Gradient term for the 4th-order symplectic integrator

似鳥啓吾

2018 年 11 月 2 日

The Poisson bracket is

$$\{A,\, B\} = \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} \right), \tag{1}$$

and for a Hamiltonian $H = T(p) + V(q)$,

$$\{X,\, V\} = \sum_i \left(\frac{\partial X}{\partial q_i} \cdot F_i \right), \tag{2}$$

where $F_i = -\partial V/\partial q_i$ is force. Thus,

$$\{T,\, V\} = \sum_i \left(\frac{p_i}{m_i} \cdot F_i \right), \tag{3}$$

and

$$\{\{T,\, V\},\, V\} = \sum_j \left[F_j \cdot \frac{\partial}{\partial p_j} \left(\frac{p_i}{m_i} \cdot F_i \right) \right] = \sum_j \left(\frac{F_j \cdot F_j}{m_j} \right), \tag{4}$$

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

$$\boldsymbol{G}_i = -\frac{\partial}{\partial \boldsymbol{r}_i} \left[\sum_{j=1}^{N} \frac{\boldsymbol{F}_j \cdot \boldsymbol{F}_j}{m_j} \right] = -2 \sum_{j=1}^{N} \left[\left(\frac{\partial}{\partial \boldsymbol{r}_i} \boldsymbol{F}_j \right) \cdot \boldsymbol{a}_j \right]. \tag{5}$$

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

$$\boldsymbol{F}_i = \sum_{j \neq i}^{N} \boldsymbol{F}_{ij} = \sum_{j \neq i}^{N} \frac{G m_i m_j}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^3} (\boldsymbol{r}_j - \boldsymbol{r}_i). \tag{6}$$

and $\boldsymbol{a}_i$ is acceleration $\boldsymbol{F}_i/m$. Thus,

$$\frac{\partial}{\partial \boldsymbol{r}_i} \boldsymbol{F}_j = \frac{\partial}{\partial \boldsymbol{r}_i} \left[\sum_{k \neq j}^{N} \boldsymbol{F}_{jk} \right] = \begin{cases} \displaystyle\sum_{k \neq i}^{N} \frac{\partial}{\partial \boldsymbol{r}_i} \boldsymbol{F}_{ik} & (i = j) \\ \displaystyle\frac{\partial}{\partial \boldsymbol{r}_i} \boldsymbol{F}_{ji} = -\frac{\partial}{\partial \boldsymbol{r}_i} \boldsymbol{F}_{ij} & (i \neq j) \end{cases}. \tag{7}$$

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

$$\boldsymbol{G}_i = -2 \sum_{j \neq i}^{N} \left[\frac{\partial}{\partial \boldsymbol{r}_i} \boldsymbol{F}_{ij} \right] \cdot \left(\boldsymbol{a}_i - \boldsymbol{a}_j \right) \tag{8}$$

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

$$\frac{\partial}{\partial \boldsymbol{r}_i} \frac{(\boldsymbol{r}_j - \boldsymbol{r}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^3} = \frac{-I}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^3} + \frac{3(\boldsymbol{r}_j - \boldsymbol{r}_i) \otimes (\boldsymbol{r}_j - \boldsymbol{r}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^5}, \tag{9}$$

where I is a unit matrix.

Finally we have

$$\boldsymbol{G}_i = -2Gm_i \sum_{j \neq i}^{N} m_j \left[\frac{(\boldsymbol{a}_j - \boldsymbol{a}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^3} - \frac{3(\boldsymbol{r}_j - \boldsymbol{r}_i) \cdot (\boldsymbol{a}_j - \boldsymbol{a}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^5} (\boldsymbol{r}_j - \boldsymbol{r}_i) \right]. \tag{10}$$

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.

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

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

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

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

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,

$$
\begin{aligned}
\{T + V_H, V_S\} &= \frac{p \cdot F_S}{m} && (11) \\
\{\{T + V_H, V_S\}, V_S\} &= \frac{F_S \cdot F_S}{m} && (12) \\
\{V_S, T + V_H\} &= -\frac{p \cdot F_S}{m} && (13) \\
\{\{V_S, T + V_H\}, T + V_H\} &= -\left\{\frac{p}{m} \cdot F_S,\ T + V_H\right\} \\
&= -\left(\left[\frac{p}{m} \cdot \frac{\partial F_S}{\partial q}\right] \frac{p}{m} + F_S \cdot F_H\right) && (14)
\end{aligned}
$$

The leading error term is (12).