Bishoy & Moaz Taha

Comparative Analysis: Metropolis, Heat Bath, Wolff Cluster, and Swendsen-Wang Algorithms for a 2D Ising Model

Summary

Section	Maximum + bonus	Your Grade + bonus
1	6+4	4+2
2	25+4	17+1
3	28+4	26+3
4	20+4	16+2
5	4+2	4+0
6	9+2	9+1
Deductions	-11	0
Total	92+20	76+9

Section 1: Introduction (6 points)

Essential Elements (6 points):

- ☑ (1 pt) Introduces the 2D square-lattice Ising model and its significance
- ☐ (1 pt) Explains the phase transition at critical temperature $T_c \approx 2.269$ J/κ_B
- ☑ (1 pt) Describes the problem with single-spin flip methods at low T (getting stuck, ergodicity issues)
- ☐ (1 pt) Introduces the Monte Carlo approach and concept of equilibrium sampling
- ☑ (1 pt) Mentions the algorithms to be compared
- ☑ (1 pt) States the objective: comparing efficiency and accuracy of different update schemes

Bonus Elements (up to 4 points):

- ☑ (+1 pt) Discusses critical slowing down near T_c
- ☐ (+1 pt) Mentions the exact analytical solution (Onsager) as reference
- ☐ (+1 pt) Explains how $\langle m \rangle = 0$ analytically but simulations show $\pm|m|$
- ☑ (+1 pt) Provides historical context or applications of the Ising model

Section 2: Methods (25 points)

Metropolis Algorithm (5 points):

- ☑ (2 pts) Describes single-spin flip proposal
- ☑ (2 pts) Explains acceptance criterion: $\min(1, e^{-\beta\Delta E})$
- ☐ (1 pt) Defines a "sweep" as N attempted flips

Heat Bath Algorithm (5 points):

- ☑ (2 pts) Describes the heat bath update rule
- ☑ (2 pts) Explains probability calculation: $P(s_i = +1) = 1/(1 + e^{-2\beta h_i})$
- ☑ (1 pt) Notes relationship/difference with Metropolis

Wolff Cluster Algorithm (6 points):

- ☑ (2 pts) Describes cluster building from random seed
- ☑ (2 pts) States the bond probability: $p_{add} = 1 - e^{-2\beta J}$
  You wrote that the addition ends when you reach a spin that's not aligned with the original one, which is wrong. (-1)
- ☐ (1 pt) Explains the cluster flip operation
- ☐ (1 pt) Discusses when Wolff may not be optimal (very low T, whole-lattice clusters)

General Methodology (9 points):

- ☑ (1 pt) Specifies boundary conditions (periodic)
- ☑ (1 pt) Lists system sizes: $L \in \{16, 32, 64, 128\}$ or similar
- ☑ (1 pt) Describes temperature grid (coarse far from Tc, fine near Tc)
- ☐ (2 pts) Explains thermalization/burn-in procedure
- ☑ (2 pts) Defines observables: $\langle|m|\rangle$, $\langle e \rangle$, χ, C, Binder cumulant UL
- ☐ (1 pt) Explains integrated autocorrelation time τ estimation
  You explained that you used an approximate to calculate it. Sure, but I have to ask, how did you determine ?
- ☐ (1 pt) Mentions use of identical random seeds for fair comparison

Bonus Elements (up to 4 points):

- ☐ (+1 pt) Includes pseudocode for each algorithm
- ☐ (+1 pt) Discusses error estimation with autocorrelation correction
- ☐ (+1 pt) Explains uncertainty
- ☑ (+1 pt) Describes Swendsen-Wang or parallel tempering

Section 3: Results (28 points)

Required Figures (18 points):

- ☑ (3 pts) CPU time per independent sample vs. Temperature (all algorithms on one plot)
- ☑ (3 pts) Integrated autocorrelation time τ vs. Temperature for each algorithm
- ☑ (3 pts) $\langle |m| \rangle$ vs. T (showing phase transition)
- ☑ (3 pts) $\langle e \rangle$, χ, C vs. T plots
- ☑ (3 pts) Binder cumulant crossings for multiple L values
- ☑ (3 pts) At least one heatmap (CPU time or τ as function of L and T)

Data Presentation (6 points):

- ☑ (2 pts) Results for multiple system sizes as specified
- ☑ (2 pts) Clear labeling of axes, legends, units
- ☐ (2 pts) Error bars accounting for autocorrelation

Algorithm-Specific Results (4 points):

- ☑ (2 pts) Cluster size distribution for Wolff algorithm
- ☑ (1 pt) Shows divergent behavior of τ or χ near Tc
- ☑ (1 pt) Results from 3-5 independent trials for heatmap cells

Bonus Elements (up to 4 points):

- ☑ (+1 pt) Finite-size scaling analysis
- ☑ (+1 pt) Tc estimation from Binder cumulant crossings
  Not *explicit* but good enough.
- ☐ (+1 pt) Comparison with exact/analytical values
- ☑ (+1 pt) Swendsen-Wang results (if implemented)

Section 4: Discussion (20 points)

Algorithm Comparison (10 points):

- ☑ (2 pts) Compares efficiency (CPU time per independent sample) across algorithms
- ☑ (2 pts) Analyzes autocorrelation time differences, especially near Tc
- ☑ (2 pts) Discusses which algorithm is best in different temperature regimes
- ☑ (2 pts) Explains why Wolff reduces critical slowing down
- ☑ (2 pts) Addresses trade-offs (per-step cost vs. decorrelation)

Physical Interpretation (6 points):

- ☑ (2 pts) Interprets the phase transition in simulation results
- ☑ (2 pts) Discusses finite-size effects on observables
- ☑ (2 pts) Explains behavior of susceptibility and heat capacity peaks

Critical Analysis (4 points):

- ☐ (2 pts) Addresses limitations or unexpected results
  P.S. I mean limitations *you* faced. Unexpected results you couldn't explain. These are the trademarks of a realllly good paper
- ☐ (2 pts) Discusses sources of error and their mitigation

Bonus Elements (up to 4 points):

- ☑ (+1 pt) Compares to literature values for Tc or critical exponents
- ☐ (+1 pt) Discusses potential improvements or optimizations
- ☐ (+1 pt) Analyzes parallel tempering results (if implemented)
- ☑ (+1 pt) Provides practical recommendations for different simulation scenarios

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Section 5: Conclusion (4 points)

Essential Elements (4 points):

- ☑ (1 pt) Summarizes key findings on algorithm performance
- ☑ (1 pt) States which algorithm is preferred and under what conditions
- ☑ (1 pt) Confirms observation of phase transition at expected Tc
- ☑ (1 pt) Suggests future work or extensions

Bonus Elements (up to 2 points):

- ☐ (+1 pt) Reflects on broader implications for Monte Carlo simulations
- ☐ (+1 pt) Proposes specific extensions (3D Ising?)

Section 6: Appendix & Code Quality (9 points)

- ☑ (3 pts) Code is included and readable
- ☑ (2 pts) Code is well-documented with comments
- ☑ (2 pts) Code organization is logical (separate functions for each algorithm)
- ☑ (2 pts) Reproducibility: random seeds, parameters documented

Bonus Elements (up to 2 points):

- ☐ (+1 pt) Includes validation tests (detailed balance check)

☑ (+1 pt) Efficient implementation (vectorization, Numba, etc.)

Overall Presentation & Writing (Deductions)

☐ (-1 to -3 pts) Poor grammar, spelling, or unclear writing
☐ (-1 to -2 pts) Inconsistent formatting
☐ (-1 to -3 pts) Missing figure captions or references
☐ (-1 to -3 pts) Plagiarism or uncited sources