



Russian Supercomputing Days 2026

Metropolis configuration overlap as a thermodynamic variable

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Algorithmic quantities as observables

- Generalized ensembles turn algorithmic quantities into observables: histogram flatness, swap probabilities, resampling factors.
- Burovski et al. (2019): the Metropolis acceptance rate is a thermodynamic function.
- 1D Ising, exact: $R = 1 + \varepsilon$, $\varepsilon = E/(JN)$. In 2D the relation is nearly linear near T_c .

Question

R is a single-sweep quantity. Does the memory between successive Metropolis states also behave as a thermodynamic variable?

Models and Metropolis updates

$$H_{\text{Ising}} = -J \sum_{\langle ij \rangle} s_i s_j, \quad s_i = \pm 1$$

$$H_{\text{Potts}} = -J \sum_{\langle ij \rangle} \delta_{s_i, s_j}, \quad s_i \in \{1, 2, 3\}$$

$$P_{\text{acc}} = \min(1, e^{-\beta \Delta E})$$

- $T_c^{\text{Ising}} = 2/\ln(1 + \sqrt{2}) \approx 2.269$, $T_c^{(3)} = 1/\ln(1 + \sqrt{3}) \approx 0.995$.
- One sweep: $N = L^2$ proposals in random site order.
- The proposed state always differs from the current one.

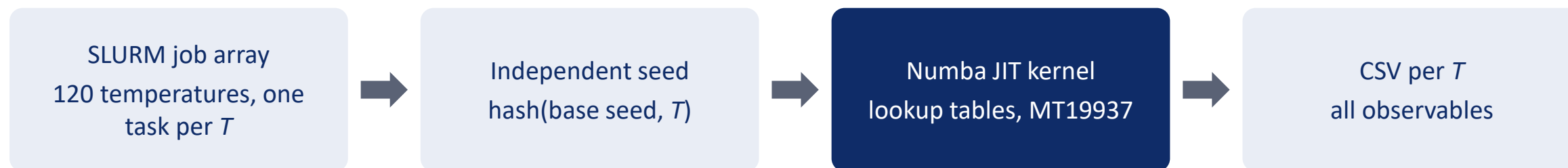
Ising lookup table

$\Delta E/J$	-8	-4	0	4	8
P_{acc}	1	1	1	$e^{-4\beta}$	$e^{-8\beta}$

Three-state Potts lookup table, $\Delta E = J(n_\alpha - n_\beta)$

$\Delta E/J$	≤ 0	1	2	3	4
P_{acc}	1	$e^{-\beta}$	$e^{-2\beta}$	$e^{-3\beta}$	$e^{-4\beta}$

Implementation on the HSE HPC cluster



- Different temperatures need no communication: embarrassingly parallel scan.
- Precomputed Boltzmann tables remove exponentials from the inner loop.
- Cluster Charisma, Intel Xeon Gold 6240.

Parameter	Value
L	64 ... 1024
N_{therm}	$2 \cdot 10^5$ sweeps
N_{meas}	10^6 sweeps
Temperatures	120 per L

Configuration overlap

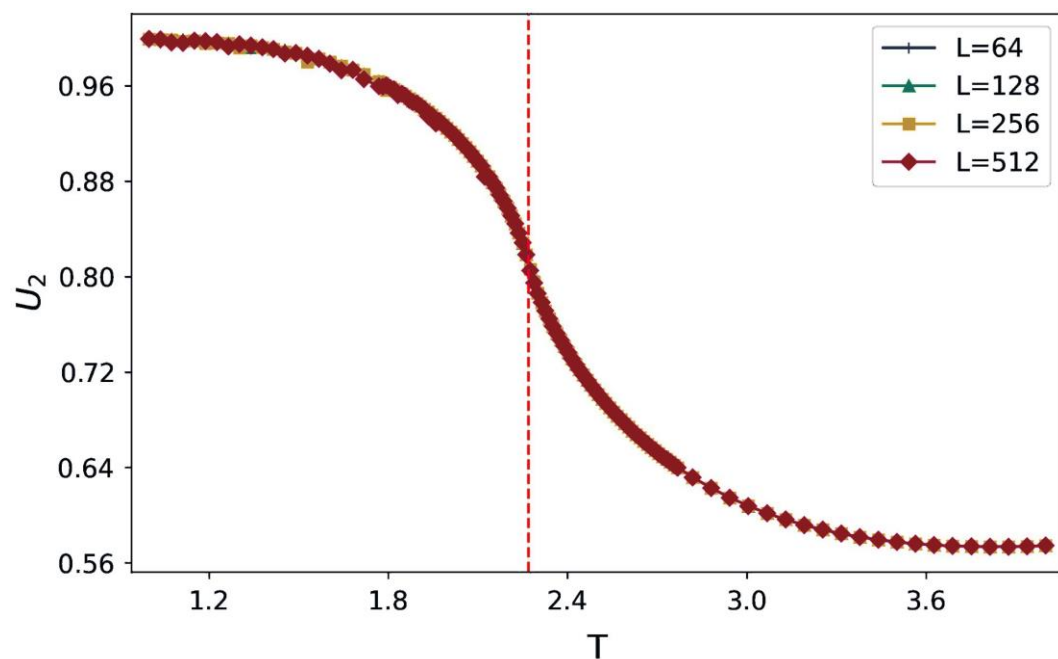
$$U_n(t) = \frac{1}{N} \sum_{i=1}^N \delta(s_i^{(t)}, s_i^{(t+n)})$$

- Fraction of spins unchanged between sweeps t and $t + n$.
- We measure $\langle U_n \rangle$ and $\text{Var}(U_n) = \langle U_n^2 \rangle - \langle U_n \rangle^2$.
- Each site is proposed once per sweep and the proposal always changes the spin, so a spin changes if and only if the move is accepted.

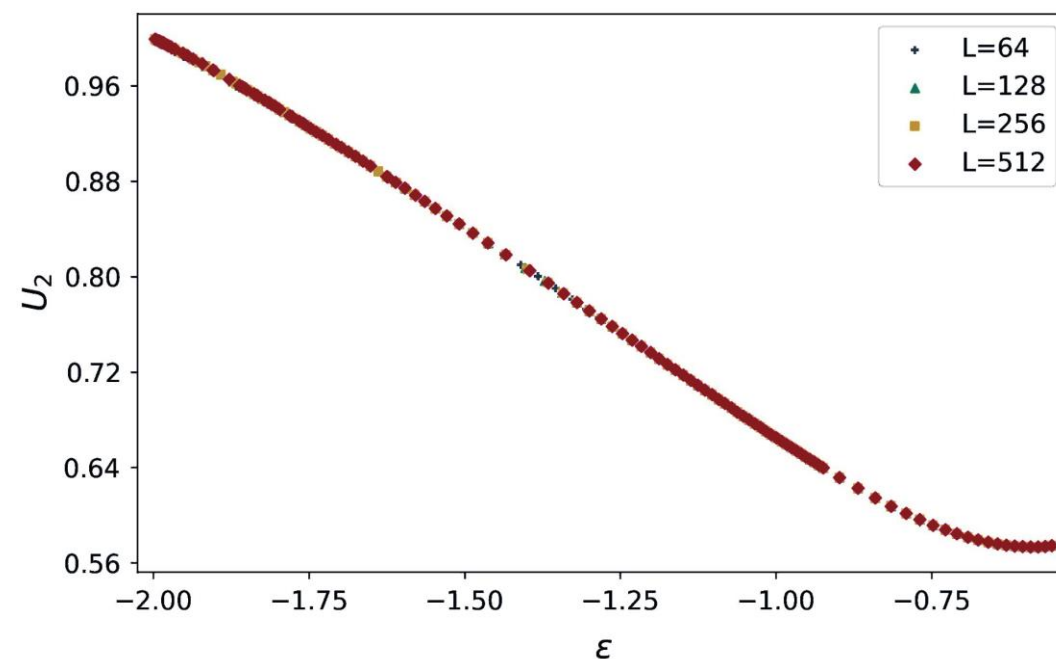
$$U_1(t) \equiv 1 - R(t) \quad \implies \quad \langle U_1 \rangle_{1D} = |\varepsilon|$$

U_1 repeats the acceptance rate sweep by sweep.
The first nontrivial object is U_2 .

Ising model: data collapse of $\langle U_2 \rangle$



$\langle U_2 \rangle$ versus T , $L = 64-512$, dashed line: T_c

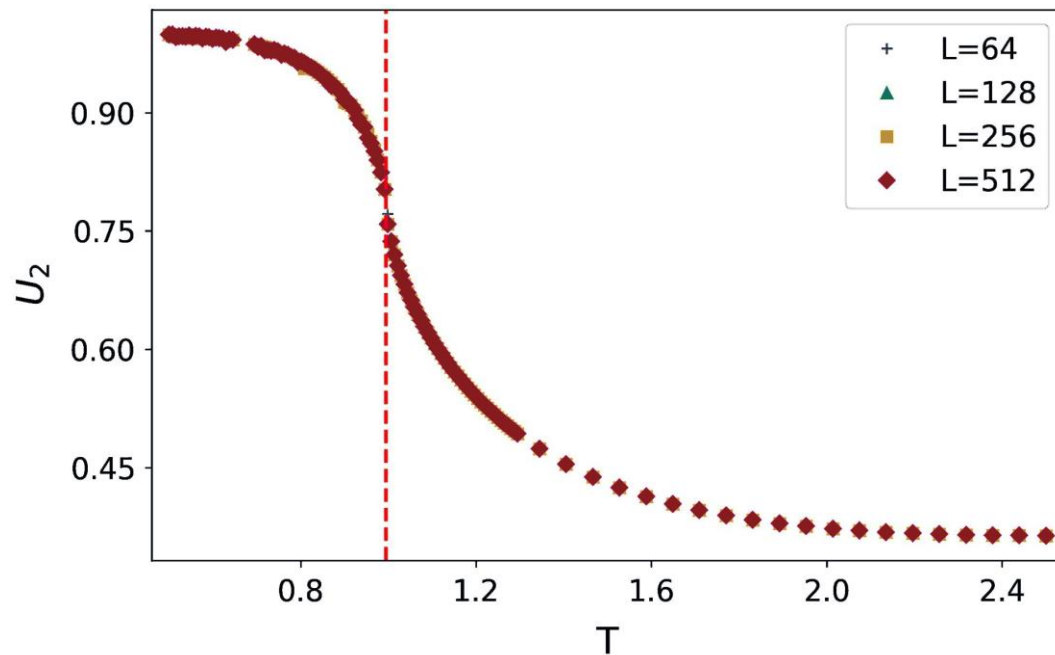


$\langle U_2 \rangle$ versus energy density ϵ

$$\langle U_2 \rangle = g(\epsilon) \approx a + b\epsilon$$

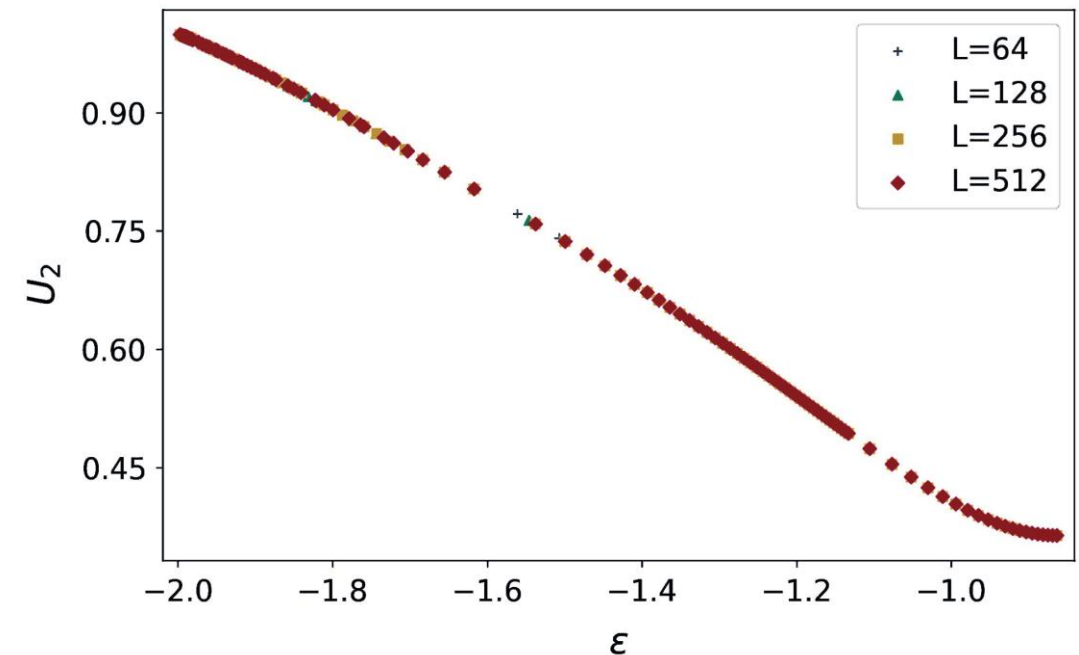
Near ϵ_c : $b = -0.348(3)$ ($L = 512$). Not derivable from $R = R(\epsilon)$.

Three-state Potts model



$\langle U_2 \rangle$ versus T , $L = 64-512$

High- T limit $\langle U_2 \rangle \rightarrow 1/3$ instead of $1/2$ for Ising.



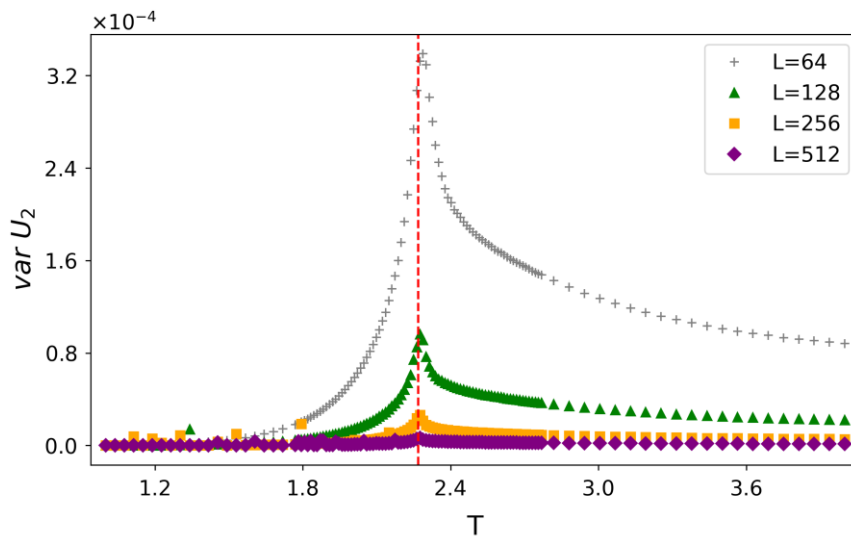
$\langle U_2 \rangle$ versus ϵ : the collapse holds

$b = -0.573(5)$ ($L = 512$), steeper than Ising

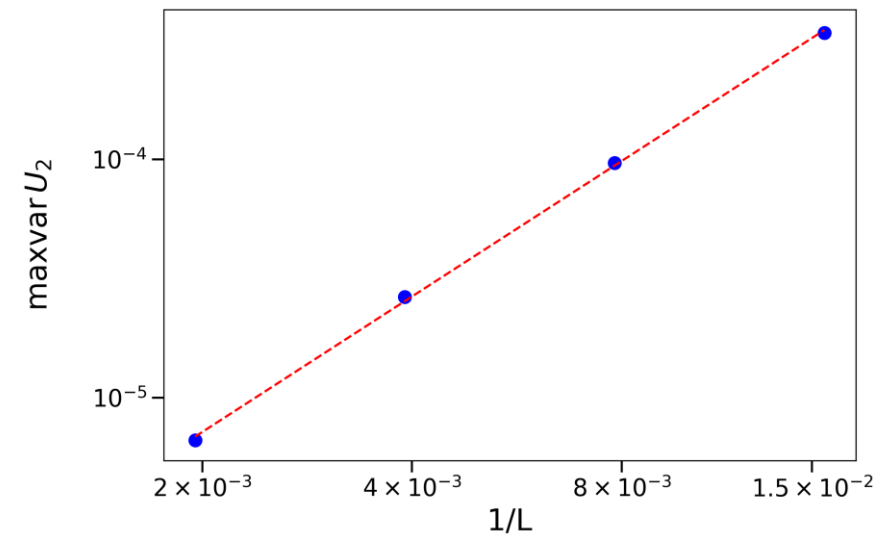
Variance and heat capacity

$$\text{Var}(U_2) = b^2 \text{Var}(\varepsilon) = b^2 \frac{C T^2}{N}$$

- Assumes $\text{Var}(U_2 \mid \varepsilon)$ is small compared with $b^2 \text{Var}(\varepsilon)$. The collapse supports this.
- The peak of $\text{Var}(U_2)$ coincides with the peak of C , i.e. with T_c .
- Peak height $b^2 C_{\max} T_c^2 / N$: close to L^{-2} , with the growth of $C_{\max}(L)$ on top.



Var(U_2) versus T , 2D Ising, Metropolis



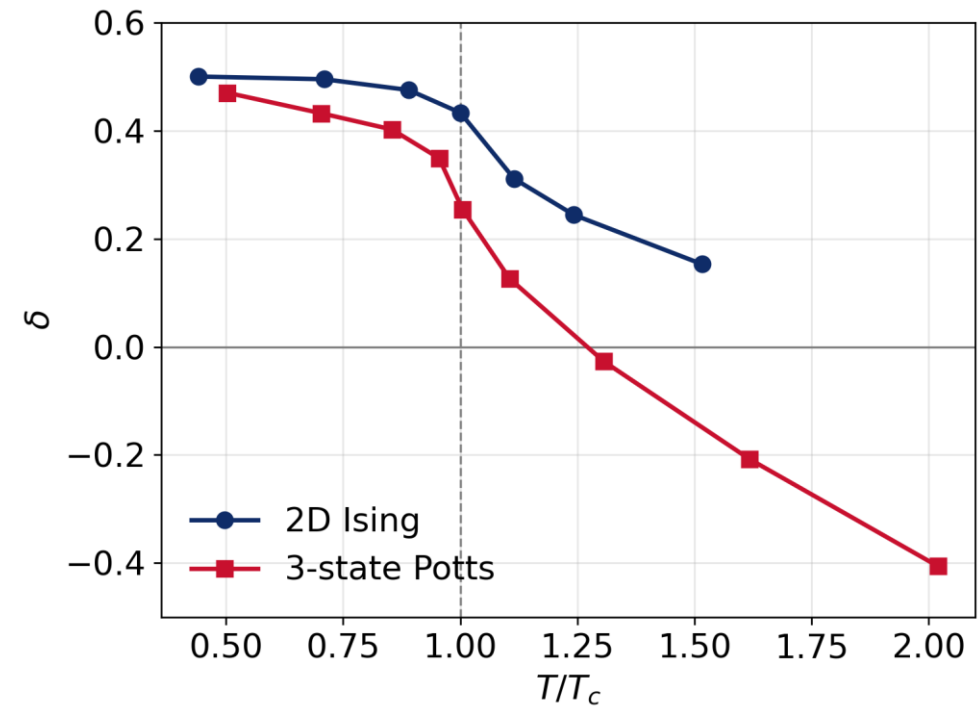
Peak height of $\text{Var}(U_2)$ versus $1/L$

Persistence parameter δ

$$\langle U_2 \rangle = 1 - 2\langle R \rangle(1 - \langle R \rangle)(1 - \delta)$$

$$\delta = \frac{R_{\text{rev}} - \langle R \rangle}{2(1 - \langle R \rangle)}$$

- $\delta = 0$: independent-sweep approximation.
- Ising: reverse flip has $\Delta E' = -\Delta E$. $\delta \rightarrow 1/2$ at $T \rightarrow 0$, $\delta \rightarrow 0$ at $T \rightarrow \infty$, $\delta \approx 0.43$ at T_c .
- Potts: the old state is proposed with probability $1/(q - 1) = 1/2$. $\delta < 0$ above T_c .



δ versus T/T_c , $L = 512$ (Tables 1 and 2 of the paper)

Exact result in 1D: parallel updates

$$P(Q_j = 1) = \frac{x}{x+1}, \quad p_{\text{flip}}(a, b) = 1 - (1 - \alpha)ab, \quad \alpha = x^{-2}$$

$$Q_j^{(1)} = Q_j^{(0)} \oplus (f_j \oplus f_{j+1})$$

- Bonds are independent in the thermodynamic limit, $x = e^{2\beta J}$.
- A bond changes if exactly one of its ends flips.
- Condition on (Q_{i-1}, Q_i) and follow spin i for two sweeps.

$$U_2^{\text{par}} = \frac{x^5 - x^4 + 2x^3 + 2x^2 - 4x + 2}{x^4(x+1)}$$

$$\delta^{\text{par}} = \frac{x^4 - x^3 + x^2 - 1}{2x^4}$$

Checks: $U_2^{\text{par}} \rightarrow 1$ at $x \rightarrow \infty$ and $x \rightarrow 1$. $\delta^{\text{par}} \rightarrow 1/2$ at low T , $\delta^{\text{par}} \geq 0$ for all $x \geq 1$.

Sequential updates: bounds

$$\mathcal{C}(2) \geq \mathcal{C}(1)^2, \quad U_2 = \frac{1}{2}(1 + \mathcal{C}(2)), \quad R = \frac{1}{2}(1 - \mathcal{C}(1))$$

- Remark: reversibility gives $\delta \geq 0$ via the spectral decomposition of the spin autocorrelation $\mathcal{C}(n)$.
- Conjecture: $\delta^{\text{seq}} \leq \delta^{\text{par}}$ for the 1D Ising chain.

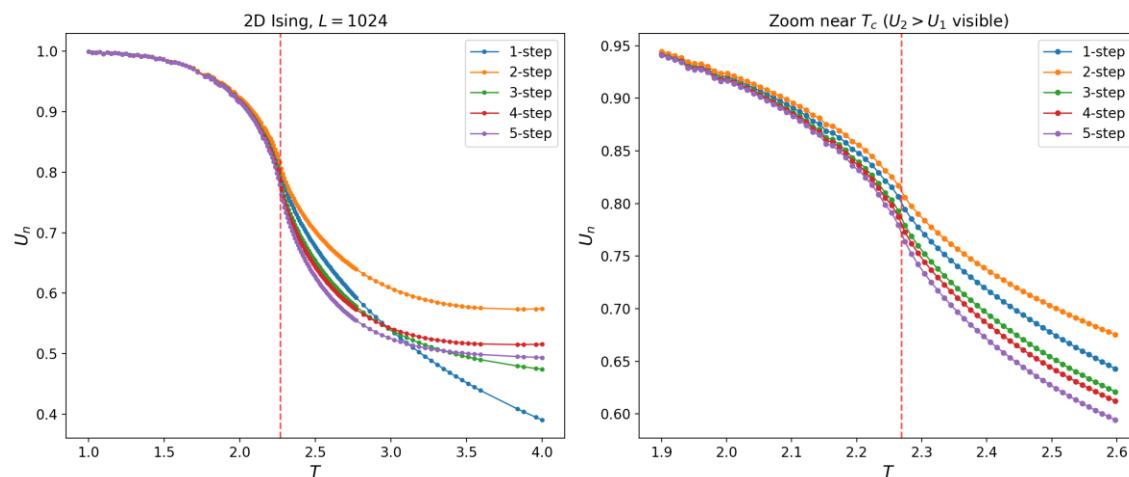
$$U_2^{\text{indep}} \leq U_2^{\text{seq}} \leq U_2^{\text{par}}$$

T/J	R	U_2^{par}	U_2^{seq}	U_2^{indep}	δ^{par}	δ^{seq}
0.5	0.036	0.965	0.955	0.931	0.491	0.347
1.0	0.238	0.797	0.727	0.637	0.441	0.250
2.0	0.538	0.689	0.552	0.503	0.375	0.099
3.0	0.678	0.712	0.585	0.564	0.340	0.049
5.0	0.803	0.775	0.690	0.683	0.289	0.020

1D Ising, $L = 500$

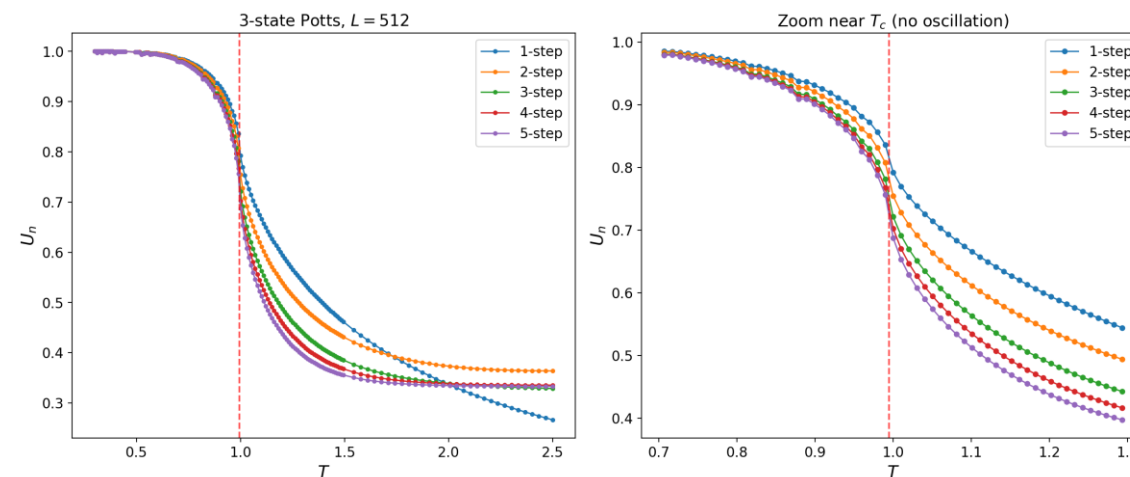
An exact U_2^{seq} is open: the causal cone of a sequential sweep reaches the start of the sweep.

Multistep overlaps



2D Ising, $L = 1024$: $\langle U_2 \rangle > \langle U_1 \rangle$ everywhere

$$\langle U_2 \rangle > \langle U_1 \rangle \iff \delta > 1 - \frac{1}{2(1 - \langle R \rangle)}$$



3-state Potts, $L = 512$: monotonic in n near T_c

Ising: the reverse flip is favoured. Potts: proposal dilution drives $\delta < 0$ above T_c .

Conclusions

1. $\langle U_2 \rangle = g(\varepsilon)$: the mean overlap collapses onto one function of the energy density.
2. $\text{Var}(U_2) = b^2 C T^2 / N$: overlap fluctuations follow the heat capacity and peak at T_c .
3. The persistence parameter δ separates Ising ($\delta \geq 0$) and Potts ($\delta < 0$ above T_c).
4. 1D Ising: closed form for parallel updates, bounds for sequential updates.

Open questions

$g(\varepsilon)$ and b from first principles.

Proof of $\delta^{\text{seq}} \leq \delta^{\text{par}}$.

First-order transitions: bimodal energy, a different $g(\varepsilon)$.



Thank you for your attention!

