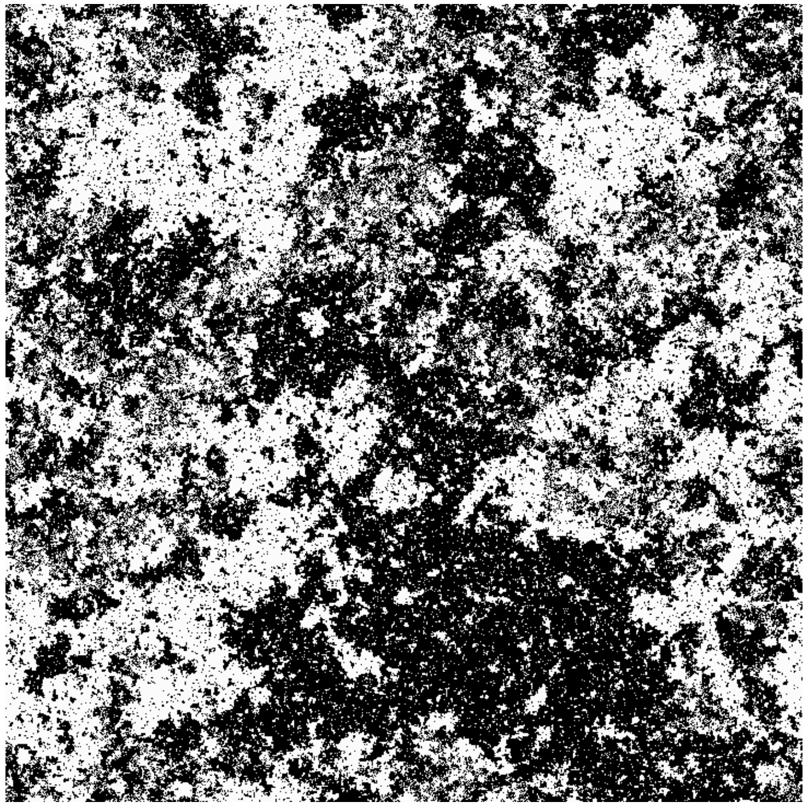
Statistical mechanics: Ising Model

Physics 682 / CIS 629: Computational Methods for Nonlinear Systems

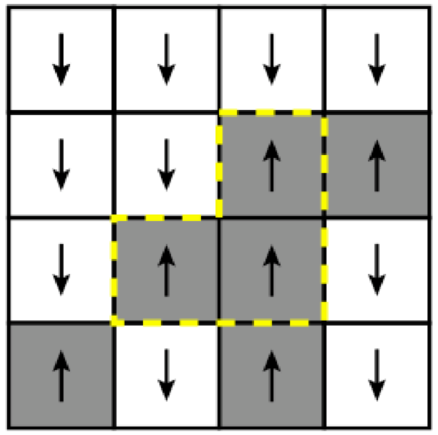
- Statistical mechanics: probability $\rho(\mathbf{S})$ to be in state $\mathbf{S}$
- Ising model: simple model of magnetic systems
  - $\mathbf{S} = \{\mathbf{S_i}\}$, sites i on a (square) lattice, i = (x,y)
  - Spins $\mathbf{S_i} = \pm 1$
- Equilibrium statistical mechanics:
  - Energy $E(\mathbf{S})$
  - Boltzmann probability distribution: $\rho(\mathbf{S}) \sim \exp(-E(\mathbf{S})/k_B T)$
  - High temperatures: states have equal weight
  - Low temperatures: low-energy states predominate
- Ising model: $\mathbf{E(S) = -J \; \Sigma_{<i,j>} \; S_i S_j - H \; \Sigma_i \; S_i}$
  - lowest energy state ($J > 0$), all spins up (+1) or down (-1)
  - Broken symmetry ferromagnetic phase
  - High temperature paramagnetic phase
  - Transition at T_c: fluctuations on all scales



- Markov chain
  - dynamics for statistical models
  - transition rate $P_{S'S}$ from S to S'
  - Markovian: independent of history

- Markov chain properties
  - detailed balance: equilibrium flux $S \to S'$ = flux $S' \to S$ $\Rightarrow$ $P_{S'S} \cdot \rho(S) = P_{SS'} \cdot \rho(S')$
  - ergodic: every state can be reached
  - A Markovian model that is ergodic and satisfies detailed balance will eventually approach equilibrium.

- Ising model dynamics
  - Heat bath Monte Carlo
    - pick a spin at random, measure flip ΔE
    - equilibrate to its current environment:
      - up with prob. $e^{-\beta E_+}/(e^{-\beta E_+} + e^{-\beta E_-})$, down with prob. $e^{-\beta E_-}/(e^{-\beta E_+} + e^{-\beta E_-})$
  - Metropolis Monte Carlo
    - pick a spin at random, measure flip ΔE
    - if $\Delta E < 0$, execute flip
    - if $\Delta E > 0$, execute flip at some probability $p \sim \exp(-\Delta E/k_B T)$
  - Wolff algorithm
    - clever generation of cluster flips
    - much faster dynamics near T_c (avoids critical slowing down)
    - satisfies detailed balance



Some variations on a theme

- Random field Ising model
  - $E(S) = -J \sum_{<i,j>} S_i S_j - \sum_i H_i S_i$ (H_i random)
  - interesting behavior even at T=0
    - avalanches on many length and time scales ("crackling noise")
    - phase transition as a function of the strength of the disorder
    - hysteresis & return-point memory
    - see "Hysteresis Exercise" (not in Python)
- Spin glasses
  - $E(S) = -\sum_{<i,j>} J_{ij} S_i S_j$ (J_{ij} random)
  - typically frustrated: cannot find spin assignment that optimally satisfies all interactions
  - rugged energy landscape: many low-energy states with roughly equal energy (and potentially large barriers)
  - replica theory and cavity methods translated to NP-complete problems (e.g., 3SAT) to provide new algorithms