Synchronous Parallel Kinetic Monte Carlo Application to Critical, billion-atom, 3D Ising Systems

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Motivation: Method

- Kinetic Monte Carlo is widely used in many scientific disciplines.
- Several methods to (more or less) efficiently parameterize kMC models.
- Not so much work on speeding up kMC itself.
- Parallelization is commonplace in MD simulations and as a way to 'slave' computationally-demanding calculations of saddle points, attempt frequencies, etc, in kMC methods.
- What about parallelization of kMC?

Motivation: Application

- Ising model can be used to map discrete-lattice systems: lattice gas, binary alloys, magnetism, etc.
- Ising system is interesting for studying second-order phase transformations.
- Belongs to a universality class for systems with long-range correlated disorder.
- Very large systems must be considered to capture the kinetic behavior, particularly in 3D.
- No analytical solution for critical kinetics in 3D, only slow converging numerical solutions.
- Many methods employed over the years.

Ising system kinetics

Master equation:

$$\frac{\partial p(\sigma,t)}{\partial t} = \sum_i \{\mathcal{W}_i(\sigma)p(\sigma,t) - \mathcal{W}_i(\sigma')p(\sigma',t)\}$$

Transition rates for Glauber dynamics:

$$\mathcal{W}_i(\sigma) = \frac{\lambda}{2}\left[1 - \sigma_i \tanh(2\beta\Delta E_i)\right]$$

ΔEi follows from the Ising Hamiltonian

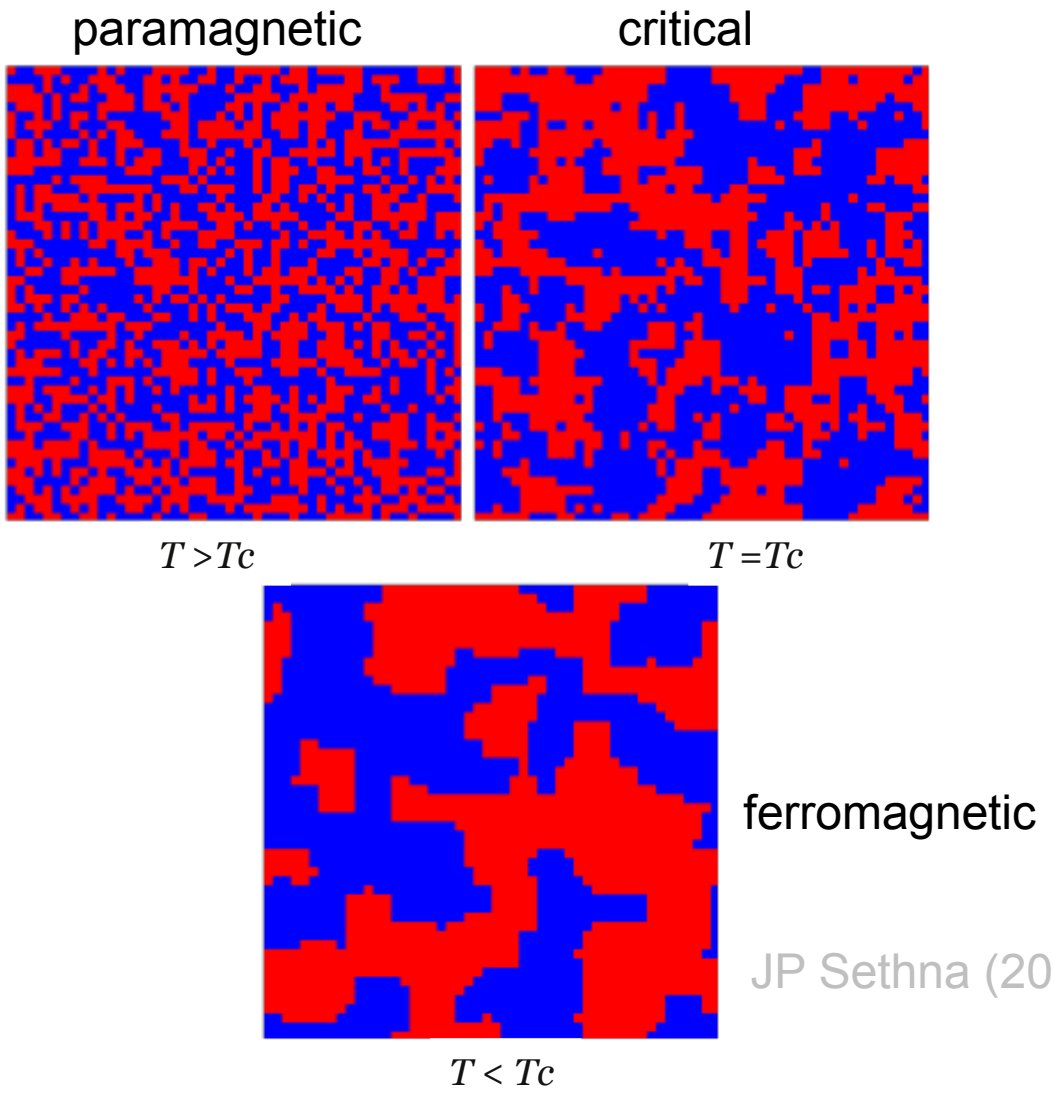
$$\mathcal{H}(\sigma) = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j \rightarrow \Delta E_i = -J\sum_{\langle i,j\rangle}\sigma_j$$

Temperature behavior of Ising systems

- At the critical temperature Tc, domains of aligned spins are created.
- These domains are defined by a correlation length ξ:

$$\xi \propto |T - T_c|^{\nu}$$

- v is the 'scale' critical exponent.
- Critical exponents not converged for 3D.



JP Sethna (2009)

The net magnetization is the order parameter of the Ising system

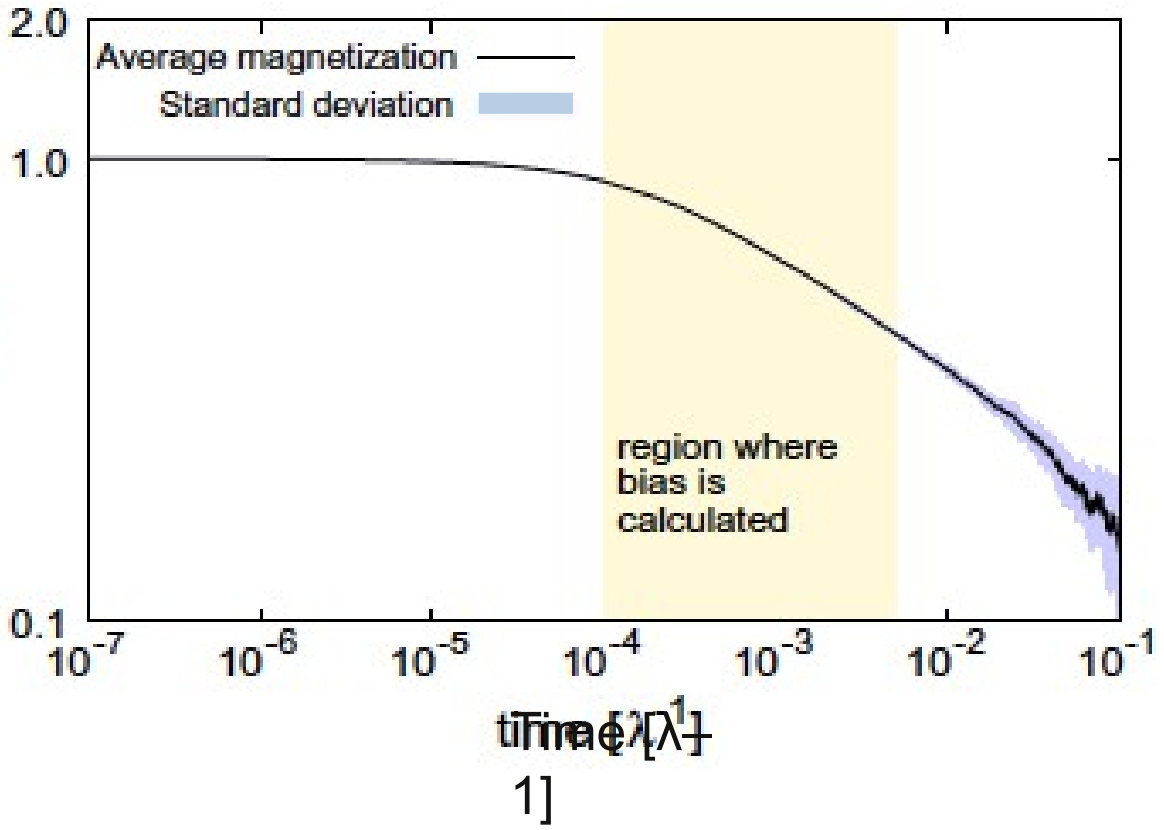
$$m(\sigma) = \frac{1}{N}\sum_i \sigma_i$$

$$m(t) \propto t^{-\kappa/z\nu}$$

The value of the critical exponents in 1D and 2D is analytically known and can be converged for 4 and higher dimensions.

In 3D: no converged numerical solution.

$$z = -\frac{\kappa}{\nu}\left[\frac{d(\log m)}{d(\log t)}\right]^{-1}$$



Serial kMC not sufficient

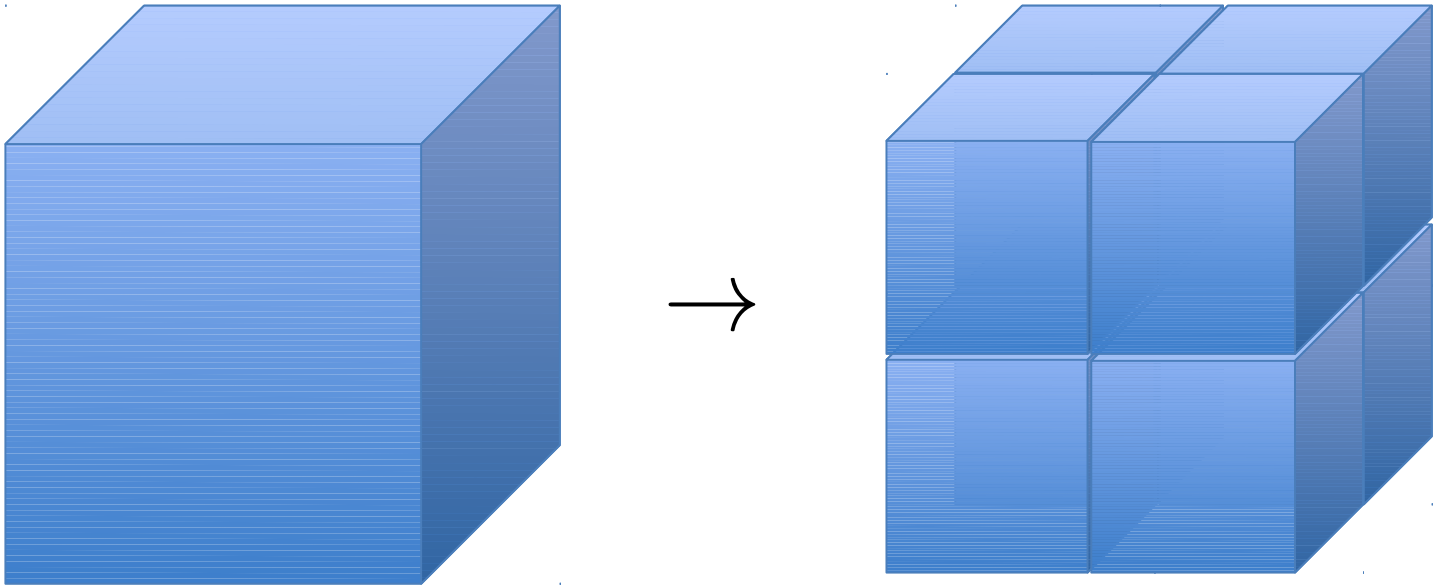
Parallel kMC algorithms to study large kinetic systems

- Discrete event kinetics are inherently difficult to parallelize.
- Traditional parallelization approaches based on **asynchronous** kinetics (Lubachevsky 1988, Jefferson 1985).
- **Causality errors** arise with these approaches: mutually affecting events occurring in different domains.
- This requires '**roll-back**' techniques to reconcile the time evolution of different processors.
- This leads to implementation complexity and regions of low efficiency.
- Rigorous and semi-rigorous algorithms have been proposed (Amar and Shim 2003, Shim and Amar 2005,

We use a novel synchronous parallel kMC algorithm to study very large systems

Assume a spatial domain containing *N* walkers:

- Each walker defined by a rate q_i, $R_{\text{tot}} = \sum_i^N q_i$
- Perform spatial domain decomposition:



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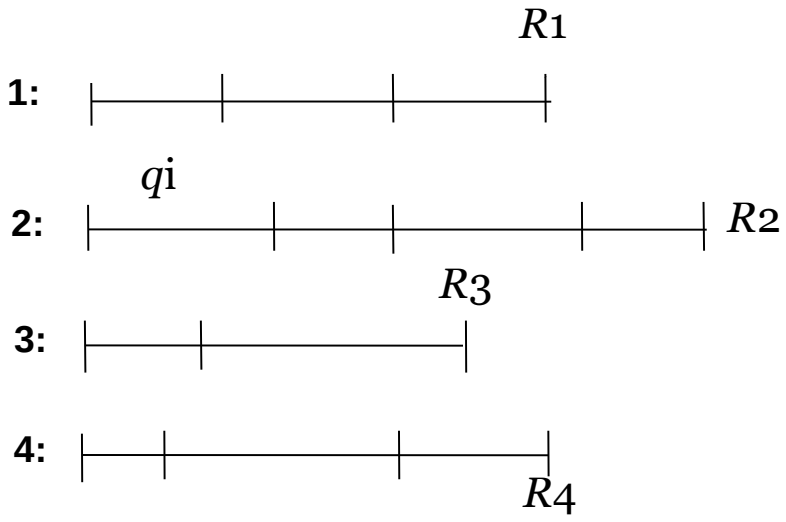
Now, for parallel kMC, perform K (4) domain partitions and construct frequency lines:



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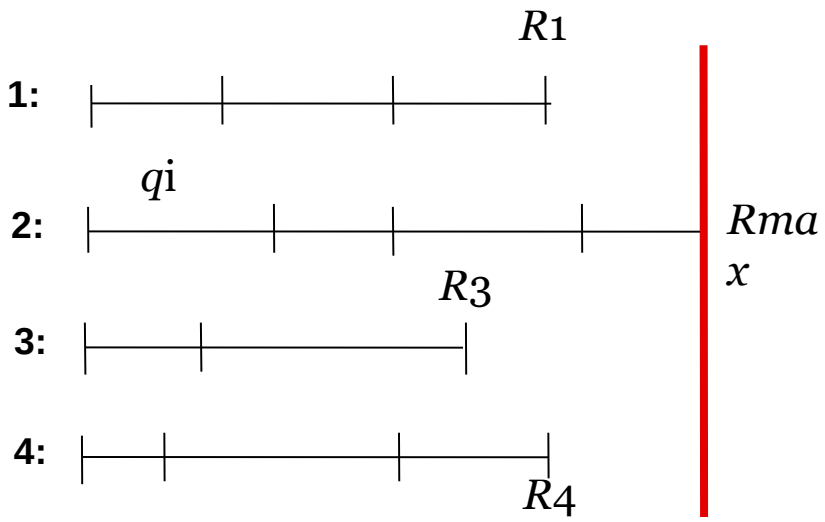

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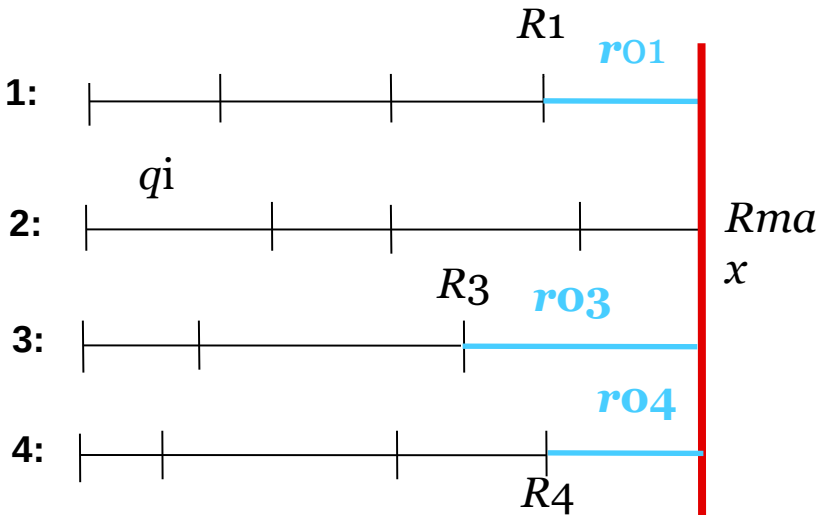

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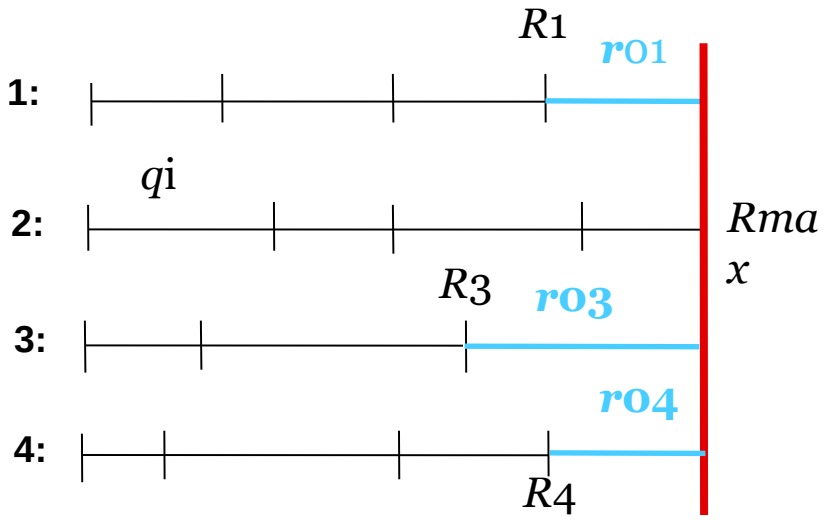

The $r0k$ are the 'dummy' rates (no event) that ensure synchronicity:

$$R_{max} = r_k + r_{0k}$$

$$R_{tot} = \sum_k r_k \leq K R_{max}$$

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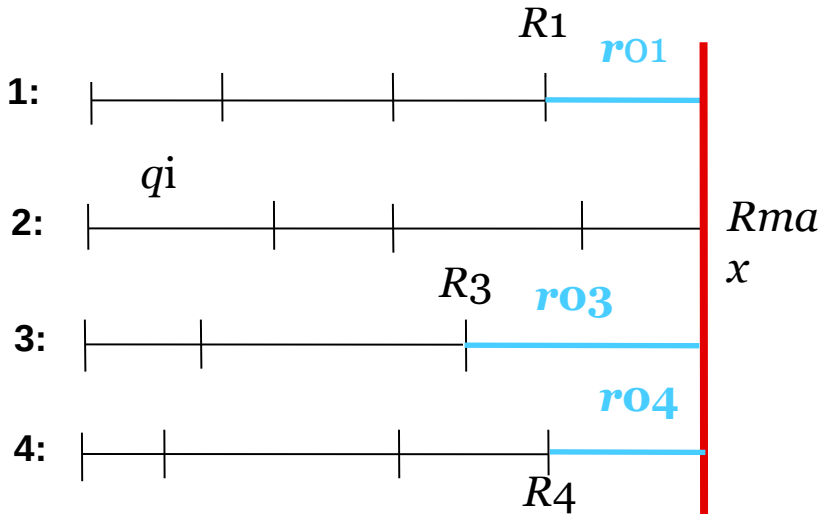

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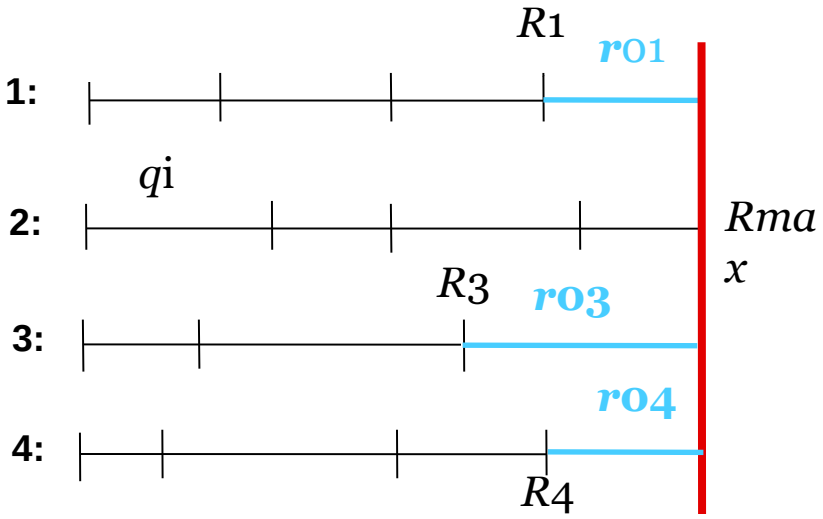

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For optimum scalability, perform domain decomposition subject to the following constraint:

$$\min \left[\sum_k r_{0k} \right]$$

Parallel kMC algorithm

1. Perform spatial decomposition into K domains.
2. Define partial aggregate rates in each Ω_k: $r_k = \sum_i^{n_k} q_{ik}$ $R_{\text{tot}} = \sum_k^{K} r_k$
3. Choose the maximum partial rate as: $R_{\text{max}} = \max_k \{r_k\}$
4. Assign 'null' rates to each Ω_k such that: $r_{k0} = R_{\text{max}} - r_k$
5. Sample event from each subdomain with probability q_{ik}/R_{max} $\delta t_p = -\frac{\ln \xi}{R_{\text{max}}}$
6. Execute event and advance time by

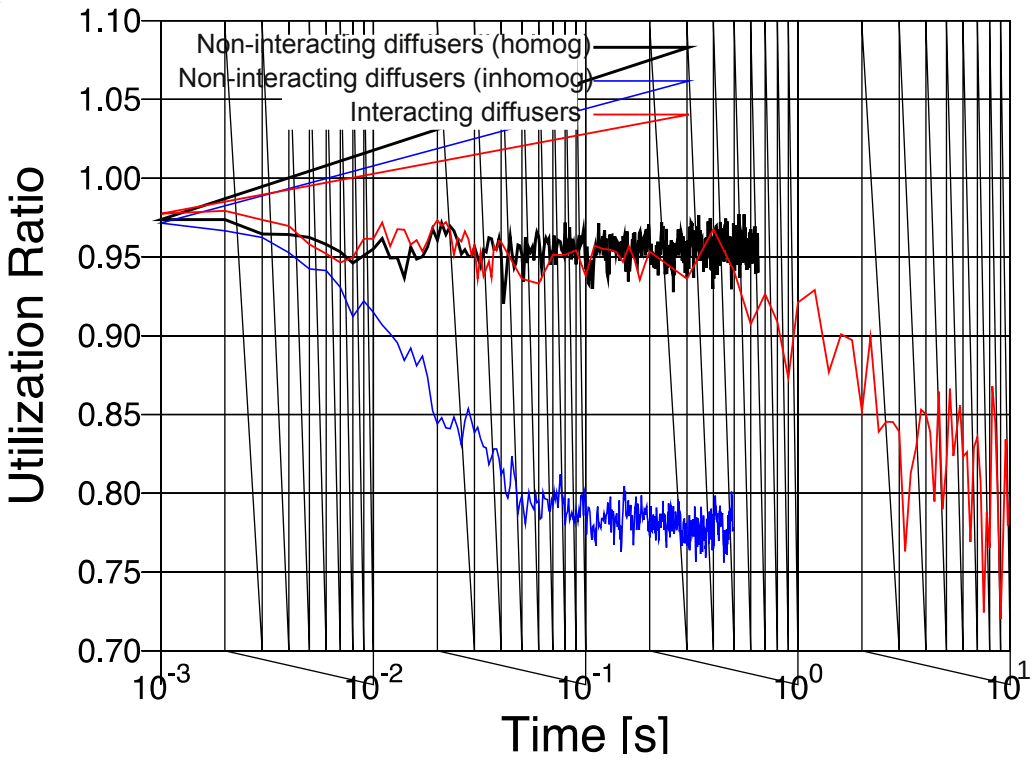
Parallel boost

Utilization Ratio (UR):
probability of not having a null event in a given kMC cycle

$$UR = 1 - \frac{\sum_k r_{k,0}}{KR_{max}}$$

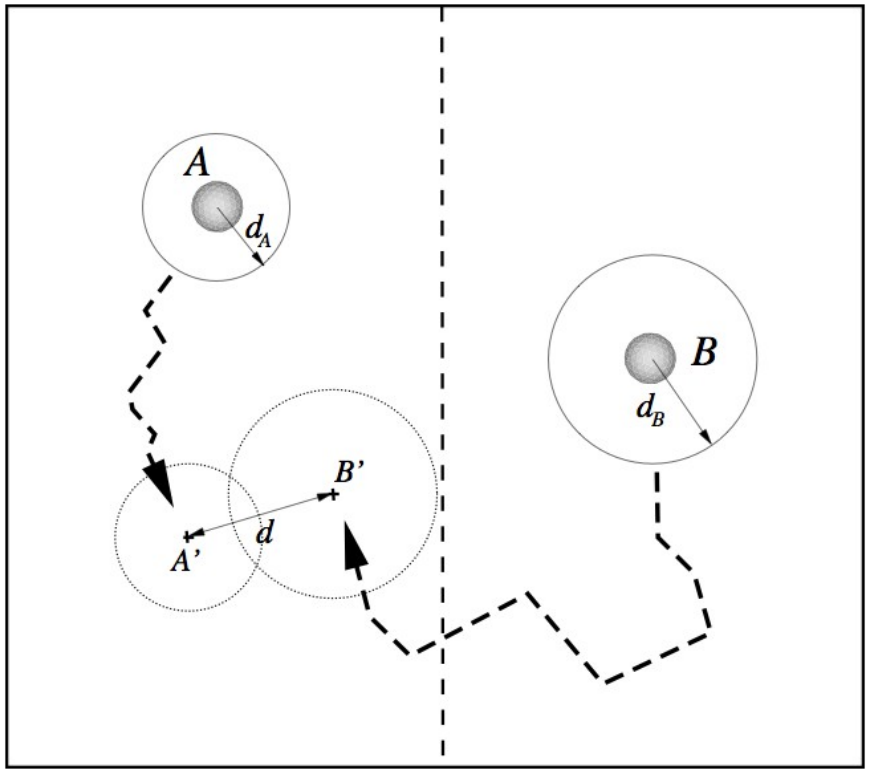
parallel timestep:
proportional to the number of processors *K* and the *UR*

$$dt_p = K \cdot UR \cdot dt_s$$

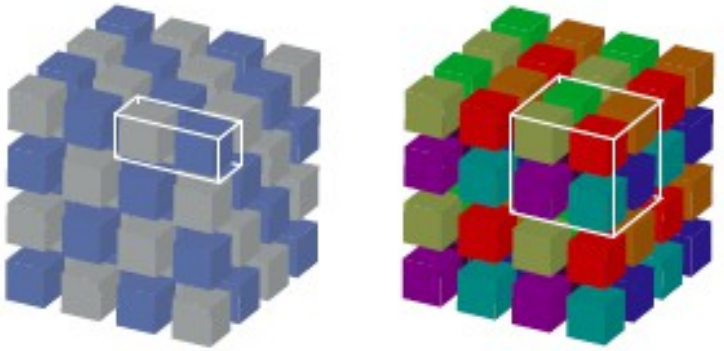


Solution of boundary conflicts via sublattice decomposition

Boundary conflicts appear when mutually-influencing events occur simultaneously on different domains



A simple solution is to use a sublattice decomposition (chess method in 2D)



Amar *et al*. (2004, 2005)

Co-occurring events only on identically-colored subcells

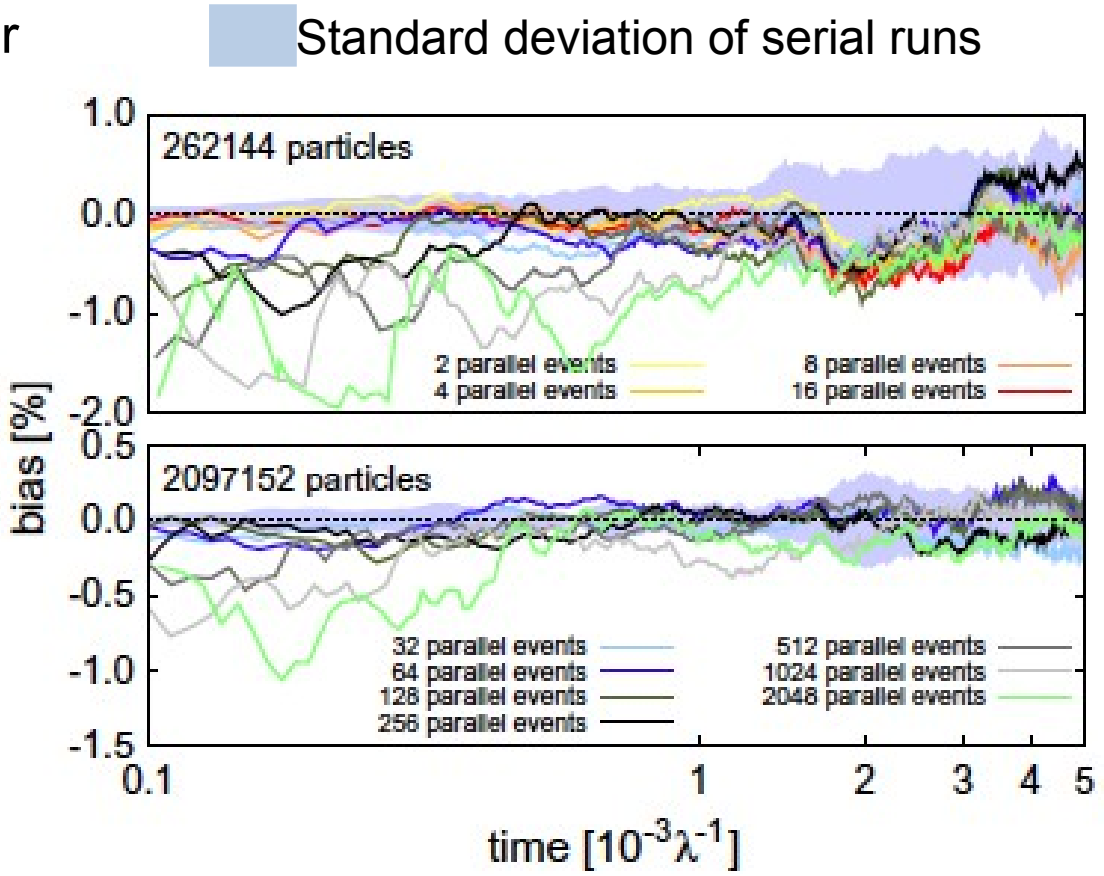
Sublattice decomposition introduces a bias

- Reduced sampling space introduces a systematic error (bias).

$$\text{bias} = \langle m(\sigma_c)\rangle_p - \langle m(\sigma_c)\rangle_s$$

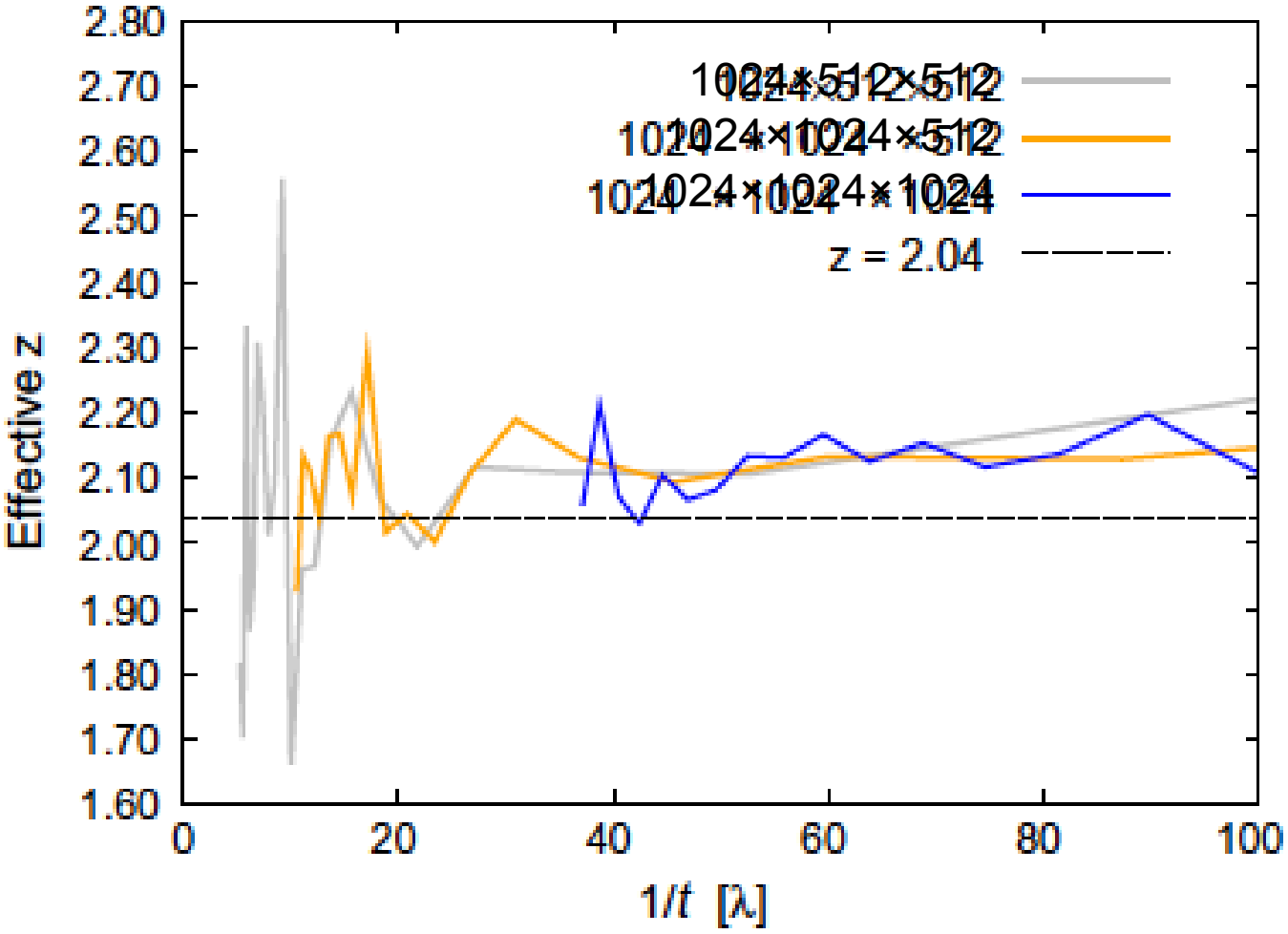
- Bias can be controlled with system size and numbers of processors.

- One must also include intrinsic statistical fluctuations of the parallel runs: $\sigma_b = \sqrt{\sigma_p^2 + \sigma_s^2}$



- We find that σb is always less than the standard deviation of the serial calculations

Calculation of critical exponent z

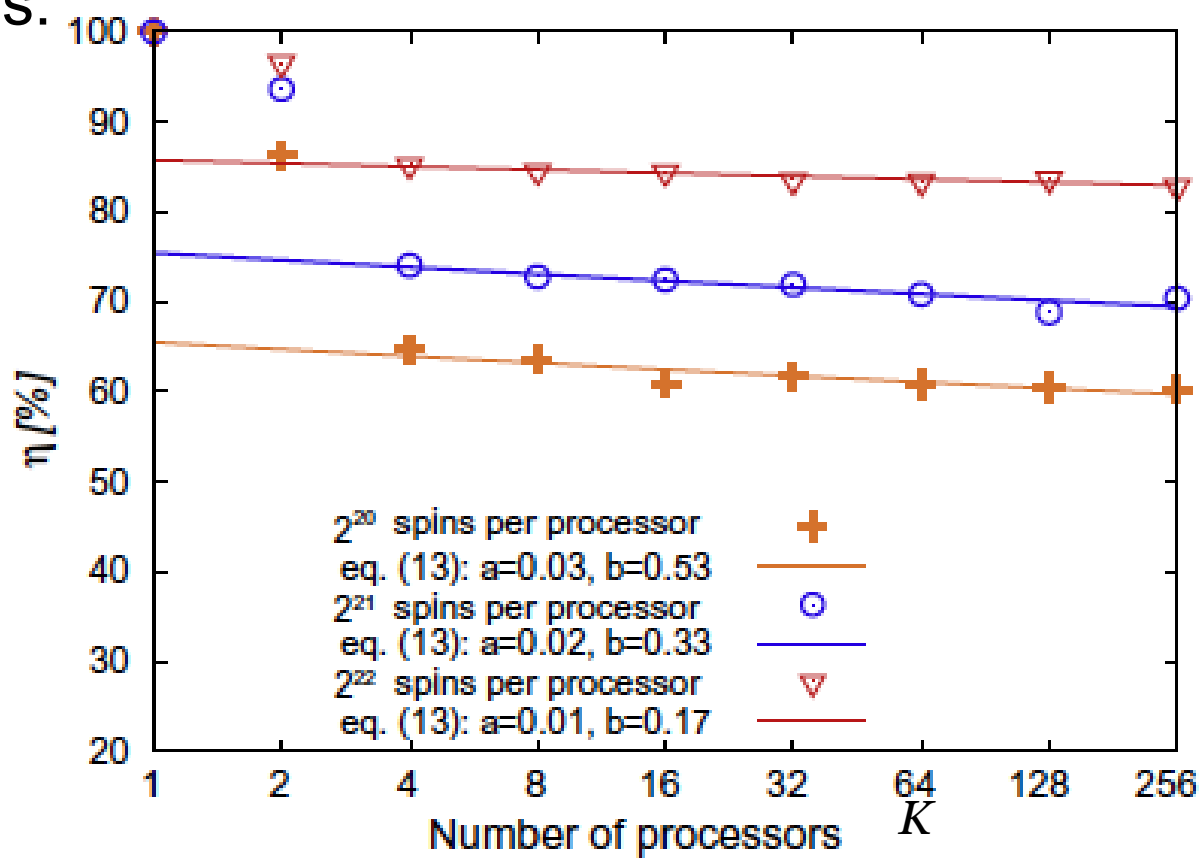


Martinez, Monasterio, Marian, JCP (2010)

Weak scaling of parallel kMC algorithm is good.

Parallel efficiency governed by local MPI calls:

$$\eta = \frac{1}{1 + a \log K + b}$$



Conclusions

· Parallel synchronous kMC algorithm suitable for large systems.

- Resolution of boundary conflicts
- Good scalability
- Controlled sampling errors

· Critical behavior of Ising systems is well reproduced and converged to the state of the art.

· Current and future applications of the method include solid solution precipitation, segregation, and in general situations where large systems are required.