A different calculation scheme for probability-dependent interaction calculation

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Assume that one has a potential that can be written in the following form:

$$U = U(\{\mathbf{r}_i\}) = U(\{p_i(\{\mathbf{r}_j\})\}, \{\mathbf{r}_i\}) \tag{1}$$

where $\{p_i\}$ is a set of per-particle probabilities of occupying a given state. In our case, the probabilities are a function of the local neighborhood and can be calculated using a normal pair neighbor list.

Then, the forces due to this can be calculated all at once, i.e.,

$$\begin{aligned}
\nabla U =& \nabla U(\{\mathbf{r}_i\}) = \nabla U(\{p_i(\{\mathbf{r}_j\})\}, \{\mathbf{r}_i\}) \qquad (2)\\
=& -\left(\sum_{\alpha}(\nabla_i p_{s_i,\alpha}) \cdot (\mu_\alpha - kT \ln p_{s_i,\alpha}) + \sum_{j\in N(i)} \sum_{\alpha} \nabla_i p_{s_j,\alpha} \cdot (\mu_\alpha - kT \ln p_{s_j,\alpha})\right) \qquad (3)\\
& - \left(\sum_{j\in N(i)} \sum_{\alpha\beta} p_{s_i,\alpha} p_{s_j,\beta} \cdot \nabla_i u_{\alpha\beta}\right)\\
& - \Bigg(\Big\{ \sum_{j\in N(i)} \sum_{\alpha\beta} (\nabla_i p_{s_i,\alpha} p_{s_j,\beta} + p_{s_i,\alpha} \nabla_i p_{s_j,\beta}) \cdot u_{\alpha\beta} \Big\}\\
& \quad + \Big\{ \Big(\sum_{\substack{j\notin N(i)\\ k\in N(i)}} \sum_{\alpha\beta} (p_{s_j,\alpha} \nabla_i p_{s_k,\beta}) + \sum_{\substack{j\in N(i)\\ k\notin N(i)}} \sum_{\alpha\beta} (\nabla_i p_{s_j,\alpha} p_{s_k,\beta}) + \sum_{\substack{j\in N(i)\\ k\in N(i)}} \sum_{\alpha\beta} (p_{s_j,\alpha} \nabla_i p_{s_k,\beta}\\
& \qquad + \nabla_i p_{s_j,\alpha} p_{s_k,\beta}) \Big) \cdot u_{\alpha\beta} \Big\} \Bigg)
\end{aligned}$$

and in our special case this has four subforce terms that are very common.

But it can also be done in a few-step procedure, like so:

$$\nabla U(\{p_i(\{\mathbf{r}_j\})\}, \{\mathbf{r}_i\}) = \nabla U(\{p_i(\{\mathbf{r}_j\})\}, \{\mathbf{r}_i\})|_{\{p_i(\{\mathbf{r}_j\})\}} + \sum_i \frac{dU(\{p_i(\{\mathbf{r}_j\})\}, \{\mathbf{r}_i\})}{dp_i}|_{\{\mathbf{r}_j\}} \nabla p_i(\{\mathbf{r}_j\}) \tag{4}$$

The advantage of this is that it is very simple to program in an extensible manner. First, calculate the $\{p_i(\{\mathbf{r}_j\})\}$ in one neighbor loop. Then, calculate $\nabla U(\{p_i(\{\mathbf{r}_j\})\}, \{\mathbf{r}_i\})|_{\{p_i(\{\mathbf{r}_j\})\}}$ and $\sum_i \frac{dU(\{p_i(\{\mathbf{r}_j\})\},\{\mathbf{r}_i\})}{dp_i}|_{\{\mathbf{r}_j\}}$ in a second neighbor loop. Finally, calculate $\{\nabla p_i(\{\mathbf{r}_j\})\}$ in a third neighbor loop.