t.b.a.

T. S.

19.12.2023

t.b.a.

t.b.a.

t.b.a.

t.b.a. t.b.a.?

t.b.a.

t.b.a.

Monte Carlo integration and importance sampling

$$\langle f \rangle_{p(x)} = \int f(x) \cdot p(x) \, \mathrm{d}x \approx \frac{1}{N} \sum_{\substack{n=1 \\ x_n \sim p(x)}}^{N} f(x_n)$$

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$$\langle f \rangle_{p(x)} = \int f(x) \frac{p(x)}{q(x)} \cdot q(x) \, \mathrm{d}x \approx \frac{1}{N} \sum_{\substack{n=1 \\ x_n \sim q(x)}}^{N} f(x_n) \frac{p(x_n)}{q(x_n)}$$

$$\langle f \rangle_{p(x)} = \langle f \cdot \frac{p(x)}{q(x)} \rangle_{q(x)}$$

Flat-histogram Monte Carlo

All points in the configurational space are equally probable, new states are accepted with probability

$$p_{\mathrm{acc}} \propto \frac{1}{g(U)}$$

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Wang-Landau-type methods

$$\ln g(U) \rightarrow \ln g(U) + \boldsymbol{\gamma_t}$$

Update on every step

$$\boldsymbol{\gamma_t = \min\{\gamma_0, \frac{t_0}{t}\}}$$

Multicanonical-type methods

$$\ln g(U) \rightarrow \ln g(U) + \boldsymbol{\ln H(U)}$$

Update after very final step

t.b.a.
to bind approximations

$$\hat{g}(U) = \int \delta(E(x) - U)\, \mathrm{d}x$$

t.b.a.
to bind approximations

$$\hat{g}(U)=\int \delta(E(x)-U)\,\mathrm{d}x$$

$$\hat{g}(U)=\int \frac{\delta(E(x)-U)}{q(E(x))}\,q(E(x))\,\mathrm{d}x \approx \sum_{x\sim q(E(x))} \frac{\delta(E(x)-U)}{q(E(x))}$$

t.b.a.
to bind approximations

$$\hat{g}(U) = \int \delta(E(x) - U)\,\mathrm{d}x \approx C \cdot \sum_{x \sim q(E(x))} \delta(E(x) - U)\, g(E(x))$$

$$\hat{g}(U) = \int \frac{\delta(E(x) - U)}{q(E(x))} q(E(x))\,\mathrm{d}x \approx \sum_{x \sim q(E(x))} \frac{\delta(E(x) - U)}{q(E(x))}$$

$$q(E) \propto \frac{1}{g(E)}$$ for flat-histogram algorithms

t.b.a.
to bind approximations

$$\hat{g}(U) = \int \delta(E(x) - U)\,\mathrm{d}x \approx C \cdot \sum_{x \sim q(E(x))} \delta(E(x) - U)\,g(E(x))$$

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t.b.a.
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Multicanonical-type methods

$$\ln g(U) \rightarrow \ln g(U) + \mathbf{\ln \boldsymbol{H}(\boldsymbol{U})}$$

$$\hat{g}(U) \approx C \cdot \sum_{x \sim q(E(x))} \delta(E(x) - U)\, g(U)$$

$$\hat{g}(U) \approx C \cdot g(U) \underbrace{\sum_{x \sim q(E(x))} \delta(E(x) - U)}_{H(U)}$$

$$\boldsymbol{\ln \hat{g}(U) \approx \ln C + \ln g(U) + \ln H(U)}$$

t.b.a.
to bind approximations

$$\hat{g}(U) = \int \delta(E(x) - U)\,\mathrm{d}x \approx C \cdot \sum_{x \sim q(E(x))} \delta(E(x) - U)\, g(E(x))$$

Multicanonical-type methods

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

Wang-Landau-type methods

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

$$g_{\mathrm{is}}(U) \approx \sum_t g(E(x_t), t)\, \delta(E(x_t) - U)$$

t.b.a. t.b.a.?
to bind approximations. trio: better approximation?

$$p_{\mathrm{acc}} \propto \frac{1}{g(U)}$$

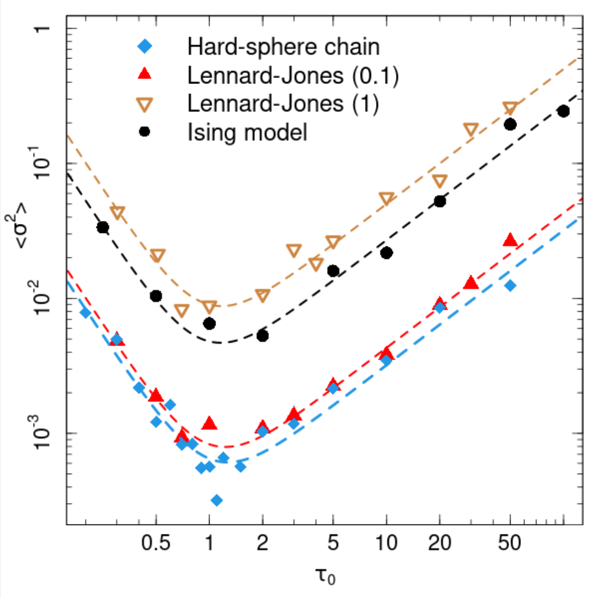
Wang-Landau-type methods

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

$$\gamma_t = \min[\gamma_0; \frac{t_0}{t}]$$

$$\tau_0 = \frac{t_0}{N_{\mathrm{bin}}}$$

How accurate is it?



t.b.a. t.b.a.?
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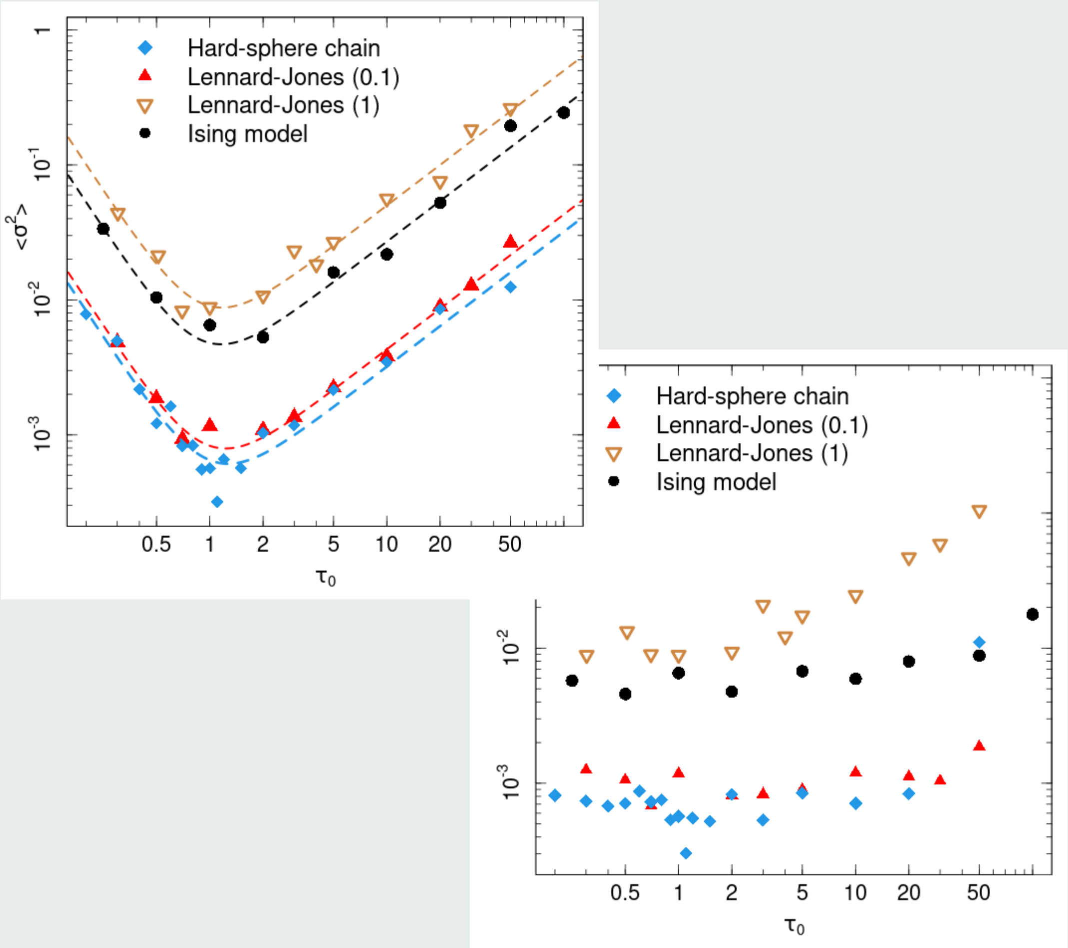
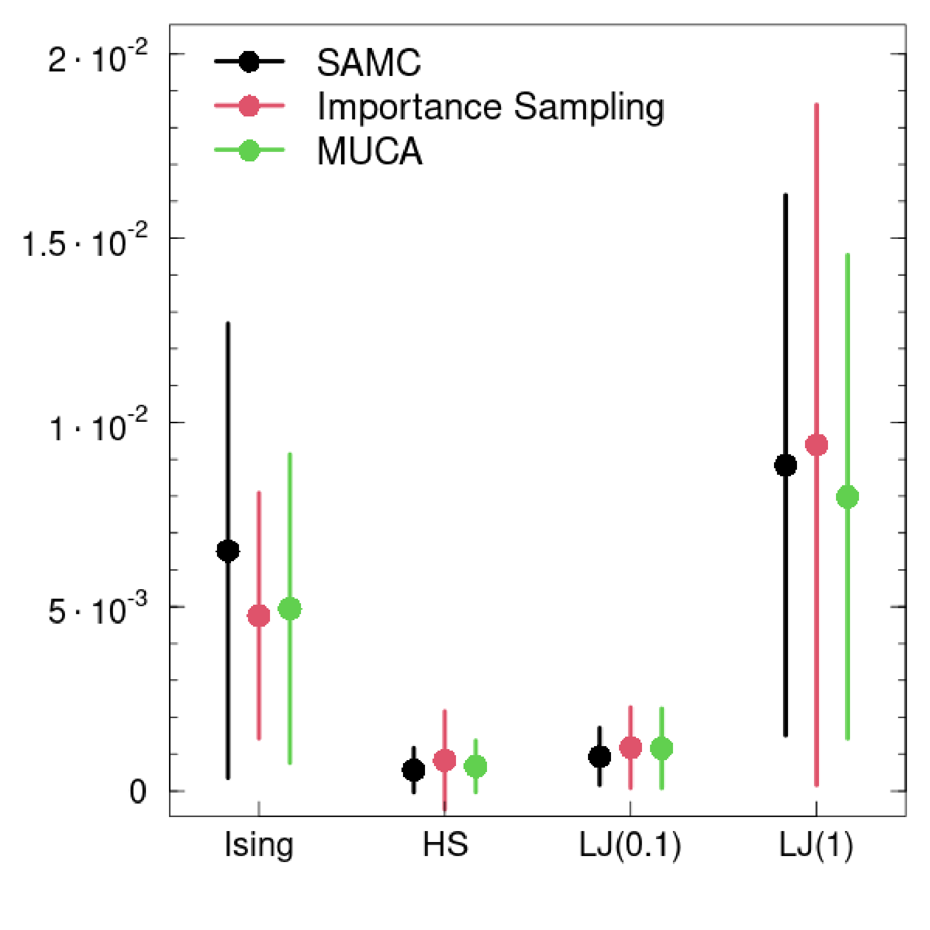


t.b.a. t.b.a.?
to bind approximations. trio: better approximation?

How accurate is it?



t.b.a.
to broaden applications

$$\hat{g}(U) \approx C \cdot \sum_{x \sim q(E(x))} \delta(E(x) - U)\, g(E(x))$$

t.b.a.
to broaden applications

$$\hat{g}(U) \approx C \cdot \sum_{x \sim q(E(x))} \delta(E(x) - U)\, g(E(x))$$

$$\hat{k}(U) \approx C \cdot \sum_{x \sim q(E(x))} \delta(K(x) - U)\, g(E(x))$$

t.b.a.
to broaden applications

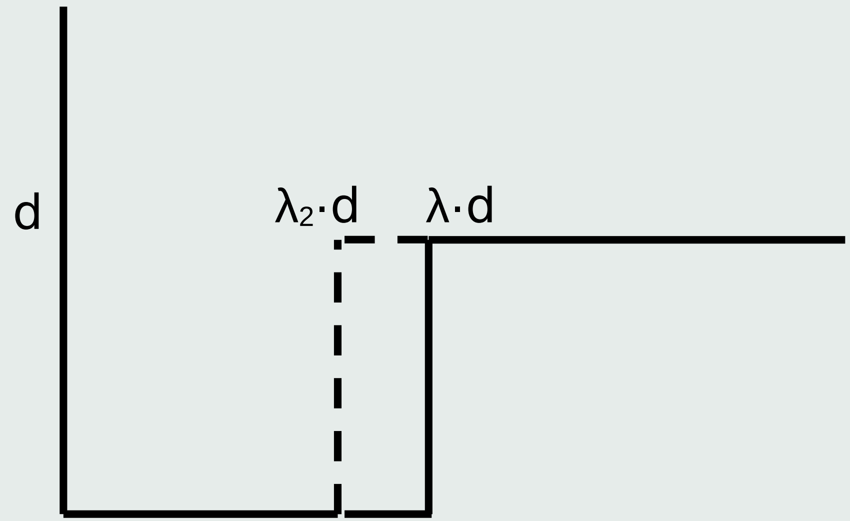
Example 1

$$\hat{g}(U) \approx C \cdot \sum_{x \sim q(E(x))} \delta(E(x) - U)\, g(E(x))$$

$$\hat{k}(U) \approx C \cdot \sum_{x \sim q(E(x))} \delta(K(x) - U)\, g(E(x))$$

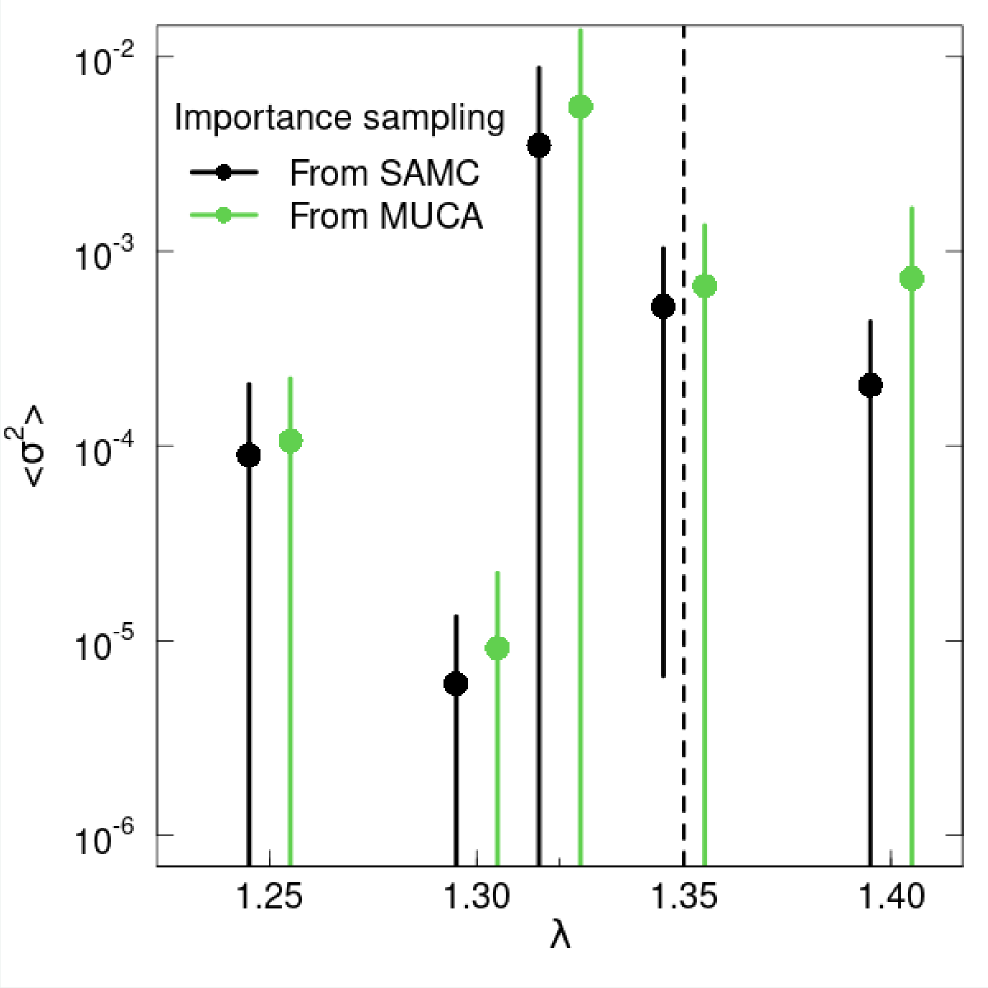
$$E(x) = -\sum_{\langle ij \rangle} \Theta(\lambda d - r_{ij})$$

$$K(x) = -\sum_{\langle ij \rangle} \Theta(\lambda_2 d - r_{ij})$$



t.b.a.
to broaden applications

Example 1

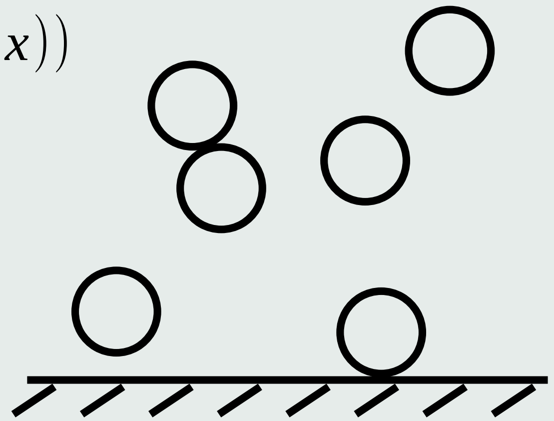


Example 2

$$\hat{g}(U) \approx C \cdot \sum_{x \sim q(E(x))} \delta(E(x) - U)\, g(E(x))$$

$$\hat{k}(U) \approx C \cdot \sum_{x \sim q(E(x))} \delta(K(x) - U)\, g(E(x))$$

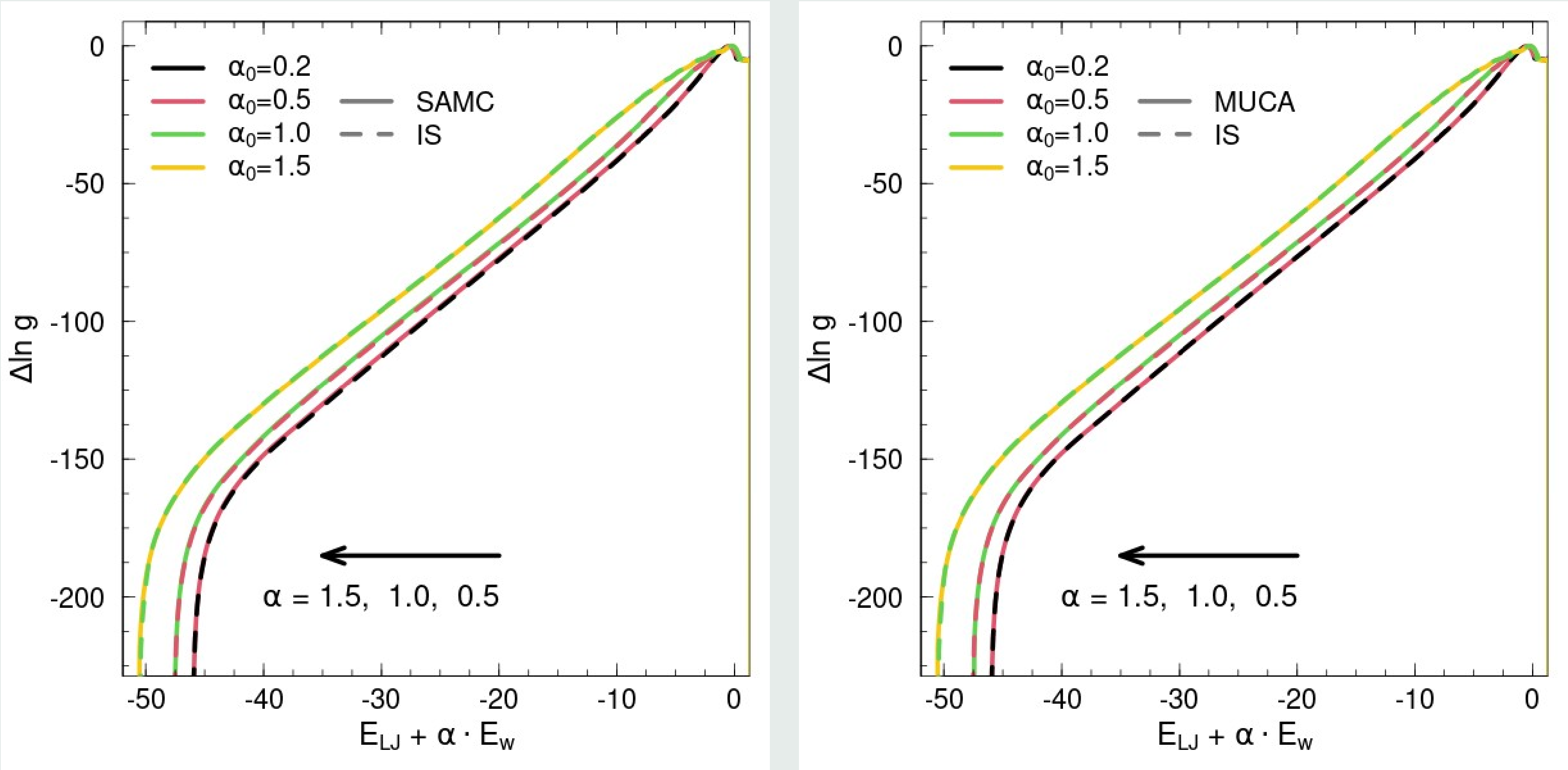
$$K(x) = \underbrace{E_{\mathrm{LJ}}(x)}_{\text{bead-bead}} + \alpha\, \underbrace{E_{\mathrm{w}}(x)}_{\text{bead-surface}}$$



13 LJ beads + LJ wall

t.b.a.
to broaden applications

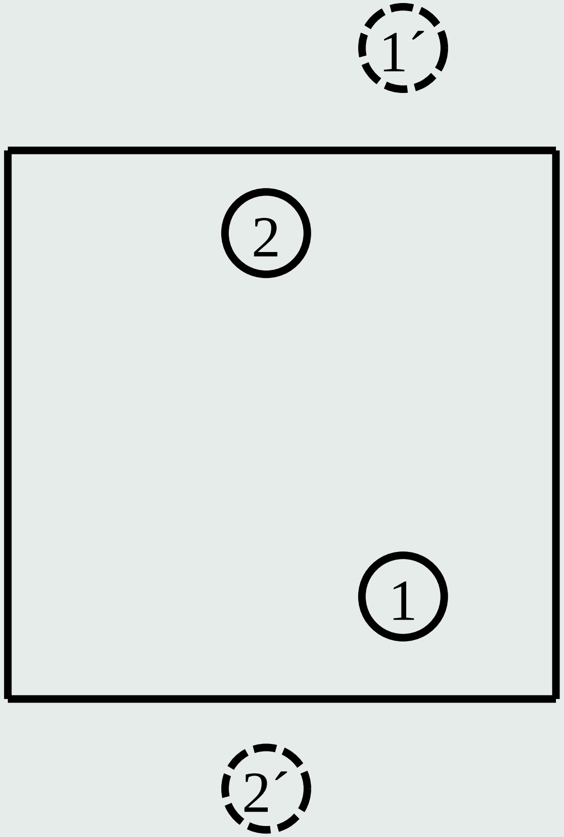
Example 2



$$K(x) = E_{\mathrm{LJ}}(x) + \alpha E_{\mathrm{w}}(x)$$

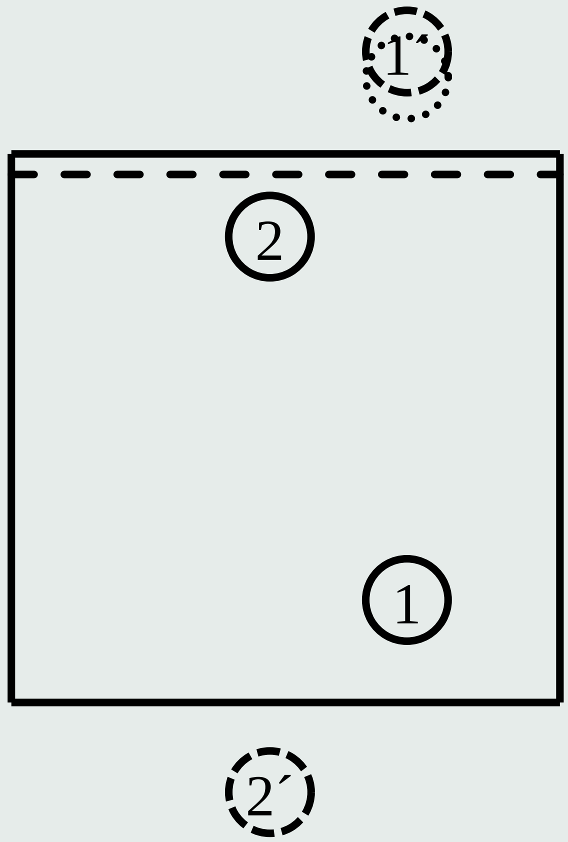
t.b.a.
trial beyond accustomed

$$E = \sum_{\langle ij \rangle} U\left(\min\left(r_{ij}\right) | L\right)$$



t.b.a.
trial beyond accustomed

$$E = \sum_{\langle ij \rangle} U\left(\min\left(r_{ij}\right) | L\right)$$

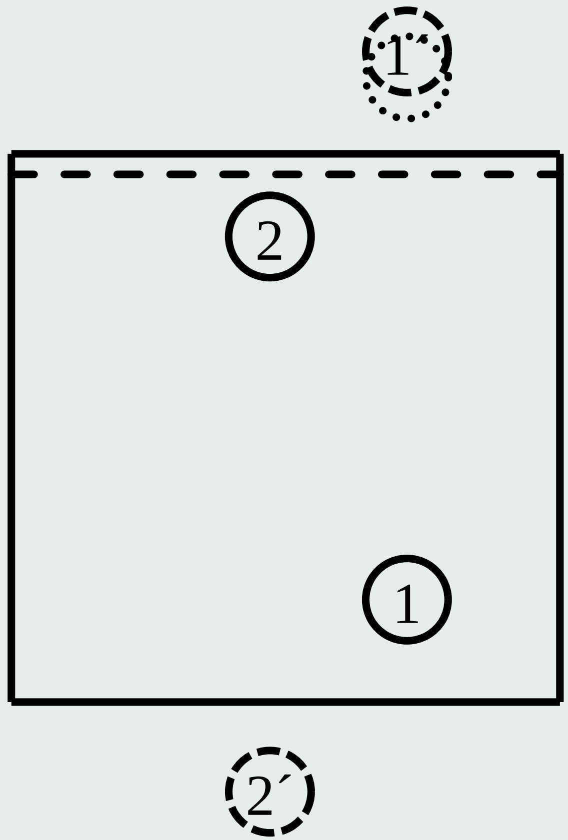


$$\beta p = \frac{\partial \ln g}{\partial V}$$

t.b.a.
trial beyond accustomed

$$E=\sum_{\langle ij\rangle} U\left(\min\left(r_{ij}\right)\middle| L\right)$$

$$K=\sum_{\langle ij\rangle} U\left(\min\left(r_{ij}\right)\middle| l<L\right)$$

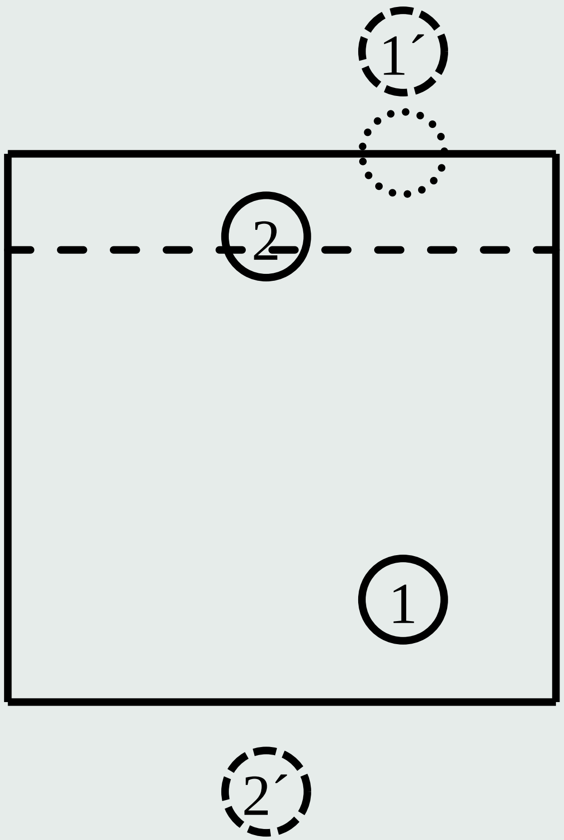


$$\beta p=\frac{\partial \ln g}{\partial V}$$

$$pV=-\frac{1}{3}\left\langle r_{ij}\cdot F\left(r_{ij}\right)\right\rangle$$

t.b.a.
trial beyond accustomed

$$E = \sum_{\langle ij \rangle} U\left(\min\left(r_{ij}\right) \middle| L\right)$$



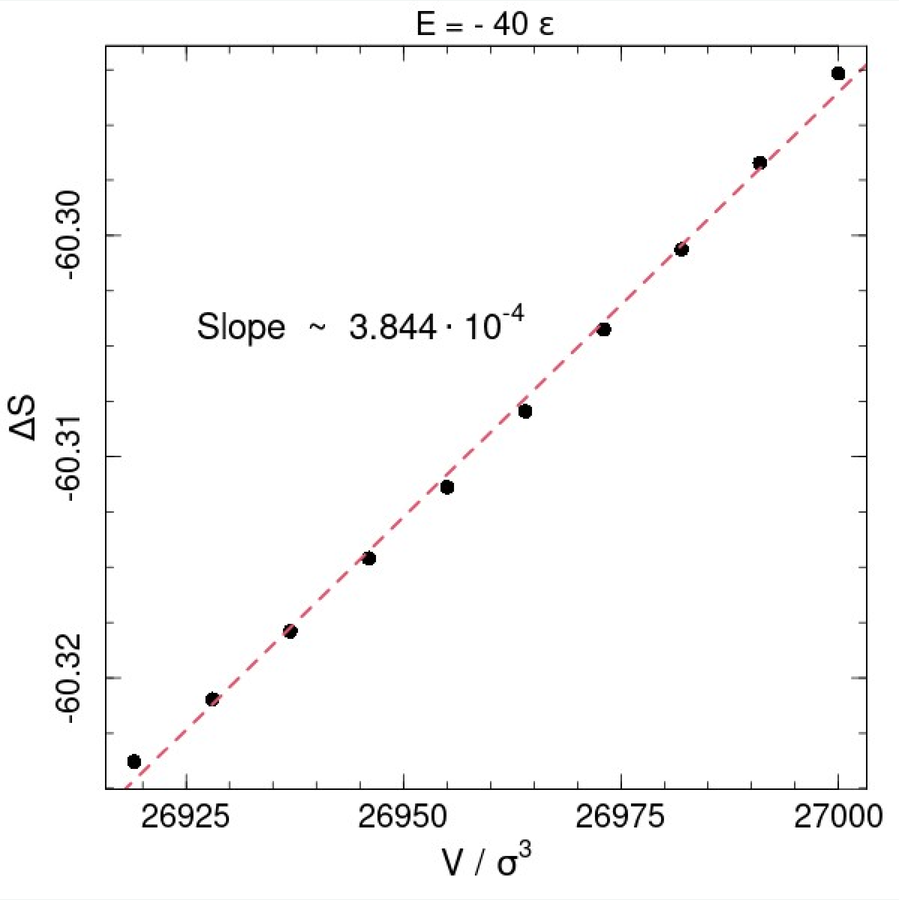
$$K = \sum_{\langle ij \rangle} U\left(\min\left(r_{ij}\right) \middle\| l < L\right)$$

$$\beta p = \frac{\partial \ln g}{\partial V}$$

$$pV = -\frac{1}{3}\left\langle r_{ij} \cdot F\left(r_{ij}\right)\right\rangle$$

t.b.a.
trial beyond accustomed

Pressure of 13 LJ particles



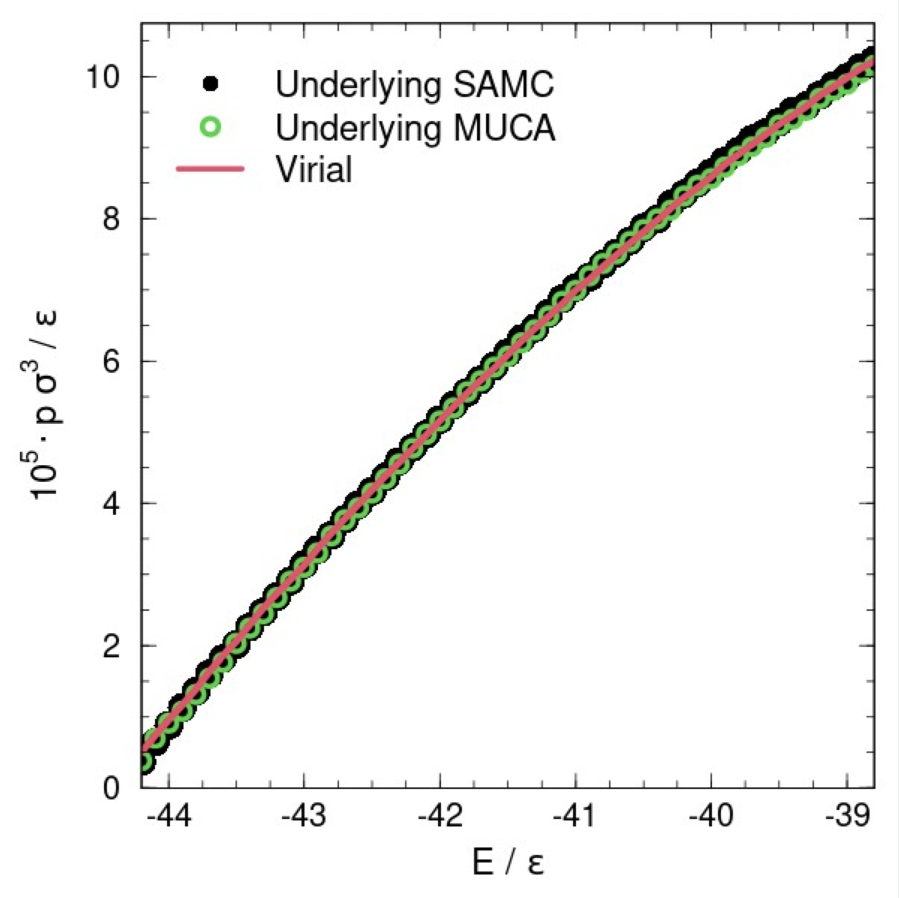
$$K = \sum_{\langle ij \rangle} U\left(\min\left(r_{ij}\right) \| l_z < L\right)$$

$$\beta p = \frac{\partial \ln g}{\partial V}$$

t.b.a.
trial beyond accustomed

Pressure of 13 LJ particles

$$\beta p = \frac{\partial \ln g}{\partial V}$$



$$K = \sum_{\langle ij \rangle} U\left(\min\left(r_{ij}\right) \| l_z < L\right)$$

$$pV = -\frac{1}{3} \langle r_{ij} \cdot F\left(r_{ij}\right) \rangle$$

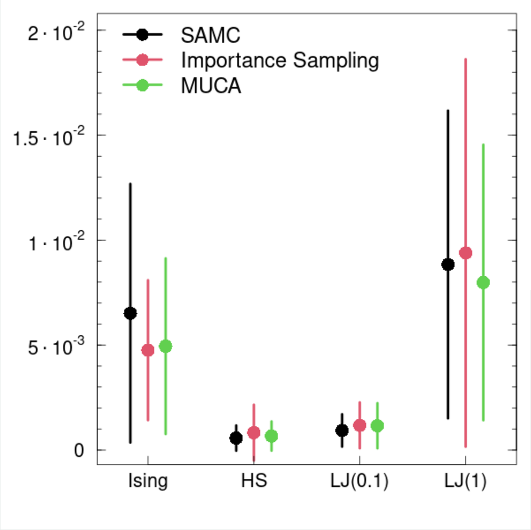
t.b.a.
Take before abroad

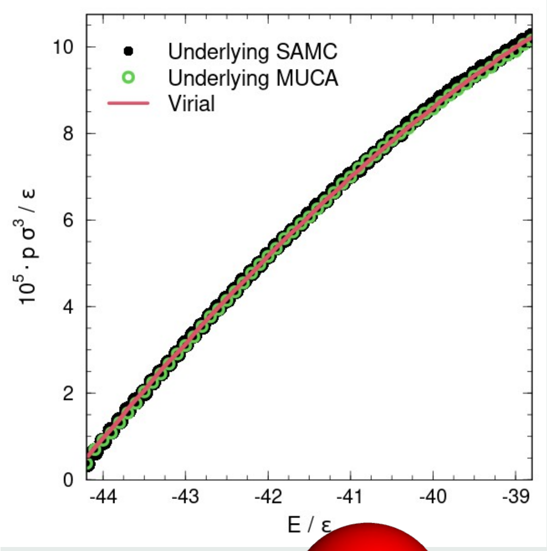
- Optimal convergence rate for SAMC is $t_0 \ / \ N_b \approx 1$

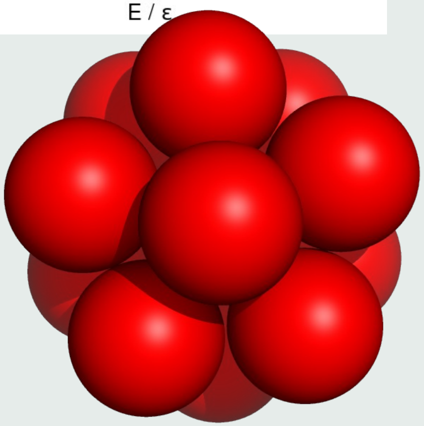
- Importance sampling error depends not on the SAMC parameters and have the same accuracy as MUCA or optimal SAMC

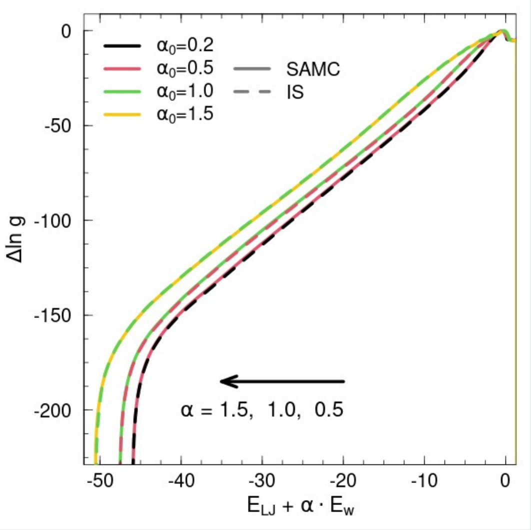
- Sampling during a single run may be efficiently provided for a series of system or potential parameters within a single SAMC or MUCA simulation (running with other values of these parameters).

Thank you for your attention!









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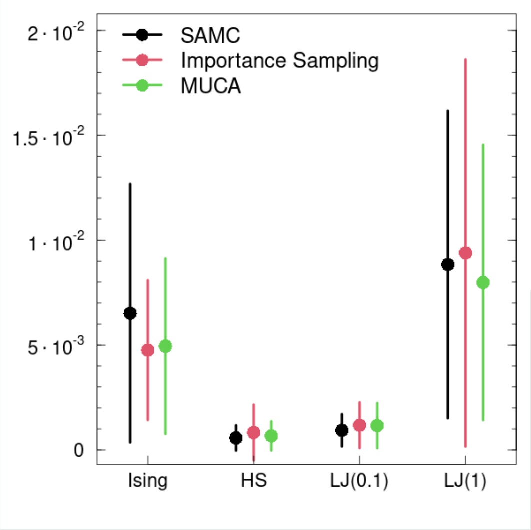

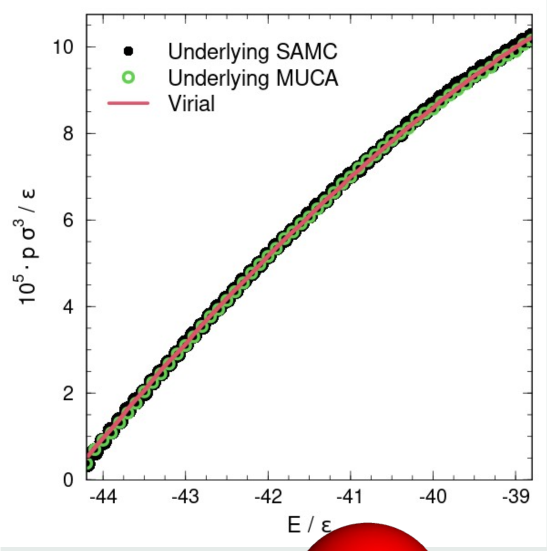

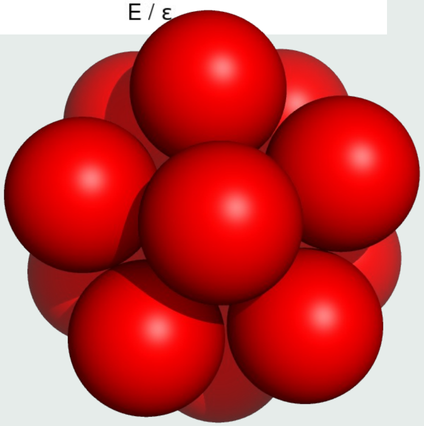

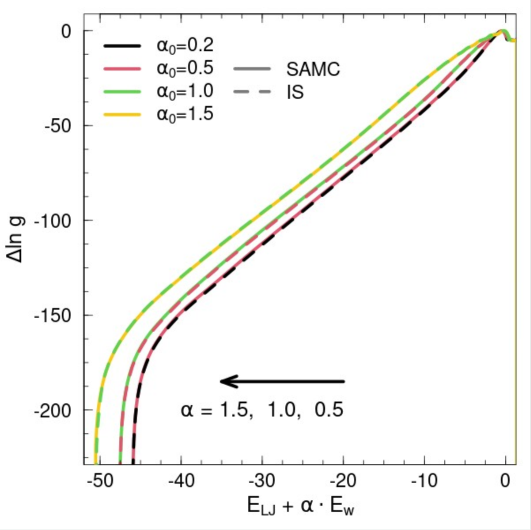

t.b.a.
to broaden applications

Example 1

TABLE III. Density of states $g_6^{(k)}$ for square-well 6-mer chains with well diameter $\lambda\sigma$ and bond length $L=\sigma$. The partition function for the related hard-sphere 6-mer chain is $Z_6^{hs}=0.257\,93$.

λ	k=0	k=1	k=2	k=3	k=4	k=5	k=6	k=7	k=8	k=9	k=10
1.10	0.196 15	0.052 77	8.02×10^{-03}	9.19×10^{-04}	8.11×10^{-05}	5.31×10^{-06}	2.56×10^{-07}	7.37×10^{-09}	0.0	0.0	0.0
1.15	0.168 42	0.070 09	0.016 18	2.81×10^{-03}	3.79×10^{-04}	3.82×10^{-05}	2.87×10^{-06}	1.32×10^{-07}	0.0	0.0	0.0
1.20	0.142 80	0.082 20	0.025 65	6.01×10^{-03}	1.10×10^{-03}	1.51×10^{-04}	1.57×10^{-05}	1.05×10^{-06}	7.0×10^{-14}	0.0	0.0
1.25	0.119 36	0.089 59	0.035 51	0.010 52	2.45×10^{-03}	4.30×10^{-04}	5.82×10^{-05}	5.38×10^{-06}	1.24×10^{-09}	0.0	0.0
1.30	0.098 13	0.092 77	0.044 99	0.016 20	4.63×10^{-03}	9.97×10^{-04}	1.69×10^{-04}	2.06×10^{-05}	6.26×10^{-08}	0.0	0.0
1.32	0.090 26	0.093 00	0.048 55	0.018 75	5.76×10^{-03}	1.34×10^{-03}	2.46×10^{-04}	3.32×10^{-05}	1.85×10^{-07}	7.2×10^{-15}	0.0
1.35	0.079 10	0.092 33	0.053 47	0.022 78	7.75×10^{-03}	2.00×10^{-03}	4.13×10^{-04}	6.44×10^{-05}	7.17×10^{-07}	9.2×10^{-11}	0.0
1.40	0.062 29	0.088 80	0.060 44	0.029 87	0.011 86	3.59×10^{-03}	8.89×10^{-04}	1.74×10^{-04}	4.73×10^{-06}	3.49×10^{-08}	0.0
1.43	0.053 26	0.085 46	0.063 72	0.034 16	0.014 79	4.89×10^{-03}	1.34×10^{-03}	2.98×10^{-04}	1.33×10^{-05}	2.97×10^{-07}	4.7×10^{-14}
1.45	0.047 68	0.082 78	0.065 52	0.036 95	0.016 90	5.93×10^{-03}	1.73×10^{-03}	4.16×10^{-04}	2.54×10^{-05}	9.07×10^{-07}	1.7×10^{-11}
1.50	0.035 24	0.074 76	0.068 60	0.043 51	0.022 62	9.15×10^{-03}	3.06×10^{-03}	8.86×10^{-04}	1.01×10^{-04}	7.34×10^{-06}	1.08×10^{-08}
1.60	0.016 65	0.054 38	0.068 71	0.053 84	0.034 75	0.018 23	7.65×10^{-03}	2.91×10^{-03}	6.98×10^{-04}	1.08×10^{-04}	4.58×10^{-06}
1.80	1.30×10^{-03}	0.012 37	0.039 52	0.058 41	0.055 81	0.042 20	0.025 24	0.014 09	6.34×10^{-03}	2.13×10^{-03}	5.07×10^{-04}