Gradient term for the 4th-order symplectic integrator

似鳥啓吾

2018 年 10 月 3 日

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.,

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

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 $\boldsymbol{G}_ih^2$ has a dimension of force (aceleration times mass).