Gradient term for the 4th-order symplectic integrator

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For the 4th-order forward symplectic integrator, we need to evaluate the gradient term,

$$\boldsymbol{G}_i = \frac{1}{m_i}\frac{\partial}{\partial \boldsymbol{r}_i}\left[\sum_{j=1}^{N} \boldsymbol{F}_j \cdot \boldsymbol{F}_j\right] = \frac{2}{m_i}\sum_{j=1}^{N}\left[\frac{\partial}{\partial \boldsymbol{r}_i}\boldsymbol{F}_j \cdot \boldsymbol{F}_j\right]. \tag{1}$$

Here, $\boldsymbol{F}_i$ is force on particle i and $\boldsymbol{F}_{ij}$ contribution from particle j, i.e.,

$$\boldsymbol{F}_i = \sum_{j \neq i}^{N} \boldsymbol{F}_{ij} = \sum_{j \neq i}^{N} \frac{G m_i m_j}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^3}(\boldsymbol{r}_j - \boldsymbol{r}_i). \tag{2}$$

Thus,

$$\frac{\partial}{\partial \boldsymbol{r}_i}\boldsymbol{F}_j = \frac{\partial}{\partial \boldsymbol{r}_i}\left[\sum_{k \neq j}^{N} \boldsymbol{F}_{jk}\right] = \begin{cases} \displaystyle\sum_{k \neq i}^{N} \frac{\partial}{\partial \boldsymbol{r}_i}\boldsymbol{F}_{ik} & (i = j) \\ \displaystyle\frac{\partial}{\partial \boldsymbol{r}_i}\boldsymbol{F}_{ji} = -\frac{\partial}{\partial \boldsymbol{r}_i}\boldsymbol{F}_{ij} & (i \neq j) \end{cases}. \tag{3}$$

The summation remains only in the diagonal term and disappears elsewhere.

$$\boldsymbol{G}_i = \frac{2}{m_i}\sum_{j \neq i}^{N}\left[\frac{\partial}{\partial \boldsymbol{r}_i}\boldsymbol{F}_{ij}\right] \cdot \left(\boldsymbol{F}_i - \boldsymbol{F}_j\right) \tag{4}$$

For the N-body system, gradient of mutual force in 3×3 matrix is given in,

$$\frac{\partial}{\partial \boldsymbol{r}_i}\frac{(\boldsymbol{r}_j - \boldsymbol{r}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^3} = \frac{-I}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^3} + \frac{3(\boldsymbol{r}_j - \boldsymbol{r}_i) \otimes (\boldsymbol{r}_j - \boldsymbol{r}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^5}, \tag{5}$$

where I is a unit matrix.

Finally we have

$$\boldsymbol{G}_i = 2G\sum_{j \neq i}^{N} m_j\left[\frac{(\boldsymbol{F}_j - \boldsymbol{F}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^3} - \frac{3(\boldsymbol{r}_j - \boldsymbol{r}_i) \cdot (\boldsymbol{F}_j - \boldsymbol{F}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^5}(\boldsymbol{r}_j - \boldsymbol{r}_i)\right]. \tag{6}$$

One can just replace the velocity by the force in the jerk formula to compute it. Note that $\boldsymbol{G}_i h^2$ has a dimension of force (aceleration times mass).

1 Materials

$$\tilde{\boldsymbol{F}}_i = \boldsymbol{F}_i + \frac{h^2}{48}\frac{1}{m_i}\frac{\partial}{\partial \boldsymbol{r}_i}\,|\boldsymbol{F}|^2$$

$$K(\tfrac{1}{6}h)D(\tfrac{1}{2}h)\tilde{K}(\tfrac{2}{3}h)D(\tfrac{1}{2}h)K(\tfrac{1}{6}h)$$

$$\begin{aligned}
&\left[\begin{pmatrix}\partial_1\\ \partial_2\\ \partial_3\end{pmatrix}\begin{pmatrix}F_1 & F_2 & F_3\end{pmatrix}\right]\begin{pmatrix}F_1\\ F_2\\ F_3\end{pmatrix}\\
&=\begin{pmatrix}\partial_1(F_{12}+F_{13}) & \partial_1 F_{21} & \partial_1 F_{31}\\ \partial_2 F_{12} & \partial_2(F_{23}+F_{21}) & \partial_2 F_{32}\\ \partial_3 F_{13} & \partial_3 F_{23} & \partial_3(F_{31}+F_{32})\end{pmatrix}\begin{pmatrix}F_1\\ F_2\\ F_3\end{pmatrix}\\
&=\begin{pmatrix}(\partial_1 F_{12})(F_1-F_2)+(\partial_1 F_{13})(F_1-F_3)\\ (\partial_2 F_{23})(F_2-F_3)+(\partial_2 F_{21})(F_2-F_1)\\ (\partial_3 F_{31})(F_3-F_1)+(\partial_3 F_{32})(F_3-F_2)\end{pmatrix}
\end{aligned}$$

$$|\boldsymbol{F}_{\mathrm{hard}}+\boldsymbol{F}_{\mathrm{soft}}|^2-|\boldsymbol{F}_{\mathrm{hard}}|^2=|\boldsymbol{F}_{\mathrm{soft}}|^2+2\boldsymbol{F}_{\mathrm{hard}}\cdot\boldsymbol{F}_{\mathrm{soft}}$$