

Errata: Boosting Free-Energy Perturbation Calculations with GPU- Accelerated NAMD

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1 Equation (4)

$$\begin{aligned}\Delta U_{\lambda_{i-1} \rightarrow \lambda_i}^{\text{LJ}} &= U_{\lambda_i}^{\text{LJ}}(\mathbf{x}) - U_{\lambda_{i-1}}^{\text{LJ}}(\mathbf{x}) \\ U_{\lambda_k}^{\text{LJ}}(\mathbf{x}) &= \lambda_k \left[\frac{A}{(r^2 + \delta(1 - \lambda_k))^6} - \frac{B}{(r^2 + \delta(1 - \lambda_k))^3} \right] \quad \forall k = i, i-1\end{aligned}$$