Calculation of the Hessian for pairwise interactions as a function of squared distance

Consider a particle system with pairwise potentials, its potential energy is:

$$U = \sum_i \sum_{j \neq i} u(r_{ij}^2)$$

where $u(\cdot)$ is a function operating on the square magnitude of vector $r_{ij} = r_j - r_i$. The force for the ith particle of the system is the negative gradient of the potential energy:

$$f_i = -\frac{\partial U}{\partial r_i} = -\sum_{j \neq i} \frac{\partial u}{\partial r_i} = -\sum_{j \neq i} u^{(1)} \frac{\partial (r_{ij})^2}{\partial r_i}$$

where $u^{(n)}$ is th nth derivative of $u(\cdot)$.

Assuming a column vector notation $r_i = (x_i, y_i, z_i)^T$,

$$\frac{\partial (r_{ij})^2}{\partial r_i} = \frac{\partial}{\partial r_i}(r_j - r_i)^T(r_j - r_i) = -2(r_j - r_i), \quad \frac{\partial (r_{ij})^2}{\partial r_j} = 2(r_j - r_i)$$

Therefore

$$f_i = 2\sum_{j \neq i} u^{(1)}(r_j - r_i)$$

For a general implicit integrator, the linear system below is solved

$$\left[\mathbf{I} + \beta \Delta t^2 M^{-1}\mathbf{H}\right]\mathbf{v}_{t+1} = \mathbf{v}_t + \Delta t M^{-1}\mathbf{f}$$

where $\mathbf{H}$ is the Hessian of the potential energy.

Each "element" in the Hessian is a 3×3 matrix:

$$H_{ij} = \frac{\partial^2 U}{\partial r_i r_j^T} = -2\frac{\partial}{\partial r_j^T}\sum_{k \neq i} u^{(1)}(r_k - r_i)$$

For diagonal terms,

$$H_{ii} = 2\sum_{k \neq i}[2u^{(2)}(r_k - r_i)(r_k - r_i)^T + u^{(1)}\mathbf{I}]$$

For off-diagonal terms,

$$H_{ij} = H_{ji} = -2[2u^{(2)}(r_j - r_i)(r_j - r_i)^T + u^{(1)}\mathbf{I}]$$

Note that the center of mass should be stationary, thus the row and column sum of $\mathbf{H}$ is zero.