Rod-Bonded Discrete Element Method

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1. Derivation of Energy Function in Orientation Level

To get an integral in orientation level, we reorganize the orientation-related part of the Newton-Euler equation as follows,

$$\mathbf{q}_i^{(n+1)} - \mathbf{q}_i^{(n)} - \frac{h}{2}\begin{bmatrix}0\\ \boldsymbol{\omega}_i^{(n)}\end{bmatrix}\mathbf{q}_i^{(n)} = \frac{h^2}{2}\begin{bmatrix}0\\ \mathbf{I}_i^{-1}\mathbf{T}_i^{(n+1)}\end{bmatrix}\mathbf{q}_i^{(n)} \quad (1)$$

Multiplying both sides of the equation by $\bar{\mathbf{q}}_i^{(n)}$,

$$\mathbf{q}_i^{(n+1)}\bar{\mathbf{q}}_i^{(n)} - \mathbf{u}_i^{(n)} = \frac{h^2}{2}\begin{bmatrix}\mathbf{0} & \\ & \mathbf{I}_i^{-1}\end{bmatrix}\begin{bmatrix}\mathbf{0}\\ \mathbf{T}_i^{(n+1)}\end{bmatrix}, \quad (2)$$

where $\mathbf{u}_i^{(n)} = \mathbf{q}_I + \frac{h}{2}\begin{bmatrix}0\\ \boldsymbol{\omega}_i^{(n)}\end{bmatrix}$.

Substituting $\begin{bmatrix}0\\ \mathbf{T}_i\end{bmatrix} = \frac{1}{2}\widetilde{\mathbf{T}}_i\bar{\mathbf{q}}_i$ into Eqn. (2) and multiplying both sides by $\mathbf{q}_i^{(n)}$, and moving the moment of inertia to the left-hand side, we get

$$\widetilde{\mathbf{I}}_i((\mathbf{q}_i^{(n+1)} - \mathbf{u}_i^{(n)})\bar{\mathbf{q}}_i^{(n)}) = \frac{h^2}{4}\widetilde{\mathbf{T}}_i\bar{\mathbf{q}}_i \quad (3)$$

for every discrete elements.

Torque parameter $\widetilde{\mathbf{T}}_i$ is conservative about E, $\widetilde{\mathbf{T}}_i = -\nabla_{\mathbf{q}_i}E$[4]. Multiplying both sides by $\mathbf{q}_i^{(n)}$, we further have:

$$(\widetilde{\mathbf{I}}_i((\mathbf{q}_i^{(n+1)} - \mathbf{u}_i^{(n)})\bar{\mathbf{q}}_i^{(n)}))\mathbf{q}_i^{(n)} = -\frac{h^2}{4}\nabla_{\mathbf{q}_i}E. \quad (4)$$

An optimization formulation can be obtained by transposing the right-hand side of Eqn. (4) to the left and integrating:

$$\min_{\mathbf{q}_i^{(n+1)}} \frac{2}{h^2}(\mathbf{q}_i^{(n+1)}\bar{\mathbf{q}}_i^{(n)} - \mathbf{u}_i^{(n)})\widetilde{\mathbf{I}}_i(\mathbf{q}_i^{(n+1)}\bar{\mathbf{q}}_i^{(n)} - \mathbf{u}_i^{(n)}) + E^{(n+1)}. \quad (5)$$

By summing i, the optimization function can be obtained.

$$\min_{\mathbf{q}^{(n+1)}} \frac{2}{h^2}\sum_i \left\|\mathbf{q}_i^{(n+1)}\bar{\mathbf{q}}_i^{(n)} - \mathbf{u}_i^{(n)}\right\|_{\widetilde{\mathbf{I}}_i} + E^{(n+1)}. \quad (6)$$

2. Gradient and Hessian of the Cosserat Energy

We should revisit the matrix multiplication form of quaternion multiplication first.

$$\mathbf{pq} = Q(\mathbf{p})\mathbf{q} = \begin{bmatrix}\Re(\mathbf{p}) & -\Im(\mathbf{p})^T\\ \Im(\mathbf{p}) & \Re(\mathbf{p})\mathbf{1}_{3\times3} + [\Im(\mathbf{p})]^\times\end{bmatrix}\begin{bmatrix}\Re(\mathbf{q})\\ \Im(\mathbf{q})\end{bmatrix}, \quad (7)$$

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where the matrix $[\mathbf{p}]^\times$ is used to represent the vector cross product as a matrix-vector product $\mathbf{p}\times\mathbf{q} = [\mathbf{p}]^\times\mathbf{q}$. Right multiplying a quaternion can also be written in the form of a matrix-vector product:

$$\mathbf{pq} = \hat{Q}(\mathbf{q})\mathbf{p} = \begin{bmatrix}\Re(\mathbf{q}) & -\Im(\mathbf{q})^T\\ \Im(\mathbf{q}) & \Re(\mathbf{q})\mathbf{1}_{3\times3} - [\Im(\mathbf{q})]^\times\end{bmatrix}\begin{bmatrix}\Re(\mathbf{p})\\ \Im(\mathbf{p})\end{bmatrix}. \quad (8)$$

According to [2], the derivative of a rotated vector $\mathbf{R}(\mathbf{q})\mathbf{p}$ w.r.t. $\mathbf{q}$ is

$$\frac{\partial(\mathbf{R}(\mathbf{q})\mathbf{p})}{\partial\mathbf{q}} = 2\hat{Q}(\mathbf{p}\bar{\mathbf{q}})_{3\times4}, \quad (9)$$

where $(\cdot)_{3\times4}$ means we only take the lower 3×4 part of the matrix.

Next, we give the specific derivatives of the strain measure and the Darboux vector. Take the derivative of $\boldsymbol{\Gamma}_{ij}$ with respect to $\mathbf{x}_i$, we get

$$\frac{\partial\boldsymbol{\Gamma}_{ij}}{\partial\mathbf{x}_i} = -\frac{1}{l}(R(\mathbf{q}_{ij})R(\mathbf{q}_{ij}^0))^T. \quad (10)$$

Take the derivative of $\boldsymbol{\Gamma}_{ij}$ w.r.t. $\mathbf{q}_i$, we get

$$\frac{\partial\boldsymbol{\Gamma}_{ij}}{\partial\mathbf{q}_i} = \frac{1}{l}R(\mathbf{q}_{ij}^0)^T\hat{Q}(\partial_s\mathbf{x}\mathbf{q}_{ij})_{3\times4}diag(1,-1,-1,-1)\frac{\partial\mathbf{q}_{ij}}{\partial\mathbf{q}_m}, \quad (11)$$

where

$$\frac{\partial\mathbf{q}_{ij}}{\partial\mathbf{q}_m} = \frac{\mathbf{1} - \mathbf{q}_{ij}\mathbf{q}_{ij}^T}{\|\mathbf{q}_m\|}. \quad (12)$$

The derivative of $\boldsymbol{\Omega}$ w.r.t. $\mathbf{q}_i$ is

$$\frac{\partial\boldsymbol{\Omega}_{ij}}{\partial\mathbf{q}_i} = -\frac{2}{l}(\frac{1}{2}\hat{Q}(\mathbf{q}_j - \mathbf{q}_i)diag(1,-1,-1,-1)\frac{\partial\mathbf{q}_{ij}}{\partial\mathbf{q}_m} - Q(\bar{\mathbf{q}}_{ij})) \quad (13)$$

The force derived from E_{SE} and the torque derived from E_{BT} have been calculated in Eqns. (Main-26, Main-27), the force derived from E_{SE} can be calculated by the following equation

$$\widetilde{\mathbf{T}}_i^{SE} = -\nabla_{\mathbf{q}_i}E_{ij}^{SE} = -(\frac{\partial E_{ij}^{SE}}{\partial\boldsymbol{\Gamma}_{ij}}\frac{\partial\boldsymbol{\Gamma}_{ij}}{\partial\mathbf{q}_i})^T = -l(\frac{\partial\boldsymbol{\Gamma}_{ij}}{\partial\mathbf{q}_i})^T C^\Gamma\boldsymbol{\Gamma}_{ij}. \quad (14)$$

It is very difficult to further derive these derivatives with respect to quaternions using the quaternion representation.

For simplicity, we use the Gauss-Newton method, using an approximate Hessian matrix to ignore the terms containing the second derivative of $\mathbf{\Gamma}$ and $\mathbf{\Omega}$. For example,

$$\begin{aligned} \mathbf{H}^{SE}_{\mathbf{x}_i,\mathbf{x}_i} &\approx l(\frac{\partial \mathbf{\Gamma}_{ij}}{\partial \mathbf{x}_i})^T C^{\Gamma} \frac{\partial \mathbf{\Gamma}_{ij}}{\partial \mathbf{x}_i}, \\ \mathbf{H}^{SE}_{\mathbf{q}_i,\mathbf{x}_i} &\approx l(\frac{\partial \mathbf{\Gamma}_{ij}}{\partial \mathbf{q}_i})^T C^{\Gamma} \frac{\partial \mathbf{\Gamma}_{ij}}{\partial \mathbf{x}_i}. \end{aligned} \tag{15}$$

The other blocks of the Hessian matrix are calculated similarly.

3. Asymmetry Introduced by Torques in [3]

In this section, we first construct a linear system in angular velocity level following Baraff et al.[1]. We take the derivative of the shear torque in [3] to show that the resulting coefficient matrix of the linear system is asymmetric. In a similar way, we explain that the twist torque in [3] is not integrable because its torque derivative matrix in orientation level is asymmetric.

For any discrete element i, the implicit Euler scheme for updating orientation is

$$\begin{cases} \Delta \mathbf{q}_i = \frac{1}{2} h \begin{bmatrix} 0 \\ \boldsymbol{\omega}_i^{(n+1)} \end{bmatrix} \mathbf{q}_i^n \\ \Delta \boldsymbol{\omega}_i = h \mathbf{I}_i^{-1} \mathbf{T}_i^{(n+1)}. \end{cases} \tag{16}$$

Here we consider a simplified case where the torque $\mathbf{T}_i$ depends only on orientation, which is sufficient to show that the coefficient matrix of the angular velocity part in the linear system is asymmetric. Applying a first-order Taylor series expansion to T_i

$$\Delta \boldsymbol{\omega}_i = h \mathbf{I}_i^{-1} (\mathbf{T}_i^{(n)} + \sum_k \frac{\partial \mathbf{T}_i}{\partial \mathbf{q}_k} \Delta \mathbf{q}_k). \tag{17}$$

Eliminating Δq from the above equation, using matrix multiplication in Eqn. (8) instead of quaternion multiplication, we obtain

$$\Delta \boldsymbol{\omega}_i = h \mathbf{I}_i^{-1} (T_i^{(n)} + \frac{h}{2} \sum_k \frac{\partial T_i}{\partial \mathbf{q}_k} \hat{Q}(\mathbf{q}_k) \begin{bmatrix} 0 \\ \boldsymbol{\omega}_k^{(n+1)} \end{bmatrix}). \tag{18}$$

After regrouping, each particle has the following equation

$$\begin{aligned} &(\mathbf{I}_i - \frac{h^2}{2} \frac{\partial T_i}{\partial \mathbf{q}_i} \hat{Q}(\mathbf{q}_i) \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix}) \Delta \boldsymbol{\omega}_i - \frac{h^2}{2} \sum_{k \neq i} \frac{\partial T_i}{\partial \mathbf{q}_k} \hat{Q}(\mathbf{q}_k) \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix} \Delta \boldsymbol{\omega}_k \\ &= h(T_i^{(n)} + \frac{h}{2} \sum_k \frac{\partial T_i}{\partial \mathbf{q}_k} \hat{Q}(\mathbf{q}_k) \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix} \boldsymbol{\omega}_k), i = 1, ..., m, \end{aligned} \tag{19}$$

, forming a linear system. $\begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix}$ is a 4×3 matrix, and its upper and lower parts are respectively a 3×3 identity matrix and a 1×3 zero vector. Defining $K_{ij} = \frac{\partial T_i}{\partial \mathbf{q}_j} \hat{Q}(\mathbf{q}_j) \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix}$ and $K_{ji} = \frac{\partial T_j}{\partial \mathbf{q}_i} \hat{Q}(\mathbf{q}_i) \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix}$, it is easy to see that K_{ij} and K_{ji} are 3×3 block matrices in the symmetrical position of the coefficient matrix(omit $\frac{h^2}{2}$).

In [3], the shear torque of the bond are obtained by calculating the rotation angle between the shear direction and the normal direction. The shear direction $\mathbf{d}_s$ is defined as

$$\begin{bmatrix} 0 \\ \mathbf{d}_s \end{bmatrix} = \frac{1}{2} (\mathbf{q}_i \begin{bmatrix} 0 \\ \mathbf{d}_0 \end{bmatrix} \bar{\mathbf{q}}_i + \mathbf{q}_j \begin{bmatrix} 0 \\ \mathbf{d}_0 \end{bmatrix} \bar{\mathbf{q}}_j). \tag{20}$$

where $\mathbf{d}_0$ is the initial bond direction. The shear torque applied to particle i is

$$\mathbf{M}_i^s = \frac{1}{2} l k_s (\mathbf{n} \times \frac{\mathbf{d}_s}{\|\mathbf{d}_s\|}), \tag{21}$$

where $\mathbf{n} = (\mathbf{x}_i - \mathbf{x}_j) / \left\|\mathbf{x}_i - \mathbf{x}_j\right\|$. The torque with respect to the opposite particle j is $\mathbf{M}_j^s = \mathbf{M}_i^s$.

Now we can substitute $\mathbf{M}^s$ into the block matrices K_{ij} and K_{ji} from the coefficient matrix in Eqn. (19)

$$\begin{aligned} K_{ij} &= \frac{\partial \mathbf{M}_i^s}{\partial \mathbf{d}_s} \frac{\partial \mathbf{d}_s}{\partial \mathbf{q}_j} \hat{Q}(\mathbf{q}_j) \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix}, \\ K_{ji} &= \frac{\partial \mathbf{M}_i^s}{\partial \mathbf{d}_s} \frac{\partial \mathbf{d}_s}{\partial \mathbf{q}_i} \hat{Q}(\mathbf{q}_i) \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix}. \end{aligned} \tag{22}$$

It can be seen that the front part of K_{ij} and K_{ji} are both $2 \frac{\partial \mathbf{M}_i^s}{\partial \mathbf{d}_s}$, while the back part is only related to $\mathbf{q}_i$ and $\mathbf{q}_j$ respectively. $\mathbf{q}_i$ and $\mathbf{q}_j$ are completely independent variables, so for any $\mathbf{q}_i$, there is a $\mathbf{q}_j$ such that $K_{ij} \neq K_{ji}^T$, i.e, the coefficient matrix is asymmetric.

For implicit integration in orientation level, we first convert the torque into the torque parameter according to Eqn. (Main-28), because the torque parameter can be considered as the first derivative of energy with respect to the quaternion. We further take derivatives of the obtained torque parameters, and find that its torque derivative matrix is asymmetric.

The torque parameter applied to the discrete element i, j has the following forms respectively,

$$2\hat{Q}(\mathbf{q}_i) \begin{bmatrix} 0 \\ \mathbf{T}_i \end{bmatrix}, 2\hat{Q}(\mathbf{q}_j) \begin{bmatrix} 0 \\ \mathbf{T}_j \end{bmatrix}. \tag{23}$$

In [3], the twist torque has the following calculation form,

$$\mathbf{M}_i^t = k_t (\theta \mathbf{a} \cdot \mathbf{n}) \mathbf{n}, \tag{24}$$

where $\mathbf{a} = \frac{\Im(\mathbf{q}_t)}{|\Im(\mathbf{q}_t)|}, \theta = 2 \arccos \Re\left(\mathbf{q}_t\right)$, and $\mathbf{q}_t = \mathbf{q}_j \bar{\mathbf{q}}_i$. And the twist torque with respect to the opposite particle j is $\mathbf{M}_j^t = -\mathbf{M}_i^t$.

Here, if we use L_{ij}, L_{ji} to represent the derivative of torque paramters in Eqn. (23), we have

$$\begin{aligned} L_{ij} &= 2\hat{Q}(\mathbf{q}_i) \begin{bmatrix} 0 \\ I \end{bmatrix} \frac{\partial \mathbf{M}_i^t}{\partial \mathbf{q}_t} \hat{Q}(\bar{\mathbf{q}}_i) \\ L_{ji} &= -2\hat{Q}(\mathbf{q}_j) \begin{bmatrix} 0 \\ I \end{bmatrix} \frac{\partial \mathbf{M}_i^t}{\partial \mathbf{q}_t} Q(q_j) diag(1, -1, -1, -1). \end{aligned} \tag{25}$$

The asymmetry of the matrix can be found like Eqn. (22), which means that the torque in [3] is not integrable in orientation level.

References

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