High Performance Computing with C++

Final Report

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Contents

Derivation of LJ-Force

Suppose we have a list of N atoms with the position vectors $\vec{r}_k := [x_k, y_k, z_k]^T$. The vector between a pair of atoms is defined as $\vec{r}_{ij} := \vec{r}_j - \vec{r}_i$. The pair distance r_{ij} is defined as the 2-norm of $\vec{r}_{ij}$:
$r_{ij} := \sqrt{(x_j - x_i)^2 + (y_j - y_i)^2 + (z_j - z_i)^2}$. The potential energy of an atom pair is given by (cite ???):

$$E_{pot_{ij}} = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right] \tag{1}$$

The parameters ϵ and σ tune the potential strength and the resting distance respectively. To get the potential energy of the whole system, we have to sum over all atom pairs:

$$E_{pot} = \frac{1}{2} \sum_{ij,\ i \neq j} E_{pot_{ij}} \tag{2}$$

The force, which the i-th atom exerts on the k-th atom is the pair force:

$$\vec{f}_{ik} = \nabla_{\vec{r}_k} E_{pot_{ik}} = \frac{\partial E_{pot_{ik}}}{\partial r_{ik}} \cdot \nabla_{\vec{r}_k} r_{ik} \tag{3}$$

Using Eq. (1), the first part of Eq. (3) reads:

$$\frac{\partial E_{pot_{ik}}}{\partial r_{ik}} = \frac{24\epsilon(\sigma^6 r_{ik}^6 - 2\sigma^{12})}{r_{ik}^{13}} \tag{4}$$

The first line of the gradient of the pair distance can be calculated as follows:

$$\frac{dr_{ik}}{dx_k} = \frac{1}{2r_{ik}} \cdot 2(x_k - x_i) \cdot (1 - \delta_{ik}) \tag{5}$$

Applying the same principle from Eq. (5) to the other two coordinate axes and plugging it, togerther with the result from Eq. (4), into Eq. (3) yields:

$$\vec{f}_{ik} = \frac{24\epsilon(\sigma^6 r_{ik}^6 - 2\sigma^{12})}{r_{ik}^{14}} \cdot (1 - \delta_{ik}) \cdot \vec{r_{ik}} \tag{6}$$