Gradient term for the 4th-order symplectic integrator

似鳥啓吾

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

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

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 (acceleration times mass).

1 Materials

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

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

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

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

2 P^{3}T

Poisson bracket is

$$\{A,B\}=\frac{\partial A}{\partial q}\frac{\partial B}{\partial p}-\frac{\partial B}{\partial q}\frac{\partial A}{\partial p}.$$

We split the Hamiltonian into a hard part and a soft part,

$$H=\underbrace{(T+V_H)}_{\text{hard}}+\underbrace{V_S}_{\text{soft}}.$$

Now,

$$\{T+V_H,V_S\}=\frac{p\cdot F_S}{m} \tag{7}$$

$$\{\{T+V_H,V_S\},V_S\}=\frac{F_S\cdot F_S}{m} \tag{8}$$

$$\{V_S,T+V_H\}=-\frac{p\cdot F_S}{m} \tag{9}$$

$$\begin{aligned}\{\{V_S,T+V_H\},T+V_H\}&=-\frac{1}{m}\{p\cdot F_S,T+V_H\}\\ &=-\frac{1}{m}\left(\frac{1}{m}\left[p\cdot\frac{\partial F_S}{\partial q}\right]p+F_S\cdot F_H\right)\end{aligned} \tag{10}$$

The leading error term is (8).