Convergence estimation of flat-histogram algorithms based on simulation results

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Flat-histogram algorithms

Multi-canonical Monte Carlo, Wang-Landau-type algorithms

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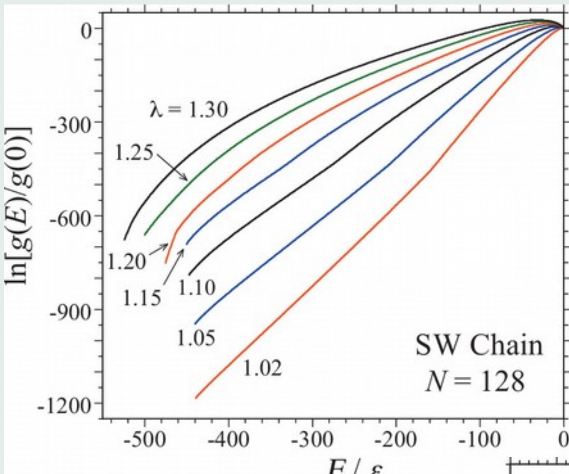

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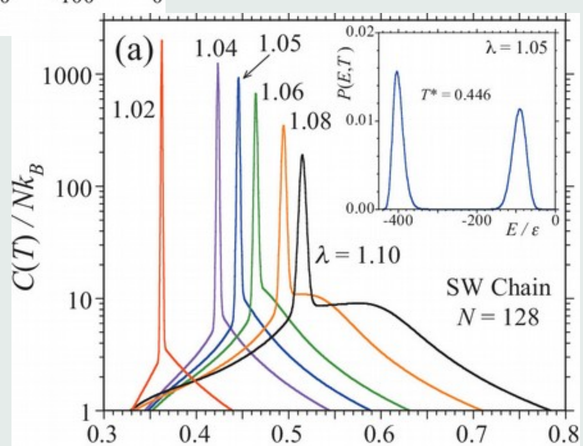

*) M.P. Taylor, W. Paul, K. Binder. JCP 131.11 (2009)

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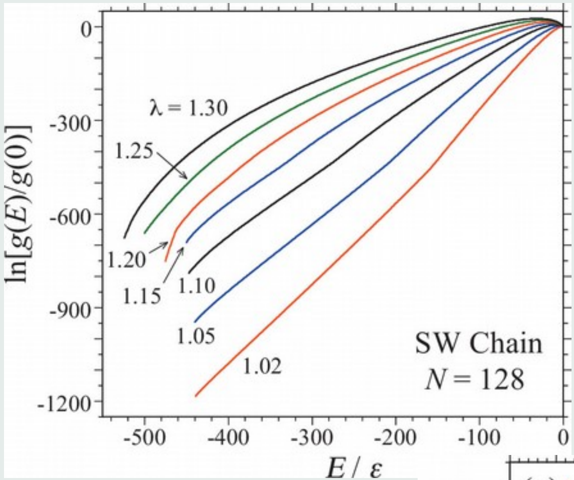

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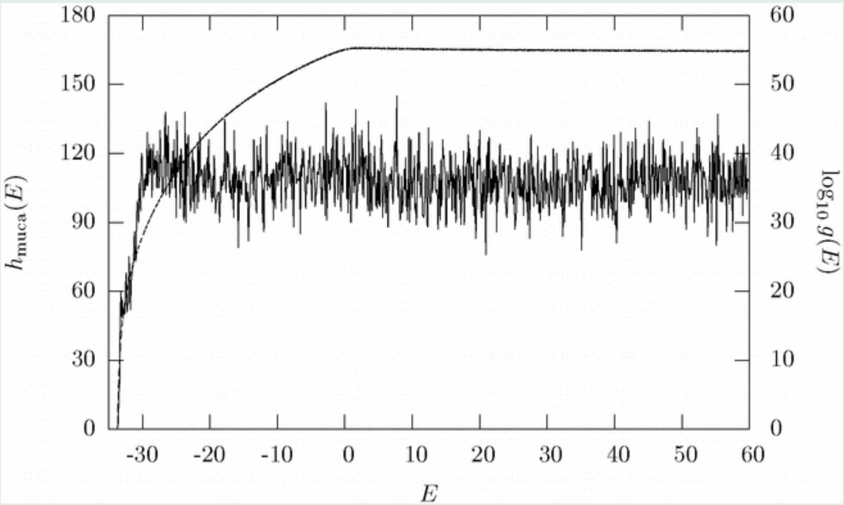

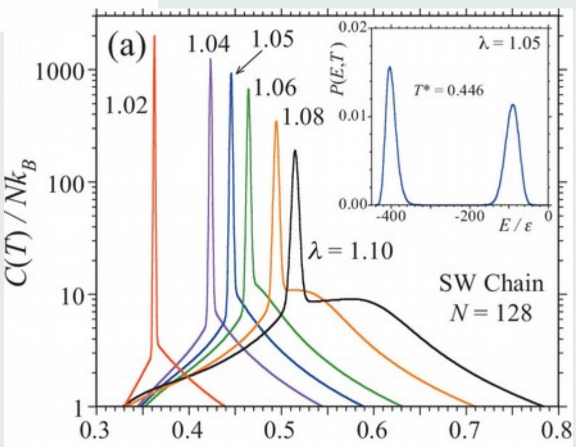

*) M.P. Taylor, W. Paul, K. Binder. JCP 131.11 (2009)

**) S. Schnabel, M. Bachmann, W. Janke. JCP 126.10 (2007)

Flat-histogram algorithms. A general scheme

Multi-canonical Monte Carlo, Wang-Landau-type algorithms

Initial configuration + initial estimation of Density of states (DOS)

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Multi-canonical Monte Carlo, Wang-Landau-type algorithms

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↓

Trial move with acceptance probability depending on the current DOS estimation

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Update (sometimes) the DOS estimation

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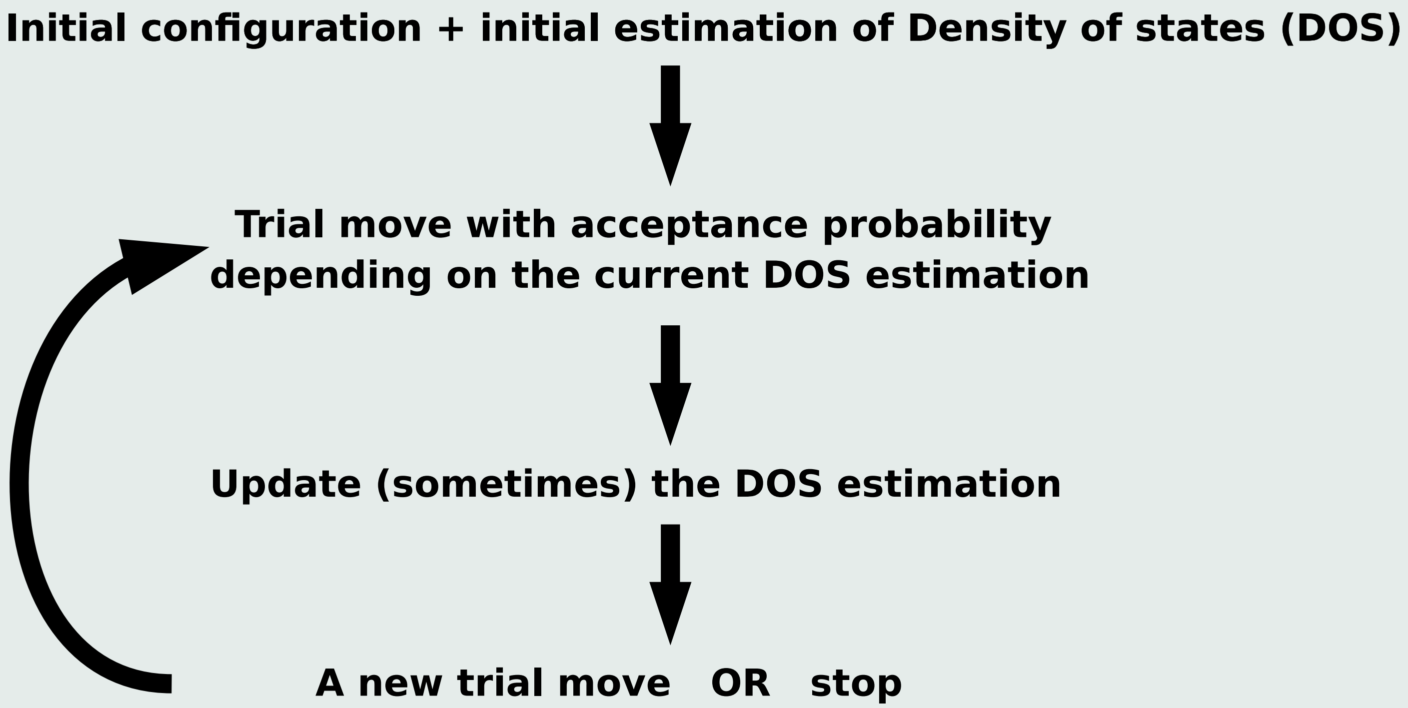

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On every step (WL)

Under some condition (MuCa)

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Update (sometimes) the DOS estimation

On every step (WL)

$$\ln g(U) \rightarrow \ln g(U) + \gamma_t$$

Under some condition (MuCa)

$$\ln g(U) \rightarrow \ln g(U) + W(U) \cdot \ln H(U)$$

Theoretical convergence

Stochastic approximation Monte Carlo

$$\sum_{t}^{\infty} \gamma_t = \infty$$

$$\sum_{t}^{\infty} \gamma_t^{\nu} < \infty$$

$$\nu \in (1,2)$$

F. Liang, C. Liu, R.J. Carroll, Journal of the American Statistical Association 102 (2007) 305-320

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Stochastic approximation Monte Carlo

$$\sum_t^{\infty} \gamma_t = \infty$$

$$\sum_t^{\infty} \gamma_t^{\nu} < \infty \quad \nu \in (1,2) \quad \Rightarrow \quad \ln g_{t \to \infty}(U) \to \ln g_{\mathrm{ex}}(U) + C$$

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Theoretical convergence

Stochastic approximation Monte Carlo

$$\sum_{t}^{\infty} \gamma_t = \infty$$

$$\sigma_{\mathrm{ex}}^2(t) = \sum_U \left(\ln g_t(U) - \ln g_{\mathrm{ex}}(U) - C\right)^2 \leqslant \lambda \cdot \gamma_t$$

$$\sum_{t}^{\infty} \gamma_t^{\nu} < \infty$$

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$$\hat{\sigma}_{\mathrm{ex}}^2(t) = \sum_U \left(\ln g_t^*(U) - \ln g_{\mathrm{ex}}(U)\right)^2 \leqslant \lambda^* \cdot \gamma_t$$

$$\ln g_t^*(U) = \ln g_t(U) - C^*$$

$$C^* = \ln g_t(U^*) - \ln g_{\mathrm{ex}}(U^*) \approx C$$

Convergence from practical point of view

$$\hat{\sigma}_{\text{ex}}^2(t) = \sum_U \left(\ln g_t^*(U) - \ln g_{\text{ex}}(U)\right)^2 \leqslant \lambda^* \cdot \gamma_t$$

Convergence from practical point of view

$$\hat{\sigma}^2_{\mathrm{ex}}(t) = \sum_U \left(\ln g^*_t(U) - \ln g_{\mathrm{ex}}(U)\right)^2$$

$$\hat{\sigma}^2_{\mathrm{av}}(t) = \sum_U \left(\ln g^*_t(U) - \langle \ln g_T(U) \rangle\right)^2$$

Convergence from practical point of view

$$\hat{\sigma}_{\mathrm{ex}}^2(t) = \sum_U \left(\ln g_t^*(U) - \ln g_{\mathrm{ex}}(U) \right)^2$$

$$\hat{\sigma}_{\mathrm{av}}^2(t) = \sum_U \left(\ln g_t^*(U) - \langle \ln g_T(U) \rangle \right)^2$$

$$\hat{\sigma}_{**,m}^2(t) = \frac{1}{m} \sum_{i=1}^{m} \hat{\sigma}_{**}^{(i)2}(t)$$

Models

Ising model (8x8 square)

P.D. Beale, Physical Review Letters 76 (1996) 78

Binomial model of 10 independent elements having energy +1 or 0

Exact solution is binomial distribution with probabilities p=0.1 and q=0.9

Hard-sphere chain having 4 tangent spheres with square-well potential

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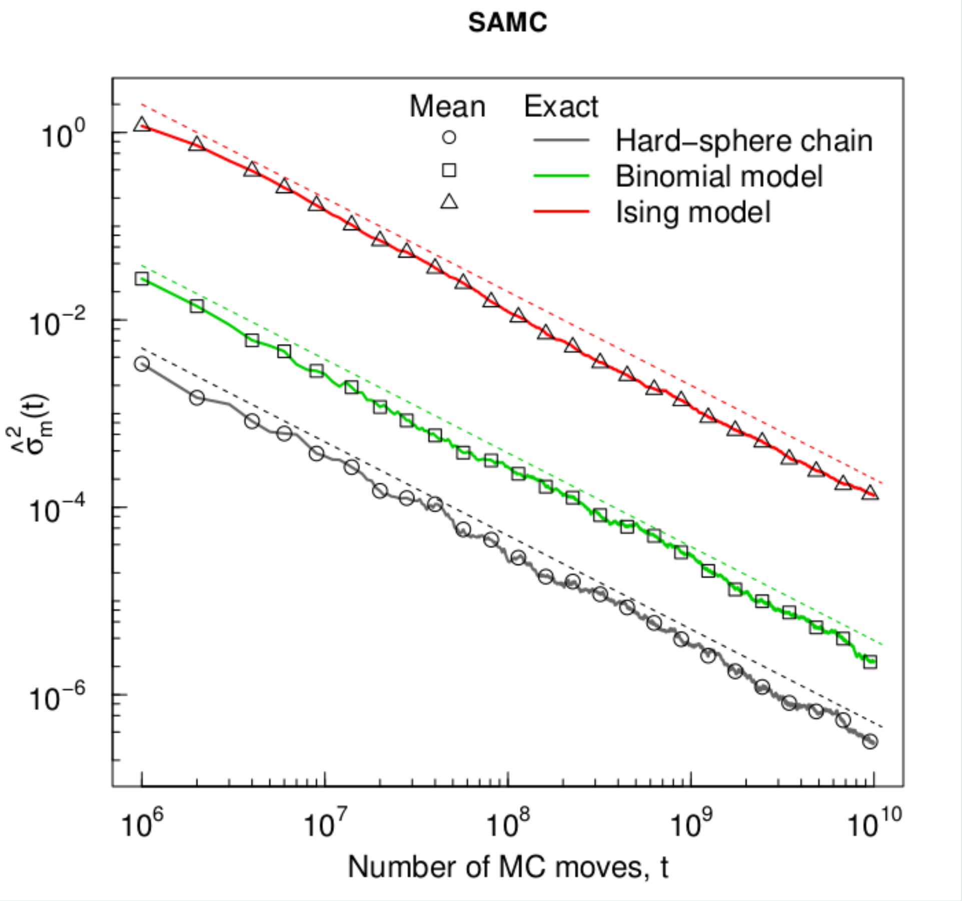

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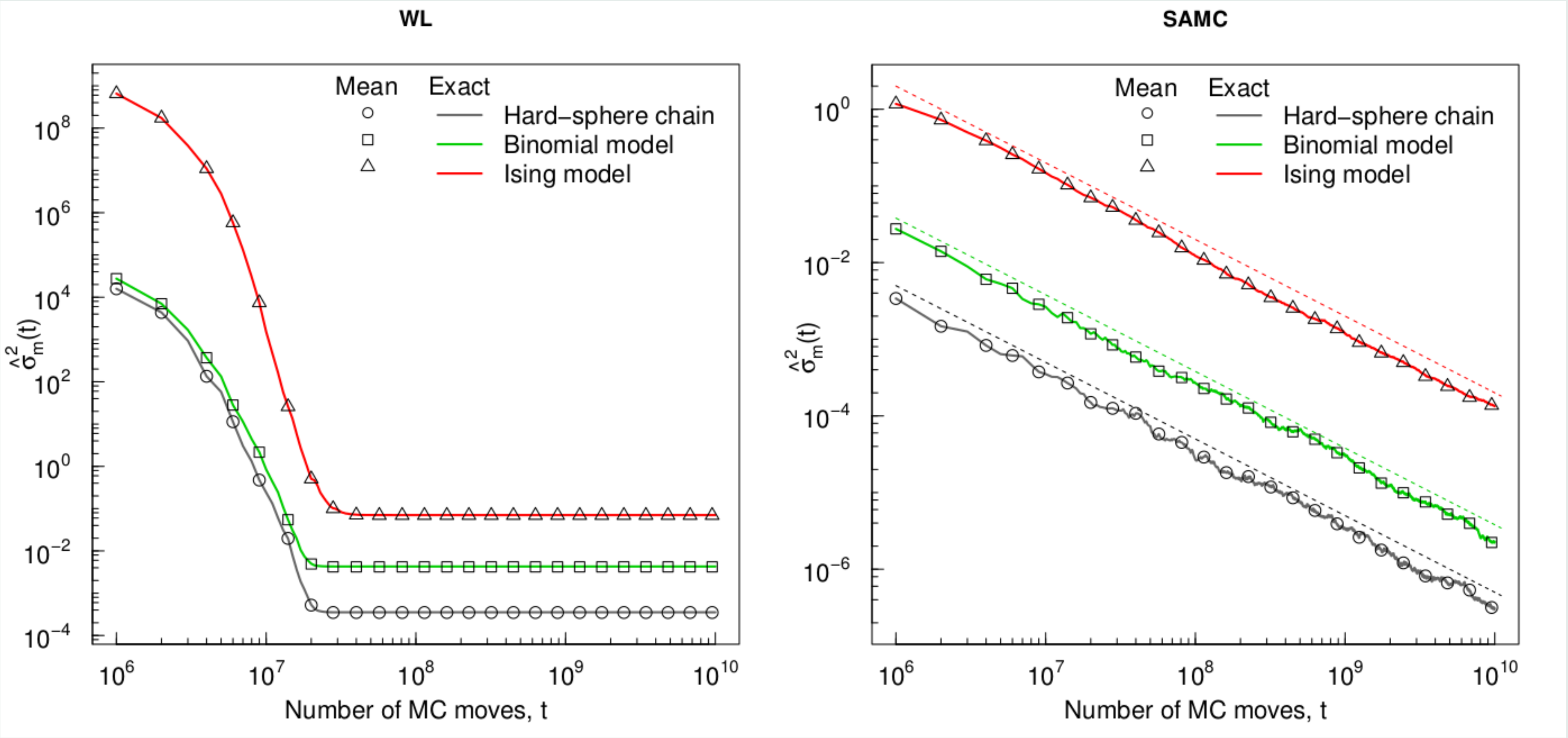

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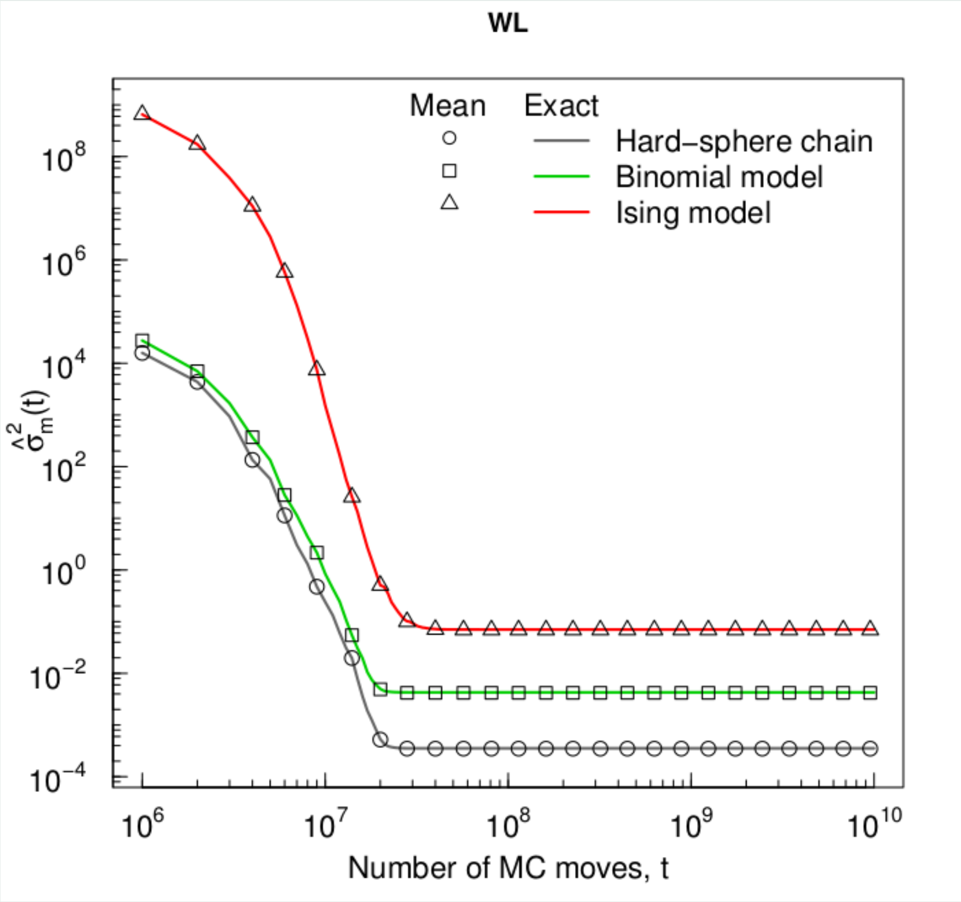


$$\ln g(U) \rightarrow \ln g(U) + \gamma_t$$

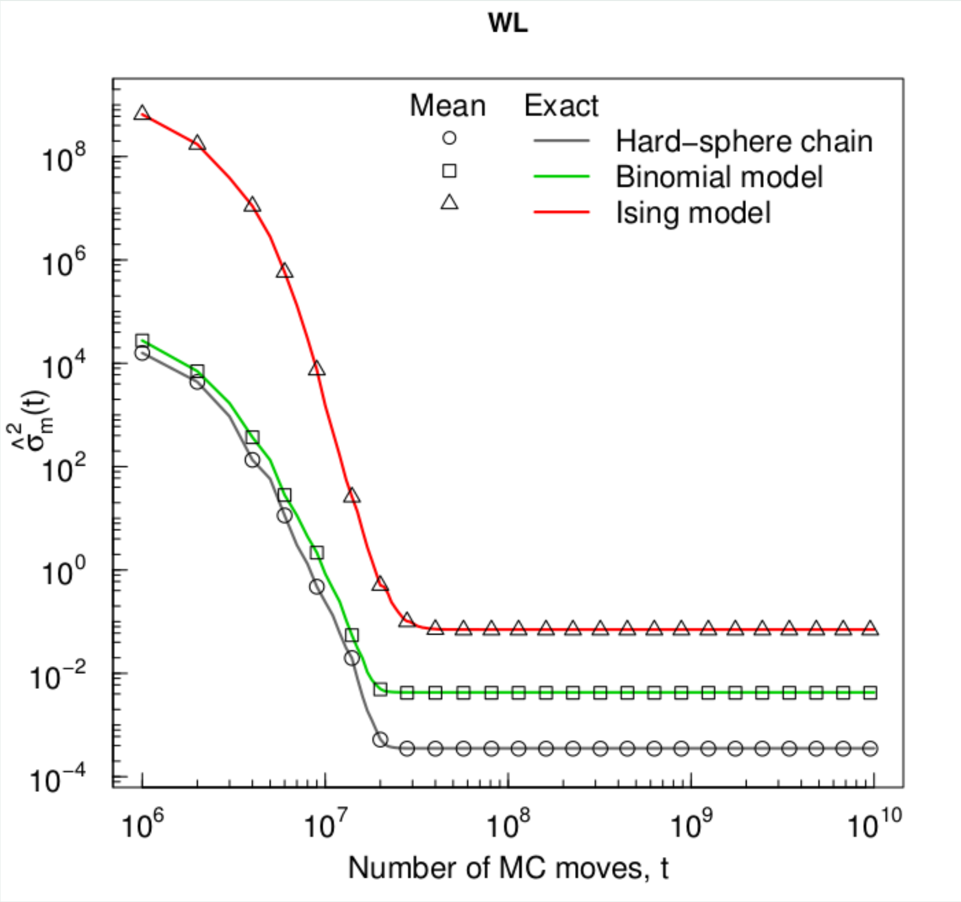
$$\sum_t^{\infty} \gamma_t = \infty$$

$$\sum_t^{\infty} \gamma_t^{\nu} < \infty$$

$$\nu \in (1,2)$$

?

Convergence of a single flat-histogram simulation



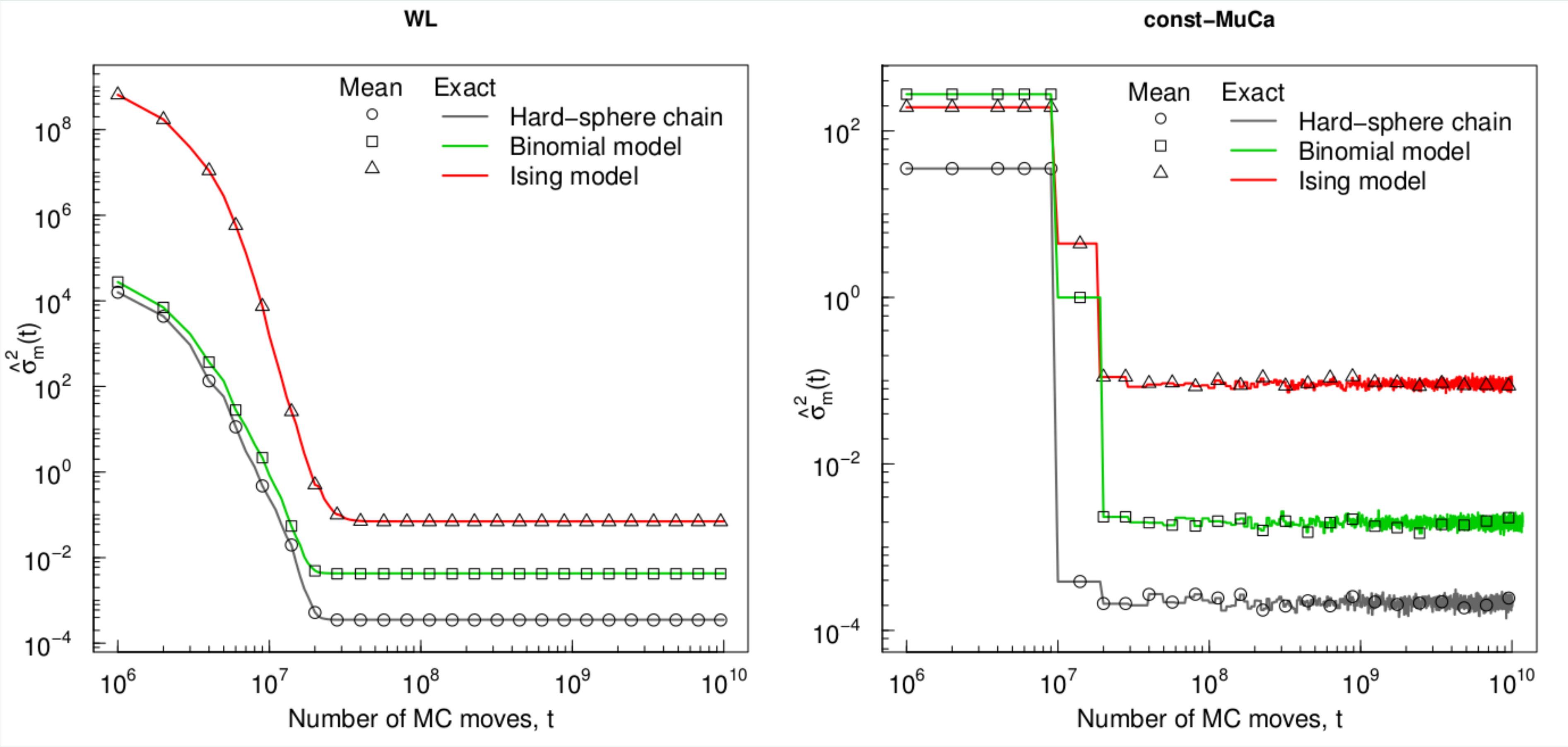
$$\ln g(U) \rightarrow \ln g(U) + \gamma_t$$

$$\sum_t^{\infty} \gamma_t = \infty$$ **No (?)**

$$\sum_t^{\infty} \gamma_t^{\nu} < \infty$$ **Yes (?)**

$$\nu \in (1,2)$$

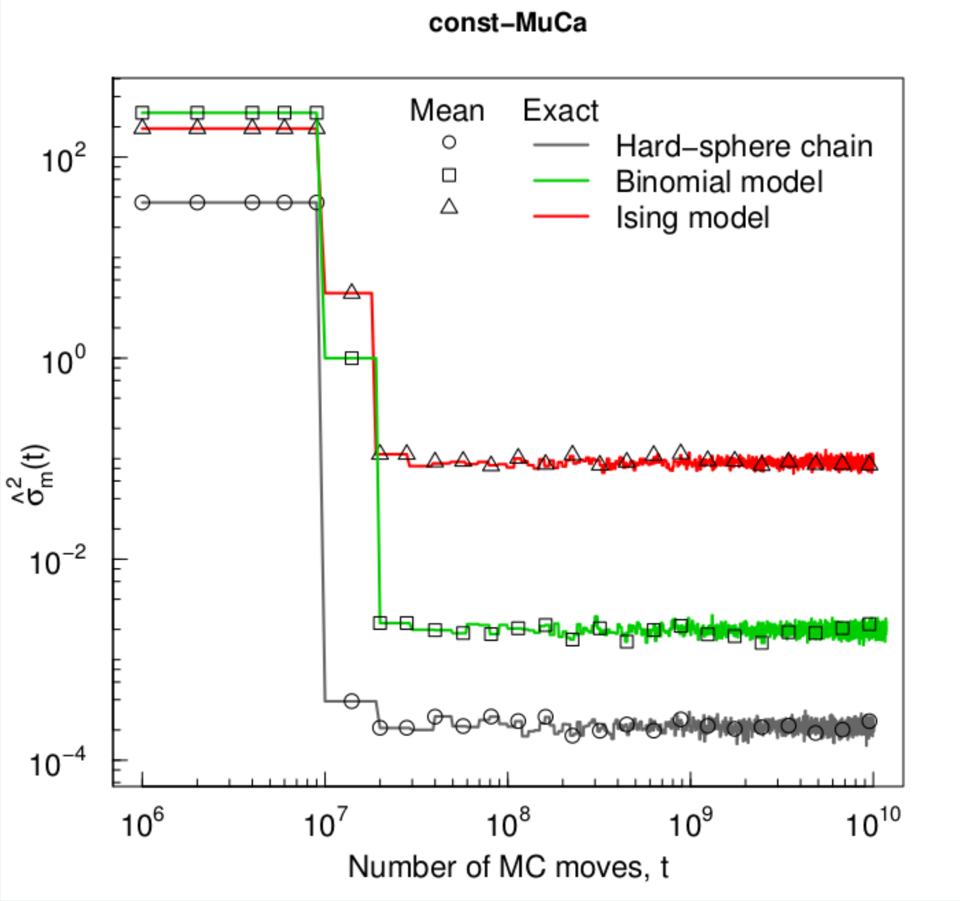
Convergence of a single flat-histogram simulation



Convergence of a single flat-histogram simulation

$$\ln g(U) \rightarrow \ln g(U) + W(U) \cdot \ln H(U)$$

$$W(U) = 1$$



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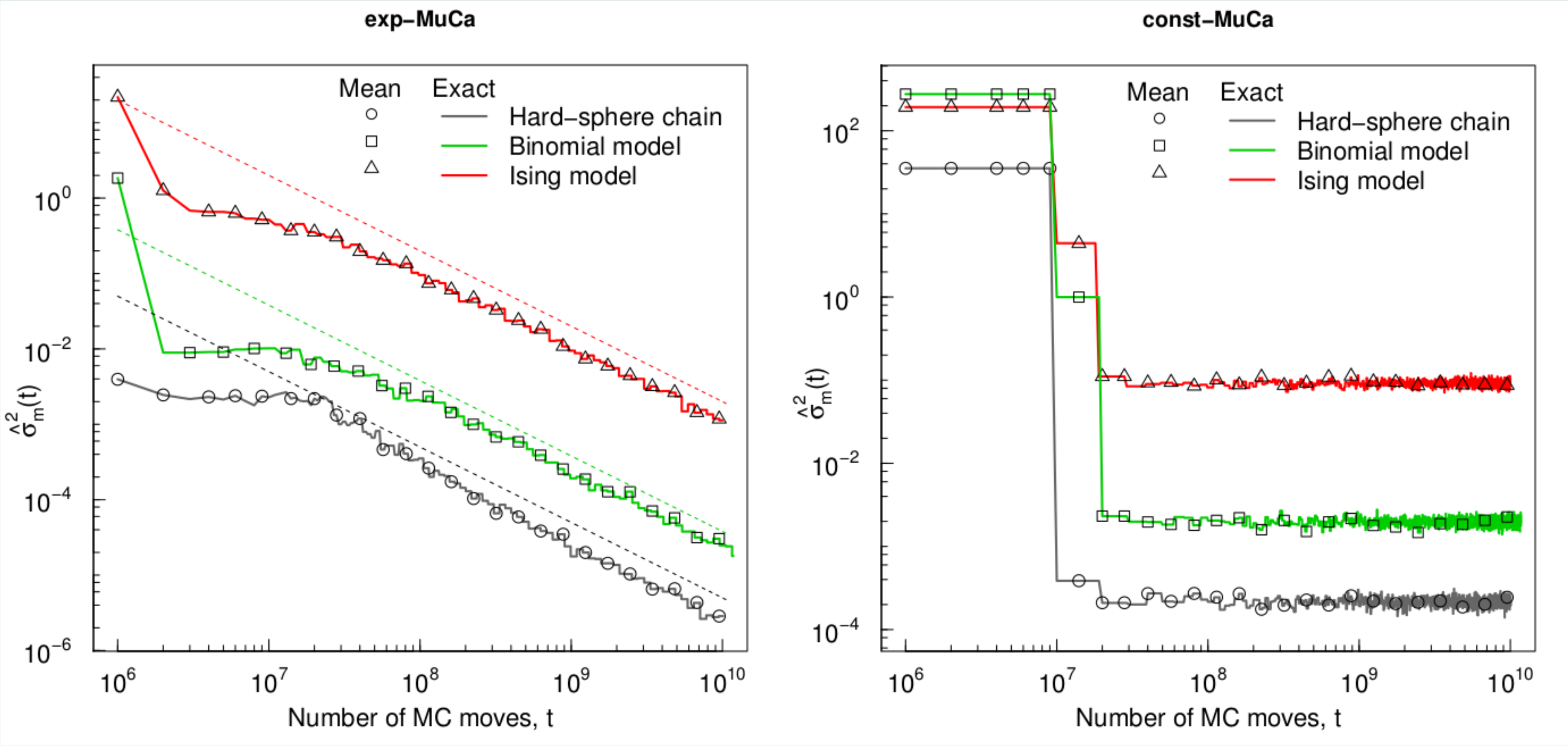

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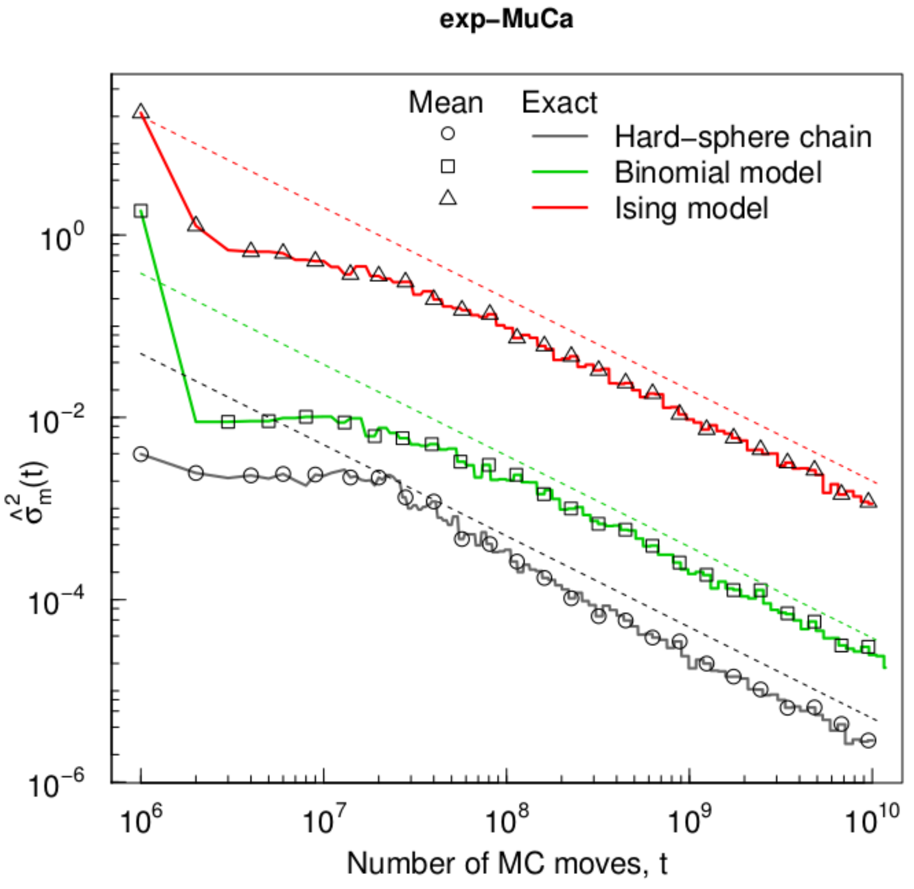
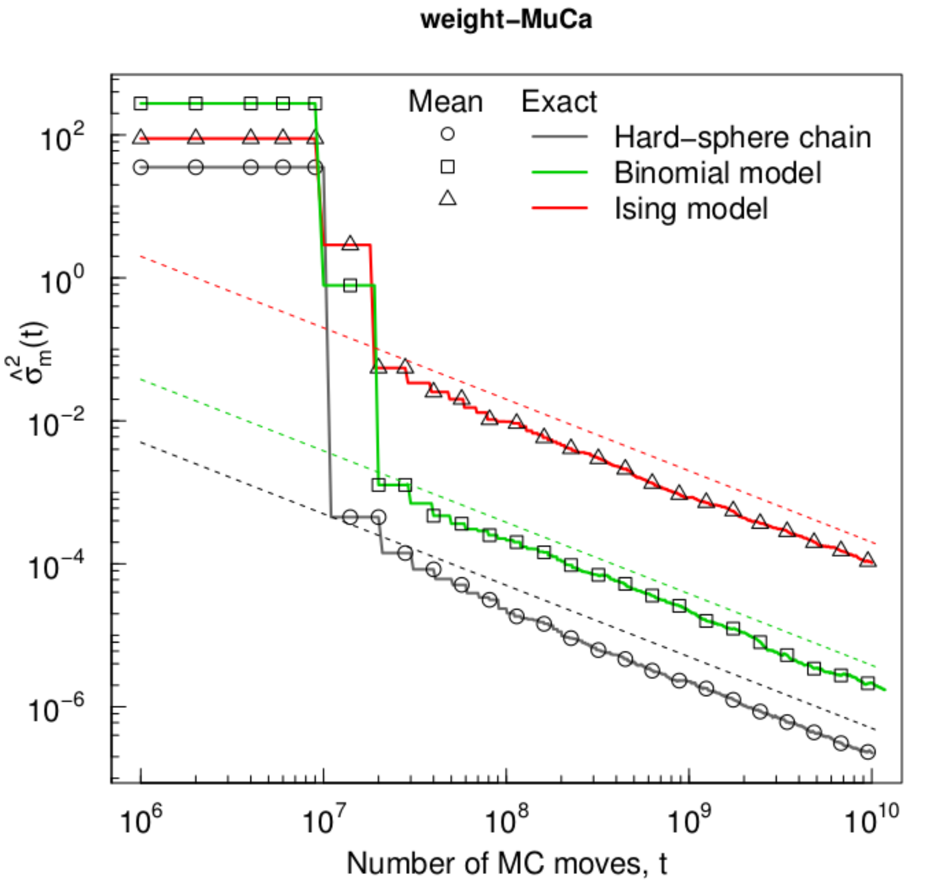




B.A. Berg, Journal of statistical physics 82 (1996) 323-342

B.A. Berg, Nuclear Physics B (Proceedings Supplements) 63 (1998) 982-984

Convergence of the averaged DOS

$$\hat{\sigma}_{\mathrm{av}}^2(t)=\sum_U \left(\langle \ln g_t(U)\rangle-\langle \ln g_T(U)\rangle\right)^2$$

Convergence of the averaged DOS

$$\hat{\sigma}^2_{\mathrm{av}}(t)=\sum_U \left(\langle \ln g_t(U)\rangle-\langle \ln g_T(U)\rangle\right)^2$$

$$\hat{\sigma}^2_{\mathrm{av},m}(t)=\frac{1}{m}\sum_{i=1}^{m}\hat{\sigma}^{(i)2}_{\mathrm{av}}(t)$$

$$\hat{s}^2_m(t)=\frac{1}{m}\hat{\sigma}^2_{\mathrm{av},m}(t)$$

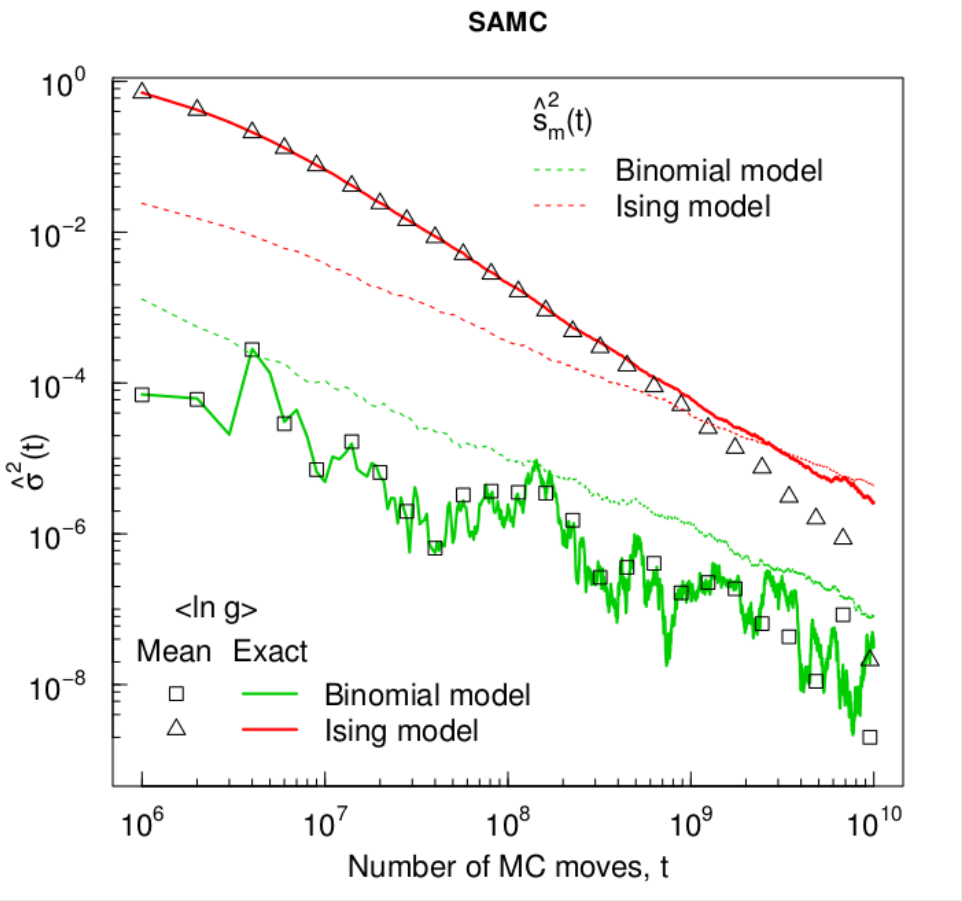
Convergence of the averaged DOS

$$\hat{\sigma}^2_{\mathrm{av}}(t) = \sum_U \left(\langle \ln g_t(U) \rangle - \langle \ln g_T(U) \rangle \right)^2$$

$$\hat{\sigma}^2_{\mathrm{av},m}(t) = \frac{1}{m} \sum_{i=1}^{m} \hat{\sigma}^{(i)2}_{\mathrm{av}}(t)$$

$$\hat{s}^2_m(t) = \frac{1}{m} \left(\hat{\sigma}^2_{\mathrm{av},m}(t) + 3\sqrt{\mathrm{Var}[\hat{\sigma}^2_{\mathrm{av},m}]} \right)$$

Convergence of the averaged DOS



Convergence of the averaged DOS

Errors

=

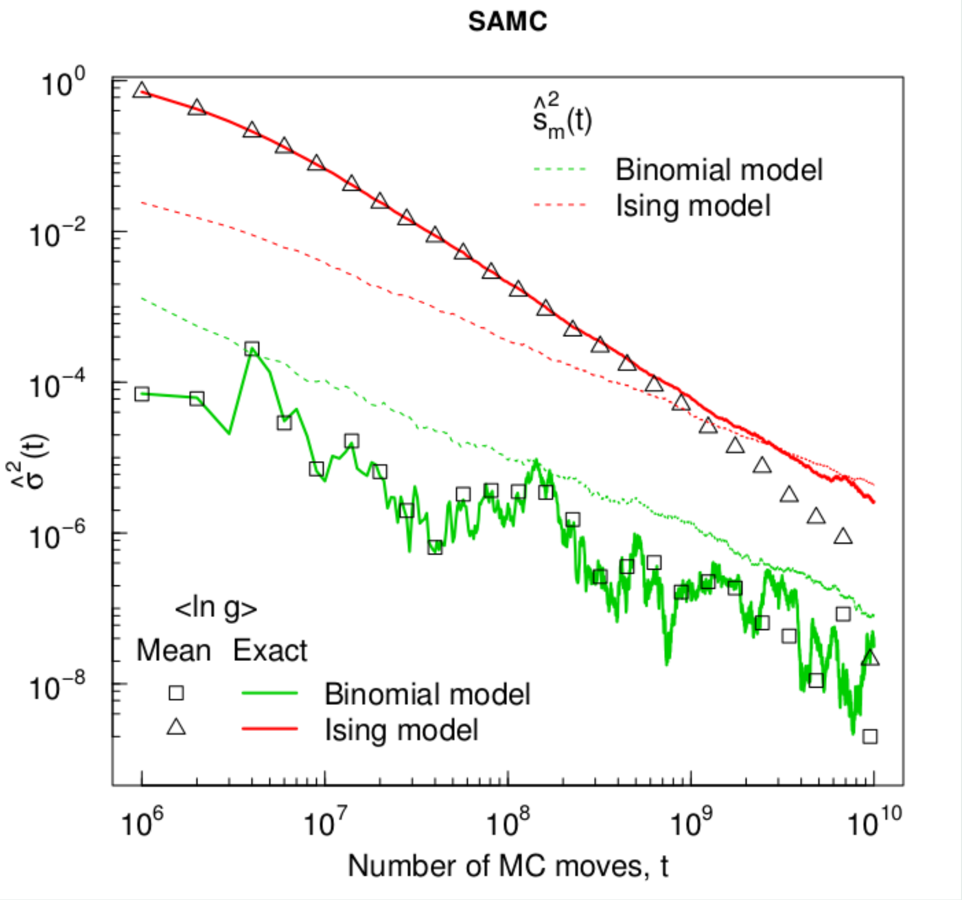
Stochastic errors

+

Systematic errors

+

Quasi-systematic errors



Convergence of the averaged DOS

Errors

=

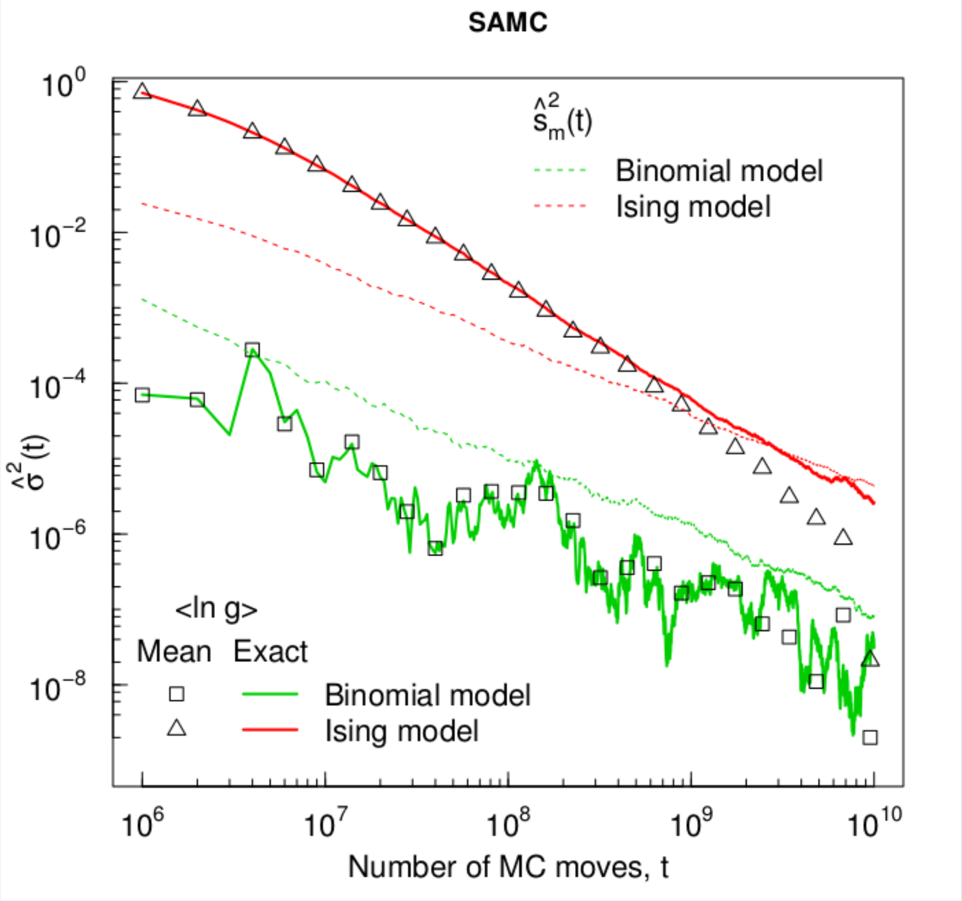
Stochastic errors — **1 / (# of runs)$^{1/2}$**

+

Systematic errors — **0**

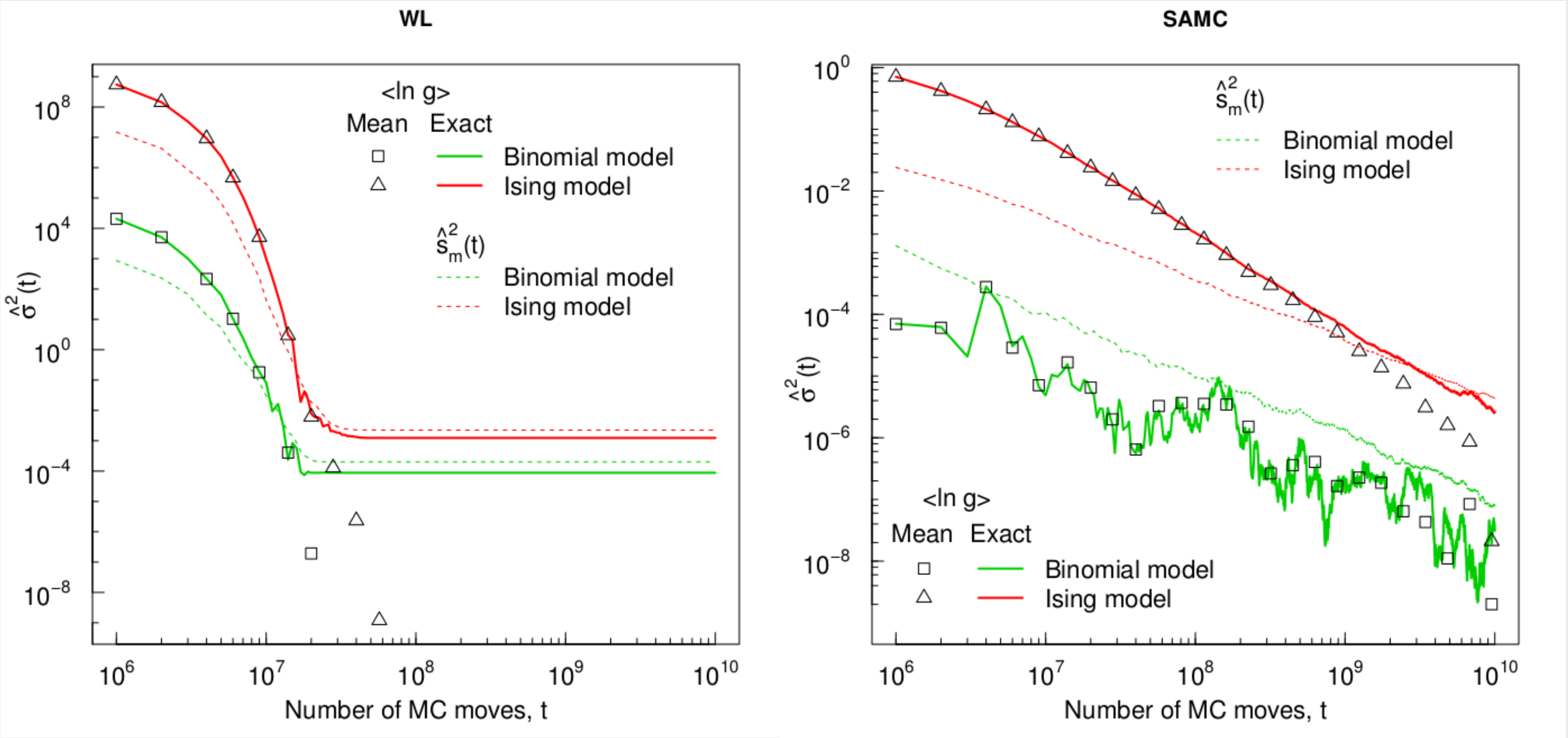
+

Quasi-systematic errors — **Saturates?** *)



*) R.E. Belardinelli, V.D. Pereyra,
"Nonconvergence of the Wang-Landau algorithms with multiple random walkers." PRE 93.5 (2016), 053306.

Convergence of the averaged DOS



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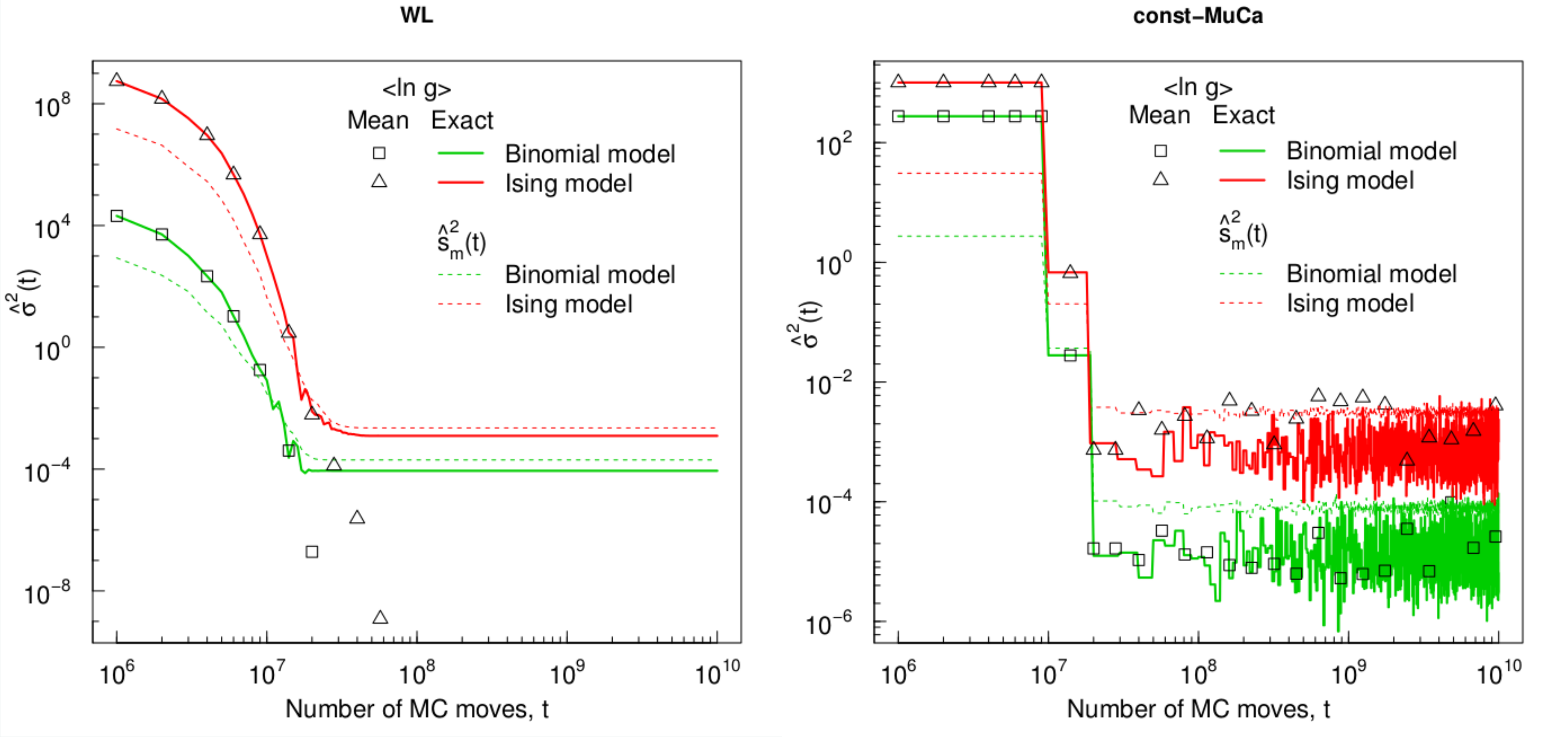

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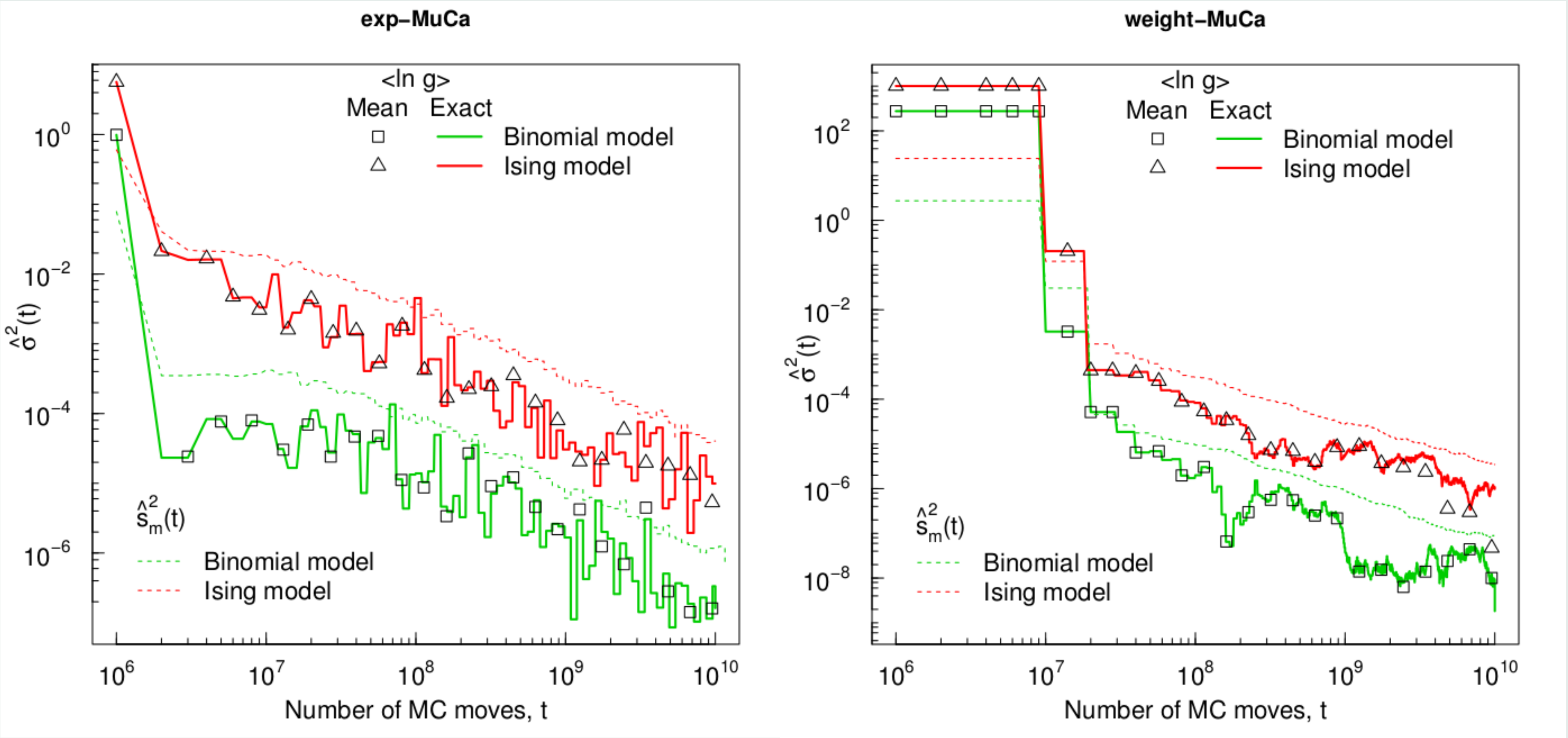

Conclusion

Convergence of a flat-histogram algorithm can be estimated by involving only the simulation results

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MuCa has similar asymptotic behavior as WL-type simulations (original or 1/t one)

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Sometimes «longer» is better than «more»?

Thank you for your attention!