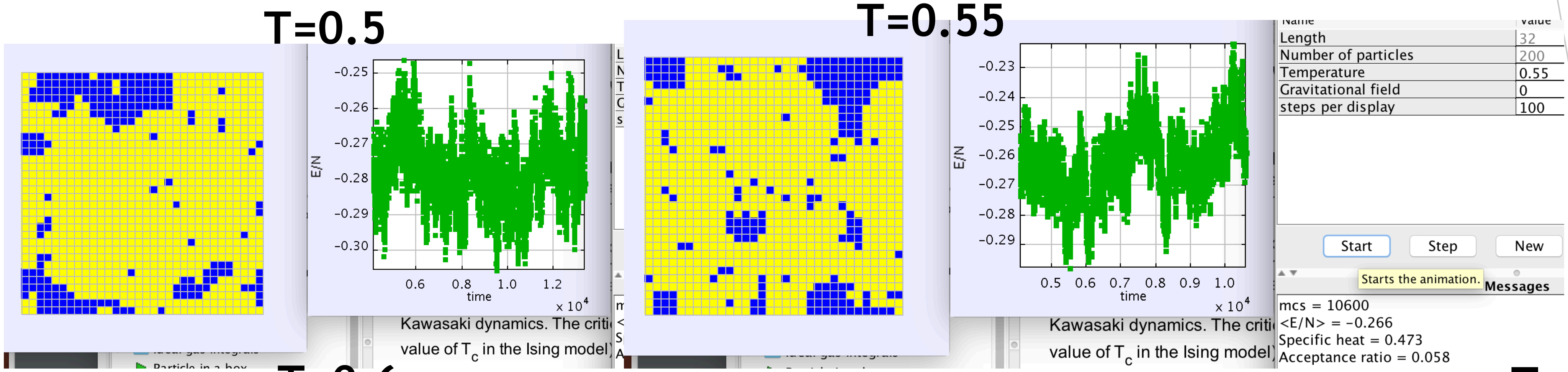
T=0.4
E/N
time
x 10^4
Kawasaki dynamics. The criti
T=0.5
E/N
time
x 10^3
Kawasaki dynamics. The criti
value of Tc in the Ising model
Number of particles 600
Temperature 0.5
Gravitational field 0
steps per display 100
Start
Step
New
Messages
mcs = 9800
<E/N> = -1.047
Specific heat = 1.26
Acceptance ratio = 0.046
Science SP
Particle in a box
T=0.55
E/N
time
T=0.6
E/N
Number of particles 600
Temperature 0.6
Gravitational field 0
steps per display 100
Start
Step
New
Messages
T=0.65
E/N
time
x 10^4
Kawasaki dynamics. The criti
value of T in the Ising model
T=0.7
E/N
time
x 10^4
Kawasaki dynamics. The criti
value of Tc in the Ising model
Length 32
Number of particles 600
Temperature 0.7
Gravitational field 0
steps per display 100
Start
Step
New
Messages
mcs = 11300
<E/N> = -0.898
Specific heat = 0.408
Acceptance ratio = 0.124

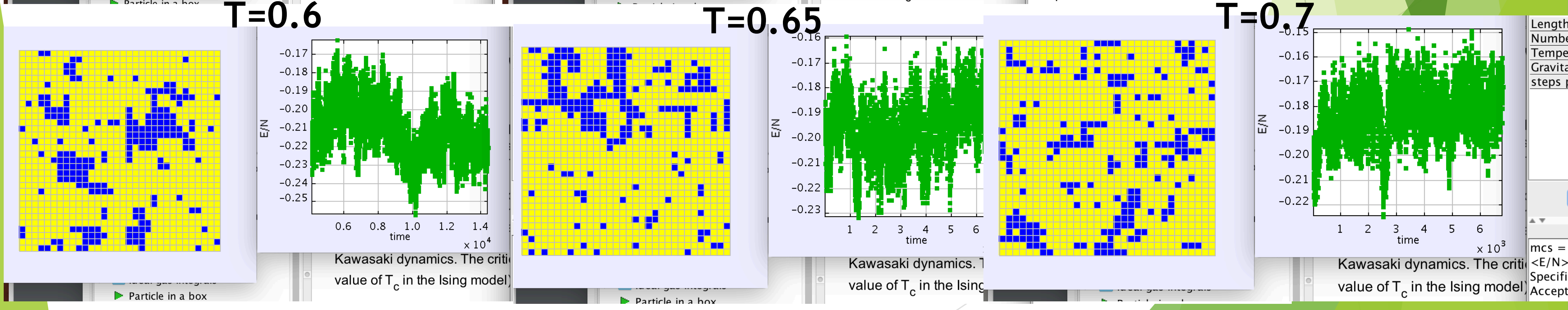
Repeating with N=200

Temperature	<E/N>
0.4	-0.326
0.45	-0.299
0.5	-0.276
0.55	-0.266
0.6	-0.214
0.65	-0.196
0.7	-0.183



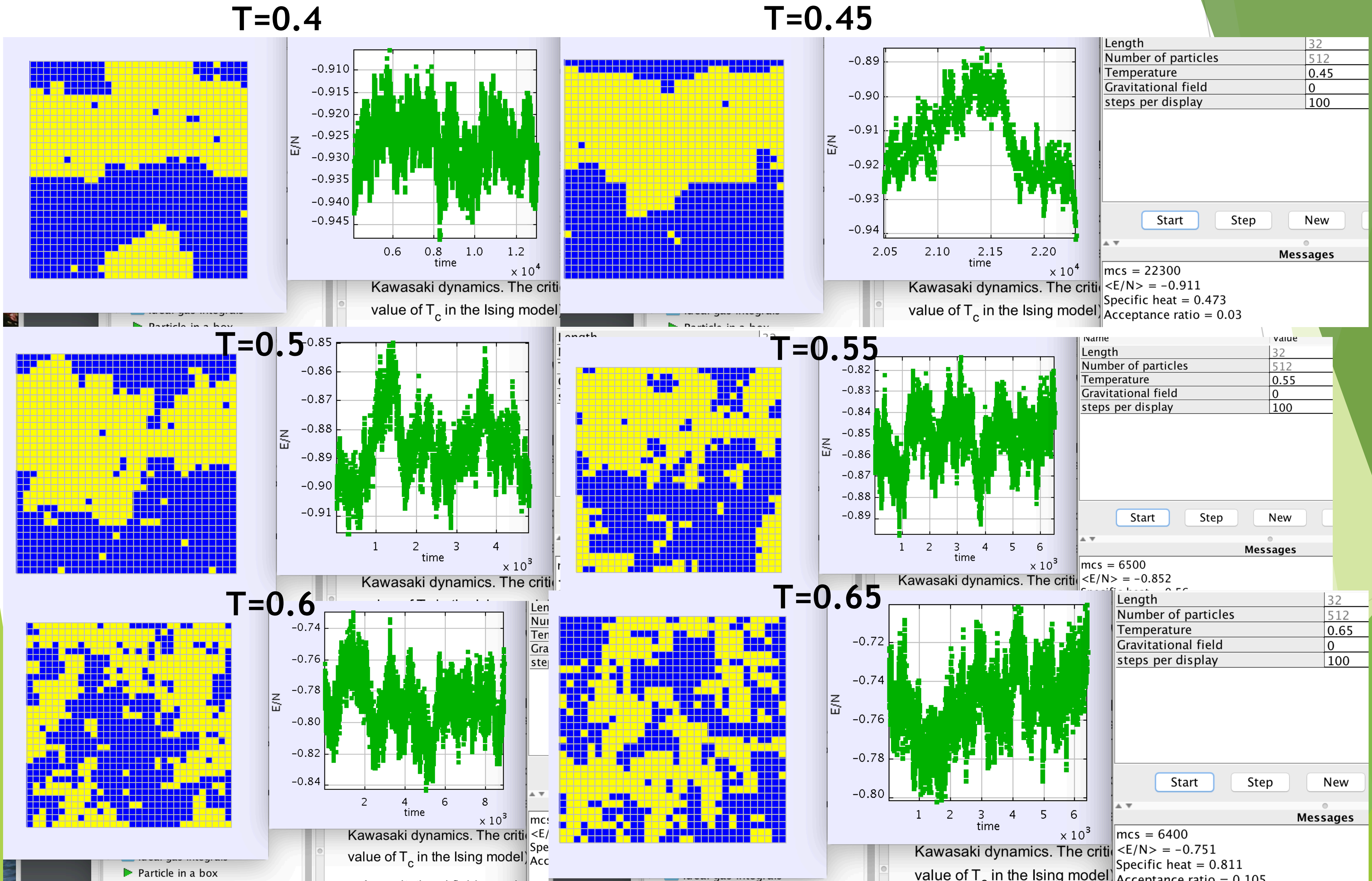
Similar results here as in the N=600 case





(d) Repeat part (c) with $N = 512$. In this case the system will pass through a critical point. The change from a one phase to a two-phase system occurs continuously in the thermodynamic limit. Can you detect this change or does the system look similar to the case in part (c)?

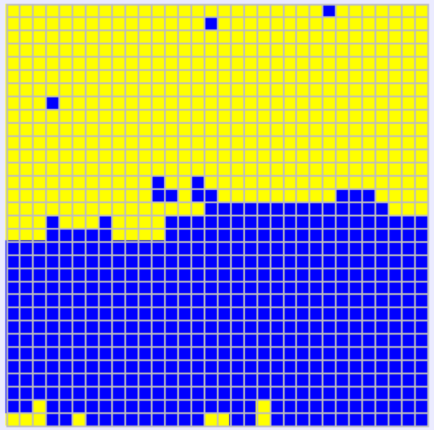
Temperature	<E/N>
0.4	-0.928
0.45	-0.911
0.5	-0.887
0.55	-0.852
0.6	-0.789
0.65	-0.751
0.7	-0.722


T=0.4
T=0.45
T=0.5
T=0.55
T=0.6
T=0.65
E/N
time
Kawasaki dynamics. The criti
value of T_c in the Ising model
Length 32
Number of particles 512
Temperature 0.45
Gravitational field 0
steps per display 100
Start
Step
New
Messages
mcs = 22300
<E/N> = −0.911
Specific heat = 0.473
Acceptance ratio = 0.03
Length 32
Number of particles 512
Temperature 0.55
Gravitational field 0
steps per display 100
mcs = 6500
<E/N> = −0.852
Length 32
Number of particles 512
Temperature 0.65
Gravitational field 0
steps per display 100
mcs = 6400
<E/N> = −0.751
Specific heat = 0.811
Particle in a box

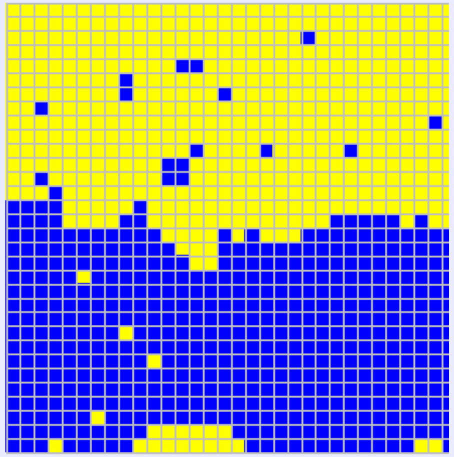
(e) If we include a gravitational field, the program removes the periodic boundary conditions in the vertical direction, and thus sites in the top and bottom rows have three neighbors instead of four. The field should help define the liquid and gas regions. Choose $g = 0.01$ and repeat the above simulations. Describe the differences you see.

Temperature	<E/N>
0.4	-0.946
0.45	-0.888
0.5	-0.867
0.55	-0.836
0.6	-0.801
0.65	-0.73
0.7	-0.724

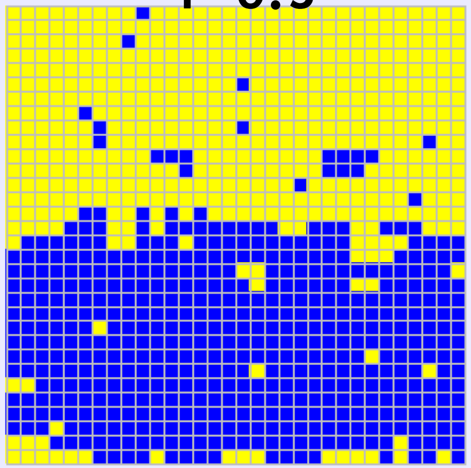
T=0.4



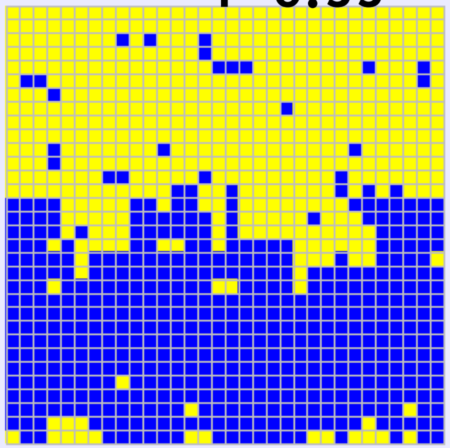
T=0.45



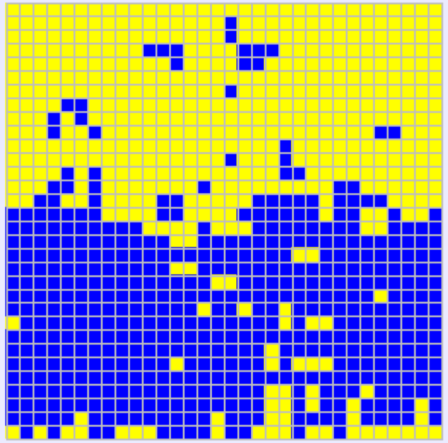
T=0.5



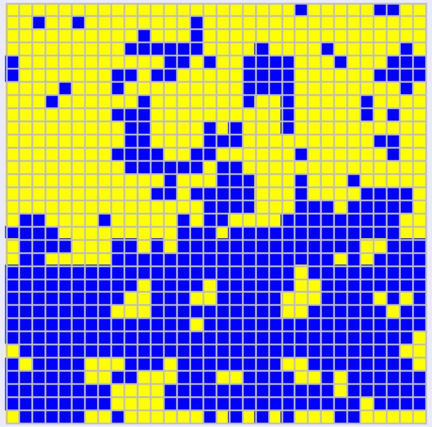
T=0.55



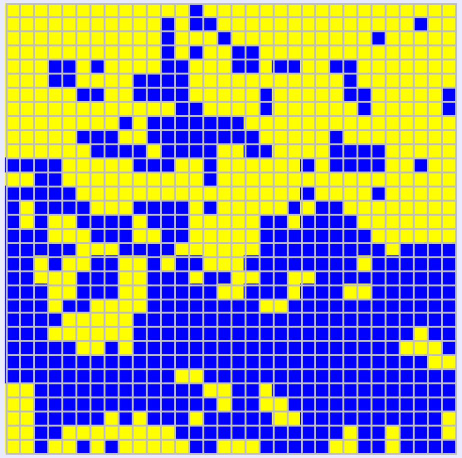
T=0.6



T=0.65



T=0.7



(f) Simulate a lattice gas of $N = 2048$ particles on a $L = 64$ lattice at $T = 2.0$ with no gravitational field for 5000 mcs. Then change the temperature to $T = 0.2$. This process is called a (temperature) quench, and the resulting behavior is called *spinodal decomposition*. The domains grow very slowly as a function of time. Discuss why it is difficult for the system to reach its equilibrium state for which there is one domain of mostly occupied sites in equilibrium with one domain of mostly unoccupied sites. □