Potts Model Simulation

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Background

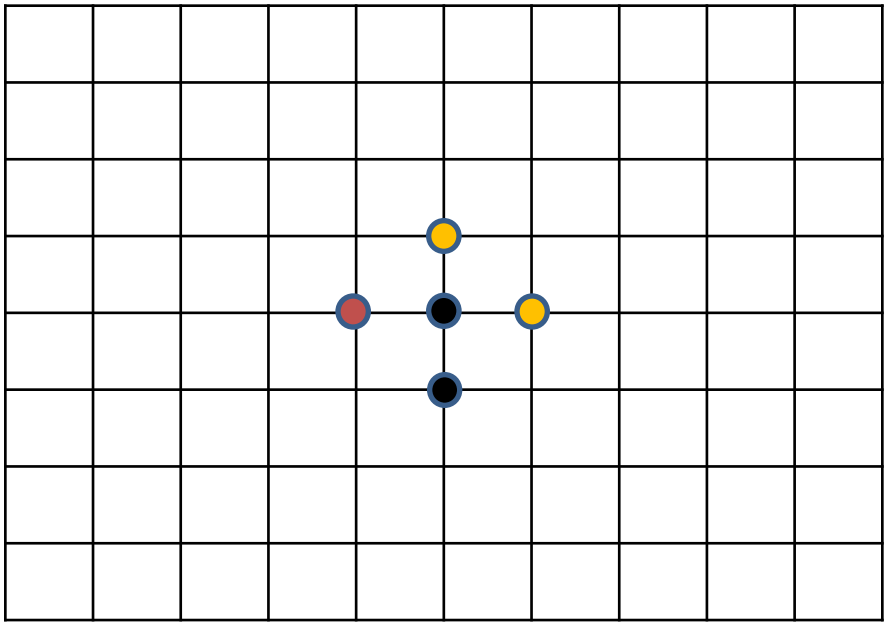
- The Potts model is a generalization of the Ising model, a model of interacting spins on a crystalline lattice - a good model to study phase transitions and critical behavior, both 1st and 2nd order transitions.

- Plus it is nice for the computational physics course because the model is not analytically solved in d>1, and usually studied numerically using Monte-Carlo methods.

The Model

$$H = -\sum_{<ij>} J\delta(\sigma_i, \sigma_j)$$

- $\sigma_i = 1..q$
- <I,j> indicates nearest - neighbours summation
- q is called the state of the model, and it gives different behaviors for different states



- For example, for q=2 we get exactly the Ising Model

The Model

- When J>0 the system simulates a ferromagnet and for J<0 an antiferromagnet.

- The Potts Model has common generalization adding on-site magnetic field, which is:

$$H = -\sum_{<ij>} J\delta(\sigma_i, \sigma_j) + \sum_i h_i \sigma_i$$

- If these h_i are random it can bring some interesting results, such as domains, even for infitesimally small h.

Phase Transitions

In 2D, lattices with $J > 0$ exhibit:

- first order transition when $q > 4$.
- a continuous transition when $q \leq 4$.

Phase Transitions

- In order to study phase transitions, we must first define our order parameter:

$$L = \sum_i \delta(\sigma_i, 0)$$

which basically counts how many of the spins are in the "zero" state.

- The order parameter behaves as T goes to Tc from below as

$$< \frac{L(T)}{N} > \sim |T - Tc|^{\beta}$$

where β is the critical exponent.

- Also the susceptibility undergoes a phase transition:

$$< \frac{\partial_h L(T)}{N} > \sim |T - Tc|^{\gamma}$$

Programing goals

- Calculate the critical exponents for q=2,4,6 with and without a random field
- Calculate domain sizes for q=2 (Ising) in a 1000*1000 lattice
- Parallel the calculation
- Generate some nice graphs and images

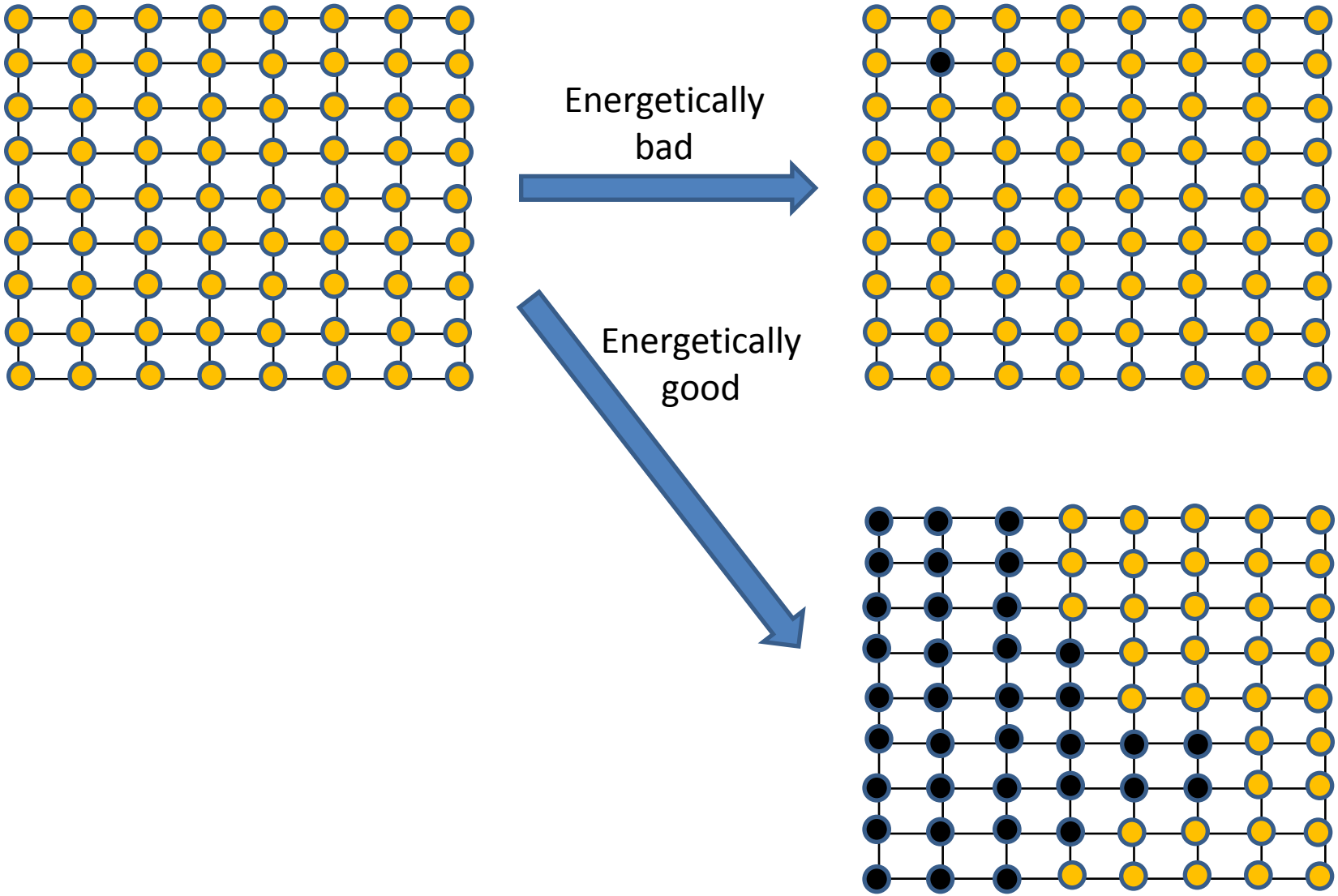
The computational difficulties

- In 2D, with an N*N lattice and a q-state model, there are $N*N*2^q$ possibilities to arrange the lattice.
  For example, 1000*1000 and q=8 gives 256 million different combinations.
- In order to find the critical exponent, one must average over many different runs with many different initial states

The computational difficulties

- Visualize the data, generating both images of the lattice and graphs of the order-parameter
- Sometimes in this model, it is energetically-favorable to flip a group (domain) of spins, instead of just a single spin, which creates a big problem for the Metropolis algorithm which flips a single spin each time

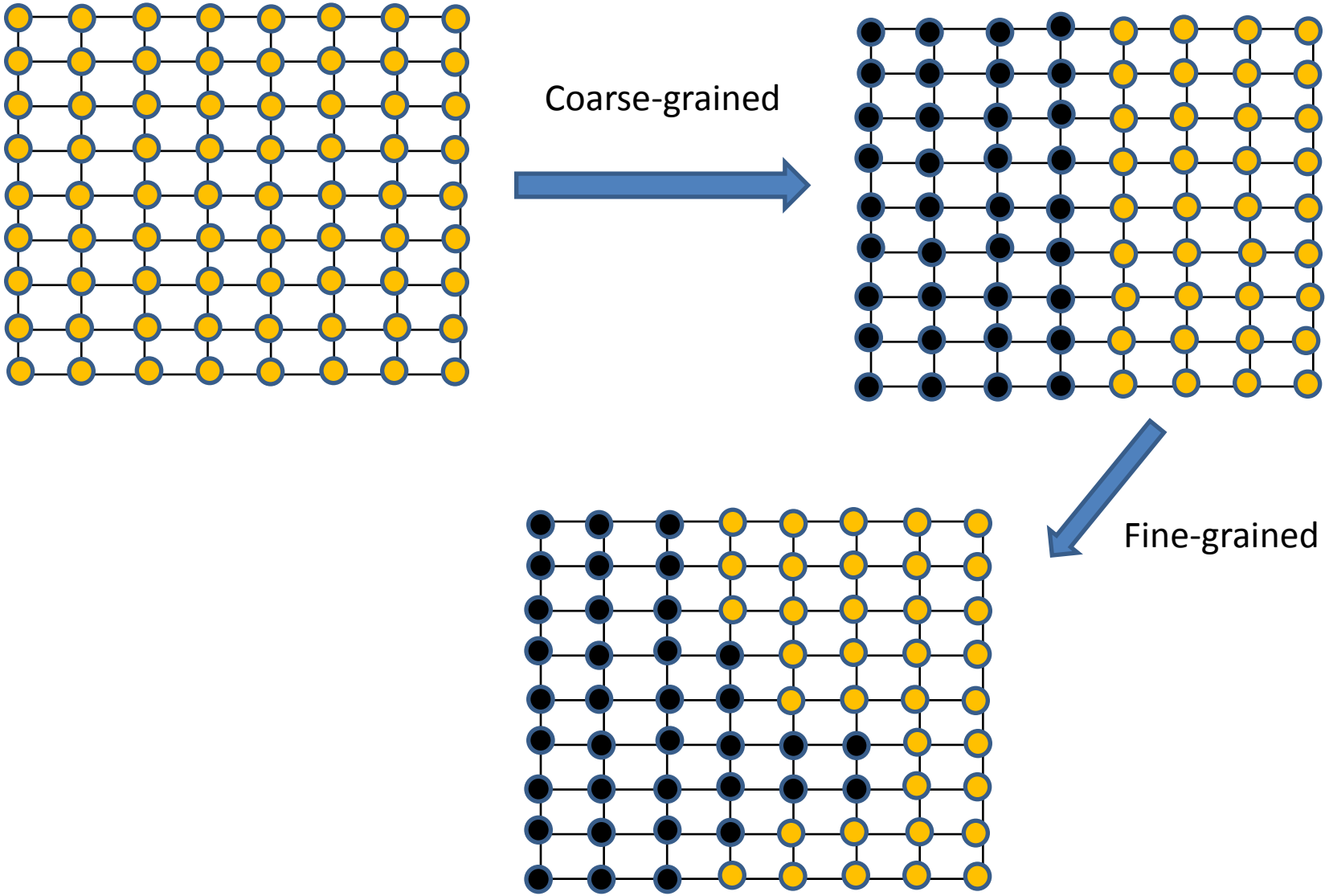
The computational difficulties



How will I attack the difficulties?

- Parallel the calculation using condor to simulate many different starting-positions, and different magnetic fields.
- Use a Multilevel Coarse-Grained Monte-Carlo algorithm: run the metropolis algorithm on the original grid, as well as on a coarse-grained grid with different resolutions, in order to deal with the domains problem
- Possibly parallel these different resolutions runs with openMP or MPI if possible in within condor

How will I attack the difficulties?



How will I attack the difficulties?

- Program in Python
- Visualize with matplotlib for the graphs and visual-python for the lattice view

Questions? Remarks?

Thank you for listening