Parallel Tempering Algorithm in Monte Carlo Simulation

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Monte Carlo Algorithms

• Motivation: Difficulty in direct sampling
• Idea: Construct a Markov chain with desired equilibrium distribution
  ➔ Estimate with Bayesian inference
• Underlying principle:
  Detailed balance condition with a certain transition probability
  \[ \pi(x)P(x,y) = \pi(y)P(y,x) \]
Boltzmann Distribution

• Canonical ensemble for systems taking discrete values of energy
• The most common ensemble in statistical mechanics
• Probability distribution: \( P(E;T) = e^{\frac{-E}{kB}} \frac{T}{Z(T)} \)

• Objective:
  Employ Monte Carlo algorithms to calculate physical quantities of interest
N-vector Model

• Mathematical model of ferromagnetism in statistical mechanics
• Square/cubic lattice containing magnetized spins with dimension N
  – \( N = 1 \) \( \rightarrow \) Ising model
  – \( N = 2 \) \( \rightarrow \) XY model
  – \( N = 3 \) \( \rightarrow \) Heisenberg model
  – \( N = 4 \) \( \rightarrow \) Standard model

• Physical Quantities
  
  Hamiltonian: \( H = -J \sum \langle \uparrow, \uparrow \rangle \langle \uparrow, \downarrow \rangle s_{i} \downarrow, s_{j} \downarrow \rangle \)

  Magnetization: \( M = \sum \langle \uparrow, \uparrow \rangle s_{i} \downarrow \)
Metropolis Algorithm

• Transition probability: \[ P_{\text{flip}} = \min\{1, e^{\Delta E / k_B T} \} \]

• Flow

1. Generate an initial state randomly

2. Equilibration time, during which at each step:
   1. Choose a spin randomly and propose a trail flip
   2. Accept the flip with a probability \( P_{\text{flip}} \), or otherwise retain the original state
Metropolis Algorithm

• Flow (Cont’d)

3. Sampling time, during which at each step:
   ① Choose a spin randomly and propose a trail flip
   ② Accept the flip with a probability $P_{\text{flip}}$ and store the physical quantities, or otherwise retain the original state

4. Calculate the average physical quantities of interest
Kraken XT5

- Located in ORNL
- Cray Linux Environment (CLE) 3.1
- 9408 computed node, each with 12 cores & 16 GB memory

http://www.nics.tennessee.edu/sites/www.nics.tennessee.edu/files/images/kraken-high-right-425.jpg
Experiment 1: 2D Ising

- \(10^9\) equilibration steps & \(10^9\) sampling steps

![Graph showing mean magnetization per spin against temperature (in [J]) with a sharp transition at around 1.7 J]

**Mean Magnetization Per Spin**

- Temperature (in [J])
- Mean Magnetization Per Spin

- \(N=0\)
Drawback of Metropolis Algorithm

• Low convergence rate at low temperatures
• Reason: For lower temperature systems,

\[
\text{For } \Delta E > 0, P_{\text{flip}} = \min\{1, e^{\Delta E/k_B T}\} \approx 0
\]
\[
\text{For } \Delta E < 0, P_{\text{flip}} = \min\{1, e^{\Delta E/k_B T}\} = 1
\]

⇒ trapped in energy minimum
⇒ fail to generate states according to Boltzmann distribution
Parallel Tempering

• Objective:
  Run Metropolis Algorithm on different temperatures & allow exchange of states every certain amount of sampling steps

→ High-temperature configurations apply to low-temperature systems & rescue them from being trapped

\[ P_{\text{exchange}} = \min\{1, e^{\Delta \beta \delta E}\} \approx 0; \beta = 1/k_B T \]
Experiment 2: 2D Ising model

- $10^9$ equilibration steps & $10^9$ sampling steps
- Varying number of evenly-distributed exchanges

![Graph showing magnetization per spin vs. temperature for 0 and 10 exchanges.](image)
Experiment 2: 2D Ising model

- $10^9$ equilibration steps & $10^9$ sampling steps
- Varying number of evenly-distributed exchanges

[Graph showing mean magnetization per spin varying with temperature for 0 and 10 exchanges.]
Experiment 2: 2D Ising model

- $10^9$ equilibration steps & $10^9$ sampling steps
- Varying number of evenly-distributed exchanges

![Graph showing mean magnetization per spin vs. temperature (J) for different numbers of exchanges: 250 exchanges, $10^4$ exchanges, $10^7$ exchanges. The graph demonstrates how the mean magnetization changes with temperature, with different curves for each number of exchanges.](image-url)
Experiment 3
Convergence of magnetic susceptibility

- 100*100 2-D Ising Model (square lattice)
- Total equilibration step = $10^9$
- Total Monte Carlo sampling step = $10^9$
- Temperature Range $K_b T = 0.5$ (J) $\sim 5.5$ (J)
- 96 processors covering the temperature range
- Second moment requires more time to converge
Experiment 3

Convergence of magnetic susceptibility
Experiment 3
Convergence of magnetic susceptibility

![Graph showing the convergence of magnetic susceptibility with respect to $k_bT$ (J)].

- **S/S**
- **S/P $10^4$**
Experiment 3
Convergence of magnetic susceptibility

![Graph showing the convergence of magnetic susceptibility with plots for S/P 10^4 and P/P 10^4. The x-axis represents k_bT (J) from 0.5 to 3.5, and the y-axis represents Magnetic Susceptibility from 0 to 200. The graph illustrates the behavior of magnetic susceptibility as a function of temperature.]
Experiment 3
Convergence of magnetic susceptibility

![Graph showing the convergence of magnetic susceptibility.](image-url)
Experiment 4
Geometric temperature spacing

• 100*100 2-D Ising Model (square lattice)

• Total equilibration step = $10^9$
• Total Monte Carlo sampling step = $10^9$
• Number of exchange = $10^6$

• Temperature Range $K_bT = 0.5$ (J) $\sim 5.0$ (J)
• 96 processors covering the temperature range
Experiment 4
Geometric temperature spacing
Experiment 4
Geometric temperature spacing

Replica exchange difficulty throughout temperature range

Exchange acceptance ratio

$k_b T$ (J)
Experiment 4
Geometric temperature spacing

Replica exchange difficulty throughout temperature range

Exchange acceptance ratio vs. $k_bT$ (J)

- A/SE
- G/SE
- Ideal
Adaptive temperature spacing
Adaptive temperature spacing
Adaptive temperature spacing
Adaptive temperature spacing
Experiment 5

Adaptive temperature spacing

- 100*100 2-D Ising Model (square lattice)
- Total equilibration step = $10^9$
- Total Monte Carlo sampling step = $10^9$
- Number of exchange = $10^4$
- Temperature Range $K_b T = 0.5 \text{ (J)} \sim 5.5 \text{ (J)}$
- 96 processors covering the temperature range
Experiment 5
Adaptive temperature spacing

Replica exchange difficulty with/without adaptive spacing

Exchange acceptance ratio

\( k_b T \) (J)

- Regular
- Adapt/9
Experiment 5
Adaptive temperature spacing

Magnetic Susceptibility with/without adaptive temp spacing

- Regular

Magnetic susceptibility vs. $k_bT$ (J)
Experiment 5
Adaptive temperature spacing

Magnetic Susceptibility with regular & adaptive spacing

- Regular
- Adaptive
Implementation on other models

2-D Heisenberg Model

- 100*100 2-D Heisenberg Model (square lattice)
- Total equilibration step = $10^9$
- Total Monte Carlo sampling step = $10^9$
- Number of exchange = $10^4$
- Temperature Range $K_b T = 0.10 \ (J) \sim 4.25 \ (J)$
- 180 processors covering the temperature range
Implementation on other models

2-D Heisenberg Model

![Graph showing magnetic susceptibility versus k_bT (J)]
Implementation on other models

2-D Heisenberg Model

Magnetic Susceptibility vs. $k_bT$ (J)

- S/P
- P/P
Implementation on other models
2-D Heisenberg Model

Magnetic Susceptibility

$k_b T (J)$
Implementation on other models

2-D Heisenberg Model

Exchange acceptance rate vs. $k_bT (J)$

- Regular
- Adaptive/9
Implementation on other models
3-D Heisenberg Model

- 25*25*25 3-D Heisenberg Model (square lattice)
- Total equilibration step = $10^9$
- Total Monte Carlo sampling step = $10^9$
- Number of exchange = $10^4$
- Temperature Range $K_b T = 0.30$ (J) ~ 4.50 (J)
- 192 processors covering the temperature range
Implementation on other models

3-D Heisenberg Model

Magnetic susceptibility vs. $k_b T (J)$
Implementation on other models

3-D Heisenberg Model

Magnetic susceptibility vs. $k_bT$ (J)

Serial
Adaptive
Future Direction:
Interoperable Executive Library (IEL)

- Software framework used for multi-physics simulations
- Designed to execute & schedule in parallel a series of physics solvers
- Objective: Run parallel tempering on different parameter spaces with data & information change on shared boundaries