Dynamical Scaling Laws During Collapse of a Polymer : lattice vs off-lattice

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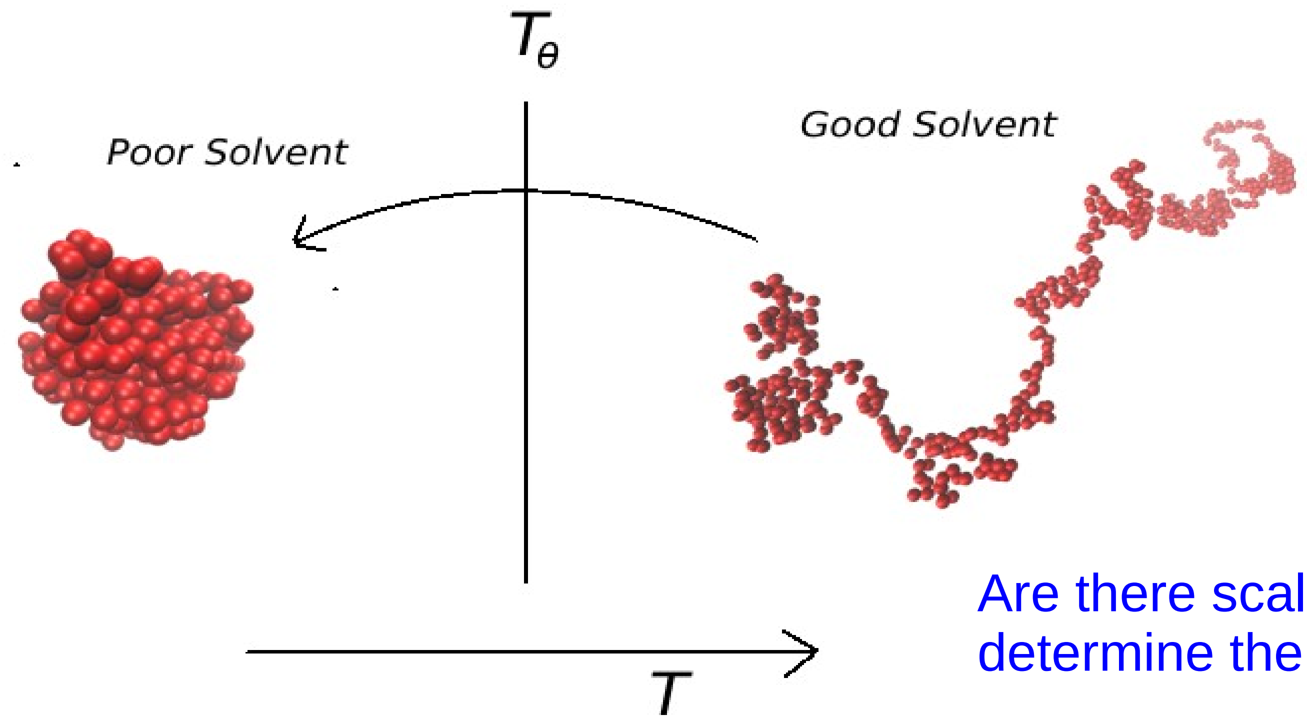
Introduction



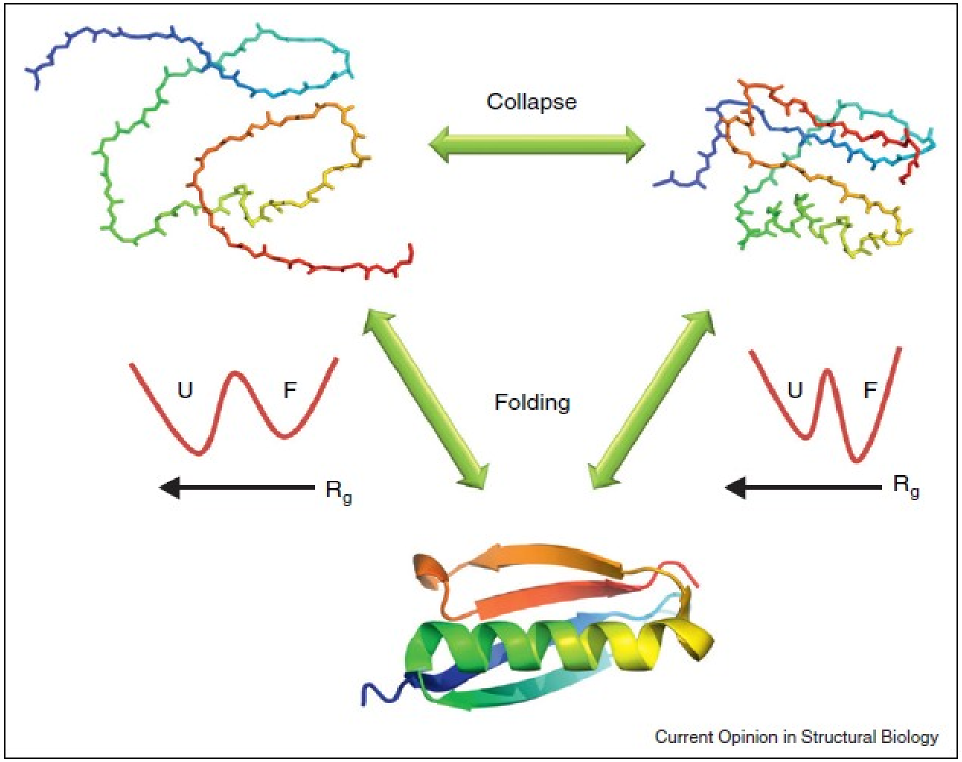
Are there scaling laws that determine the dynamics ?

Temperature quench has been used extensively to study the *phase ordering* in ferromagnets as well for the kinetics of phase separation in solids and fluids

A. J. Bray, Adv. Phys., (2002)

Motivation

Connection with the folding process of protein ???



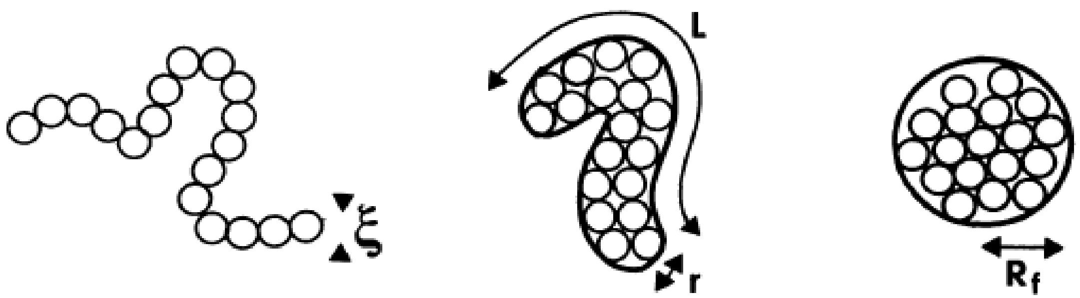
G. Haran, Curr. Opin. Struct. Biol. **22**, 14 (2012)

Collapse precedes or occurs simulataneously with the folding of protein to its native structure

Simulations: C.J. Camacho and D. Thirumalai, PNAS **90**, 6369 (1993).

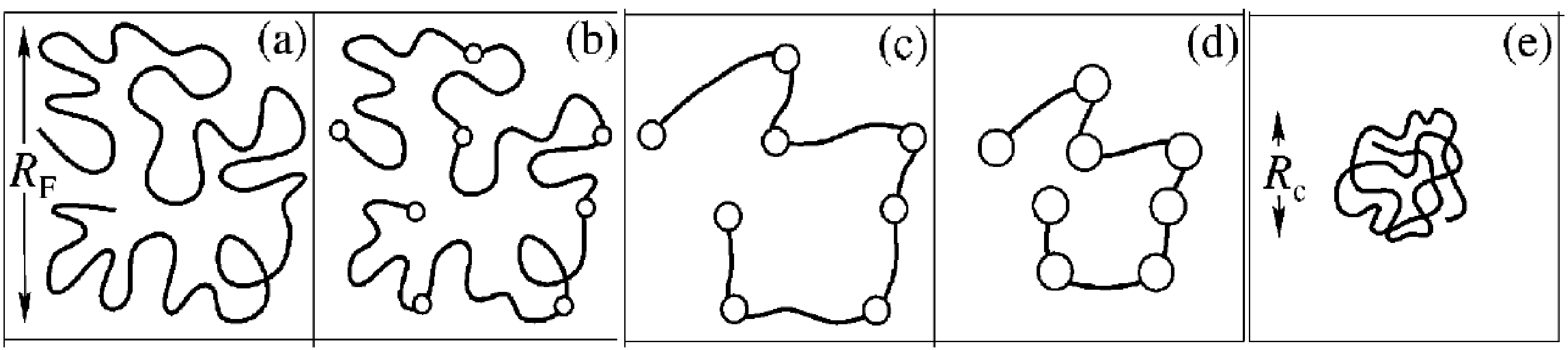
Experiments: B. Schuler, E.A. Lipman, and W.A. Eaton, Nature **419**, 743 (2002).

Phenomenological theory of Collapse



De Gennes' sausage model (1985)

“pear-necklace”



Rapid formation of primary clusters

Coarsening of clusters

Rearrangements to form a compact globule

A.Halperin and P.M.Goldbart, *Phys. Rev. E* **61**, 565 (2000)

Scaling to look for

1. Scaling of the collapse time: $\tau_c \sim N^z$

2. Scaling of the cluster growth: $C_s(t) \sim t^{\alpha_c}$

3. Aging and related scaling: $C(t, t_w) = A x^{-\lambda_c}; x = C_s(t) / C_s(t_w)$

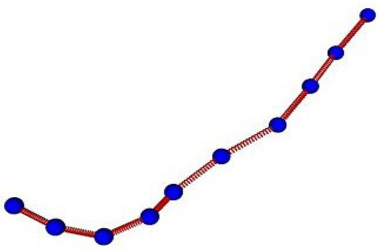
$$C(t, t_w) = \langle O_i(t) . O_i(t_w) \rangle - \langle O_i(t) \rangle . \langle O_i(t_w) \rangle$$

Two-time correlation function

Off-lattice Model

non-bonded interaction

$$E_{nb}(r) = E_{LJ}(r) - E_{LJ}(r_c); \quad r \le r_c$$
$$= 0 \quad ; \quad r > r_c$$
$$E_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$



bead spring model

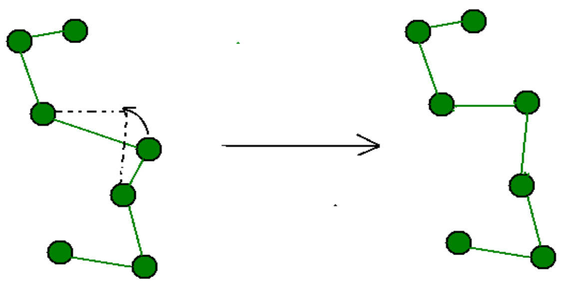
$$E_b(r) = \frac{-K}{2} R^2 \ln\left[1 - \left(\frac{r - r_0}{R}\right)^2\right]$$

FENE bonds

$$K = 40, \quad r_0 = 0.7, \quad \sigma = r_0/2^{1/6}, R = 0.3$$

Monte Carlo simulations with Metropolis algorithm

$$T_h = 10\,\epsilon/k_B; T_q = 1.0\,\epsilon/k_B$$



single-monomer moves

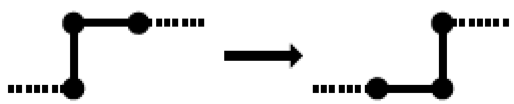
S. Majumder and W. Janke, *EPL* **110**, 58001 (2015)
S. Majumder, J. Zierenberg and W. Janke, Leipzig preprint

Lattice Model

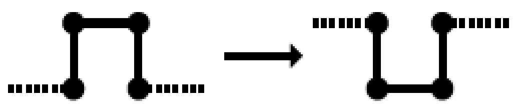
Hamiltonian of a interactive self avoiding walk:

$$H = -\frac{1}{2} \sum_{i \neq j, j \pm 1} w(r_{ij}) \qquad w(r_{ij}) = \begin{cases} 1, & r_{ij} = 1 \\ 0, & r_{ij} \neq 1 \end{cases}$$

Monte Carlo moves (local updates)

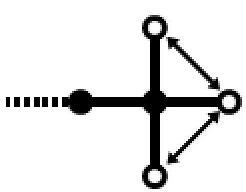


Corner moves



Crankshaft moves

Metropolis algorithm



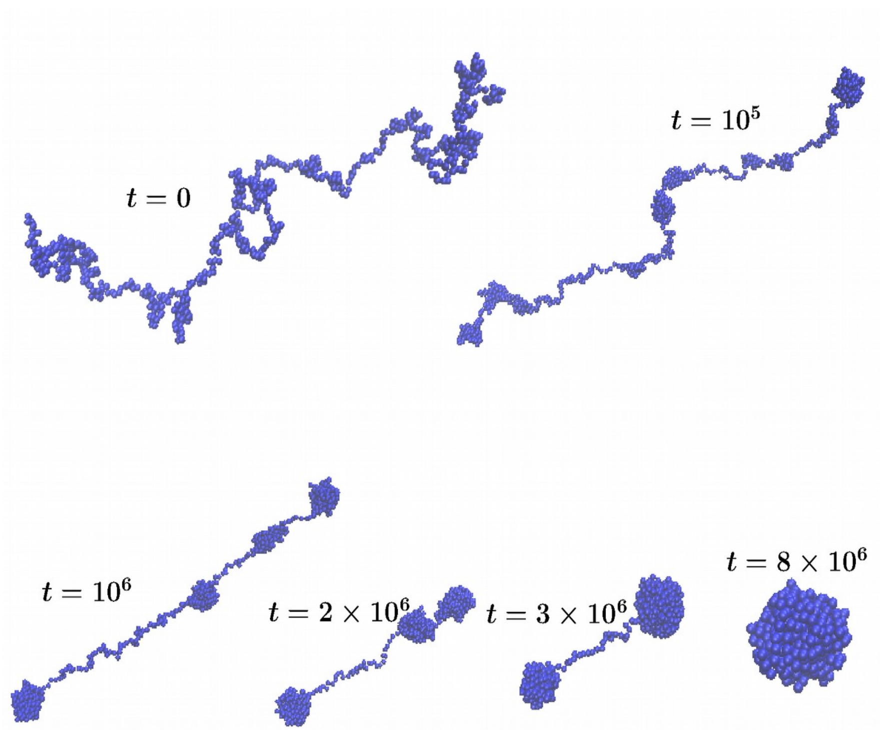
End moves

$$T_h = 10\,\epsilon / k_B ; T_q = 1.0\,\epsilon / k_B$$

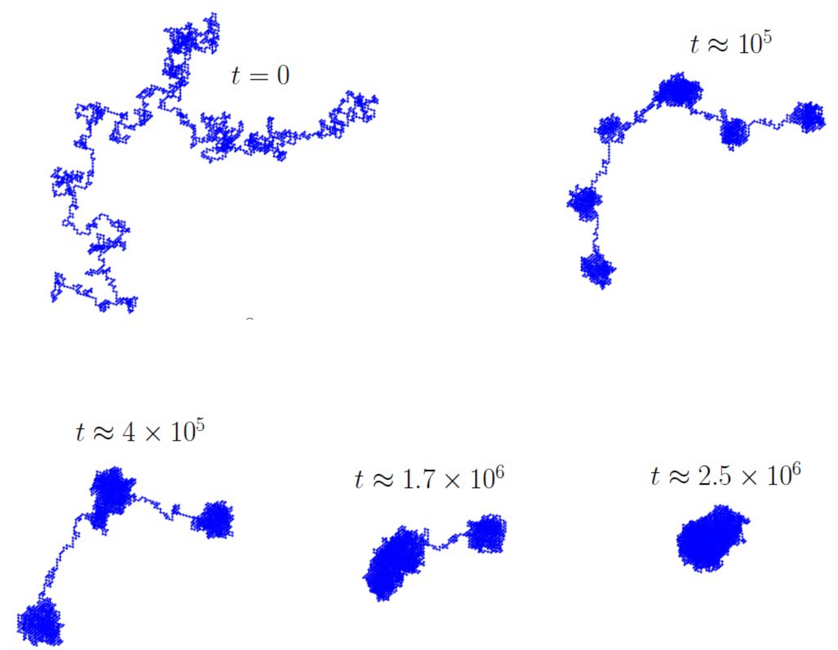
Results

Time evolution after the quench

Off-lattice



Lattice



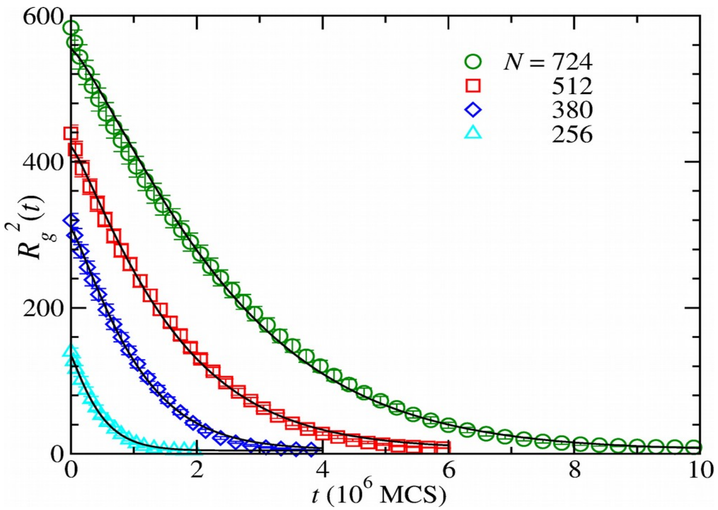
consistent with the pearl-necklace picture

S. Majumder and W. Janke,
J. Phys.: Conf. Ser. **750**, 012020 (2016)

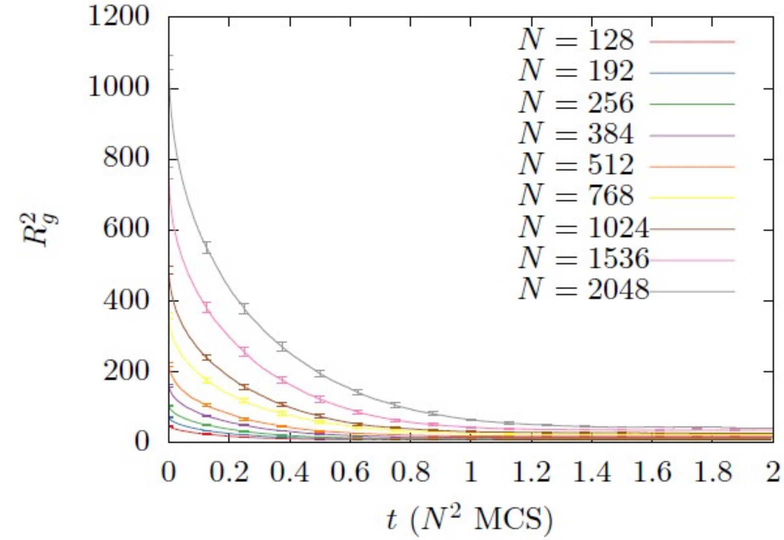
H. Christiansen, S. Majumder and W. Janke, in preparation (2016)

Scaling of Collapse time

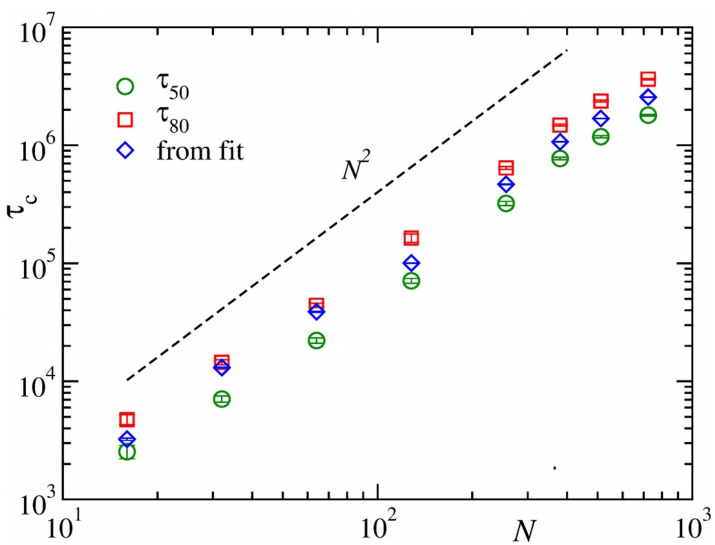
Off-lattice



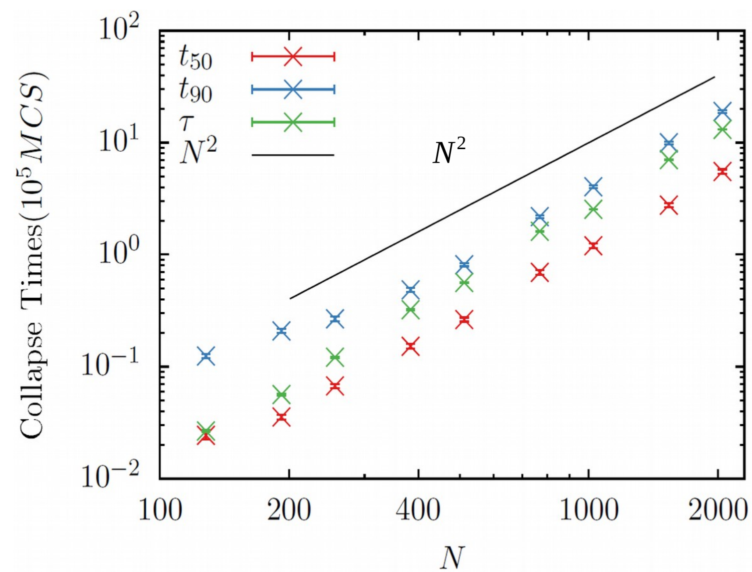
Lattice



$$R_g^2 = b_0 + b_1 \exp[(-t/\tau_c)^\beta]$$



Apparently consistent with Rouse scaling

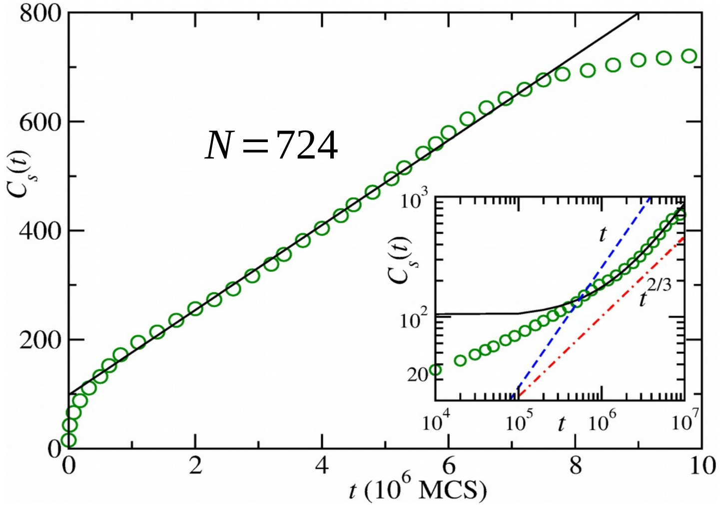


S. Majumder, J. Zierenberg and W. Janke, Leipzig preprint (2016)

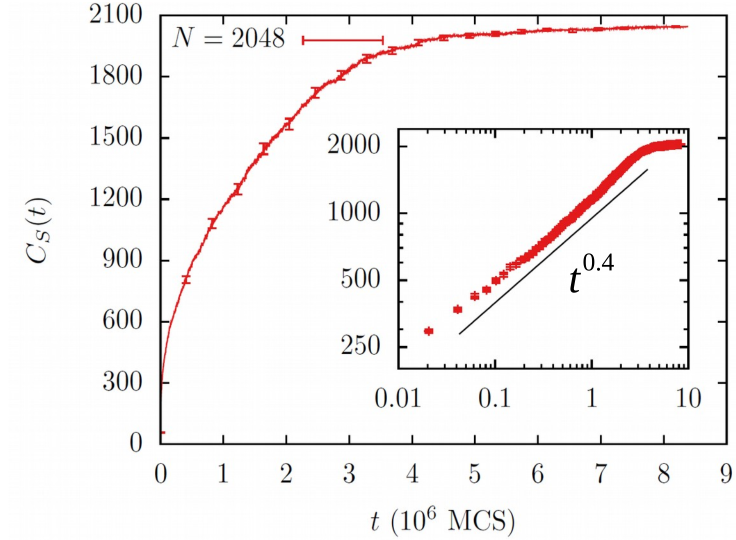
H. Christiansen, S. Majumder and W. Janke, in preparation (2016)

Scaling of Cluster Growth

Off-lattice

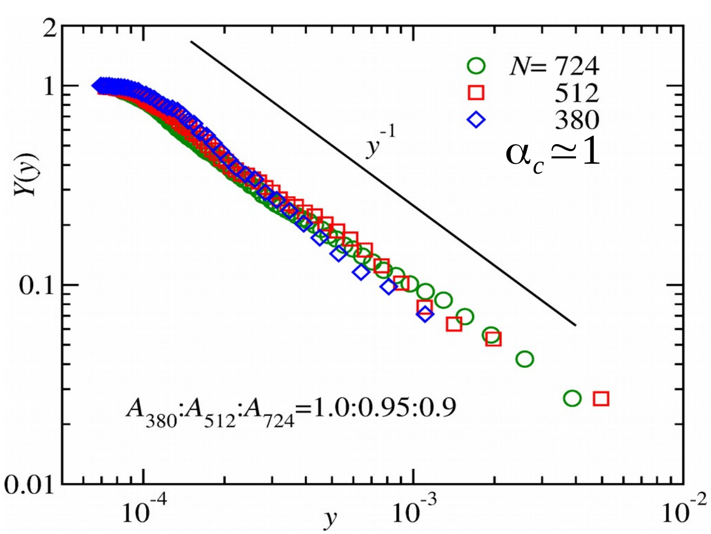


Lattice



$$C_s(t) = C_0 + A_N t^{\alpha}$$

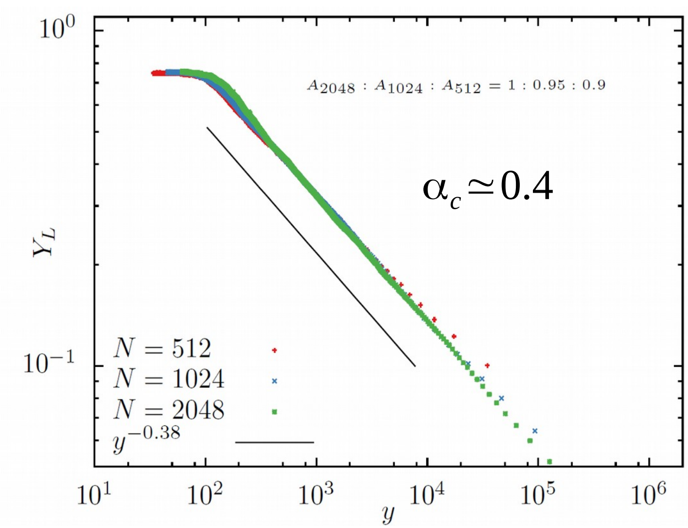
Finite-Size Scaling Analysis



Linear Growth in the coarsening phase

Finite-Size Scaling Analysis

non-linear growth



S. Majumder and W. Janke, *EPL* **110**, 58001 (2015)

H. Christiansen, S. Majumder and W. Janke, in preparation (2016)

Aging and related Scaling

$$C(t,t_w)=\langle O_i(t).O_i(t_w)\rangle-\langle O_i(t)\rangle.\langle O_i(t_w)\rangle ; t>t_w$$

t_w → waiting time

For coarsening dynamics this shows scaling w.r.t the growing lengthscale

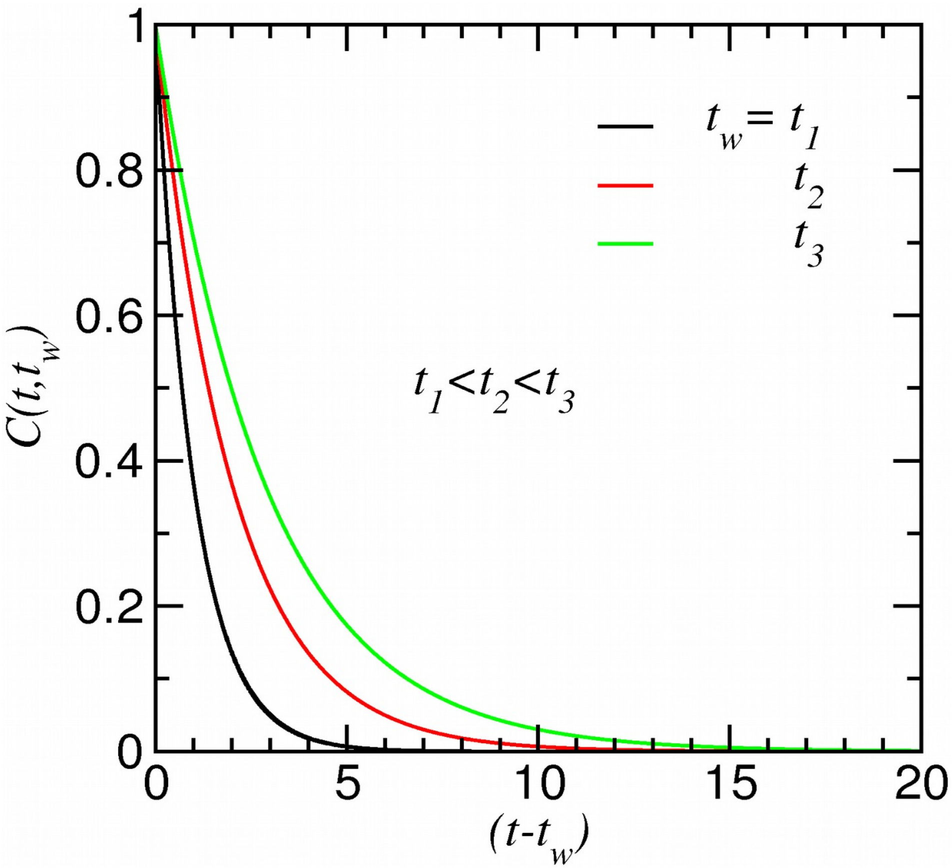
$$C(t,t_w)\sim\left(\frac{\ell}{\ell_w}\right)^{-\lambda}$$

Fisher-Huse (FH) bound: $d/2\leq\lambda\leq d$

For a collapsing polymer

$O_i=\pm 1$ whether the monomer belongs to cluster

An analog to the density-density autocorrelation function



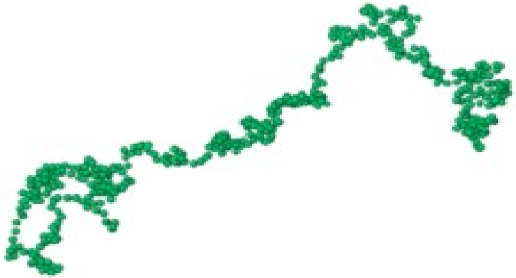
waiting time behavior

S. Majumder and W. Janke, *Phys. Rev. E* **93**, 032506 (2016)

Aging and related Scaling

$$C(t,t_w)=Ax^{-\lambda_c};\, x=C_s(t)/C_s(t_w)$$

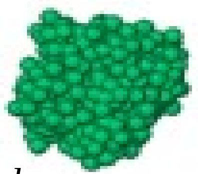
$$C(t,t_w)\approx\rho(t)\rho(t_w)$$



$$R_g \sim C_s^{\nu} \Longrightarrow \rho(t_w)=C_s/C_s^{d\nu}$$

Case1:

$$C(t,t_w)\approx 1.(C_s/C_s^{d\nu})=C_s^{-(\nu d-1)}$$



Case2: $\rho(t)=\rho(t_w)=C_s/C_s^{d\nu}$

$$C(t,t_w)\approx(C_s/C_s^{d\nu}).(C_s/C_s^{d\nu})=C_s^{-2(\nu d-1)}$$

$$R_g \sim C_s^{1/d} \Longrightarrow \rho(t)=1$$

$$(\nu d-1)\le\lambda_c\le 2(\nu d-1)$$

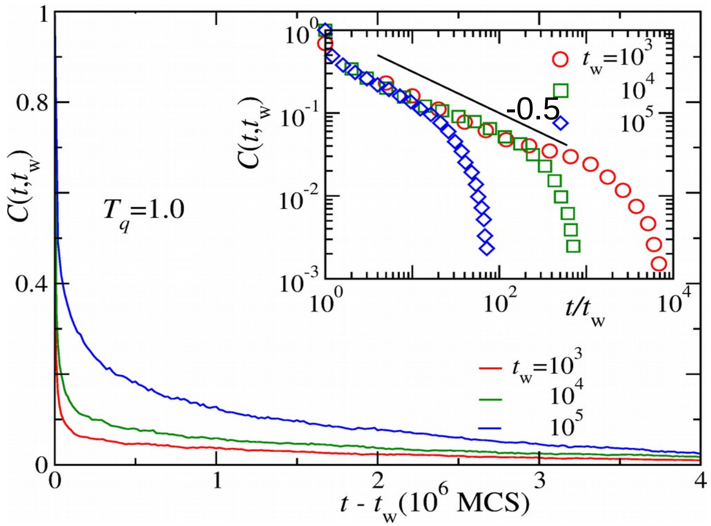
Inserting precise numerical estimate $\nu=\nu_F=0.587597$

$$0.762791\le\lambda_c\le 1.525528$$

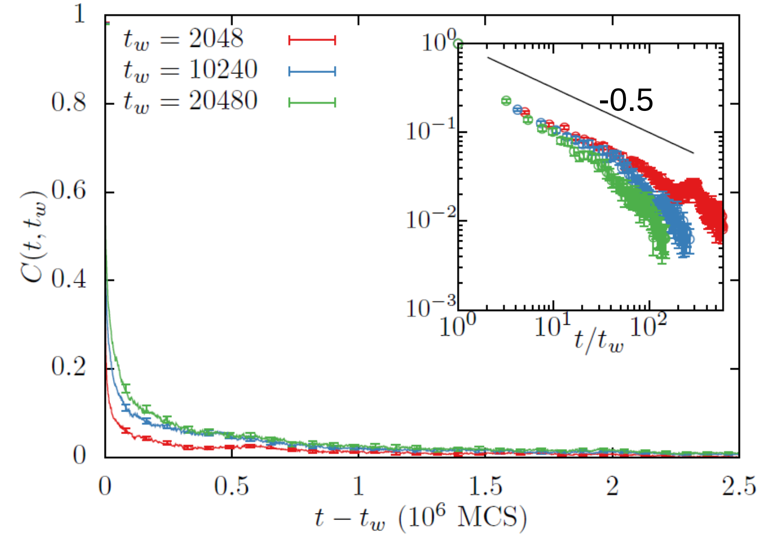
S. Majumder and W. Janke, *Phys. Rev. E* **93**, 032506 (2016)

Aging and related Scaling

Off-lattice

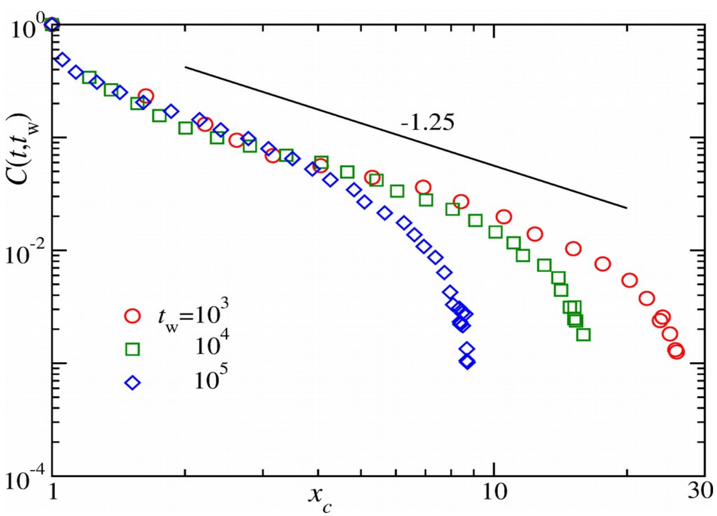


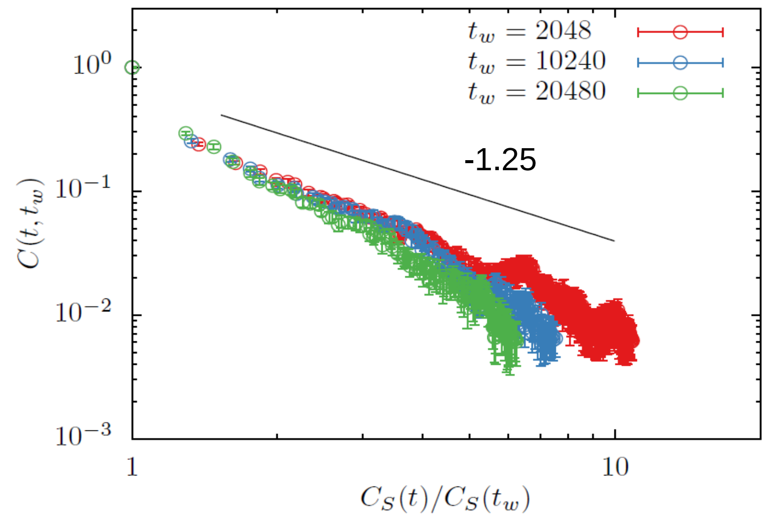
Lattice



Evidence of aging

Scaling of the autocorrelation functions apparently are the same





S. Majumder and W. Janke, *Phys. Rev. E* **93**, 032506 (2016)

H. Christiansen, S. Majumder and W. Janke, in preparation (2016)

Conclusions

1. The dynamics is faster for the continuum model with power-law scaling of the collpase time in both the cases

2. Scaling of the cluster growth seem to be different in the models compared

3. Aging and related scaling found to be universal with both the models following the same theoretical bound

Acknowledgements

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Please visit the poster by **Henrik** for more details