Efficient Method of Simulating with Long-Range Interactions: The Case of Coarsening in the Ising Model

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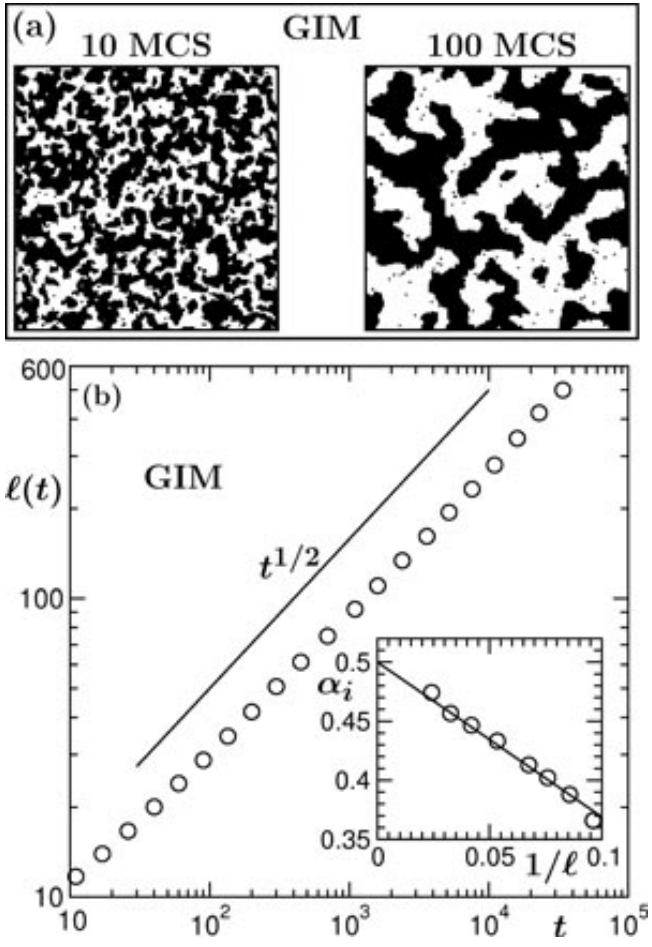
Coarsening

- In coarsening one is interested in the growth of ordered structures when a system is quenched from a "random" high temperature state to a "ordered" low temperature/energy state.
- The driving force is the reduction of energetically unfavored interfaces.
- This process can be quantified by calculating the average "size" $\ell(t)$ of oriented regions for different times during the process.
- Even though the observed structures may be quite complex, $\ell(t)$ is in most cases a simple function of time; typically a power law.



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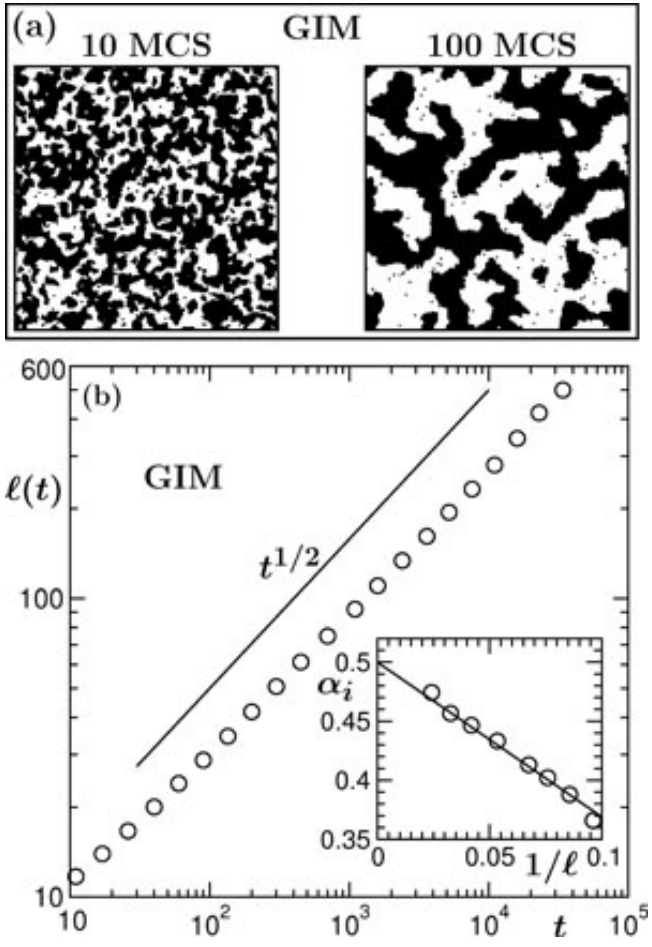

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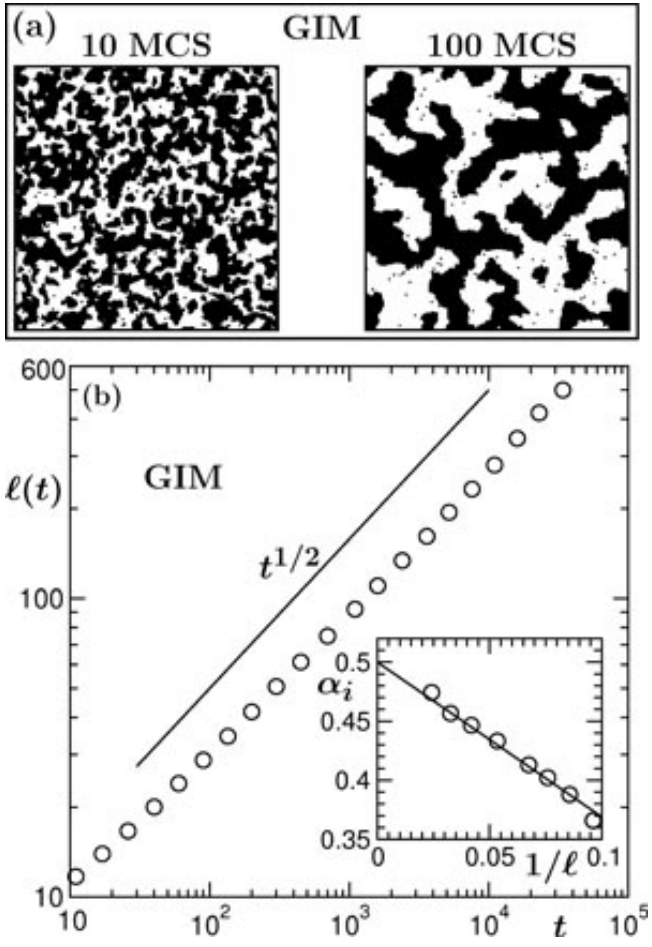

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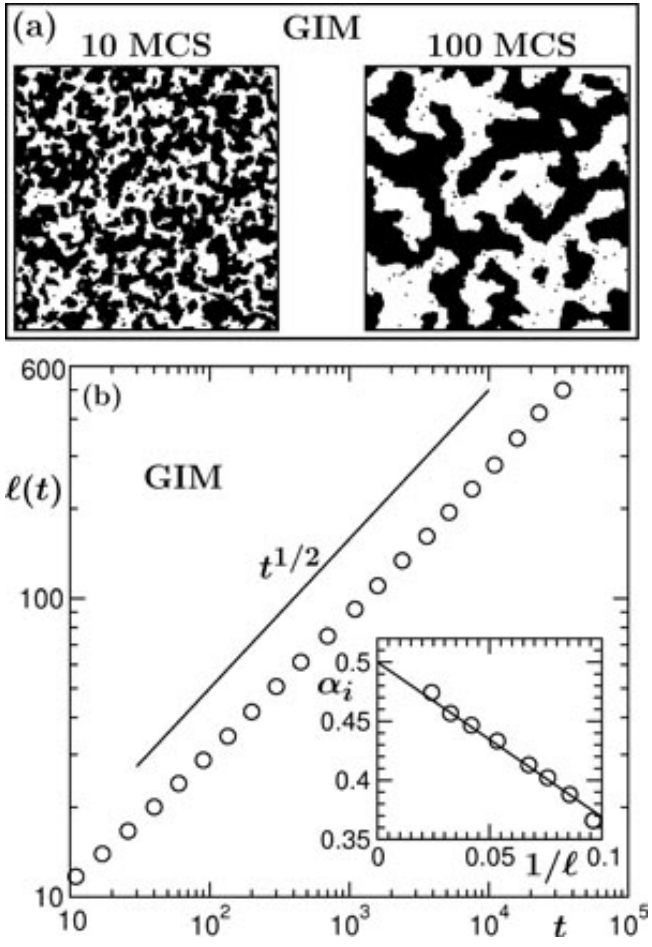

2D Long-Range Ising model

Until now, most of the studies were conducted on short-range interacting systems, because long-range interacting systems were not feasible.

The model considered here now is the long-range 2D Ising model with Hamiltonian

$$H = -\sum_{i \neq j} J(|\mathbf{r}_i - \mathbf{r}_j|) s_i s_j,$$

where

$$J(r) = \frac{1}{r^{d+\sigma}}.$$

In the simulation only local (and thereby "physical") moves are allowed $\rightarrow$ cluster-algorithms cannot be used $\rightarrow$ standard local Metropolis simulation

$\rightarrow$Possible application of long-range Ising model in modelling of the dynamics of neuron activity patterns

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Growth of Lengthscale

For the growth of the characteristic length scale $\ell(t)$ there exists a prediction in dependence on the value of σ in $J(r)$[1]:

$$\ell(t) \propto \begin{cases} t^{\frac{1}{1+\sigma}} & \sigma < 1 \\ (t \ln(t))^{\frac{1}{2}} & \sigma \equiv 1 \\ t^{\frac{1}{2}} & \sigma > 1 \end{cases}$$

Previous studies of this problem for the long-range Ising model relied on a cut-off ($r_c = 2.5^{6/(2+\sigma)}$) for the long-range interactions to make the problem tractable.
This, however, gives the short-range behaviour of[2]

$$\ell(t) \propto t^{1/2}$$

independent of σ.

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Calculation of Local Energy Change

Short-Range Ising Model:

$$\Delta E(x,y) = -2S(x,y)J(\underbrace{S(x+1,y)+S(x,y+1)+S(x-1,y)+S(x,y-1)}_{\text{A Number}})$$

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Basic Idea

Using the *pseudo heatbath* $h(x, y)$, the local energy change can now be written as

$$\Delta E(x, y) = -2S(x, y)h(x, y).$$

But how can we efficiently calculate h when using long-range interactions?

Idea: Store *pseudo heatbath* $h(x, y)$ for every spin.

During the quench only a subset of the system changes
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Algorithm

Start the simulation with an aligned lattice and calculate the starting *pseudo heatbath* $h(x, y) = h_0 \forall x, y$.

Set $h(x, y) = h_0 \forall (x, y)$

Then flip 50% of spins to arrive at random start configuration.
Whenever a spin flipped, update the heatbath of **all** other spins.

In the actual simulation then:

- Choose random spin with coordinates (x, y)
- Calculate $\Delta E(x, y) = -2S(x, y)h(x, y)$
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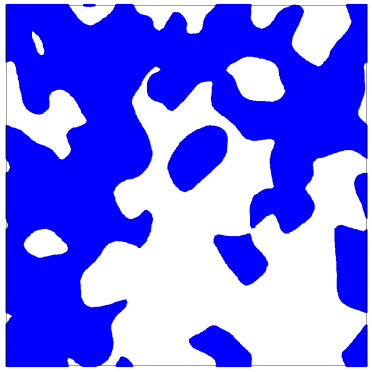
Runtime for different σ

Table: Table of clocks needed for a simulation of length $t = 2500$ (MCS) and $L = 128$ in both algorithm.

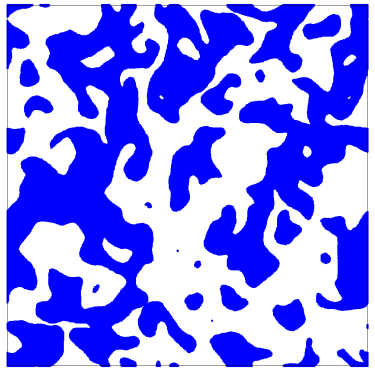
σ	Clocks New Algorithm (10^6)	Clocks Old Algorithm (10^6)
0.25	7.5 ± 0.1	1382 ± 4
0.50	8.3 ± 0.2	1386 ± 7
0.75	10.4 ± 0.5	1398 ± 6
1.00	13.2 ± 0.8	1403 ± 6
1.50	22.8 ± 1.7	1461 ± 14

Speed up of a factor of ≈ 180!

Snapshots of Evolution



(a) $\sigma = 0.5$
$t = 100$ (MCS)



(b) $\sigma = 1.0$
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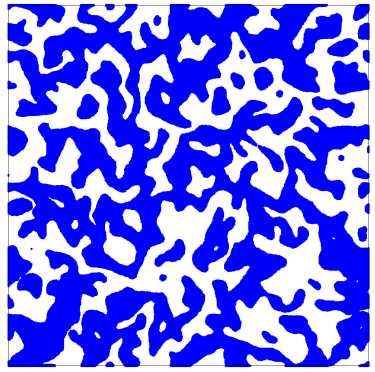

(c) $\sigma = 1.5$
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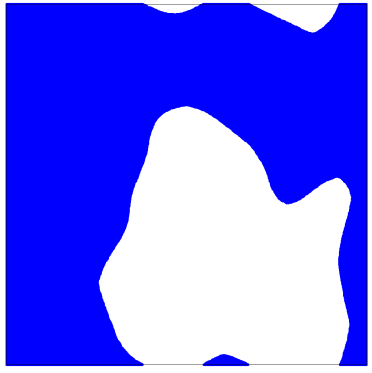
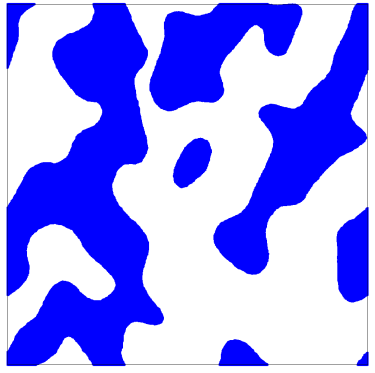


(d) $\sigma = 0.5$
$t = 400$ (MCS)



(e) $\sigma = 1.0$
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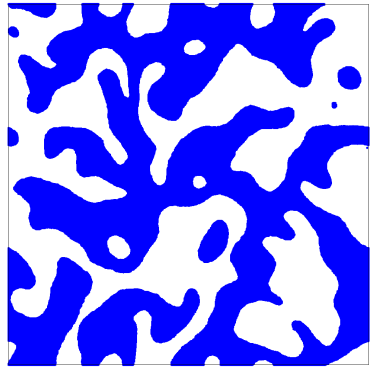
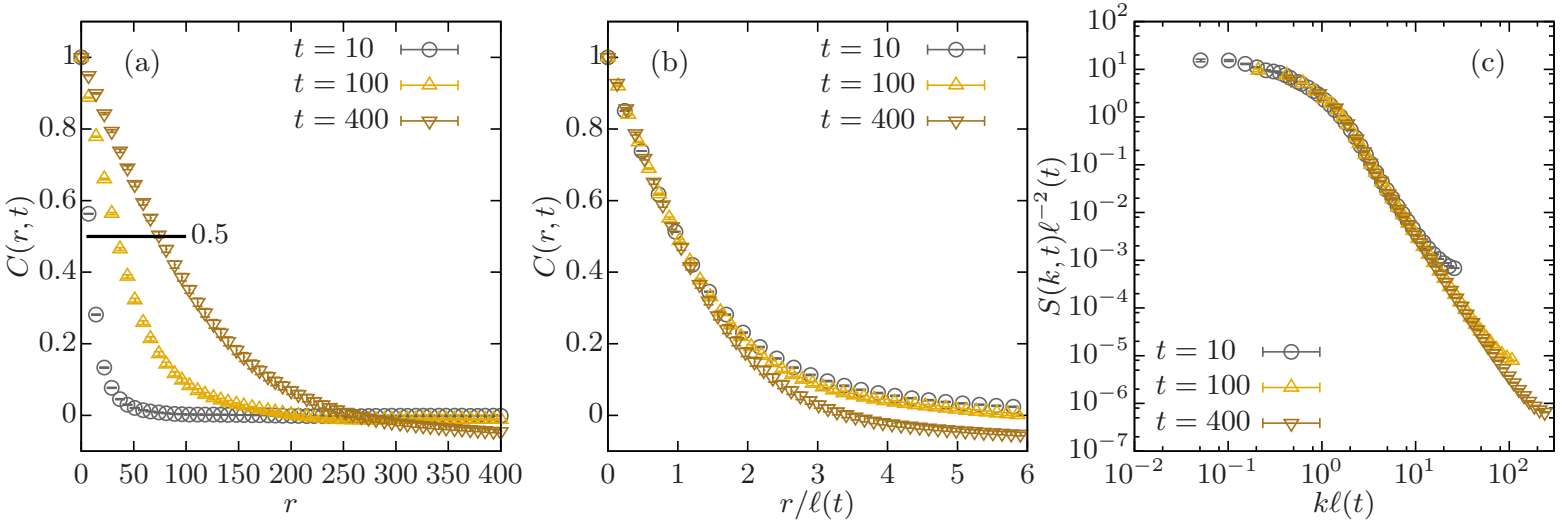


(f) $\sigma = 1.5$
$t = 400$ (MCS)

Correlation Function and Structure Factor - for different times

$$C(r,t) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle,\ S(k,t) = \int dr C(r,t) e^{ikr}$$

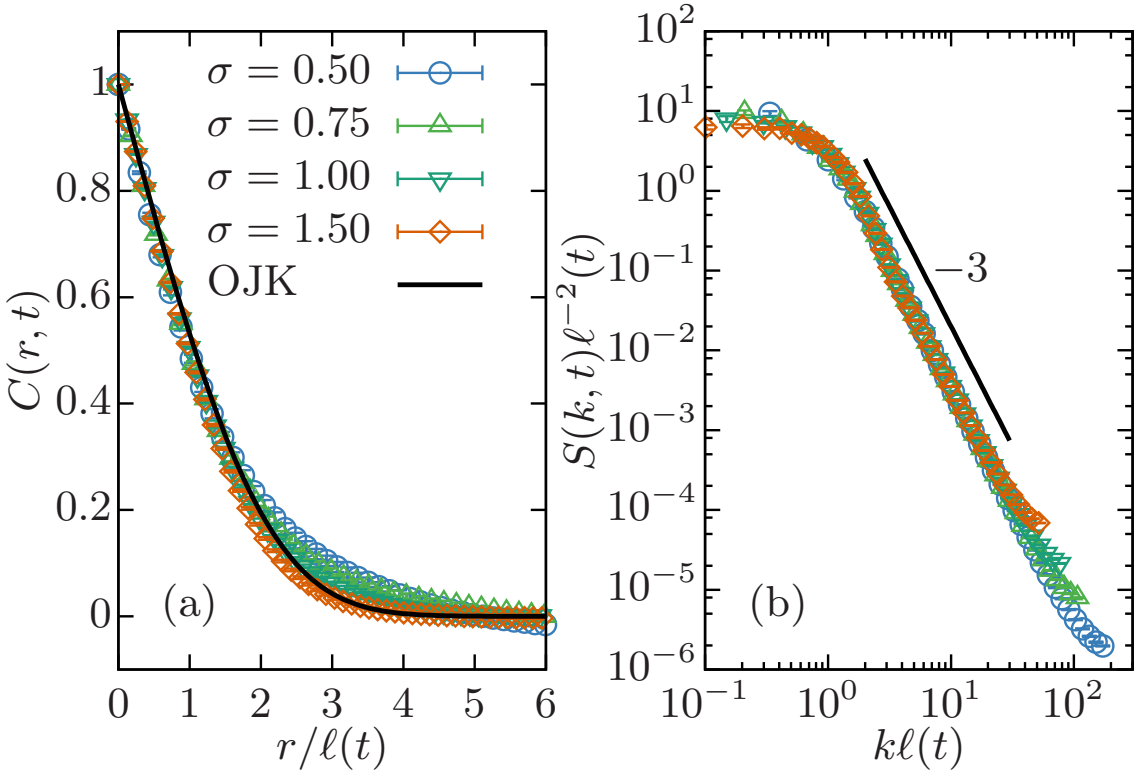


Extract characteristic length from intersection of $C(r,t)$ with 0.5
Here the graphs have constant $\sigma = 0.75$.

Correlation Function and Structure Factor - for different σ

OJK: $C(r,t) = \frac{2}{\pi}\sin^{-1}(e^{-r^2/\ell(t)^2})$

Porod's law: $S(k,t) \sim k^{-(d+1)}$



With constant time $t = 100$

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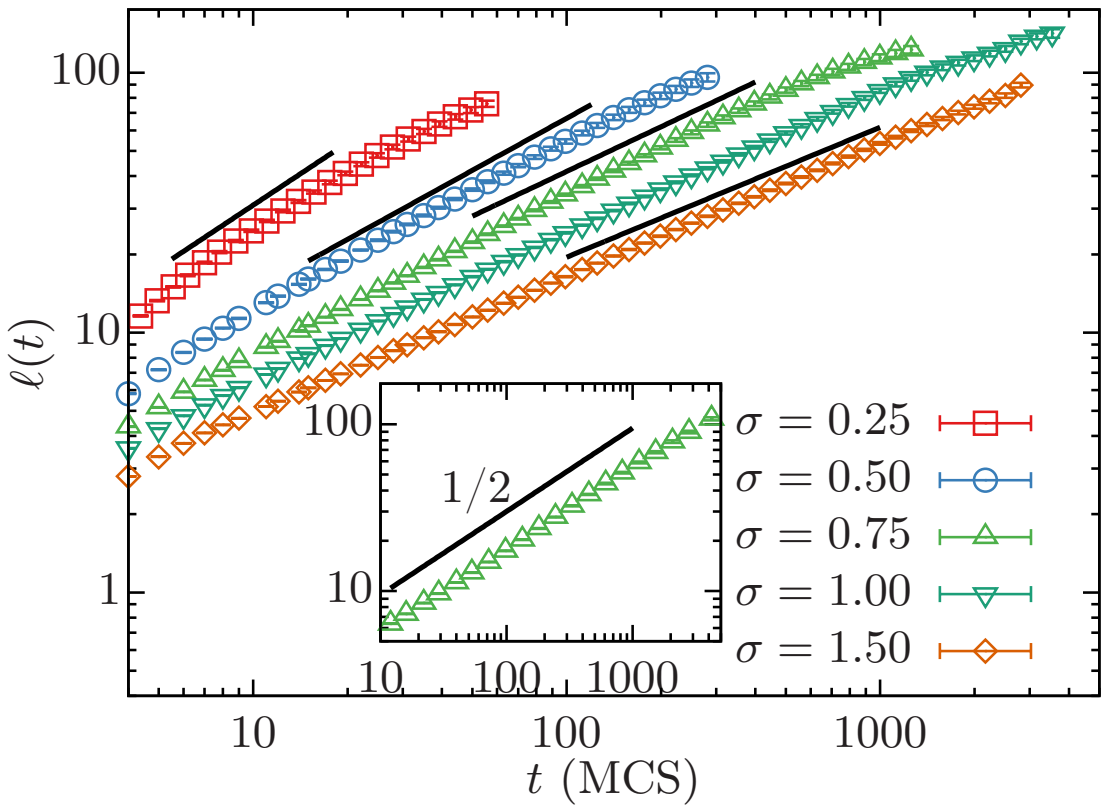
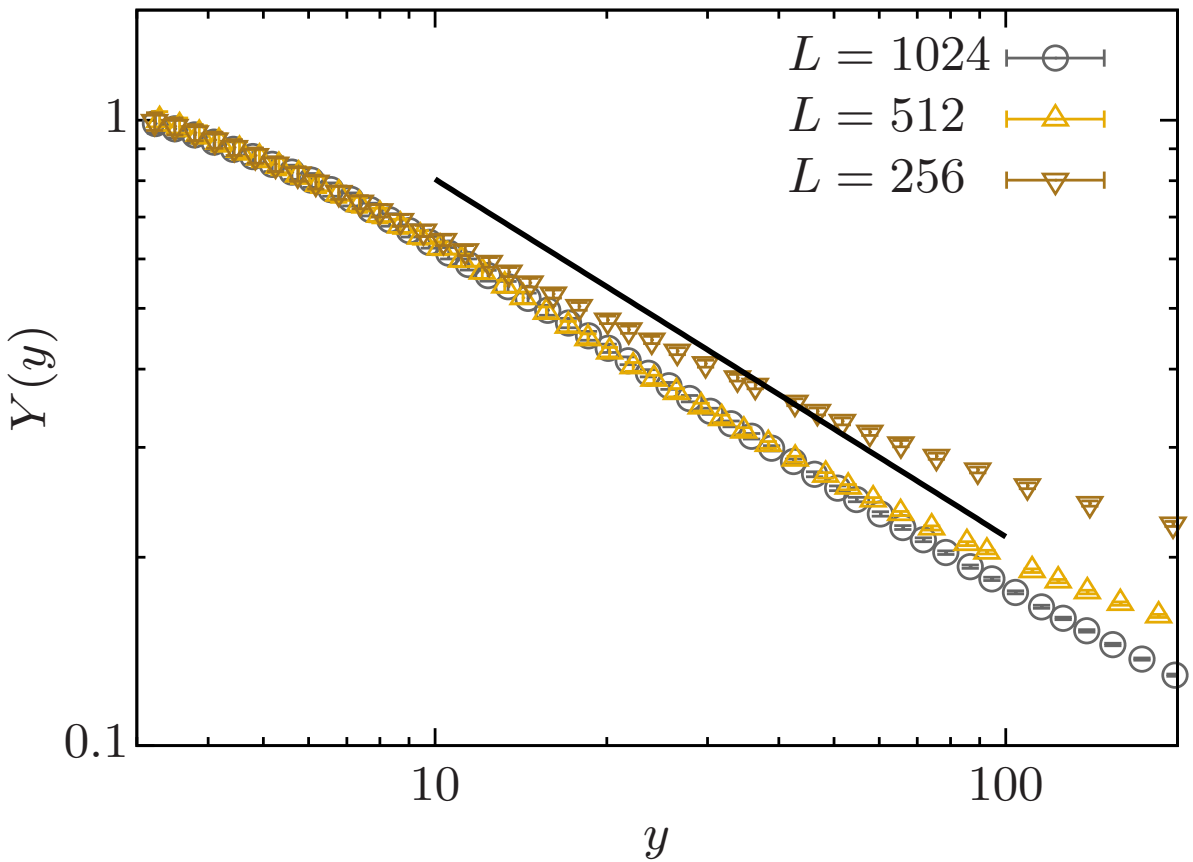


In inset result with cut-off $r_c = 2.5^{6/(2+\sigma)}$ and $\sigma = 0.75$

Finite Size Scaling

$$\ell(t) = \ell_0 + A(t - t_0)^{\frac{1}{1+\sigma}} \Rightarrow Y(y) = \frac{\ell(t)}{\ell_{\max}},\ y = f_s \frac{(\ell_{\max} - \ell_0)^{1/(1+\sigma)}}{t - t_0}$$



With $\sigma = 0.75$

Concluding Remarks

- First conformation of theoretical prediction of

$$\ell(t) = \begin{cases} t^{\frac{1}{1+\sigma}} & \sigma < 1 \\ (t \ln(t))^{\frac{1}{2}} & \sigma \equiv 1 \\ t^{\frac{1}{2}} & \sigma > 1 \end{cases}$$

  by using the full potential $J(r) = (r^{(d+\sigma)})^{-1}$ instead of a cut-off
- Introduction of (too small) cut-off changes the dynamics of the model to be effectively short-ranged
- $\rightarrow$ the use of the full potential is made possible by the introduction of a new way of looking at the local energy change calculation
- Adaptation to models with "discrete" states quite "straight-forward", e.g. q-state Potts model or q-state Clock model

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