Direct shape optimization for strengthening 3D printable objects - Supplementary Material

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A Analytic Gradient and Hessian of strain tensor $\boldsymbol{\varepsilon}$

Similar to Equation 7 and Equation 8, we can express the partial derivatives of the strain tensor $\frac{\partial \boldsymbol{\varepsilon}(i,j)}{\partial x_{v,k}}$ wrt the coordinates of a vertex in the optimized shape (here r, s are matrix element indices):

$$\frac{\partial \boldsymbol{\varepsilon}(i,j)}{\partial x_{v,k}} = \mathbf{U}^T \bar{\mathbf{P}} \frac{\partial \bar{\mathbf{X}}^{-1}}{\partial x_{v,k}} \mathbf{V}$$

$$\frac{\partial \bar{\mathbf{X}}^{-1}(i,j)}{\partial \bar{\mathbf{X}}(r,s)} = -\bar{\mathbf{X}}^{-1}(i,r)\bar{\mathbf{X}}^{-1}(s,j)$$

$$\frac{\partial \bar{\mathbf{X}}(i,j)}{\partial x_{v,k}} = \begin{cases} 1 & \text{if } v = v_i \text{ and } k = j \\ -1 & \text{if } v = v_0 \text{ and } u = j \\ 0 & \text{otherwise} \end{cases}$$

The Hessian of $\boldsymbol{\varepsilon}$ contains three parts: $\frac{\partial^2 \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{P}}^2}$, $\frac{\partial^2 \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{P}} \partial \bar{\mathbf{X}}}$ and $\frac{\partial^2 \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{X}}^2}$, expressed as follows (here w refers to another vertex index, l is a coordinate index):

$$\frac{\partial^2 \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{P}}^2} = \mathbf{0}$$

$$\frac{\partial^2 \boldsymbol{\varepsilon}}{\partial p_{v,k} \partial x_{w,l}} = \mathbf{U}^T \frac{\partial \bar{\mathbf{P}}}{\partial p_{v,k}} \frac{\partial (\bar{\mathbf{X}}^{-1})}{\partial x_{w,l}} \mathbf{V}$$

$$\frac{\partial^2 \boldsymbol{\varepsilon}}{\partial x_{v,k} \partial x_{w,l}} = \mathbf{U}^T \bar{\mathbf{P}} \frac{\partial^2 (\bar{\mathbf{X}}^{-1})}{\partial x_{v,k} \partial x_{w,l}} \mathbf{V}$$

We also need to compute the second order derivatives of $\mathbf{X}^{-1}$. Let us denote $\mathbf{X}(i,*)$ as the i^{th} row in matrix $\mathbf{X}$, and $\mathbf{X}(*,j)$ as the j^{th} column. Then we will have:

$$\frac{\partial^2 (\bar{\mathbf{X}}^{-1})}{\partial \bar{\mathbf{X}}(r,s) \partial \bar{\mathbf{X}}(t,u)} = \bar{\mathbf{X}}^{-1}(s,t) \cdot \bar{\mathbf{X}}^{-1}(*,r) \cdot \bar{\mathbf{X}}^{-1}(u,*) + \bar{\mathbf{X}}^{-1}(t,s) \cdot \bar{\mathbf{X}}^{-1}(*,u) \cdot \bar{\mathbf{X}}^{-1}(r,*)$$

B Analytic Hessian of elastic energy U

The analytic Hessian of elastic energy U gives the gradient of the force, which is actually the Jacobian of the force equilibrium constraints. It can be computed as follows:

$$\frac{\partial^2 U(\bar{\mathbf{X}}, \bar{\mathbf{P}})}{\partial \bar{\mathbf{P}}^2} = \mathcal{V} \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{P}}} : \mathbf{E} \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{P}}}$$

$$\frac{\partial^2 U(\bar{\mathbf{X}}, \bar{\mathbf{P}})}{\partial \bar{\mathbf{X}} \partial \bar{\mathbf{P}}} = \mathcal{V} \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{P}}} : E \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{X}}} + \mathcal{V} \boldsymbol{\varepsilon} : E \frac{\partial^2 \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{X}} \partial \bar{\mathbf{P}}} + \frac{\partial \mathcal{V}}{\partial \bar{\mathbf{X}}} \boldsymbol{\varepsilon} : E \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{P}}}$$

where : refers to double dot product between tensors, and the partial derivatives of the volume $\frac{\partial \mathcal{V}}{\partial \bar{\mathbf{X}}}$ can be computed as:

$$\frac{\partial \mathcal{V}}{\partial \bar{\mathbf{X}}(i,j)} = \frac{1}{6} \big(\bar{\mathbf{X}}(i+1,j+1) * \bar{\mathbf{X}}(i+2,j+2) - \bar{\mathbf{X}}(i+1,j+2) * \bar{\mathbf{X}}(i+2,j+1) \big)$$

Here the indices of the matrix should wrap around when $i+2 > 3$ or $j+2 > 3$. Notice that $\frac{\partial^2 U(\bar{\mathbf{X}}, \bar{\mathbf{P}})}{\partial^2 \bar{\mathbf{X}}}$ is not needed when computing the Jacobian.

C Analytic Gradient and Hessian of $\hat{\sigma}$

If we rewrite $\boldsymbol{\sigma}$ in vector form:

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \end{bmatrix} \quad (18)$$

One might easily notice that Equation 10 can be written in the form:

$$\hat{\sigma}^2 = \frac{1}{2} \boldsymbol{\sigma}^T \mathbf{M} \boldsymbol{\sigma} \quad (19)$$

Where $\mathbf{M}$ is a constant matrix:

$$\mathbf{M} = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6 \end{bmatrix} \quad (20)$$

Thus, Equation 10 can be further rewritten into the form:

$$\hat{\sigma}^2 = \frac{1}{2} \boldsymbol{\varepsilon}_t : \mathbf{EME} \boldsymbol{\varepsilon}_t \quad (21)$$

Which is very similar to Equation 3. Thus its analytic gradient also has a similar form:

$$\frac{\partial \hat{\sigma}^2(\bar{\mathbf{X}}, \bar{\mathbf{P}})}{\partial \bar{\mathbf{P}}} = \left(\mathbf{U}^T \bar{\mathbf{P}} \bar{\mathbf{X}}^{-1} \mathbf{V} - \mathbf{I} \right) : \mathbf{EME} \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{P}}}$$

$$\frac{\partial \hat{\sigma}^2(\bar{\mathbf{X}}, \bar{\mathbf{P}})}{\partial \bar{\mathbf{X}}} = \left(\mathbf{U}^T \bar{\mathbf{P}} \bar{\mathbf{X}}^{-1} \mathbf{V} - \mathbf{I} \right) : \mathbf{EME} \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{X}}}$$

The Hessian is expressed as follows:

$$\frac{\partial^2 \hat{\sigma}(\bar{\mathbf{X}}, \bar{\mathbf{P}})}{\partial \bar{\mathbf{P}}^2} = \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{P}}} : \mathbf{EME} \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{P}}}$$

$$\frac{\partial^2 \hat{\sigma}(\bar{\mathbf{X}}, \bar{\mathbf{P}})}{\partial \bar{\mathbf{X}} \partial \bar{\mathbf{P}}} = \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{P}}} : \mathbf{EME} \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{X}}} + \boldsymbol{\varepsilon} : \mathbf{EME} \frac{\partial^2 \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{X}} \partial \bar{\mathbf{P}}}$$

$$\frac{\partial^2 \hat{\sigma}(\bar{\mathbf{X}}, \bar{\mathbf{P}})}{\partial \bar{\mathbf{X}}^2} = \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{X}}} : \mathbf{EME} \frac{\partial \boldsymbol{\varepsilon}}{\partial \bar{\mathbf{X}}} + \boldsymbol{\varepsilon} : \mathbf{EME} \frac{\partial^2 \boldsymbol{\varepsilon}}{\partial^2 \bar{\mathbf{X}}}$$

D Singularity in Affine Transformation Computation

Computing Equation 14 involves calculating a transformation matrix from $\mathbf{X}^0$ to $\mathbf{X}$ within a neighborhood $\mathcal{N}(i)$. Such transformation requires a matrix inverse in the form of $(\mathbf{A}_i^T \mathbf{A}_i)^{-1}$, where $\mathbf{A}_i$ contains the position of the neighbor vertices [SCOL*04]. In our problem, $\mathbf{A}_i^T \mathbf{A}_i$ will become singular when neighbor vertices are coplanar in the original shape. To compute its pseudo-inverse, we perform SVD on $\mathbf{A}_i^T \mathbf{A}_i$. The near-zero singular value corresponds to the surface normal direction. To better preserve its coplanarity, we set the near-zero singular value to be a very small positive value (10^{-8} in our implementation), then compute its inverse matrix. This forces vertex $\mathbf{x}_i$ to stay at the center of its neighbors in its normal direction, thus it will remain coplanar with its neighbors.