Parallel Tempering Algorithm in Monte Carlo Simulation

Tony Cheung (CUHK)
Kevin Zhao (CUHK)

Mentors:
Ying Wai Li (ORNL)
Markus Eisenbach (ORNL)
Kwai Wong (UTK/ORNL)
Metropolis Algorithm on Ising Model

- Reason: difficulty of direct sampling
- Objective: compute average physical quantities of interest
- Idea: generate microstates according to Boltzmann distribution (canonical ensemble) after sufficient number of steps
- Boltzmann distribution: $P(s; T) = \frac{\exp(-\beta E_s)}{Z}$, $\beta = \frac{1}{KT}$
- Underlying principle: detailed balance
Metropolis Algorithm on Ising Model

• Simulation process
  1. Randomly initialize the model
  2. Choose a spin at random & make a trial flip
  3. Accept the flip with probability

\[ P_{flip} = \min\{1, \exp(-\beta \Delta E)\}, \beta = \frac{1}{KT} \]

  4. If the flip is accepted, determine the desired physical quantities
  5. Repeat steps 2-4 to obtain a sufficient number of microstates
  6. Calculate the ensemble average of quantities
Parallel Tempering

• Recall: \( P_{\text{flip}} = \min\{1, \exp(-\beta \Delta E)\}, \beta = \frac{1}{KT} \)

• Drawback: Low temperature
  ➞ Unlikely to accept flips with positive energy difference
  ➞ Trapped in energy local minimum

• Motivation: Run Metropolis algorithm on different temperatures & allow exchange of microstates
  ➞ High-temperature configuration at low-temperature system

• The probability of accepting an exchange is given by
  \( P_{\text{exchange}} = \min\{1, \exp(\Delta \beta \Delta E)\} \)
Temperature dependence of mean magnetization per spin with various replica exchange frequency

\[ N = \# \text{ of replica exchange} \]

Total \# of MC steps fixed to be \(10^9\); equilibration time set to \(10^9\)
Temperature dependence of mean magnetization per spin with various replica exchange frequency

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Mean Magnetization Per Spin

Temperature
Temperature dependence of energy fluctuation (SD) with various replica exchange frequency

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Running Time Dependence on # of Replica Exchanges

Monte Carlo Simulation takes up most of the time, while Parallel tempering is becoming the dominant factor.
Coming soon

• Parallel tempering Metropolis running with:
  – Various temperature spacing (# of processors)
  – Different exchange patterns
  – Geometric temperature sequence

• Implementation on other models

• Goal: optimize the algorithm
  – Better convergence with less time
  – Self adjusting algorithms