

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,

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

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

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

Thus,

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

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

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

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

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

where I is a unit matrix.

Finally we have

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

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

1 Materials

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

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

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

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

2 P³T

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,

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

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

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

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

The leading error term is (8).