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.,

$$\nabla U = \nabla U(\{\mathbf{r}_i\}) = \nabla U(\{p_i(\{\mathbf{r}_j\})\}, \{\mathbf{r}_i\}) \tag{2}$$

$$\tag{3}$$

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.