

Studying soft matter with “soft” potentials: fast lattice Monte Carlo simulations and corresponding lattice self-consistent field calculations

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A few mistakes in the lattice self-consistent field (LSCF) calculations in our original paper need to be corrected. First, the initial condition for the one-end-integrated propagator $q_s(\mathbf{r})$ in eqn (6) there should be $q_{s=1}(\mathbf{r}) = \exp[-\omega(\mathbf{r})/N]$. Due to the boundary conditions for impenetrable walls (*i.e.*, $q_s(x=0) = q_s(x=L_x+1) = 0$ for all s) used in the paper, this slightly changes the LSCF results of the segmental density profile $\phi_{\text{LSCF}}(x)$, non-bonded interaction energy per chain $\langle \beta \mathcal{H}^E/n \rangle_{\text{LSCF}}$ (which should be about 0.08466) and thus $\langle n_{\text{pair}}/nC \rangle_{\text{LSCF}}$; the differences can hardly be seen in Fig. 1 and 2. Similarly, the initial condition for the propagator $Q_{p,s}(x|x')$ should be $Q_{p,s=0}(x|x') = \delta_{x,x'} \exp[-\omega(x)/N]$.

Second, the mean-square chain radius of gyration in the x direction should be computed as

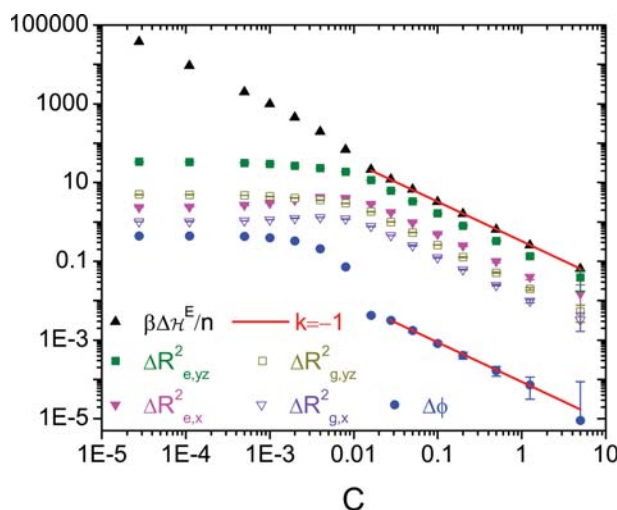
$$\langle R_{g,x}^2 \rangle_{\text{LSCF}} = \frac{1}{N^2} \sum_{s'=1}^{N-1} \sum_{s=s'+1}^N \frac{\sum_x \sum_{x'} \exp\left[\frac{\omega(x) + \omega(x')}{N}\right] q_{N-s+1}(x) Q_{p,s-s'}(x|x') q_{s'}(x') (x-x')^2}{VQ}$$

where the term in the summation with $s' = 1$ and $s = N$ is the mean-square chain end-to-end distance in the x direction, $\langle R_{e,x}^2 \rangle_{\text{LSCF}}$.

While the formula in the paper gives correct $\langle R_{e,x}^2 \rangle_{\text{LSCF}} \approx 10.591$, $\langle R_{g,x}^2 \rangle_{\text{LSCF}}$ reported there is incorrect and should be about 2.2384.

Finally, while our system is homogeneous in the directions parallel to the confining walls, the LSCF results of chain dimensions in these directions are not the same as those of random walk in the bulk, *i.e.*, $\langle R_{e,i}^2 \rangle_{\text{LSCF}} \neq (N-1)/3$ and $\langle R_{g,i}^2 \rangle_{\text{LSCF}} \neq (N^2-1)/18N$ for $i = y$ and z . With the simple cubic lattice model used in the paper, this can be understood by the fact that, for segments in the lattice layers closest to a wall (*i.e.*, at $x = 1$ and L_x), the probability for the next step of the (confined) random walk being along the y (or z) direction is $2/5$, larger than the value of $1/3$ in the bulk. Taking into account that $\phi_{\text{LSCF}}(x=1) = \phi_{\text{LSCF}}(x=L_x) \approx 0.92647$, this gives $\langle R_{e,i}^2 \rangle_{\text{LSCF}} \approx 20.395$ and $\langle R_{g,i}^2 \rangle_{\text{LSCF}} \approx 3.4559$ for $i = y$ and z .

Fig. 3 should therefore be replaced by the figure below, showing that, at large chain number density $C \gtrsim 0.02$, the differences between our fast lattice Monte Carlo (FLMC) and LSCF results in $\langle \beta \mathcal{H}^E/n \rangle$, $\langle R_{e,i}^2 \rangle$ ($i = x, y, z$), $\langle R_{g,i}^2 \rangle$ ($i = x, y, z$), and $\phi(x)$ all scale with $1/C$.



The differences between FLMC and LSCF results in various quantities as a function of chain number density C , where $\beta\Delta\mathcal{H}^E/n \equiv \langle \beta\mathcal{H}^E/n \rangle_{\text{FLMC}} - \langle \beta\mathcal{H}^E/n \rangle_{\text{LSCF}}$, $\Delta R_{e,yz}^2 \equiv \left(\langle R_{e,y}^2 + R_{e,z}^2 \rangle_{\text{FLMC}} - \langle R_{e,y}^2 + R_{e,z}^2 \rangle_{\text{LSCF}} \right) / 2$ with $\Delta R_{g,yz}^2$ similarly defined, $\Delta R_{e,x}^2 \equiv \langle R_{e,x}^2 \rangle_{\text{FLMC}} - \langle R_{e,x}^2 \rangle_{\text{LSCF}}$ with $\Delta R_{g,x}^2$ similarly defined, $\Delta\phi \equiv \sqrt{\sum_{x=1}^{L_x} [\phi_{\text{FLMC}}(x) - \phi_{\text{LSCF}}(x)]^2 / L_x}$, and the two straight lines have a slope of -1 . Note that the error bar for $\beta\Delta\mathcal{H}^E/n$ is smaller than the symbol size and thus not shown. See the original paper for more details.
