

How to optimize Configurational Bias Monte Carlo? Corrections

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Owing to a data transmission problem with this article from the last newsletter, the equations were not printed with correct superscript characters. The corrected equations are printed below. A complete copy of the corrected article is available by ftp or from the WWW server.

The contribution of each i^{th} segment to this Rosenbluth weight is equal to the average of the Boltzmann factors of the trial positions for this segment:

$$W_{\Gamma_i} = \frac{1}{k_i} \sum_{j=1}^{k_i} e^{-\beta U_{\Gamma_{ij}}^{\text{nb}}}, \quad (1)$$

where $\beta = 1/k_B T$ and $U_{\Gamma_{ij}}^{\text{nb}}$ is the non-bonded energy of the j^{th} trial direction for the i^{th} segment. The Rosenbluth weight of the total configuration Γ , is the product of the weights of the individual segments, including the Boltzmann factor of the energy of the first segment, U_{Γ_0} :

$$W_{\Gamma} = e^{-\beta U_{\Gamma_0}} \prod_{i=1}^{\ell} W_{\Gamma_i}, \quad (2)$$

where ℓ is the chain length.

$$\langle P_{\text{add}}(\mathbf{k}_{\ell+1}) \rangle = 1 - \langle (1 - P_{\text{add}}(1))^{\mathbf{k}_{\ell+1}} \rangle. \quad (8)$$

$$\langle P_{\text{add}}(\mathbf{k}_{\ell+1}) \rangle = 1 - (1 - \langle P_{\text{add}}(1) \rangle)^{\mathbf{k}_{\ell+1}}. \quad (9)$$

Figure 1: The efficiency, as defined by equation 7, for inserting a hard dimer (—) and a fully flexible trimer of hard spheres (---) into a fluid of hard spheres at several densities $\rho\sigma^3$, over a range of k -values.