Projective Peridynamic Modeling of Hyperelastic Membranes with Contact: Supplementary Technical Document

April 7, 2023

This material serves as a supplementary technical document, so we suppose readers have read the original article. Some notation will not be repeated and share the same definition if it is not being mentioned again.

1 Extended Shape tensor and deformation tensor

We will first show that the extended shape tensor $\mathbf{K}_i$ is non-singular, so that deformation gradient can be calculated as Eq.(15) in the article.

1.1 Non-singularity of Extended Shape Tensor

Silling and Lehoucq [3] demonstrate that if the deformation is sufficiently smooth, the peridynamic stress tensor converges to a Piola-Kirchhoff stress tensor, which is a function only of the local deformation gradient tensor, as in the classical theory. Originally, the 3×3 deformation gradient tensor $\mathbf{F}_i$ has

$$\mathbf{F}_i = \left(\sum_j \omega_{ij} (\mathbf{y}_j - \mathbf{y}_i)(\mathbf{x}_j - \mathbf{x}_i)^T \right) \mathbf{K}_i^{-1}, \tag{1}$$

the 3×3 shape tenson $\mathbf{K}_i$ calculated as

$$\mathbf{K}_i = \sum_j \omega_{ij} (\mathbf{x}_j - \mathbf{x}_i)(\mathbf{x}_j - \mathbf{x}_j)^T, \tag{2}$$

where ω is a **scalar non-negative state** acting as a weighting function, $\mathbf{x}, \mathbf{y}$ represented the rest shape and currently deformed shape.

As for a co-dimensional membrane/plane model, it is possible that the rest shape remains to lay on a plane of $\mathbb{R}^3$. Denoted the plane as

$$\mathbf{v} + \mathbf{X} \tag{3}$$

where $\mathbf{v}$ is a transform and $\mathbf{X}$ is hyperplane with two chosen orthonormal vector bases in $\mathbb{R}^3$ as $\mathbf{e}_1, \mathbf{e}_2$ (**distincted from the conventional orthonormal vector bases of** $\mathbb{R}^3$, e.g., $\mathbf{e}_1 = (1,0,0)^T$, which are not necessarily or able to be chosen for the hyperplane we discussed above), then we have $\mathbf{X} = \{q^1\mathbf{e}_1 + q^2\mathbf{e}_2 | \forall q^1, q^2 \in \mathbb{R}\}$, and $\mathbb{R}^3 = \mathbf{X} \oplus \mathbf{X}^\perp, \mathbf{X} \cap \mathbf{X}^\perp = \varnothing$, where $\mathbf{X}^\perp$ is the orthogonal complement space of $\mathbf{X}$, and $\oplus$ denotes the direct sum operator. It is simple to show that, with the concept of orthogonal complement space and direct sum, by denoting the orthonormal vector base of $\mathbf{X}^\perp$ as $\mathbf{e}_3$, we then have $\mathbf{X}^\perp = \{q^3\mathbf{e}_3 | \forall q^3 \in \mathbb{R}, \mathbf{e}_3 = \pm\mathbf{e}_1 \times \mathbf{e}_2\}$, since only $\mathbf{e}_3 = \pm\mathbf{e}_1 \times \mathbf{e}_2$ provides orthogonality to $\mathbf{e}_1$ and $\mathbf{e}_2$ with unit length. To make a convention, we use the defininition of $\mathbf{e}_3 = \mathbf{e}_1 \times \mathbf{e}_2$.

Extended shape tensor

$$\mathbf{K}_i = \sum_j \omega_{ij} (\mathbf{x}_j - \mathbf{x}_i)(\mathbf{x}_j - \mathbf{x}_i)^T + \mathbf{x}_i^\perp \otimes \mathbf{x}_i^\perp, \tag{4}$$

where $\mathbf{x}_i^\perp = \xi \text{norm} \left(\frac{\sum_J \theta_J \mathbf{n}_J}{\sum_J \theta_J} \right)$, J denotes triangle contained vertex i with index J, θ_J is the inner angle of triangle J at vertex i, $\mathbf{n}_J$ is the normal of triangle J represented as $\text{norm}\left((\mathbf{x}_J^2 - \mathbf{x}_J^0) \times (\mathbf{x}_J^1 - \mathbf{x}_J^0) \right)$, where the superscript $(\cdot)^{\{1,2,3\}}$ denotes three related vertexes in triangle and $\text{norm}(\cdot)$ denotes normalization operator.

We use $\{\mathbf{x}\}$ to denote all vertexes in the neighborhood of vertex i on rest shape, and $\{\mathbf{y}\}$ on the deformed shape. The adjacency relation is chosen as 1-neighborhood, which means that $\{\mathbf{x}\}$ collects all vertexes connected to vertex i with an edge, so that any vertex in $\{\mathbf{x}\}$ will be in a triangle which contain vertex i. (The generality will not get limited by such neighborhood chosen, since if a minimal neighborhood can guarantee the non-singularity of shape tensor, so does an expanded one). As $\{\mathbf{x}\}$ is a point set, $\{\mathbf{x}-\mathbf{x}_i\} := \{\mathbf{x}-\mathbf{x}_i|\forall \mathbf{x}\in\{\mathbf{x}\}\}$ provides the corresponding vector set. With the above illustration, if neighbors of vertex i lay on a plane, the Eq. (3) can be describe as $(\mathbf{x}_i - \mathbf{o}) + \mathbf{X}_i$, where $\mathbf{X}_i$ is the spanning space of $\{\mathbf{x}-\mathbf{x}_i\}$ and $\mathbf{o}$ the original point. Also we have $\mathbf{X}_i$ is a hyperplane of $\mathbb{R}^3$, i.e. $\forall \mathbf{u}\in\mathbf{X}_i = \{q^1\mathbf{e}_1 + q^2\mathbf{e}_2|\forall q^1, q^2\in\mathbb{R}\}$. An illustrative diagram on Fig. 1 will outline such case.

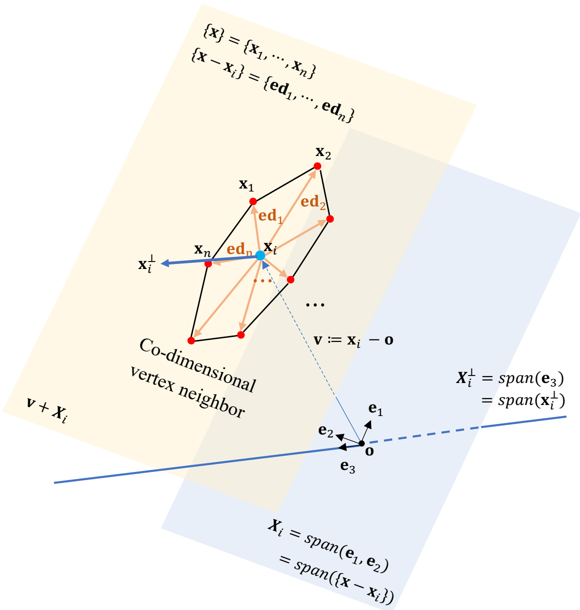

Figure 1: Illustrative diagram of the co-dimensional case.

We show that, in this case, the extended shape tensor is non-singluar.

On the other hand, we also show that if $\{\mathbf{x}-\mathbf{x}_i\}$ span $\mathbb{R}^3$, the extended shape tensor will also keep its non-singluarity.

We use some mathematical convention if not mentioned, e.g., $\otimes$ the Kronecker product and concepts on linear algebra.

Given Eq. (4), we proof the following two lemmas:

Lemma 1 *$span(\{\mathbf{x}-\mathbf{x}_i\}) := \mathbf{X}_i = \{q^1\mathbf{e}_1 + q^2\mathbf{e}_2|\forall q^1, q^2\in\mathbb{R}\}$, then we have $span(\{\mathbf{x}-\mathbf{x}_i\}\cup\{\mathbf{x}_i^\perp\}) = \mathbb{R}^3$, as $\mathbf{x}_i^\perp$ is given to be $\mathbf{x}_i^\perp = \xi\mathrm{norm}\left(\frac{\sum_J \theta_J\mathbf{n}_J}{\sum_J\theta_J}\right)$.*

Proof. Because of the adjacency relationship chosen above, we have that the collection set of vertexes of any triangle J which contain vertex i is the same as $\{\mathbf{x}\}\cup\{\mathbf{x}_i\}$ (See the diagram and the above discussion for an outline). Then we have $\mathbf{n}_J = \mathrm{norm}\left((\mathbf{x}_J^2-\mathbf{x}_J^0)\times(\mathbf{x}_J^1-\mathbf{x}_J^0)\right)$, the superscript denotes inner vertexes of triangle and they also in set $\{\mathbf{x}\}\cup\{\mathbf{x}_i\}$. If $\mathbf{x}_J^0 = \mathbf{x}_i$, then we will always have $(\mathbf{x}_J^2-\mathbf{x}_J^0)\in\{\mathbf{x}-\mathbf{x}_i\}$, $(\mathbf{x}_J^1-\mathbf{x}_J^0)\in\{\mathbf{x}-\mathbf{x}_i\}$. If $\mathbf{x}_J^0$ is not $\mathbf{x}_i$, then we will have, i.e., like $\mathbf{x}_J^2 = \mathbf{x}_i$, then $(\mathbf{x}_J^2-\mathbf{x}_J^0)\in\mathrm{span}(\{\mathbf{x}-\mathbf{x}_i\})$, $(\mathbf{x}_J^2-\mathbf{x}_J^1)\in\mathrm{span}(\{\mathbf{x}-\mathbf{x}_i\})$, and thus $\mathbf{x}_J^1-\mathbf{x}_J^0 = (\mathbf{x}_J^1-\mathbf{x}_J^2)-(\mathbf{x}_J^0-\mathbf{x}_J^2)\in\mathrm{span}(\{\mathbf{x}-\mathbf{x}_i\})$.

This gives the edges of triangle J, i.e., $\mathbf{ed}_{(\cdot)} := \mathbf{x}_J^{(\cdot)}-\mathbf{x}_J^0\in\mathrm{span}(\{\mathbf{x}-\mathbf{x}_i\})$, so that $\mathbf{ed}_1 = q_1^1\mathbf{e}_1 + q_1^2\mathbf{e}_2$, $\mathbf{ed}_2 = q_2^1\mathbf{e}_1 + q_2^2\mathbf{e}_2$. Then $\mathbf{n}_J = \mathrm{norm}(\mathbf{ed}_1\times\mathbf{ed}_2) = \mathrm{norm}((q_1^1\mathbf{e}_1+q_1^2\mathbf{e}_2)\times(q_2^1\mathbf{e}_1+q_2^2\mathbf{e}_2)) = \mathrm{norm}((q_1^1q_2^2 - q_1^2q_2^1)\mathbf{e}_3)$. As the term $(q_1^1q_2^2 - q_1^2q_2^1)$ is the determinant, i.e., double area of the planar triangle, if the triangle keeps non-degenerated, then this term will keep non-zero. If all triangle degenerated to a segment, then the co-dimensional material will remain to be a line, which is not the cases we design. Then we have $\mathbf{n}_J = \mathrm{norm}((q_1^1q_2^2 - q_1^2q_1^2)\mathbf{e}_3) = \mathbf{e}_3$. Here our primitive are manipulated through an algorithm to keep the vertex and triangle norm remain outer.

Then following $\mathbf{x}_i^\perp = \xi \text{norm}(\sum_J \theta_J \mathbf{n}_J / \sum_J \theta_J)$, it is simply to verify that $\mathbf{x}_i^\perp = \xi \mathbf{e}_3$, so that we have $\text{span}(\{\mathbf{x} - \mathbf{x}_i\} \cup \{\mathbf{x}_i^\perp\}) = \mathbb{R}^3$.

$\square$

Lemma 2 *Spectral Representation.*
*Given a vector set (with n vectors) $\{\mathbf{u}_i\}$ spanning $\mathbb{R}^3$, i.e., span$(\{\mathbf{u}_i\}) = \mathbb{R}^3 = \{q^1\mathbf{e}_1 + q^2\mathbf{e}_2 + q^3\mathbf{e}_3 | \forall q^1, q^2, q^3 \in \mathbb{R}\}$, its generated second-order tensor $\mathbf{U} = \sum_{i=1}^n \omega_i \mathbf{u}_i \otimes \mathbf{u}_i$, $\omega_i > 0$ has **spectral representation** as $\mathbf{U} = \sum_{k=1}^3 \lambda_k \mathbf{n}_k \otimes \mathbf{n}_k$, where $\lambda_k \neq 0$ and $\{\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3\}$ are orthonormal vertor basis.*

Proof. As $\sum_{i=1}^n \omega_i \mathbf{u}_i \otimes \mathbf{u}_i$ is a real-symmetric matrix, it has spectral representation (from spectral theorem) as $\sum_{i=1}^n \omega_i \mathbf{u}_i \otimes \mathbf{u}_i = \sum_{k=1}^3 \lambda_k \mathbf{n}_k \otimes \mathbf{n}_k$, where $\{\mathbf{n}_k\}$ are three orthonormal vectors. We have to show that each $\lambda_k \neq 0$. When $\{\mathbf{u}_i\}$ spanning $\mathbb{R}^3$, we have $\mathbf{u}_i = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)\mathbf{q}_i = \mathbf{E} \cdot \mathbf{q}_i$, where $\mathbf{E} = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ are chosen orthonormal vertor basis and $\mathbf{q}_i$ are the coordinate of $\mathbf{u}_i$ at such basis. We then have: $\sum_{i=1}^n \omega_i \mathbf{u}_i \otimes \mathbf{u}_i = \mathbf{E}\left(\sum_{i=1}^n \omega_i \mathbf{q}_i \otimes \mathbf{q}_i\right)\mathbf{E}^T$.

Now, consider if exists $\lambda_k = 0$. Then we have $\left(\sum_{k=1}^3 \lambda_k \mathbf{n}_k \otimes \mathbf{n}_k\right) \cdot \mathbf{n}_k = \mathbf{0}, \mathbf{n}_k \neq \mathbf{0}$ and $\left(\sum_{i=1}^n \omega_i \mathbf{u}_i \otimes \mathbf{u}_i\right) \cdot \mathbf{n}_k = \mathbf{0}$. Expresses $\mathbf{n}_k$ as $\mathbf{n}_k = \mathbf{E} \cdot \mathbf{q}_k$ in vector basis $\mathbf{E}$ and its coordinate $\mathbf{q}_k$. The above equation becomes:

$$\mathbf{E}\left(\sum_{i=1}^n \omega_i \mathbf{q}_i \otimes \mathbf{q}_i\right)\mathbf{E}^T \cdot \mathbf{E} \cdot \mathbf{q}_k = \mathbf{0}, \tag{5}$$

which gives: $\mathbf{E}\left(\sum_{i=1}^n \omega_i \mathbf{q}_i \otimes \mathbf{q}_i\right) \cdot \mathbf{q}_k = \mathbf{0}$. Because $\mathbf{E}$ is a vector basis matrix of $\mathbb{R}^3$, the only solution exists that $\mathbf{E} \cdot \mathbf{q} = \mathbf{0}$ as $\mathbf{q} = \mathbf{0}$, so that we must have $\left(\sum_{i=1}^n \omega_i \mathbf{q}_i \otimes \mathbf{q}_i\right) \cdot \mathbf{q}_k = \mathbf{0}$.

Now, we denote $\mathbf{N} = \sum_{i=1}^n \omega_i \mathbf{q}_i \otimes \mathbf{q}_i$ and show that $\mathbf{N} \cdot \mathbf{q}_k = \mathbf{0}$, if and only $\mathbf{q}_k = \mathbf{0}$ or $\forall \mathbf{q}_i, \mathbf{q}_k \cdot \mathbf{q}_i = 0$. Firstly, the sufficient condition is simple: if $\mathbf{q}_k = \mathbf{0}$, then it is obviously to show $\mathbf{N} \cdot \mathbf{q}_k = \mathbf{0}$ and if $\forall \mathbf{q}_i$, $\mathbf{q}_i \cdot \mathbf{q}_k = 0$, then $\mathbf{N} \cdot \mathbf{q}_k = \mathbf{0}$.

Now we want to show the necessary condition: if $\mathbf{N} \cdot \mathbf{q}_k = \mathbf{0}$, then $\mathbf{q}_k = \mathbf{0}$ or $\forall \mathbf{q}_i$, $\mathbf{q}_i \cdot \mathbf{q}_k = 0$. Assume $\mathbf{q}_k \neq \mathbf{0}$ and there exists some $\{\mathbf{q}_i\}$ s.t. $\mathbf{q}_i \cdot \mathbf{q}_k \neq 0$, then we at most choose three orthonormal vectors, s.t. $\mathbf{q}_1 \cdot \mathbf{q}_k \neq 0, \mathbf{q}_2 \cdot \mathbf{q}_k \neq 0, \mathbf{q}_3 \cdot \mathbf{q}_k \neq 0$ to represent $\mathbf{q}_i$. Denoted $\mathbf{q}_i = \alpha_i \mathbf{q}_1 + \beta_i \mathbf{q}_2 + \gamma_i \mathbf{q}_3$, we then have:

$$\begin{aligned} \mathbf{N} \cdot \mathbf{q}_k &= \left(\sum_{i=1}^n \omega_i(\alpha_i \mathbf{q}_1 + \beta_i \mathbf{q}_2 + \gamma_i \mathbf{q}_3) \otimes (\alpha_i \mathbf{q}_1 + \beta_i \mathbf{q}_2 + \gamma_i \mathbf{q}_3)\right) \cdot \mathbf{q}_k \\ &= \sum_{i=1}^n \omega_i \alpha_i (\mathbf{q}_i \cdot \mathbf{q}_k)\mathbf{q}_1 + \sum_{i=1}^n \omega_i \beta_i (\mathbf{q}_i \cdot \mathbf{q}_k)\mathbf{q}_2 + \sum_{i=1}^n \omega_i \gamma_i (\mathbf{q}_i \cdot \mathbf{q}_k)\mathbf{q}_3 = \mathbf{0}, \end{aligned} \tag{6}$$

which gives three parameter equations of $\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3$ correspondingly to be zero, since $\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3$ are chosen orthonormal.

We look at the equations (also remind $\omega_i > 0$):

$$\begin{cases} \sum_{i=1}^n \omega_i \alpha_i (\mathbf{q}_i \cdot \mathbf{q}_k) = 0 \\ \sum_{i=1}^n \omega_i \beta_i (\mathbf{q}_i \cdot \mathbf{q}_k) = 0 \\ \sum_{i=1}^n \omega_i \gamma_i (\mathbf{q}_i \cdot \mathbf{q}_k) = 0. \end{cases} \tag{7}$$

Case 1. If $\{\mathbf{q}_i\}$ lays on span$(\{\mathbf{q}_1\})$ (this chosen of one basis does not limit general cases), then $\alpha_i \neq 0, \beta_i = 0$, $\gamma_i = 0$. As $\sum_{i=1}^n \omega_i \alpha_i (\mathbf{q}_i \cdot \mathbf{q}_k) = \sum_{i=1}^n \omega_i \alpha_i^2 (\mathbf{q}_1 \cdot \mathbf{q}_k) = 0$, which gives $\mathbf{q}_1 \cdot \mathbf{q}_k = 0$. Then we have $\mathbf{q}_i \cdot \mathbf{q}_k = 0$.

Case 2. If $\{\mathbf{q}_i\}$ lays on span$(\{\mathbf{q}_1, \mathbf{q}_2\})$ (this chosen of two basises does not limit general cases), then $\gamma_i = 0$. Then we will have :

$$\begin{cases} \sum_{i=1}^n \omega_i \alpha_i^2 (\mathbf{q}_1 \cdot \mathbf{q}_k) + \sum_{i=1}^n \omega_i \alpha_i \beta_i (\mathbf{q}_2 \cdot \mathbf{q}_k) = 0 \\ \sum_{i=1}^n \omega_i \alpha_i \beta_i (\mathbf{q}_1 \cdot \mathbf{q}_k) + \sum_{i=1}^n \omega_i \beta_i^2 (\mathbf{q}_2 \cdot \mathbf{q}_k) = 0. \end{cases} \tag{8}$$

If $\sum_{i=1}^n \omega_i \alpha_i \beta_i = 0$, then we have $\mathbf{q}_1 \cdot \mathbf{q}_k = 0, \mathbf{q}_2 \cdot \mathbf{q}_k = 0$, since $\{\mathbf{q}_i\}$ lays on span$(\{\mathbf{q}_1, \mathbf{q}_2\})$ gives that $\exists \mathbf{q}_i, \mathbf{q}_j$, *s.t.* $\alpha_i, \beta_j \neq 0$ and thus $\sum_i \omega_i \alpha_i^2 > 0, \sum_i \omega_i \beta_i^2 > 0$. If $\sum_i \omega_i \alpha_i \beta_i \neq 0$, the above equation can be deduced as $\left((\sum_i \omega_i \alpha_i \beta_i)^2 - (\sum_i \omega_i \alpha_i^2)(\sum_i \omega_i \beta_i^2)\right) \cdot (\mathbf{q}_2 \cdot \mathbf{q}_k) = 0$. As the first term is a classical equation which gives $\left((\sum_i \omega_i\alpha_i\beta_i)^2 - (\sum_i \omega_i\alpha_i^2)(\sum_i \omega_i\beta_i^2)\right) = 0$ if and only if $\forall i,\ \alpha_i = \beta_i$, then we have $\{\mathbf{q}_i\}$ lays on space spanning by a single vector $\mathbf{q}_1 + \mathbf{q}_2$, which is discussed on Case 1. Then we have the equation has to stand for other cases with arbitrary $\omega_i, \alpha_i, \beta_i$ gives $\mathbf{q}_1 \cdot \mathbf{q}_k = 0, \mathbf{q}_2 \cdot \mathbf{q}_k = 0$. Then we have $\mathbf{q}_i \cdot \mathbf{q}_k = 0$.

Case 3. If $\mathbf{q}_i$ lays on span($\{\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3\}$), the above equation set with three equations has unique solution, since $\mathbf{q}_k$ has three unknowns, then the number of equations is the same as the number of unknowns. It is simple to verify that this unique solution is $\mathbf{q}_k = \mathbf{0}$. Then we have $\mathbf{q}_i \cdot \mathbf{q}_k = 0$.

Now we have already verified that $\mathbf{N} \cdot \mathbf{q}_k = \mathbf{0}$ if and only if $\mathbf{q}_k = \mathbf{0}$ or $\forall \mathbf{q}_i,\ \mathbf{q}_i \cdot \mathbf{q}_k = 0$. As $\{\mathbf{u}_i\}$ span $\mathbb{R}^3$, then its coordinate $\{\mathbf{q}_i\}$ on vector basis $\mathbf{E}$ also span $\mathbb{R}^3$, which means that $\forall \mathbf{q}_i,\ \mathbf{q}_i \cdot \mathbf{q}_k = 0$ gives $\mathbf{q}_k = \mathbf{0}$.

Above Eq. (5) we assume that there exist $\lambda_k = 0$. By showing that $\mathbf{q}_k = \mathbf{0}$ uniquely, which means that the solution of $\left(\sum_i^n \omega_i \mathbf{u}_i \otimes \mathbf{u}_i\right)\mathbf{n} = \mathbf{0}$ only have zero trivial solution $\mathbf{n} = \mathbf{0}$, so that $\mathbf{U} = \sum_{k=1}^3 \lambda_k \mathbf{n}_k \otimes \mathbf{n}_k$ is of full rank. Then the assumption of existing $\lambda_k = 0$ is not stand. So we have $\lambda_k \neq 0, \forall k = 1, 2, 3$.

□

Theorem 1 *For a* 3×3 *second-order tensor of* $\mathbf{U} = \lambda_1 \mathbf{n}_1 \otimes \mathbf{n}_1 + \lambda_2 \mathbf{n}_2 \otimes \mathbf{n}_2 + \lambda_3 \mathbf{n}_3 \otimes \mathbf{n}_3$*, where* $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$ *are orthonormal vector basis and* $\lambda_k \neq 0,\ k = 1, 2, 3$*. Then the tensor is non-singular, with inverse* $\mathbf{U}^{-1} = \lambda_1^{-1}\mathbf{n}_1 \otimes \mathbf{n}_1 + \lambda_2^{-1}\mathbf{n}_2 \otimes \mathbf{n}_2 + \lambda_3^{-1}\mathbf{n}_3 \otimes \mathbf{n}_3$.

Proof. Yet simple to verify $\mathbf{U}\mathbf{U}^{-1} = \mathbf{U}^{-1}\mathbf{U} = \mathbf{I}$, where $\mathbf{I}$ is the 3×3 identity matrix.

□

From Lem. (1), Lem. (2) and Theo. (1), it is shown that as if the vertex neighborhood remains to be of full dimension, i.e., either by extending the neighborhood with $\mathbf{x}_i^{\perp}$ or the neighborhood originally keeping full dimension (e.g., of some complex configuration embeded in $\mathbb{R}^3$), then our extended shape tensor will always keep its non-singularity (from Lem. (2) and Theo. (1)), so that its inverse $\mathbf{K}_i^{-1}$ exists. The full-dimensional (extended) neighborhood has been a sufficient condition. So even if original shape tensor has already kept non-singularity, adding the $\mathbf{x}_i^{\perp} \otimes \mathbf{x}_i^{\perp}$ part will not change this.

In the next section, we show that, such extension will also guarantee rest and affine transform stability.

1.2 Rest and Rigid-body deformation stability for the Extended Deformation Gradient

Extended deformation gradient

$$\mathbf{F}_i = \left(\sum_j \omega_{ij}(\mathbf{y}_j - \mathbf{y}_i)(\mathbf{x}_j - \mathbf{x}_i)^T + \mathbf{y}_i^{\perp} \otimes \mathbf{x}_i^{\perp}\right)\mathbf{K}_i^{-1}. \tag{9}$$

We shown that, if the deformation configuration $\{\mathbf{y}\} = \{\mathbf{x}\}$, which should give $\mathbf{F}_i = \mathbf{I}$, and the affine transform configuration $\{\mathbf{y}\} = \mathbf{R}\{\mathbf{x}\} + \mathbf{v}$, where $\mathbf{R}$ is a rotational matrix and $\mathbf{v}$ a movement, which should gives $\mathbf{F}_i = \mathbf{R}$.

When $\{\mathbf{y}\} = \{\mathbf{x}\}$, $\mathbf{D}_i := \left(\sum_j \omega_{ij}(\mathbf{y}_j - \mathbf{y}_i)(\mathbf{x}_j - \mathbf{x}_i)^T + \mathbf{y}_i^{\perp} \otimes \mathbf{x}_i^{\perp}\right)$ is exactly the same as $\mathbf{K}_i$, so that we will simply get $\mathbf{F}_i = \mathbf{D}_i\mathbf{K}_i^{-1} = \mathbf{K}_i\mathbf{K}_i^{-1} = \mathbf{I}$.

When $\{\mathbf{y}\} = \mathbf{R}\{\mathbf{x}\} + \mathbf{v}$, $\mathbf{y}_j - \mathbf{y}_i = \mathbf{R}(\mathbf{x}_j - \mathbf{x}_i)$. Now we look at the extended term $\mathbf{y}_i^{\perp} \otimes \mathbf{x}_i^{\perp}$. As

$$\mathbf{x}_i^{\perp} = \xi \mathrm{norm}\left(\frac{\sum_J \theta_J \mathbf{n}_J}{\sum_J \theta_J}\right), \mathbf{y}_i^{\perp} = \xi \mathrm{norm}\left(\frac{\sum_J \theta'_J \mathbf{n}'_J}{\sum_J \theta'_J}\right), \tag{10}$$

where ξ represents the thickness of the membrane measured from surface to the mid-surface; J is the index of all neighboring triangles; θ_J is inner angle of triangle J with apex of vertex i; $\mathbf{n}_J$ is the triangle normal, and norm$(\cdot)$ is used to normalize a vector. The superscript $'$ for θ and $\mathbf{n}$ is used to denote quantities in the deformed configuration. As θ_J remains to be unchanged through affine transform, the only condition we have to verify is that $\forall J,\ \mathbf{n}'_J = \mathbf{R}\mathbf{n}_J$. Then we have: $\mathbf{n}'_J = \mathrm{norm}\left((\mathbf{y}_J^2 - \mathbf{y}_J^0) \times (\mathbf{y}_J^1 - \mathbf{y}_J^0)\right) = \mathrm{norm}\left((\mathbf{R}(\mathbf{x}_J^2 - \mathbf{x}_J^0)) \times (\mathbf{R}(\mathbf{x}_J^1 - \mathbf{x}_J^0))\right) = \mathrm{norm}\left(\mathbf{R}\left((\mathbf{x}_J^2 - \mathbf{x}_J^0) \times (\mathbf{x}_J^1 - \mathbf{x}_J^0)\right)\right) = \mathbf{R}\ \mathrm{norm}\left((\mathbf{x}_J^2 - \mathbf{x}_J^0) \times (\mathbf{x}_J^1 - \mathbf{x}_J^0)\right)$ from basic vertor analysis rule, where the superscript $(\cdot)^{\{1,2,3\}}$ denotes three related vertex in triangle.

Together we have

$\mathbf{D}_i = \left(\sum_j \omega_{ij}(\mathbf{y}_j - \mathbf{y}_i)(\mathbf{x}_j - \mathbf{x}_i)^T + \mathbf{y}_i^{\perp} \otimes \mathbf{x}_i^{\perp}\right) = \left(\sum_j \omega_{ij}\mathbf{R}(\mathbf{x}_j - \mathbf{x}_i)(\mathbf{x}_j - \mathbf{x}_i)^T + \mathbf{R}\mathbf{x}_i^{\perp} \otimes \mathbf{x}_i^{\perp}\right) = \mathbf{R}\mathbf{K}_i$. Then we have $\mathbf{F}_i = \mathbf{D}_i\mathbf{K}_i^{-1} = \mathbf{R}$.

2 Handle Contact Through Local Projection

2.1 Step Length of Gradient Method

In this section we will analysis how to choose step length λ to guarantee descending of the objective function in local step, i.e.,

$$\mathcal{B}(\mathbf{z}^m + \lambda\mathbf{g}) < \mathcal{B}(\mathbf{z}^m) \tag{11}$$

where

$$\mathcal{B}(\mathbf{z}) := \left(\sum_i \frac{1}{2} \left\| \mathbf{z}_i - \mathbf{y}_i^k \right\|_2^2 + \mu \sum_c B_c(\mathbf{z}) \right), \quad B(d(\mathbf{z})) = \begin{cases} -(d-\hat{d})^2 \log(\frac{d}{\hat{d}}), & 0 < d < \hat{d} \\ 0, & d \geq \hat{d} \end{cases}. \tag{12}$$

For such barrier energy function modeling the contact, since it is at least second-order smooth when actived (when $0 < d < \hat{d}$), the first-order partial derivative and second-order partial derivative are calculated and can be refered from [1](Supplement A) as:

$$\frac{\partial B(d)}{\partial d} := B'(d) = -\left(2(d-\hat{d}) \log\left(\frac{d}{\hat{d}}\right) + \frac{(d-\hat{d})^2}{d} \right) < 0, \tag{13}$$

and

$$\frac{\partial^2 B(d)}{\partial d^2} := B''(d) = -\left(2\log\left(\frac{d}{\hat{d}}\right) + (d-\hat{d})\frac{\hat{d}+3d}{d^2} \right) > 0, \tag{14}$$

for $0 < d < \hat{d}$. After the mapping of $\hat{d}_{IJ} = d_{IJ} - \xi$, show on Fig. (9) and Eq. (51), we have both d, $-B' = |B'|$ and B'' get bounded, as $\lfloor d \rfloor = \varepsilon\xi$, $\lceil |B'(d)| \rceil = 2(\hat{d}-\varepsilon\xi)\log\left(\frac{\hat{d}}{\varepsilon\xi}\right) + \frac{(\varepsilon\xi-\hat{d})^2}{\varepsilon\xi}$ and $\lceil B''(d) \rceil = 2\log\left(\frac{\hat{d}}{\varepsilon\xi}\right) + (\hat{d}-\varepsilon\xi)\frac{\hat{d}+3\varepsilon\xi}{(\varepsilon\xi)^2}$, where $\lfloor \cdot \rfloor$ denotes the lower bound and $\lceil \cdot \rceil$ denotes the upper bound.

We start to show that, the above condition makes the objective function $\mathcal{B}$ has a *Lipschitz continuous gradient* with constant L as the Lipschitz parameter, so that a fixed step with constant step length λ can be chosen as if $0 < \lambda \leq 1/L$ to guarantee convergency. We would like to provide generally definition and theorem and then look inside to the previous contact problem.

Definition 1 *L-smooth Function.*
A function f has a Lipschitz continuous gradient with constant $L > 0$, when

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2 \leq L \|\mathbf{x} - \mathbf{y}\|_2, \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n.$$

We denote this kind function as $\mathcal{C}_L^1(\mathbb{R}^n)$ and L-smooth function.

Theorem 2 *For any $f \in \mathcal{C}_L^1(\mathbb{R}^n)$, we have:*

$$f(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{y}-\mathbf{x}) + \frac{L}{2}\|\mathbf{y}-\mathbf{x}\|_2^2, \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n.$$

Since the proof of Theo. (2) can be found in any Mathematical Analysis textbook, we would like to show it directly.

Theorem 3 *Fixed step convergency for gradient method.*
For gradient method and a L-smooth objective function $f \in \mathcal{C}_L^1(\mathbb{R}^n)$, GM guaranteed to converge for any $0 < \lambda \leq 1/L$, i.e.,

$$\mathbf{x}^+ = \mathbf{x} - \lambda\nabla f(\mathbf{x}),$$
$$f(\mathbf{x}^+) \leq f(\mathbf{x}), \quad \forall\lambda, 0 < \lambda \leq 1/L.$$

Since the proof of Theo. (3) can also be found in any optimization textbook, here we woule like to provide a yet simple proof.

Proof. Consider a single iteration

$$\mathbf{x}^+ = \mathbf{x} - \lambda \nabla f(\mathbf{x}).$$

Then for any $\mathbf{x} \in \mathbb{R}^n$ and $\lambda \in (0, 1/L]$, we have:

$$\begin{aligned}
f(\mathbf{x}^+) &\leq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{x}^+ - \mathbf{x}) + \frac{L}{2}\left\|\mathbf{x}^+ - \mathbf{x}\right\|_2^2 \qquad \text{(Theo. (2))} \\
&= f(\mathbf{x}) + \nabla f(\mathbf{x})^T(-\lambda \nabla f(\mathbf{x})) + \frac{L\lambda^2}{2}\left\|\nabla f(\mathbf{x})\right\|_2^2 \\
&\leq f(\mathbf{x}) - \lambda \left\|\nabla f(\mathbf{x})\right\|_2^2 + \frac{\lambda}{2}\left\|\nabla f(\mathbf{x})\right\|_2^2 \\
&= f(\mathbf{x}) - \frac{\lambda}{2}\left\|\nabla f(\mathbf{x})\right\|_2^2 \\
&\leq f(\mathbf{x}).
\end{aligned}$$

□

Following the above theorem, the question remains to be, how to find L constant for our objective function $\mathcal{B}$. As $\mathcal{B}$ is second-order differentialable, then we have $L = \max(|\lambda_i|) = \left\|\nabla^2 \mathcal{B}\right\|_2$, $\forall \lambda_i$ are the eigenvalue of $\nabla^2 \mathcal{B}$, deduced from the inequation $\left\|\nabla \mathcal{B}(\mathbf{y}) - \nabla \mathcal{B}(\mathbf{x})\right\|_2 \leq \left\|\nabla^2 \mathcal{B}\right\|_2 \cdot \left\|\mathbf{y} - \mathbf{x}\right\|_2$.

Look inside to the Hessian of the objective function $\mathcal{B}$, since the gradient method is done for each vertex $\mathbf{z}_i$, we only need to estimate a maximal absolute eigenvalue of Hessian derivative for each $\mathbf{z}_i$, then we can get an upper bound of the step length.

As

$$\begin{aligned}
\nabla_{\mathbf{z}_i} \mathcal{B} =& - \mathbf{g}_i \\
=& - \mu \sum_I \alpha_I^i \left[\frac{(d_{IJ} - \hat{d})^2}{d_{IJ}} + 2(d_{IJ} - \hat{d}) \log\left(\frac{d_{IJ}}{\hat{d}}\right)\right] \operatorname{norm}(\mathbf{d}_{IJ}) - \mathbf{y}_i^k + \mathbf{z}_i \\
=& \mu \sum_I \alpha_I^i B'(d_{IJ}) \operatorname{norm}(\mathbf{d}_{IJ}) - \mathbf{y}_i^k + \mathbf{z}_i,
\end{aligned} \tag{15}$$

where α_I^i represents the barycentric coordinate for vertex i in triangle I, and $\mathbf{d}_{IJ} = \alpha_I^i \mathbf{z}_i + \alpha_I^j \mathbf{z}_j + \alpha_I^k \mathbf{z}_k - \alpha_J^a \mathbf{z}_a - \alpha_J^b \mathbf{z}_b - \alpha_J^c \mathbf{z}_c$, where (i, j, k) and (a, b, c) are the corresponding vertex indexes of triangle I and J. Here we explicitly describe the proximal directional distance $\mathbf{d}_{IJ}$ because we will then make derivative of $\mathbf{z}_i$ on it. The proximal distance length $d_{IJ} = \left\|\mathbf{d}_{IJ}\right\|_2$, and $\operatorname{norm}(\mathbf{d}_{IJ}) = \mathbf{d}_{IJ}/d_{IJ}$. Then we have

$$\nabla_{\mathbf{z}_i}^2 \mathcal{B} = \mu \sum_I \alpha_I^i \left(B''(d_{IJ}) \frac{\partial d_{IJ}}{\partial \mathbf{z}_i} \otimes \operatorname{norm}(\mathbf{d}_{IJ}) + B'(d_{IJ}) \frac{\partial \operatorname{norm}(\mathbf{d}_{IJ})}{\partial \mathbf{z}_i}\right) + \mathbf{I}, \tag{16}$$

where $\mathbf{I}$ is an identity matrix of dimension $\mathbf{z}_i \times$dimension $\mathbf{z}_i$, i.e., 3×3, and $\otimes$ denotes the Kronecker product.

As we have (which can be found in [2] or simply make deduction)

$$\frac{\partial d_{IJ}}{\partial \mathbf{z}_i} = \frac{\partial d_{IJ}}{\partial \mathbf{d}_{IJ}} \cdot \frac{\partial \mathbf{d}_{IJ}}{\partial \mathbf{z}_i} = \alpha_I^i \operatorname{norm}(\mathbf{d}_{IJ}),$$

$$\frac{\partial \operatorname{norm}(\mathbf{d}_{IJ})}{\partial \mathbf{z}_i} = \frac{\partial \operatorname{norm}(\mathbf{d}_{IJ})}{\partial \mathbf{d}_{IJ}} \cdot \frac{\partial \mathbf{d}_{IJ}}{\partial \mathbf{z}_i} = \frac{\alpha_I^i}{d_{IJ}}\left(\mathbf{I} - \operatorname{norm}(\mathbf{d}_{IJ}) \otimes \operatorname{norm}(\mathbf{d}_{IJ})\right),$$

which gives:

$$\begin{aligned}
\nabla_{\mathbf{z}_i}^2 \mathcal{B} &= \mu \sum_I \alpha_I^i \left(B''(d_{IJ}) \frac{\partial d_{IJ}}{\partial \mathbf{z}_i} \otimes \operatorname{norm}(\mathbf{d}_{IJ}) + B'(d_{IJ}) \frac{\partial \operatorname{norm}(\mathbf{d}_{IJ})}{\partial \mathbf{z}_i}\right) + \mathbf{I} \\
&= \left(\mu \sum_I (\alpha_I^i)^2 \frac{B'(d_{IJ})}{d_{IJ}} + 1\right) \mathbf{I} + \mu \sum_I \left[(\alpha_I^i)^2 \left(B''(d_{IJ}) + \frac{B'(d_{IJ})}{d_{IJ}}\right) \operatorname{norm}(\mathbf{d}_{IJ}) \otimes \operatorname{norm}(\mathbf{d}_{IJ})\right] \\
&= FT + ST,
\end{aligned} \tag{17}$$

where FT denotes the 'first term' and ST the 'second term'.

Since the d_{IJ} to active barrier energy is actually transformed to $\hat{d}_{IJ} = d_{IJ} - \xi$ when considering thickness modeling, such linear transform does change derivative and hessian, only changing the B', B'' terms. Then this d will go through our mapping function and get $\lfloor d \rfloor = \varepsilon\xi$ as minimal separation. In such mapping, we literally consider d as a calulated coefficient free of $\mathbf{z}_i$ (so that there will be no $\frac{\partial f(d)}{\partial d}$ exist in the Chain Rule).

Although this analyical representation of Eq. (17) can be calculated to get $L = \left\|\nabla^2_{\mathbf{z}_i}\mathcal{B}\right\|_2$, such process will be unnecessarily time costing. We choose to estimate an upper bound of $\left\|\nabla^2_{\mathbf{z}_i}\mathcal{B}\right\|_2$. As $\left\|\nabla^2_{\mathbf{z}_i}\mathcal{B}\right\|_2 \leq \|FT\|_2 + \|ST\|_2$, we will look inside to these terms each by each.

From FT, we have:

$$
\begin{aligned}
\|FT\|_2 &\leq \left|\mu \sum_I (\alpha_I^i)^2 \frac{B'}{d} + 1\right| \cdot \|\mathbf{I}\|_2 \\
&\leq \left|\mu \sum_I (\alpha_I^i)^2 \frac{B'}{d} + 1\right| \\
&< \left|\mu \sum_I (\alpha_I^i)^2 \frac{B'}{d}\right| + |1| \\
&\leq \left|\mu \sum_I \alpha_I^i \frac{B'}{d}\right| + \left|\frac{\hat{d}}{\lfloor d \rfloor}\right| \qquad (\text{since } 0 \leq \alpha_I^i \leq 1 \text{ and } 0 < d < \hat{d}) \\
&\leq \mu\alpha_0 \left|\frac{B'}{\lfloor d \rfloor}\right| + \frac{\hat{d}}{\lfloor d \rfloor} \qquad (\text{here denotes } \alpha_0 := \left\lceil \sum_I \alpha_I^i \right\rceil) \\
&\leq \frac{1}{\lfloor d \rfloor}\left(\mu\alpha_0 \lceil |B'(d)| \rceil + \hat{d}\right) =: \lceil \|FT\|_2 \rceil.
\end{aligned}
\tag{18}
$$

Although the $\|ST\|_2$ can also get an upper bound $\mu\alpha_0\left(\frac{\lceil |B'| \rceil}{\lfloor d \rfloor} + \lceil B'' \rceil\right)$ through similar deduction, however, this upper bound possess too large expansion, since '=' can only be reached when all $\alpha_I^i = 1$ and $\mathbf{d}_{IJ}$ are paralleled, because of the existence of $\|\sum_I \mathrm{norm}(\mathbf{d}_{IJ}) \otimes \mathrm{norm}(\mathbf{d}_{IJ})\|_2$. A too large expansion will make the estimation of Lipschitz constant L expanded and yet make the step length unnecessarily get smaller, so that the convergence process will be unnecessarily slow.

We will simply abandon the $\|ST\|_2$ term, since $\|FT\|_2$ has already provided enough expansion in estimation of L and thus will give a enough step length upper bound. So that the estimation of L become $L \leq \left\|\nabla^2_{\mathbf{z}_i}\mathcal{B}\right\|_2 \leq \lceil \|FT\|_2 \rceil$. Then we have $1/L \geq 1/\lceil \|FT\|_2 \rceil$.

From Theo. (3) and Eq. (18), then we have:

$$
\begin{gathered}
0 < \lambda \leq 1/L \\
\text{which means } \lambda \leq \lfloor 1/L \rfloor = \frac{\varepsilon\xi}{\mu\alpha_0 \lceil |B'(d)| \rceil + \hat{d}}.
\end{gathered}
\tag{19}
$$

This condition has a more intuitive illustration, i.e., requiring the maximum position change at each iteration of each vertex no greater than minimal separation $\varepsilon\xi$, i.e., $\max_i \|\lambda \mathbf{g}_i\|_2 \leq \varepsilon\xi$.

References

[1] Minchen Li, Zachary Ferguson, Teseo Schneider, Timothy Langlois, Denis Zorin, Daniele Panozzo, Chenfanfu Jiang, and Danny M. Kaufman. Incremental potential contact: Intersection- and inversion-free large deformation dynamics. *ACM Trans. Graph. (SIGGRAPH)*, 39(4), 2020.

[2] Kaare Brandt Petersen, Michael Syskind Pedersen, et al. The matrix cookbook. *Technical University of Denmark*, 7(15):510, 2008.

[3] Stewart A Silling and Richard B Lehoucq. Convergence of peridynamics to classical elasticity theory. *Journal of Elasticity*, 93:13–37, 2008.