X-Shells Supplementary Material

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This supplementary document presents the detailed formulas used in our X-Shells simulation and optimization framework. In particular, we first give the formulas needed to relate the constrained elastic rod quantities (centerline positions and material frame angles incident the joints) to our reduced parameters and derive gradients and Hessians of these formulas. Next, we detail our approach for optimizing over rotation variables. Then we give formulas for evaluating the gradients and Hessian-vector products for our design optimization. Finally, we revisit the popular discrete elastic rods model, pointing out an error in the approach used to compute gradients and Hessians of the bending and twisting energies and deriving correct expressions for these quantities.

1 Rod Linkages

We describe how to model the static equilibria of linkages formed by elastic rods connecting at scissor joints. Our linkage model builds on the popular discrete elastic rods model of [Bergou et al., 2010].

1.1 Rod Linkage Graph

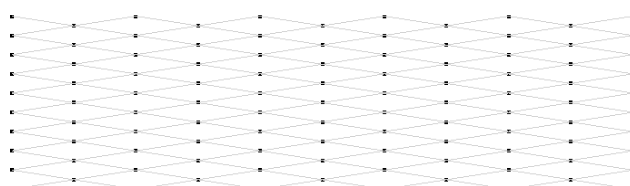

Figure 1 *An example graph defining a rod linkage.*

The linkage's initial configuration is defined by an embedded graph (i.e., a line mesh) with vertices and edges (V, E). Each edge of this graph is referred to as a *rod segment*, and generally these segments continue across the vertices to form a complete rod as shown in Figure 1.

Each graph vertex represents either a scissor joint or a rod's free end. Vertex valences can be one (free end), two (two rod ends pinned together), three (one rod's end pinned to another's interior), or four (two rods pinned together at interior points); we prohibit valences above four. Figure 1 has examples of each of these valences.

Each rod segment is modeled as a *distinct* discrete elastic rod with n_s subdivisions. We will see how to properly couple the segments making up a full rod so that they behave identically to one large elastic rod. We label the n^{th} segment s_n for $n \in \{0 \ldots |E|-1\}$ and the i^{th} joint $\jmath_i$ for $i \in \{0 \ldots |J|-1\}$, where $J \subset V$ is the set of vertices of valence 2–4.

1.2 Rod and Joint Representation

Recall that a discrete elastic rod's configuration is defined by its centerline positions and its material frame angles (expressed relative to the rod's hidden reference frame state). The material frame is used to express the orientation/twist of the rod's cross sections, which is particularly important for anisotropic rods.

The rod segments meeting at a joint can be partitioned into two sets, one for each full rod passing through the joint. This partitioning is done by determining which segments connect to form the straightest path across the vertex in the rest configuration. We need to glue together the segments making up a rod and allow the two incident rods pivot around the vertex. We accomplish this gluing by making the joint impose the exact same terminal edge vector for the segments connecting to form a single rod. Also, the joint constrains the orientation of all incident segments' cross-sections: the second material axis $\mathbf{d}_2$ must be normal to the plane spanned by both incident centerline edges. See Figure 2 for an example joint configuration.

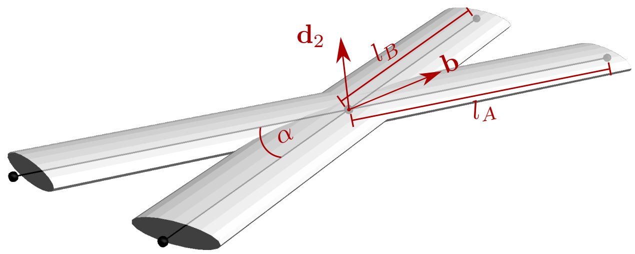

Figure 2 *The geometry of rod scissor linkages. Here we visualize the linkage graph for a single scissor linkage (comprising four rod segments) and the corresponding rod geometry. The joint parameters determine the edge vectors and material frames for the terminal edges of all incident rod segments.*

1.3 Linkage Degrees of Freedom

Our rod linkage model incorporates the constraints imposed by the joints by constructing a reduced set of variables that parametrize all admissible rod configurations. These reduced variables consist of (in order):

- For each rod segment $s \in E$:
  - Centerline positions for all interior and free-end nodes of s. The x, y, and z coordinates of the first interior/free node come first, followed by the coordinates for all subsequent nodes.
  - Material frame angles θ for all interior and free-end edges of s.
- Parameters for each joint $\jmath \in J$: position $\mathbf{p} \in \mathbb{R}^3$, orientation $\omega \in \mathbf{so}(3)$, opening angle α, and edge lengths for the two incident rods l_A and l_B.

This parameter choice for the joints allows us to easily pin a joint's rigid motion without also constraining its opening angle. Also, since the opening angles are explicit parameters, it is easy to formulate opening-angle-based deployment actuations (e.g., applied torques or angle constraints).

See Figure 2 for a visualization of how the joint's degrees of freedom determine the geometry of the incident rod edges. Each joint has an attached frame $\{\mathbf{b}, \mathbf{n} \times \mathbf{b}, \mathbf{n}\}$, which is a function of the joint's orientation variables $\boldsymbol{\omega}$. The material director $\mathbf{d}_2$ (and thus the material frame angle variable θ) for all terminal edges attached to a joint is given directly by $\mathbf{n}$.

Specifically, the joint's incident edge vectors $\mathbf{e}_A$ and $\mathbf{e}_B$ and joint normal are:

$$\mathbf{e}_A = R(\boldsymbol{\omega}) \underbrace{\left(\hat{\mathbf{b}} \cos(\alpha/2) - (\hat{\mathbf{n}} \times \hat{\mathbf{b}}) \sin(\alpha/2)\right)}_{:=\hat{\mathbf{t}}_A(\alpha)} l_A, \quad \mathbf{e}_B = R(\boldsymbol{\omega}) \underbrace{\left(\hat{\mathbf{b}} \cos(\alpha/2) + (\hat{\mathbf{n}} \times \hat{\mathbf{b}}) \sin(\alpha/2)\right)}_{:=\hat{\mathbf{t}}_B(\alpha)} l_B, \quad \mathbf{n} = R(\boldsymbol{\omega})\hat{\mathbf{n}},$$

where $\hat{\mathbf{b}}$ and $\hat{\mathbf{n}}$ are the joint's "source" bisector and normal unit vectors. These can be interpreted as defining a reference rotation matrix $R_0 := \left(\hat{\mathbf{b}} \;\middle|\; \hat{\mathbf{n}} \times \hat{\mathbf{b}} \times \mathbf{n} \;\middle|\; \hat{\mathbf{n}} \right)$ so that orientation variable $\boldsymbol{\omega}$ is a vector in the tangent space of $SO(3)$ at R_0 (see Section 2). The edge vectors $\mathbf{e}_A$ and $\mathbf{e}_B$ control the two centerline positions of the incident rod edges, placing them at, e.g., $\mathbf{p} \pm \frac{1}{2}\mathbf{e}_A$.

1.4 Elastic Energy, Gradients, and Hessians

Our model's joints store no energy, so the elastic energy of the full linkage is computed by summing the energy from each rod segment:

$$E(\mathbf{x}) := \sum_{r=1}^{|\mathcal{R}|} E_s(\mathbf{v}_r(\mathbf{x})) + E_b(\mathbf{v}_r(\mathbf{x})) + E_t(\mathbf{v}_r(\mathbf{x})), \tag{A1}$$

where $\mathbf{v}_r$ is a nonlinear function computing the full vector of centerline position and material angle variables for discrete elastic rod r from the reduced variables $\mathbf{x}$. For the energy expressions and derivatives for a single unconstrained rod, see Section 4.

In the following gradient and Hessian derivations, we focus on the energy stored in a single rod segment r, whose corresponding function $\mathbf{v}_r$ is broken down into scalar component functions v_k. We construct the full linkage's derivatives by summing these formulas over the rod segments.

1.5 Gradients

The gradient of the elastic energy with respect to the linkage variables is:

$$\frac{\partial E}{\partial x_i} = \left(\frac{\partial E_s}{\partial v_k} + \frac{\partial E_b}{\partial v_k} + \frac{\partial E_t}{\partial v_k}\right)\frac{\partial v_k}{\partial x_i},$$

where summation over repeated unreduced variable index k is implied. Note that we have effectively gathered all the full, unreduced variables (i.e., the components of functions $\mathbf{v}_r$ for all r) into a single vector indexed by k here.

The *nonzero* blocks of the Jacobian $\frac{\partial v_k}{\partial x_i}$ consist of the following terms:

$$\frac{\partial \mathbf{e}_A}{\partial \boldsymbol{\omega}} = \frac{\partial (R(\boldsymbol{\omega})\hat{\mathbf{t}}_A(\alpha))}{\partial \boldsymbol{\omega}} l_A, \quad \frac{\partial \mathbf{e}_A}{\partial \alpha} = R(\boldsymbol{\omega})\underbrace{\Big(-\hat{\mathbf{b}}\sin(\alpha/2) - (\hat{\mathbf{n}}\times\hat{\mathbf{b}})\cos(\alpha/2)\Big)}_{-\hat{\mathbf{t}}_A^{\perp}(\alpha) := -\hat{\mathbf{n}}\times\hat{\mathbf{t}}_A} l_A/2, \quad \frac{\partial \mathbf{e}_A}{\partial l_A} = R(\boldsymbol{\omega})\hat{\mathbf{t}}_A(\alpha),$$

$$\frac{\partial \mathbf{e}_B}{\partial \boldsymbol{\omega}} = \frac{\partial \left(R(\boldsymbol{\omega})\hat{\mathbf{t}}_B(\alpha)\right)}{\partial \boldsymbol{\omega}} l_B, \quad \frac{\partial \mathbf{e}_B}{\partial \alpha} = R(\boldsymbol{\omega})\underbrace{\Big(-\hat{\mathbf{b}}\sin(\alpha/2) + (\hat{\mathbf{n}}\times\hat{\mathbf{b}})\cos(\alpha/2)\Big)}_{\hat{\mathbf{t}}_B^{\perp}(\alpha) := \hat{\mathbf{n}}\times\hat{\mathbf{t}}_B} l_B/2, \quad \frac{\partial \mathbf{e}_B}{\partial l_B} = R(\boldsymbol{\omega})\hat{\mathbf{t}}_B(\alpha)$$

$$\left(\frac{\partial \theta^j}{\partial \boldsymbol{\omega}}\right)^T = -\mathbf{d}_1^j \cdot \frac{\partial \mathbf{n}}{\partial \boldsymbol{\omega}} + \underline{\mathbf{d}_1^j} \cdot \left(s_{jA}\frac{\partial P_{\widehat{\mathbf{t}^j}}^{\mathbf{t}_A}\widehat{\underline{\mathbf{d}_2^j}}}{\partial \mathbf{t}_A}\frac{\partial \mathbf{t}_A}{\partial \boldsymbol{\omega}} + s_{jB}\frac{\partial P_{\widehat{\mathbf{t}^j}}^{\mathbf{t}_B}\widehat{\underline{\mathbf{d}_2^j}}}{\partial \mathbf{t}_B}\frac{\partial \mathbf{t}_B}{\partial \boldsymbol{\omega}}\right),$$

$$\frac{\partial \theta^j}{\partial \alpha} = \underline{\mathbf{d}_1^j} \cdot \left(s_{jA}\frac{\partial P_{\widehat{\mathbf{t}^j}}^{\mathbf{t}_A}\widehat{\underline{\mathbf{d}_2^j}}}{\partial \mathbf{t}_A}\frac{\partial \mathbf{t}_A}{\partial \alpha} + s_{jB}\frac{\partial P_{\widehat{\mathbf{t}^j}}^{\mathbf{t}_B}\widehat{\underline{\mathbf{d}_2^j}}}{\partial \mathbf{t}_B}\frac{\partial \mathbf{t}_B}{\partial \alpha}\right) = \underline{\mathbf{d}_1^j} \cdot \left(\frac{s_{jB}}{2}\frac{\partial P_{\widehat{\mathbf{t}^j}}^{\mathbf{t}_B}\widehat{\underline{\mathbf{d}_2^j}}}{\partial \mathbf{t}_B}\hat{\mathbf{t}}_B^{\perp}(\alpha) - \frac{s_{jA}}{2}\frac{\partial P_{\widehat{\mathbf{t}^j}}^{\mathbf{t}_A}\widehat{\underline{\mathbf{d}_2^j}}}{\partial \mathbf{t}_A}\hat{\mathbf{t}}_A^{\perp}(\alpha)\right),$$

where the terms involving reference frame vector $\underline{\mathbf{d}_1^j}$ subtract off the rotation of the reference frame due to parallel transport. The notation $\widehat{\mathbf{t}^j}$ refers to the edge j's *source tangent vector* and $P_{\widehat{\mathbf{t}^j}}^{\mathbf{t}^j}$ is the parallel transport operator from the source edge tangent to the current edge tangent; these concepts are introduced along with their corresponding derivatives in Section 4. Note that these parallel transport terms vanish if the source frame has been updated. The terms here like $\frac{\partial(R(\boldsymbol{\omega})\hat{\mathbf{t}}_A)}{\partial \boldsymbol{\omega}}$ can be evaluated with the gradient-of-rotated-vector formulas from Section 2. The scalars s_{jA} and s_{jB} are given by:

$$s_{jX} = \begin{cases} 0 & \text{if terminal edge } j \text{ isn't part of rod } X, \\ 1 & \text{if terminal edge } j\text{'s orientation agrees with joint edge vector } \mathbf{e}_X, \text{ or} \\ -1 & \text{if terminal edge } j\text{'s orientation disagrees with joint edge vector } \mathbf{e}_X. \end{cases}$$

1.5.1 Hessian

The Hessian of the elastic energy with respect to the linkage variables is:

$$\frac{\partial^2 E}{\partial x_i \partial x_j} = \frac{\partial v_k}{\partial x_i} \frac{\partial^2 E}{\partial v_k \partial v_l} \frac{\partial v_l}{\partial x_j} + \frac{\partial E}{\partial v_k} \frac{\partial^2 v_k}{\partial x_i \partial x_j}.$$

For all the unconstrained variables (rod segments' interior/free end quantities), $\frac{\partial v_k}{\partial x_i}$ is essentially just a "permuted" Kronecker delta (1 if reduced variable x_i corresponds to unconstrained variable v_k, 0 otherwise). The Hessians of these v_k are zero, and all that remains is the first term, which is just a permutation of the sub-block of the unreduced Hessian corresponding to the unconstrained variables. We implement this term by re-indexing the sparse matrix entries.

For the constrained variables, we need to evaluate the parametrization's Hessian $\frac{\partial^2 v_k}{\partial x_i \partial x_j}$, which essentially amounts to computing the Hessians of $\mathbf{e}_A$, $\mathbf{e}_B$, and θ^j. The Hessian blocks of the edge vectors are:

$$\boxed{\begin{aligned}
&\frac{\partial^2 \mathbf{e}_A}{\partial \boldsymbol{\omega} \partial \boldsymbol{\omega}} = \frac{\partial^2 \left(R(\boldsymbol{\omega})\hat{\mathbf{t}}_A(\alpha)\right)}{\partial \boldsymbol{\omega} \partial \boldsymbol{\omega}} l_A, \quad \frac{\partial^2 \mathbf{e}_A}{\partial \boldsymbol{\omega} \partial l_A} = \frac{\partial \left(R(\boldsymbol{\omega})\hat{\mathbf{t}}_A(\alpha)\right)}{\partial \boldsymbol{\omega}}, \quad \frac{\partial^2 \mathbf{e}_A}{\partial \boldsymbol{\omega} \partial \alpha} = -\frac{\partial \left(R(\boldsymbol{\omega})\hat{\mathbf{t}}_A^{\perp}(\alpha)\right)}{\partial \boldsymbol{\omega}} \frac{l_A}{2}, \\
&\frac{\partial^2 \mathbf{e}_B}{\partial \boldsymbol{\omega} \partial \boldsymbol{\omega}} = \frac{\partial^2 \left(R(\boldsymbol{\omega})\hat{\mathbf{t}}_B(\alpha)\right)}{\partial \boldsymbol{\omega} \partial \boldsymbol{\omega}} l_B, \quad \frac{\partial^2 \mathbf{e}_B}{\partial \boldsymbol{\omega} \partial l_B} = \frac{\partial \left(R(\boldsymbol{\omega})\hat{\mathbf{t}}_B(\alpha)\right)}{\partial \boldsymbol{\omega}}, \quad \frac{\partial^2 \mathbf{e}_B}{\partial \boldsymbol{\omega} \partial \alpha} = \frac{\partial \left(R(\boldsymbol{\omega})\hat{\mathbf{t}}_B^{\perp}(\alpha)\right)}{\partial \boldsymbol{\omega}} \frac{l_B}{2}, \\
&\frac{\partial^2 \mathbf{e}_A}{\partial l_A \partial \alpha} = -\frac{1}{2} R(\boldsymbol{\omega})\hat{\mathbf{t}}_A^{\perp}(\alpha), \quad \frac{\partial^2 \mathbf{e}_A}{\partial \alpha \partial \alpha} = -R(\boldsymbol{\omega})\hat{\mathbf{t}}_A(\alpha)\frac{l_A}{4} = -\frac{\mathbf{e}_A}{4} \\
&\frac{\partial^2 \mathbf{e}_B}{\partial l_B \partial \alpha} = \frac{1}{2} R(\boldsymbol{\omega})\hat{\mathbf{t}}_B^{\perp}(\alpha), \quad \frac{\partial^2 \mathbf{e}_B}{\partial \alpha \partial \alpha} = -R(\boldsymbol{\omega})\hat{\mathbf{t}}_B(\alpha)\frac{l_B}{4} = -\frac{\mathbf{e}_B}{4}
\end{aligned}}$$

To simplify the Hessian of θ^j, we assume that the source frame has been updated (i.e., we evaluate at $\mathbf{t}^j = \widehat{\mathbf{t}^j}$); see Section 4. Recall the derivative with respect to the edge tangent of the (negated) reference frame rotation:

$$\left.\frac{\partial}{\partial \mathbf{t}^j}\right|_{\mathbf{t}^j = \widehat{\mathbf{t}^j}} \left[\underline{\mathbf{d}_1^j} \cdot \left(\frac{\partial P_{\widehat{\mathbf{t}^j}}^{\mathbf{t}^j} \underline{\widehat{\mathbf{d}_2^j}}}{\partial \mathbf{t}^j}\right)\right] = (\underline{\mathbf{d}_2^j} \otimes - \mathbf{t}^j) \cdot (-\mathbf{t}^j \otimes \underline{\mathbf{d}_1^j}) + \mathbf{d}_1^j \cdot \left.\frac{\partial^2 P_{\widehat{\mathbf{t}^j}}^{\mathbf{t}^j} \underline{\widehat{\mathbf{d}_2^j}}}{\partial \mathbf{t}^j \partial \mathbf{t}^j}\right|_{\mathbf{t}^j = \widehat{\mathbf{t}^j}} = \underline{\mathbf{d}_2^j} \otimes \underline{\mathbf{d}_1^j} - \frac{\underline{\mathbf{d}_2^j} \otimes \underline{\mathbf{d}_1^j} + \underline{\mathbf{d}_1^j} \otimes \underline{\mathbf{d}_2^j}}{2} = \frac{[\mathbf{t}^j]_\times}{2}.$$

$$\boxed{\begin{aligned}
\frac{\partial^2 \theta^j}{\partial \boldsymbol{\omega} \partial \boldsymbol{\omega}} &= -\left(\frac{\partial \mathbf{n}}{\partial \boldsymbol{\omega}}\right)^T \frac{\partial \mathbf{d}_1^j}{\partial \boldsymbol{\omega}} - \mathbf{d}_1^j \cdot \frac{\partial^2 \mathbf{n}}{\partial \boldsymbol{\omega} \partial \boldsymbol{\omega}} + \delta_{jA} \left(\frac{\partial \mathbf{t}_A}{\partial \boldsymbol{\omega}}\right)^T \frac{[\mathbf{t}^j]_\times}{2} \frac{\partial \mathbf{t}_A}{\partial \boldsymbol{\omega}} + \delta_{jB} \left(\frac{\partial \mathbf{t}_B}{\partial \boldsymbol{\omega}}\right)^T \frac{[\mathbf{t}^j]_\times}{2} \frac{\partial \mathbf{t}_B}{\partial \boldsymbol{\omega}} \\
&= -\operatorname{sym}\left(\left(\frac{\partial \mathbf{n}}{\partial \boldsymbol{\omega}}\right)^T \frac{\partial \mathbf{d}_1^j}{\partial \boldsymbol{\omega}}\right) - \mathbf{d}_1^j \cdot \frac{\partial^2 \mathbf{n}}{\partial \boldsymbol{\omega} \partial \boldsymbol{\omega}}, \\
\frac{\partial^2 \theta^j}{\partial \alpha \partial \boldsymbol{\omega}} &= \delta_{jA} \left(\frac{\partial \mathbf{t}_A}{\partial \alpha}\right)^T \frac{[\mathbf{t}^j]_\times}{2} \frac{\partial \mathbf{t}_A}{\partial \boldsymbol{\omega}} + \delta_{jB} \left(\frac{\partial \mathbf{t}_B}{\partial \alpha}\right)^T \frac{[\mathbf{t}^j]_\times}{2} \frac{\partial \mathbf{t}_B}{\partial \boldsymbol{\omega}} \\
&= -\frac{\delta_{jA}}{2} \left(\frac{\partial \mathbf{t}_A}{\partial \boldsymbol{\omega}}\right)^T \left(\mathbf{t}_A \times \frac{\partial \mathbf{t}_A}{\partial \alpha}\right) - \frac{\delta_{jB}}{2} \left(\frac{\partial \mathbf{t}_B}{\partial \boldsymbol{\omega}}\right)^T \left(\mathbf{t}_B \times \frac{\partial \mathbf{t}_B}{\partial \alpha}\right) \\
&= \frac{\delta_{jA}}{2} \left(\frac{\partial \mathbf{t}_A}{\partial \boldsymbol{\omega}}\right)^T \mathbf{n} - \frac{\delta_{jB}}{2} \left(\frac{\partial \mathbf{t}_B}{\partial \boldsymbol{\omega}}\right)^T \mathbf{n}, \\
\frac{\partial^2 \theta^j}{\partial \alpha \partial \alpha} &= \delta_{jB} \left(\frac{\partial \mathbf{t}_B}{\partial \alpha}\right)^T \frac{[\mathbf{t}^j]_\times}{2} \frac{\partial \mathbf{t}_B}{\partial \alpha} = 0.
\end{aligned}}$$

Here $\delta_{jX} = s_{jX}^2$ is the Kronecker delta, $[\cdot]_\times$ constructs the skew symmetric cross product matrix for a vector, and $\operatorname{sym}(\cdot)$ extracts the symmetric part of a 3×3 matrix.

2 Optimizing Rotations

To optimize our joints' rotational degrees of freedom, we first need to choose a representation for rotations. Our goal is to select a parametrization of $SO(3)$ that avoids singularities to the extent possible and that makes our optimizer's job easier.

We could use unit quaternions, which would solve the problem of singularities, but would require us to impose unit norm constraints during the optimization. We could use Euler angles, but these will run into singularities (gimbal lock) after just a $\frac{\pi}{2}$ rotation. Instead, we use the tangent space to $SO(3)$ (infinitesimal rotations) at some "reference" rotation R_0. In this representation, the additional rotation to be applied after R_0 is encoded as a vector pointing along the rotation axis with length equal to the rotation angle. The rotation is then obtained by the exponential map (more precisely, we construct the skew-symmetric cross-product matrix "X" for this vector and calculate $e^X R_0$).

This representation is nice because it allows rotations of up to π before running into singularities. We can avoid singularities entirely by setting bound constraints on our infinitesimal rotation components and then updating the parametrization (changing R_0 to the current rotation) if the optimizer terminates with one of these bounds active. We could even update R_0 at every step of the optimization, which would greatly simplify the gradient and Hessian formulas as we'll see in Section 2.4 (and as exploited in [Kugelstadt et al., 2018] and [Taylor and Kriegman, 1994]). However, we derive the full formulas for the gradient and Hessian away from the identity, since updating the parametrization—changing the optimization variables—at every step isn't supported in off-the-shelf optimization libraries (e.g. Knitro or IPOPT). Note that [Grassia, 1998] proposes using the same parametrization, though they only provide gradient formulas, not Hessian formulas (and work with quaternions instead of Rodrigues' rotation formula).

2.1 Representation and Exponential Map

We denote our infinitesimal rotation by vector $\boldsymbol{\omega}$, which encodes the rotation axis $\frac{\boldsymbol{\omega}}{\|\boldsymbol{\omega}\|}$ and angle $\|\boldsymbol{\omega}\|$. We can apply the rotation computed by the exponential map to a vector $\mathbf{v}$ using Rodrigues' rotation formula. For simplicity, we assume $R_0 = I$; this simplification can be applied in practice by first rotating $\mathbf{v}$ by R_0.

$$\tilde{\mathbf{v}} = R(\boldsymbol{\omega})\mathbf{v} := \mathbf{v}\cos(\|\boldsymbol{\omega}\|) + \boldsymbol{\omega}\boldsymbol{\omega}^T\mathbf{v}\frac{1-\cos(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^2} + (\boldsymbol{\omega}\times\mathbf{v})\frac{\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|}.$$

(We could obtain the entire rotation matrix by substituting the canonical basis vectors $\mathbf{e}^0$, $\mathbf{e}^1$, $\mathbf{e}^2$ in for $\mathbf{v}$.)

2.2 Gradients and Hessians

Now we compute derivatives of the rotated vector with respect to $\boldsymbol{\omega}$:

$$\begin{aligned}\frac{\partial\tilde{\mathbf{v}}}{\partial\boldsymbol{\omega}} = &-(\mathbf{v}\otimes\boldsymbol{\omega})\frac{\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|} + \left[(\boldsymbol{\omega}\cdot\mathbf{v})I + \boldsymbol{\omega}\otimes\mathbf{v}\right]\left(\frac{1-\cos(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^2}\right) + (\boldsymbol{\omega}\otimes\boldsymbol{\omega})\left((\boldsymbol{\omega}\cdot\mathbf{v})\frac{2\cos(\|\boldsymbol{\omega}\|) - 2 + \|\boldsymbol{\omega}\|\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^4}\right)\\ &- [\mathbf{v}]_\times\frac{\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|} + [(\boldsymbol{\omega}\times\mathbf{v})\otimes\boldsymbol{\omega}]\frac{\|\boldsymbol{\omega}\|\cos(\|\boldsymbol{\omega}\|) - \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^3}\end{aligned}$$

$$\boxed{\begin{aligned}= &-(\mathbf{v}\otimes\boldsymbol{\omega} + [\mathbf{v}]_\times)\frac{\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|} + \left[(\boldsymbol{\omega}\cdot\mathbf{v})I + \boldsymbol{\omega}\otimes\mathbf{v}\right]\left(\frac{1-\cos(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^2}\right)\\ &+ (\boldsymbol{\omega}\otimes\boldsymbol{\omega})\left((\boldsymbol{\omega}\cdot\mathbf{v})\frac{2\cos(\|\boldsymbol{\omega}\|) - 2 + \|\boldsymbol{\omega}\|\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^4}\right) + [(\boldsymbol{\omega}\times\mathbf{v})\otimes\boldsymbol{\omega}]\frac{\|\boldsymbol{\omega}\|\cos(\|\boldsymbol{\omega}\|) - \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^3},\end{aligned}}$$

where $[\mathbf{v}]_\times$ is the cross product matrix for $\mathbf{v}$. Next, we differentiate again to get the Hessian (a third order tensor whose two "rightmost" slots correspond to the differentiation variables):

$$
\begin{aligned}
\frac{\partial^2 \tilde{\mathbf{v}}}{\partial \boldsymbol{\omega}^2} = &-(\mathbf{v} \otimes I)\frac{\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|} - \big[(\mathbf{v} \otimes \boldsymbol{\omega} + [\mathbf{v}]_\times) \otimes \boldsymbol{\omega}\big] \left(\frac{\|\boldsymbol{\omega}\| \cos(\|\boldsymbol{\omega}\|) - \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^3}\right) \\
&+ \big[I \otimes \mathbf{v} + \mathbf{e}^i \otimes \mathbf{v} \otimes \mathbf{e}^i\big] \left(\frac{1 - \cos(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^2}\right) + \big[(\boldsymbol{\omega} \cdot \mathbf{v}) I + \boldsymbol{\omega} \otimes \mathbf{v}\big] \otimes \boldsymbol{\omega} \left(\frac{2\cos(\|\boldsymbol{\omega}\|) - 2 + \|\boldsymbol{\omega}\| \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^4}\right) \\
&+ \big[\mathbf{e}^i \otimes \boldsymbol{\omega} \otimes \mathbf{e}^i + \boldsymbol{\omega} \otimes \mathbf{e}^i \otimes \mathbf{e}^i\big] \left((\boldsymbol{\omega} \cdot \mathbf{v})\frac{2\cos(\|\boldsymbol{\omega}\|) - 2 + \|\boldsymbol{\omega}\| \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^4}\right) \\
&+ \boldsymbol{\omega} \otimes \boldsymbol{\omega} \otimes \mathbf{v} \left(\frac{2\cos(\|\boldsymbol{\omega}\|) - 2 + \|\boldsymbol{\omega}\| \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^4}\right) \\
&+ \boldsymbol{\omega} \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega} \left((\boldsymbol{\omega} \cdot \mathbf{v})\frac{8 + (\|\boldsymbol{\omega}\|^2 - 8)\cos(\|\boldsymbol{\omega}\|) - 5\|\boldsymbol{\omega}\| \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^6}\right) \\
&+ \big[-\mathbf{e}^i \otimes \boldsymbol{\omega} \otimes [\mathbf{v}]^i_\times + (\boldsymbol{\omega} \times \mathbf{v}) \otimes I\big] \left(\frac{\|\boldsymbol{\omega}\| \cos(\|\boldsymbol{\omega}\|) - \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^3}\right) \\
&+ \big[(\boldsymbol{\omega} \times \mathbf{v}) \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega}\big] \left(-\frac{3\|\boldsymbol{\omega}\| \cos(\|\boldsymbol{\omega}\|) + (\|\boldsymbol{\omega}\|^2 - 3)\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^5}\right),
\end{aligned}
$$

were we sum over repeated superscripts ($i \in 0, 1, 2$) and defined $[\mathbf{v}]^i_\times$ to be the vector holding the i^{th} *row* of the cross product matrix $[\mathbf{v}]_\times$:

$$
[\mathbf{v}]_\times = \begin{pmatrix} 0 & -v_2 & v_1 \\ v_2 & 0 & -v_0 \\ -v_1 & v_0 & 0 \end{pmatrix} \implies [\mathbf{v}]^0_\times = \begin{pmatrix} 0 \\ -v_2 \\ v_1 \end{pmatrix}, \ [\mathbf{v}]^1_\times = \begin{pmatrix} v_2 \\ 0 \\ -v_0 \end{pmatrix}, \ [\mathbf{v}]^2_\times = \begin{pmatrix} -v_1 \\ v_0 \\ 0 \end{pmatrix}.
$$

We can simplify this Hessian into a form that reveals the expected symmetry with respect to the two rightmost indices:

$$
\boxed{
\begin{aligned}
\frac{\partial^2 \tilde{\mathbf{v}}}{\partial \boldsymbol{\omega}^2} = &-(\mathbf{v} \otimes I)\frac{\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|} - \big[(\mathbf{v} \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega} + \mathbf{e}^i \otimes ([\mathbf{v}]^i_\times \otimes \boldsymbol{\omega} + \boldsymbol{\omega} \otimes [\mathbf{v}]^i_\times) + (\mathbf{v} \times \boldsymbol{\omega}) \otimes I\big] \left(\frac{\|\boldsymbol{\omega}\| \cos(\|\boldsymbol{\omega}\|) - \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^3}\right) \\
&+ \big[\mathbf{e}^i \otimes (\mathbf{e}^i \otimes \mathbf{v} + \mathbf{v} \otimes \mathbf{e}^i)\big] \left(\frac{1 - \cos(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^2}\right) \\
&+ \Big[(\boldsymbol{\omega} \cdot \mathbf{v})\Big(\mathbf{e}^i \otimes (\mathbf{e}^i \otimes \boldsymbol{\omega} + \boldsymbol{\omega} \otimes \mathbf{e}^i) + \boldsymbol{\omega} \otimes I\Big) + \boldsymbol{\omega} \otimes (\mathbf{v} \otimes \boldsymbol{\omega} + \boldsymbol{\omega} \otimes \mathbf{v})\Big] \left(\frac{2\cos(\|\boldsymbol{\omega}\|) - 2 + \|\boldsymbol{\omega}\| \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^4}\right) \\
&+ \boldsymbol{\omega} \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega} \left((\boldsymbol{\omega} \cdot \mathbf{v})\frac{8 + (\|\boldsymbol{\omega}\|^2 - 8)\cos(\|\boldsymbol{\omega}\|) - 5\|\boldsymbol{\omega}\| \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^6}\right) \\
&+ \big[(\mathbf{v} \times \boldsymbol{\omega}) \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega}\big] \left(\frac{3\|\boldsymbol{\omega}\| \cos(\|\boldsymbol{\omega}\|) + (\|\boldsymbol{\omega}\|^2 - 3)\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^5}\right).
\end{aligned}
}
$$

2.3 Numerically Robust Formulas

The rotation formula and its derivatives must be evaluated with care: around $\boldsymbol{\omega} = 0$, a naive implementation would attempt to calculate (approximately) $\frac{0}{0}$ for several of the expressions. In particular, we must use the following Taylor expansions to evaluate the problematic terms for $\|\boldsymbol{\omega}\| \ll 1$:

$$
\begin{aligned}
\frac{\sin \|\boldsymbol{\omega}\|}{\|\boldsymbol{\omega}\|} &= 1 - \frac{\|\boldsymbol{\omega}\|^2}{6} + O(\|\boldsymbol{\omega}\|^4) \\
\frac{1 - \cos(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^2} &= \frac{1}{2} - \frac{\|\boldsymbol{\omega}\|^2}{24} + O(\|\boldsymbol{\omega}\|^4) \\
\frac{\|\boldsymbol{\omega}\| \cos(\|\boldsymbol{\omega}\|) - \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^3} &= -\frac{1}{3} + \frac{\|\boldsymbol{\omega}\|^2}{30} + O(\|\boldsymbol{\omega}\|^4)
\end{aligned}
$$

$$\frac{2\cos(\|\boldsymbol{\omega}\|] - 2 + \|\boldsymbol{\omega}\|\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^4} = -\frac{1}{12} + \frac{\|\boldsymbol{\omega}\|^2}{180} + O(\|\boldsymbol{\omega}\|^4)$$
$$\frac{8 + (\|\boldsymbol{\omega}\|^2 - 8)\cos(\|\boldsymbol{\omega}\|) - 5\|\boldsymbol{\omega}\|\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^6} = \frac{1}{90} - \frac{\|\boldsymbol{\omega}\|^2}{1680} + O(\|\boldsymbol{\omega}\|^4)$$
$$\frac{3\|\boldsymbol{\omega}\|\cos(\|\boldsymbol{\omega}\|) + (\|\boldsymbol{\omega}\|^2 - 3)\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^5} = -\frac{1}{15} + \frac{\|\boldsymbol{\omega}\|^2}{210} + O(\|\boldsymbol{\omega}\|^4).$$

We determined empirically that switching over to the Taylor expansion for $\|\boldsymbol{\omega}\| < 2 \times 10^{-6}$ is a good trade-off between catastrophic cancellation in the direct calculation and truncation error in the Taylor series approximation.

2.4 Variations around the Identity

Most of the terms in the gradient and Hessian formulas vanish when we evaluate at $\boldsymbol{\omega} = 0$. This means that if we update the parametrization at every iteration of Newton's method, we can use much simpler formulas:

$$\left.\frac{\partial \tilde{\mathbf{v}}}{\partial \boldsymbol{\omega}}\right|_{\boldsymbol{\omega}=0} = -[\mathbf{v}]_\times, \qquad \left.\frac{\partial^2 \tilde{\mathbf{v}}}{\partial \boldsymbol{\omega}^2}\right|_{\boldsymbol{\omega}=0} = -(\mathbf{v} \otimes I) + \frac{1}{2}\left[\mathbf{e}^i \otimes (\mathbf{e}^i \otimes \mathbf{v} + \mathbf{v} \otimes \mathbf{e}^i)\right].$$

2.5 Full Rotation Matrix and its Derivatives

As mentioned in Section 2.1, we could evaluate the rotation matrix and its derivatives using the formulas derived above for a single rotated vector: apply them to each of the three canonical basis vectors $\mathbf{e}^0, \mathbf{e}^1, \mathbf{e}^2$. However, due to the basis vectors' sparsity, we can derive more efficient expressions. The rotation matrix is:

$$R(\boldsymbol{\omega}) = I\cos(\|\boldsymbol{\omega}\|) + (\boldsymbol{\omega} \otimes \boldsymbol{\omega})\frac{1 - \cos(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^2} + [\boldsymbol{\omega}]_\times \frac{\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|}.$$

The gradients and Hessians are now 3^{rd} and 4^{th} order tensors, respectively. The left two indices of these tensors pick a component of R and the remaining indices pick differentiation variables from $\boldsymbol{\omega}$.

$$\begin{aligned}
\frac{\partial R}{\partial \boldsymbol{\omega}} &= ([\mathbf{e}^i]_\times \otimes \mathbf{e}^i - I \otimes \boldsymbol{\omega})\frac{\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|} + \left[(\mathbf{e}^i \otimes \boldsymbol{\omega} + \boldsymbol{\omega} \otimes \mathbf{e}^i) \otimes \mathbf{e}^i\right]\left(\frac{1 - \cos(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^2}\right) \\
&\quad + (\boldsymbol{\omega} \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega})\left(\frac{2\cos(\|\boldsymbol{\omega}\|) - 2 + \|\boldsymbol{\omega}\|\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^4}\right) + \left([\boldsymbol{\omega}]_\times \otimes \boldsymbol{\omega}\right)\frac{\|\boldsymbol{\omega}\|\cos(\|\boldsymbol{\omega}\|) - \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^3}, \\
\frac{\partial^2 R}{\partial \boldsymbol{\omega}^2} &= -(I \otimes I)\frac{\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|} + \left([\mathbf{e}^i]_\times \otimes \mathbf{e}^i - I \otimes \boldsymbol{\omega}\right) \otimes \boldsymbol{\omega}\left(\frac{\|\boldsymbol{\omega}\|\cos(\|\boldsymbol{\omega}\|) - \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^3}\right) \\
&\quad + \left[(\mathbf{e}^i \otimes \mathbf{e}^k + \mathbf{e}^k \otimes \mathbf{e}^i) \otimes \mathbf{e}^i \otimes \mathbf{e}^k\right]\left(\frac{1 - \cos(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^2}\right) \\
&\quad + \left[(\mathbf{e}^i \otimes \boldsymbol{\omega} + \boldsymbol{\omega} \otimes \mathbf{e}^i) \otimes \mathbf{e}^i \otimes \boldsymbol{\omega}\right]\left(\frac{2\cos(\|\boldsymbol{\omega}\|) - 2 + \|\boldsymbol{\omega}\|\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^4}\right) \\
&\quad + \left[\mathbf{e}^i \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega} + \boldsymbol{\omega} \otimes \mathbf{e}^i \otimes \boldsymbol{\omega} + \boldsymbol{\omega} \otimes \boldsymbol{\omega} \otimes \mathbf{e}^i\right] \otimes \mathbf{e}^i\left(\frac{2\cos(\|\boldsymbol{\omega}\|) - 2 + \|\boldsymbol{\omega}\|\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^4}\right) \\
&\quad + \left(\boldsymbol{\omega} \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega}\right)\left(\frac{8 + (\|\boldsymbol{\omega}\|^2 - 8)\cos(\|\boldsymbol{\omega}\|) - 5\|\boldsymbol{\omega}\|\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^6}\right) \\
&\quad + \left([\mathbf{e}^i]_\times \otimes \boldsymbol{\omega} \otimes \mathbf{e}^i + [\boldsymbol{\omega}]_\times \otimes \mathbf{e}^i \otimes \mathbf{e}^i\right)\frac{\|\boldsymbol{\omega}\|\cos(\|\boldsymbol{\omega}\|) - \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^3} \\
&\quad - \left([\boldsymbol{\omega}]_\times \otimes \boldsymbol{\omega}\right) \otimes \boldsymbol{\omega}\left(\frac{3\|\boldsymbol{\omega}\|\cos(\|\boldsymbol{\omega}\|) + (\|\boldsymbol{\omega}\|^2 - 3)\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^5}\right)
\end{aligned}$$

$$
\begin{aligned}
&= -(I \otimes I)\frac{\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|} + \left([\mathbf{e}^i]_\times \otimes (\mathbf{e}^i \otimes \boldsymbol{\omega} + \boldsymbol{\omega} \otimes \mathbf{e}^i) - I \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega} + [\boldsymbol{\omega}]_\times \otimes I\right)\left(\frac{\|\boldsymbol{\omega}\|\cos(\|\boldsymbol{\omega}\|) - \sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^3}\right) \\
&\quad + \left[\mathbf{e}^i \otimes \mathbf{e}^k \otimes (\mathbf{e}^i \otimes \mathbf{e}^k + \mathbf{e}^k \otimes \mathbf{e}^i)\right]\left(\frac{1-\cos(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^2}\right) \\
&\quad + \left[(\mathbf{e}^i \otimes \boldsymbol{\omega} + \boldsymbol{\omega} \otimes \mathbf{e}^i) \otimes (\mathbf{e}^i \otimes \boldsymbol{\omega} + \boldsymbol{\omega} \otimes \mathbf{e}^i) + \boldsymbol{\omega} \otimes \boldsymbol{\omega} \otimes I\right]\left(\frac{2\cos(\|\boldsymbol{\omega}\|) - 2 + \|\boldsymbol{\omega}\|\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^4}\right) \\
&\quad + \left(\boldsymbol{\omega} \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega} \otimes \boldsymbol{\omega}\right)\left(\frac{8 + (\|\boldsymbol{\omega}\|^2 - 8)\cos(\|\boldsymbol{\omega}\|) - 5\|\boldsymbol{\omega}\|\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^6}\right) \\
&\quad - \left([\boldsymbol{\omega}]_\times \otimes \boldsymbol{\omega}\right) \otimes \boldsymbol{\omega}\left(\frac{3\|\boldsymbol{\omega}\|\cos(\|\boldsymbol{\omega}\|) + (\|\boldsymbol{\omega}\|^2 - 3)\sin(\|\boldsymbol{\omega}\|)}{\|\boldsymbol{\omega}\|^5}\right).
\end{aligned}
$$

3 Design Optimization Derivatives

We describe how to compute the full derivative information required to apply Newton CG to the design optimization (5) proposed in Section 5 of the main X-shells paper. The notation here follows that in the main paper.

For gradients, we solve for the adjoint deployed and flat state vectors $\mathbf{w}$, $\mathbf{y}$, and $\mathbf{s}$ needed for the target fitting objective, the flatness constraint c, and the minimum angle constraint on $\alpha_{\min}$:

$$
\begin{aligned}
\underbrace{\begin{bmatrix} H_{3D} & \mathbf{a} \\ \mathbf{a}^T & 0 \end{bmatrix}}_{K_{3D}} \begin{bmatrix} \mathbf{w} \\ w_\lambda \end{bmatrix} &= \begin{bmatrix} W\left(\mathbf{x}^*_{3D} - \mathbf{x}_{\text{tgt}}\right) + W_{\text{surf}}\left(\mathbf{x}^*_{3D} - P_{\text{surf}}\left(\mathbf{x}^*_{3D}\right)\right) \\ 0 \end{bmatrix}, \\
\underbrace{\begin{bmatrix} H_{2D} & \mathbf{a} \\ \mathbf{a}^T & 0 \end{bmatrix}}_{K_{2D}} \begin{bmatrix} \mathbf{y} \\ y_\lambda \end{bmatrix} &= \begin{bmatrix} 2S_z^T S_z \mathbf{x}^*_{2D} \\ 0 \end{bmatrix}, \\
K_{2D} \begin{bmatrix} \mathbf{s} \\ s_\lambda \end{bmatrix} &= \begin{bmatrix} S_\alpha^T \frac{\partial KS}{\partial \alpha}(S_\alpha \mathbf{x}^*_{2D}) \\ 0 \end{bmatrix},
\end{aligned}
$$

where $H_{2D} = \frac{\partial^2 E}{\partial \mathbf{x} \partial \mathbf{x}}(\mathbf{x}^*_{2D}(\mathbf{p}), \mathbf{p})$ and $H_{3D} = \frac{\partial^2 E}{\partial \mathbf{x} \partial \mathbf{x}}(\mathbf{x}^*_{3D}(\mathbf{p}), \mathbf{p})$ are the elastic energy Hessians for the deployed and flat equilibria, and scalars w_λ, y_λ, and s_λ are ignored. With these adjoint states, we can efficiently evaluate the objective and constraints' gradients:

$$
\begin{aligned}
\frac{\partial J}{\partial \mathbf{p}} &= \frac{\gamma}{E_0}\frac{\partial E}{\partial \mathbf{p}}(\mathbf{x}^*_{2D}, \mathbf{p}) + \frac{(1-\gamma)}{E_0}\frac{\partial E}{\partial \mathbf{p}}(\mathbf{x}^*_{3D}, \mathbf{p}) - \frac{\beta}{l_0^2}\mathbf{w}^T\frac{\partial^2 E}{\partial \mathbf{x} \partial \mathbf{p}}(\mathbf{x}^*_{3D}, \mathbf{p}), \\
\frac{\partial c}{\partial \mathbf{p}} &= -\mathbf{y}^T\frac{\partial^2 E}{\partial \mathbf{x} \partial \mathbf{p}}(\mathbf{x}^*_{2D}(\mathbf{p}), \mathbf{p}), \\
\frac{\partial \alpha_{\min}}{\partial \mathbf{p}} &= -\mathbf{s}^T\frac{\partial^2 E}{\partial \mathbf{x} \partial \mathbf{p}}(\mathbf{x}^*_{2D}(\mathbf{p}), \mathbf{p}).
\end{aligned}
$$

To evaluate Hessian-vector products, we compute the variations of forward and adjoint state vectors $\delta\mathbf{x}^*_{2D}$, $\delta\mathbf{x}^*_{3D}$, $\delta\mathbf{w}$, $\delta\mathbf{y}$, and $\delta\mathbf{s}$ that arise from parameter perturbation $\delta\mathbf{p}$ by solving:

$$
\begin{aligned}
K_{2D}\begin{bmatrix} \delta\mathbf{x}^*_{2D} \\ \delta\lambda_{2D} \end{bmatrix} &= \begin{bmatrix} -\frac{\partial^2 E}{\partial \mathbf{x} \partial \mathbf{p}}(\mathbf{x}^*_{2D}(\mathbf{p}), \mathbf{p})\delta\mathbf{p} \\ 0 \end{bmatrix}, \\
K_{3D}\begin{bmatrix} \delta\mathbf{x}^*_{3D} \\ \delta\lambda_{3D} \end{bmatrix} &= \begin{bmatrix} -\frac{\partial^2 E}{\partial \mathbf{x} \partial \mathbf{p}}(\mathbf{x}^*_{3D}, \mathbf{p})\delta\mathbf{p} \\ 0 \end{bmatrix}, \\
K_{3D}\begin{bmatrix} \delta\mathbf{w} \\ \delta w_\lambda \end{bmatrix} &= \begin{bmatrix} W\delta\mathbf{x}^*_{3D} + W_{\text{surf}}\left(\delta\mathbf{x}^*_{3D} - \frac{\partial P_{\text{surf}}}{\partial \mathbf{x}}\delta\mathbf{x}^*_{3D}\right) \\ 0 \end{bmatrix} - \begin{bmatrix} \left(\frac{\partial^3 E}{\partial \mathbf{x} \partial \mathbf{x} \partial \mathbf{x}}(\mathbf{x}^*_{3D}, \mathbf{p})\delta\mathbf{x}^*_{3D} + \frac{\partial^3 E}{\partial \mathbf{x} \partial \mathbf{x} \partial \mathbf{p}}(\mathbf{x}^*_{3D}, \mathbf{p})\delta\mathbf{p}\right)\mathbf{w} \\ 0 \end{bmatrix},
\end{aligned}
$$

$$K_{2\mathrm{D}}\begin{bmatrix}\delta\mathbf{y}\\ \delta y_\lambda\end{bmatrix} = \begin{bmatrix}2S_z^T S_z \delta\mathbf{x}^*_{2\mathrm{D}}\\ 0\end{bmatrix} - \begin{bmatrix}\left(\frac{\partial^3 E}{\partial\mathbf{x}\partial\mathbf{x}\partial\mathbf{x}}(\mathbf{x}^*_{2\mathrm{D}}(\mathbf{p}),\mathbf{p})\delta\mathbf{x}^*_{2\mathrm{D}} + \frac{\partial^3 E}{\partial\mathbf{x}\partial\mathbf{x}\partial\mathbf{p}}(\mathbf{x}^*_{2\mathrm{D}}(\mathbf{p}),\mathbf{p})\delta\mathbf{p}\right)\mathbf{y}\\ 0\end{bmatrix},$$

$$K_{2\mathrm{D}}\begin{bmatrix}\delta\mathbf{s}\\ \delta s_\lambda\end{bmatrix} = \begin{bmatrix}S_\alpha^T \frac{\partial^2 KS}{\partial\alpha\partial\alpha} S_\alpha \delta\mathbf{x}^*_{2\mathrm{D}}\\ 0\end{bmatrix} - \begin{bmatrix}\left(\frac{\partial^3 E}{\partial\mathbf{x}\partial\mathbf{x}\partial\mathbf{x}}(\mathbf{x}^*_{2\mathrm{D}},\mathbf{p})\delta\mathbf{x}^*_{2\mathrm{D}} + \frac{\partial^3 E}{\partial\mathbf{x}\partial\mathbf{x}\partial\mathbf{p}}(\mathbf{x}^*_{2\mathrm{D}},\mathbf{p})\delta\mathbf{p}\right)\mathbf{s}\\ 0\end{bmatrix},$$

where the derivative of the closest point projection $\frac{\partial P_{\mathrm{surf}}}{\partial\mathbf{x}}$ can be computed as $I - \mathbf{n}\otimes\mathbf{n}$ when the closest point lies on a surface triangle with normal $\mathbf{n}$, $\mathbf{e}\otimes\mathbf{e}$ when it lies on a surface edge with normalized edge vector $\mathbf{e}$, and 0 when it lies on a vertex.

The Hessian-vector products for the objective and constraints can now be calculated:

$$\begin{aligned}
\frac{\partial^2 J}{\partial\mathbf{p}\partial\mathbf{p}}\delta\mathbf{p} =& \frac{\gamma}{E_0}\left(\frac{\partial^2 E}{\partial\mathbf{p}\partial\mathbf{x}}(\mathbf{x}^*_{2\mathrm{D}},\mathbf{p})\delta\mathbf{x}^*_{2\mathrm{D}} + \frac{\partial^2 E}{\partial\mathbf{p}\partial\mathbf{p}}(\mathbf{x}^*_{2\mathrm{D}},\mathbf{p})\delta\mathbf{p}\right)\\
&+\frac{(1-\gamma)}{E_0}\left(\frac{\partial^2 E}{\partial\mathbf{p}\partial\mathbf{x}}(\mathbf{x}^*_{3\mathrm{D}},\mathbf{p})\delta\mathbf{x}^*_{3\mathrm{D}} + \frac{\partial^2 E}{\partial\mathbf{p}\partial\mathbf{p}}(\mathbf{x}^*_{3\mathrm{D}},\mathbf{p})\delta\mathbf{p}\right)\\
&-\frac{\beta}{l_0^2}\begin{bmatrix}\frac{\partial^2 E}{\partial\mathbf{p}\partial\mathbf{x}}(\mathbf{x}^*_{3\mathrm{D}},\mathbf{p})\\ 0\end{bmatrix}\delta\mathbf{w} - \frac{\beta}{l_0^2}\begin{bmatrix}\frac{\partial^3 E}{\partial\mathbf{p}\partial\mathbf{x}\partial\mathbf{x}}(\mathbf{x}^*_{3\mathrm{D}},\mathbf{p})\delta\mathbf{x}^*_{3\mathrm{D}} + \frac{\partial^3 E}{\partial\mathbf{p}\partial\mathbf{x}\partial\mathbf{p}}(\mathbf{x}^*_{3\mathrm{D}},\mathbf{p})\delta\mathbf{p}\\ 0\end{bmatrix}\mathbf{w},\\
\frac{\partial^2 c}{\partial\mathbf{p}\partial\mathbf{p}}\delta\mathbf{p} =& -\frac{\partial^2 E}{\partial\mathbf{p}\partial\mathbf{x}}(\mathbf{x}^*_{2\mathrm{D}}(\mathbf{p}),\mathbf{p})\delta\mathbf{y} - \left(\frac{\partial^3 E}{\partial\mathbf{p}\partial\mathbf{x}\partial\mathbf{x}}(\mathbf{x}^*_{2\mathrm{D}}(\mathbf{p}),\mathbf{p})\delta\mathbf{x}^*_{2\mathrm{D}} + \frac{\partial^3 E}{\partial\mathbf{p}\partial\mathbf{x}\partial\mathbf{p}}(\mathbf{x}^*_{2\mathrm{D}}(\mathbf{p}),\mathbf{p})\delta\mathbf{p}\right)\mathbf{y},\\
\frac{\partial^2 \alpha_{\min}}{\partial\mathbf{p}\partial\mathbf{p}}\delta\mathbf{p} =& -\frac{\partial^2 E}{\partial\mathbf{p}\partial\mathbf{x}}(\mathbf{x}^*_{2\mathrm{D}}(\mathbf{p}),\mathbf{p})\delta\mathbf{s} - \left(\frac{\partial^3 E}{\partial\mathbf{p}\partial\mathbf{x}\partial\mathbf{x}}(\mathbf{x}^*_{2\mathrm{D}}(\mathbf{p}),\mathbf{p})\delta\mathbf{x}^*_{2\mathrm{D}} + \frac{\partial^3 E}{\partial\mathbf{p}\partial\mathbf{x}\partial\mathbf{p}}(\mathbf{x}^*_{2\mathrm{D}}(\mathbf{p}),\mathbf{p})\delta\mathbf{p}\right)\mathbf{s}.
\end{aligned}$$

Notice that we can reuse the factorizations of $K_{2\mathrm{D}}$ and $K_{3\mathrm{D}}$ that were computed to solve the adjoint equations, so the added cost for computing these Hessian-vector products for a given $\delta\mathbf{p}$ is simply five additional back substitutions for $\delta\mathbf{x}^*_{2\mathrm{D}}$, $\delta\mathbf{x}^*_{3\mathrm{D}}$, $\delta\mathbf{w}$, $\delta\mathbf{y}$, and $\delta\mathbf{s}$.

4 Discrete Elastic Rods

We use the discrete stretching and twisting energies from [Bergou et al., 2010], however we prefer the original bending energy from [Bergou et al., 2008]. The stretching energy is given by:

$$E_s = \frac{1}{2}\sum_{j=0}^{\mathtt{ne}-1} k_s^j \left(\frac{|\mathbf{e}^j|}{|\bar{\mathbf{e}}^j|} - 1\right)^2 |\bar{\mathbf{e}}^j|.$$

The twisting energy is reproduced in (A2), the bending energy from [Bergou et al., 2010] in (A3), and the bending energy from [Bergou et al., 2008] in (A4). The notation in these energies and throughout the rest of this supplement is from [Bergou et al., 2010], except where we need to introduce the new concept of source frames to properly compute gradients and Hessians for finite, discrete steps.

4.1 Errors in [Bergou et al., 2010]

The primary objective of the remainder of this supplement is to identify and correct errors in the gradient and Hessian formulas given in [Bergou et al., 2010]. The fundamental issue lies in how reference frames are parallel transported from a previous curve configuration to construct an adapted frame for a new deformed curve. In short, the formulas in [Bergou et al., 2010] assume that the reference frames are always parallel transported from the previous instant in time, and thus, when these expressions are differentiated, no distinction is made between the current curve's frame and the *source frame* used for parallel transport.

The implication of this assumption is that the bending and twisting energies are now path dependent: traversing a closed loop in the rod variable space will lead to a different energy value as the parallel-transported reference frame (i.e., the "hidden state") will have rotated by some holonomy angle. This path dependence means that the Hessians for "infinitesimal transport" are actually *not symmetric*. We compute the correct asymmetric Hessian formulas for the twisting and bending energies in Section 4.5 and Section 4.6. The inaccurate Hessian formulas in [Bergou et al., 2010] can be obtained by symmetrizing these expressions.

To leverage efficient symmetric sparse factorizations, we prefer to use a symmetric Hessian, which can be obtained by holding the source reference frame from which we parallel transport fixed within each Newton iteration; then we have a well-defined, path-independent energy landscape to minimize at each iteration. The energy landscape now changes at discrete instants in time—whenever the source frame is updated. The resulting "finite transport" Hessian *and gradient* formulas involve additional terms missing in [Bergou et al., 2010]. To simplify the Hessian formulas and stay far away from singularities in the parallel transport operator (which occur when transporting from a vector to its negation), we update the source frame at the end of each Newton iteration, before the next Hessian is evaluated.

4.2 Preliminary derivations

First, we give some useful derivative expressions. The derivative of length with respect to an edge vector is $\frac{\partial \|\mathbf{e}^j\|}{\partial \mathbf{e}^j} = \mathbf{t}^j$. Derivatives with respect to edge vectors can easily be expressed with respect to centerline vertex positions. For example:

$$\frac{\partial \|\mathbf{e}^j\|}{\partial \mathbf{x}_a} = \mathbf{t}^j(\delta_{a(j+1)} - \delta_{aj}),$$

recalling that edge vector $\mathbf{e}^j$ points from vertex $\mathbf{x}_j$ to $\mathbf{x}_{j+1}$.

The derivative of a tangent vector $\mathbf{t}^j$ with respect to its corresponding edge vector is:

$$\frac{\partial \mathbf{t}^j}{\partial \mathbf{e}^j} = \frac{\partial(\mathbf{e}^j/\|\mathbf{e}^j\|)}{\partial \mathbf{e}^j} = \frac{I}{\|\mathbf{e}^j\|} - \frac{\mathbf{e}^j}{\|\mathbf{e}^j\|^2} \otimes \frac{\partial \|\mathbf{e}^j\|}{\partial \mathbf{e}^j} = \frac{I - \mathbf{t}^j \otimes \mathbf{t}^j}{\|\mathbf{e}^j\|},$$

which also has a clear geometric interpretation.

Recall that the curvature binormal on vertex i is given by:

$$(\kappa \mathbf{b})_i = \frac{2\mathbf{t}^{i-1} \times \mathbf{t}^i}{1 + \mathbf{t}^{i-1} \cdot \mathbf{t}^i} := \frac{2\mathbf{t}^{i-1} \times \mathbf{t}^i}{\chi},$$

where we defined $\chi = 1 + \mathbf{t}^{i-1} \cdot \mathbf{t}^i$ for convenience.

We now compute the derivative of $\kappa \mathbf{b}$ with respect to an edge vector:

$$\begin{aligned}
\frac{\partial(\kappa \mathbf{b})_i}{\partial \mathbf{e}^a} &= \left[\frac{2[\mathbf{t}^{i-1}]_\times}{\chi} - \frac{(\kappa \mathbf{b})_i}{\chi} \otimes \mathbf{t}^{i-1}\right] \frac{\partial \mathbf{t}^i}{\partial \mathbf{e}^a} + \left[-\frac{2[\mathbf{t}^i]_\times}{\chi} - \frac{(\kappa \mathbf{b})_i}{\chi} \otimes \mathbf{t}^i\right] \frac{\partial \mathbf{t}^{i-1}}{\partial \mathbf{e}^a} \\
&= \left[\frac{2[\mathbf{t}^{i-1}]_\times}{\chi} - \frac{(\kappa \mathbf{b})_i}{\chi} \otimes \mathbf{t}^{i-1}\right] \frac{I - \mathbf{t}^i \otimes \mathbf{t}^i}{\|\mathbf{e}^i\|} \delta_{ai} \\
&\quad + \left[-\frac{2[\mathbf{t}^i]_\times}{\chi} - \frac{(\kappa \mathbf{b})_i}{\chi} \otimes \mathbf{t}^i\right] \frac{I - \mathbf{t}^{i-1} \otimes \mathbf{t}^{i-1}}{\|\mathbf{e}^{i-1}\|} \delta_{a(i-1)} \\
&= \frac{\delta_{ai}}{\|\mathbf{e}^i\|} \left[\frac{2[\mathbf{t}^{i-1}]_\times}{\chi} - \underbrace{\frac{2\mathbf{t}^{i-1} \times \mathbf{t}^i}{\chi} \otimes \mathbf{t}^i}_{\cancel{(\kappa \mathbf{b})_i \otimes \mathbf{t}^i}} - \frac{(\kappa \mathbf{b})_i}{\chi} \otimes \mathbf{t}^{i-1} + \frac{(\kappa \mathbf{b})_i}{\chi} \underbrace{(\mathbf{t}^{i-1} \cdot \mathbf{t}^i)}_{\cancel{\chi} - 1} \otimes \mathbf{t}^i\right] \\
&\quad + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|} \left[-\frac{2[\mathbf{t}^i]_\times}{\chi} - \underbrace{\frac{2\mathbf{t}^{i-1} \times \mathbf{t}^i}{\chi} \otimes \mathbf{t}^{i-1}}_{\cancel{(\kappa \mathbf{b})_i \otimes \mathbf{t}^{i-1}}} - \frac{(\kappa \mathbf{b})_i}{\chi} \otimes \mathbf{t}^i + \frac{(\kappa \mathbf{b})_i}{\chi} \underbrace{(\mathbf{t}^{i-1} \cdot \mathbf{t}^i)}_{\cancel{\chi} - 1} \otimes \mathbf{t}^{i-1}\right] \\
&= \boxed{\frac{\delta_{ai}}{\|\mathbf{e}^i\|} \left[\frac{2[\mathbf{t}^{i-1}]_\times}{\chi} - \frac{(\kappa \mathbf{b})_i}{\chi} \otimes (\mathbf{t}^{i-1} + \mathbf{t}^i)\right] + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|} \left[-\frac{2[\mathbf{t}^i]_\times}{\chi} - \frac{(\kappa \mathbf{b})_i}{\chi} \otimes (\mathbf{t}^{i-1} + \mathbf{t}^i)\right].}
\end{aligned}$$

4.3 Derivative of Parallel Transport

We will need the derivative of parallel transport with respect to the target vector, and we begin with an explicit formula for parallel transport of a vector $\mathbf{v}$ from unit tangent $\mathbf{t}_1$ to unit tangent $\mathbf{t}_2$:

$$P_{\mathbf{t}_1}^{\mathbf{t}_2}\mathbf{v} = \left(\frac{(\mathbf{t}_1 \times \mathbf{t}_2) \otimes (\mathbf{t}_1 \times \mathbf{t}_2)}{1 + \mathbf{t}_1 \cdot \mathbf{t}_2} + \mathbf{t}_2 \otimes \mathbf{t}_1 - \mathbf{t}_1 \otimes \mathbf{t}_2 + \mathbf{t}_1 \cdot \mathbf{t}_2 I\right)\mathbf{v}.$$

$$\boxed{\frac{\partial P_{\mathbf{t}_1}^{\mathbf{t}_2}\mathbf{v}}{\partial \mathbf{t}_2} = \frac{\big((\mathbf{t}_1 \times \mathbf{t}_2)\cdot \mathbf{v}\big)[\mathbf{t}_1]_\times + (\mathbf{t}_1 \times \mathbf{t}_2) \otimes (\mathbf{v} \times \mathbf{t}_1)}{1 + \mathbf{t}_1 \cdot \mathbf{t}_2} - \frac{(\mathbf{t}_1 \times \mathbf{t}_2)\cdot \mathbf{v}}{(1 + \mathbf{t}_1 \cdot \mathbf{t}_2)^2}(\mathbf{t}_1 \times \mathbf{t}_2) \otimes \mathbf{t}_1 + (\mathbf{t}_1 \cdot \mathbf{v})I - \mathbf{t}_1 \otimes \mathbf{v} + \mathbf{v} \otimes \mathbf{t}_1.}$$

Notice that the initial rate of change of a time-parallel material frame vector $\mathbf{d}_1$ as the tangent rotates *from its source configuration* is:

$$\delta \mathbf{d}_1 = \left.\frac{\partial P_{\mathbf{t}_1}^{\mathbf{t}_2}\mathbf{d}_1}{\partial \mathbf{t}_2}\right|_{\mathbf{t}_2 = \mathbf{t}_1} \delta \mathbf{t}_2 = \cancel{(\mathbf{t}_1 \cdot \mathbf{d}_1)}\delta \mathbf{t}_2 - (\mathbf{t}_1 \otimes \mathbf{d}_1)\delta \mathbf{t}_2 + (\mathbf{d}_1 \otimes \cancel{\mathbf{t}_1)\delta \mathbf{t}_2} = -(\mathbf{t}_1 \otimes \mathbf{d}_1)\delta \mathbf{t}_2,$$

meaning the material frame is initially perturbed only along the tangent direction

4.4 Hessian of Twist

We can now compute the Hessian of twist m_i, whose derivatives with respect to the incident edges' vectors are:

$$\frac{\partial m_i}{\partial \mathbf{e}^i} = \frac{(\kappa \mathbf{b})_i}{2\|\mathbf{e}^i\|}, \quad \frac{\partial m_i}{\partial \mathbf{e}^{i-1}} = \frac{(\kappa \mathbf{b})_i}{2\|\mathbf{e}^{i-1}\|}.$$

Note that the twist is only linear with respect to the θ variables, so only edge vector/position variables have nonzero Hessian entries.

$$\begin{aligned}
\frac{\partial^2 m_i}{\partial \mathbf{e}^i \partial \mathbf{e}^a} &= \frac{1}{2\|\mathbf{e}^i\|}\frac{\partial (\kappa \mathbf{b})_i}{\partial \mathbf{e}^a} - \frac{(\kappa \mathbf{b})_i}{2\|\mathbf{e}^i\|^2} \otimes \mathbf{t}^i \delta_{ai} \\
&= \frac{\delta_{ai}}{2\|\mathbf{e}^i\|^2}\left[\frac{2[\mathbf{t}^{i-1}]_\times}{\chi} - \frac{(\kappa \mathbf{b})_i}{\chi} \otimes (\mathbf{t}^{i-1} + \mathbf{t}^i)\right] + \frac{\delta_{a(i-1)}}{2\|\mathbf{e}^i\|\|\mathbf{e}^{i-1}\|}\left[-\frac{2[\mathbf{t}^i]_\times}{\chi} - \frac{(\kappa \mathbf{b})_i}{\chi} \otimes (\mathbf{t}^{i-1} + \mathbf{t}^i)\right] - \frac{(\kappa \mathbf{b})_i}{2\|\mathbf{e}^i\|^2} \otimes \mathbf{t}^i \delta_{ai} \\
&= \frac{\delta_{ai}}{2\|\mathbf{e}^i\|^2}\left[\frac{2[\mathbf{t}^{i-1}]_\times}{\chi} - (\kappa \mathbf{b})_i \otimes \left(\frac{\mathbf{t}^{i-1} + \mathbf{t}^i}{\chi} + \mathbf{t}^i\right)\right] + \frac{\delta_{a(i-1)}}{2\|\mathbf{e}^i\|\|\mathbf{e}^{i-1}\|}\left[-\frac{2[\mathbf{t}^i]_\times}{\chi} - (\kappa \mathbf{b})_i \otimes \left(\frac{\mathbf{t}^{i-1} + \mathbf{t}^i}{\chi}\right)\right].
\end{aligned}$$

Similarly,

$$\begin{aligned}
\frac{\partial^2 m_i}{\partial \mathbf{e}^{i-1} \partial \mathbf{e}^a} &= \frac{1}{2\|\mathbf{e}^{i-1}\|}\frac{\partial (\kappa \mathbf{b})_i}{\partial \mathbf{e}^a} - \frac{(\kappa \mathbf{b})_i}{2\|\mathbf{e}^{i-1}\|^2} \otimes \mathbf{t}^{i-1} \delta_{a(i-1)} \\
&= \frac{\delta_{ai}}{2\|\mathbf{e}^{i-1}\|\|\mathbf{e}^i\|}\left[\frac{2[\mathbf{t}^{i-1}]_\times}{\chi} - (\kappa \mathbf{b})_i \otimes \left(\frac{\mathbf{t}^{i-1} + \mathbf{t}^i}{\chi}\right)\right] + \frac{\delta_{a(i-1)}}{2\|\mathbf{e}^{i-1}\|^2}\left[-\frac{2[\mathbf{t}^i]_\times}{\chi} - (\kappa \mathbf{b})_i \otimes \left(\frac{\mathbf{t}^{i-1} + \mathbf{t}^i}{\chi} + \mathbf{t}^{i-1}\right)\right].
\end{aligned}$$

From these expressions, we can extract:

$$\begin{aligned}
\frac{\partial^2 m_i}{\partial \mathbf{e}^i \partial \mathbf{e}^i} &= \frac{1}{2\|\mathbf{e}^i\|^2}\left[\frac{2[\mathbf{t}^{i-1}]_\times}{\chi} - (\kappa \mathbf{b})_i \otimes \left(\frac{\mathbf{t}^{i-1} + \mathbf{t}^i}{\chi} + \mathbf{t}^i\right)\right] \\
\frac{\partial^2 m_i}{\partial \mathbf{e}^i \partial \mathbf{e}^{i-1}} &= \frac{1}{2\|\mathbf{e}^i\|\|\mathbf{e}^{i-1}\|}\left[-\frac{2[\mathbf{t}^i]_\times}{\chi} - (\kappa \mathbf{b})_i \otimes \left(\frac{\mathbf{t}^{i-1} + \mathbf{t}^i}{\chi}\right)\right] \\
\frac{\partial^2 m_i}{\partial \mathbf{e}^{i-1} \partial \mathbf{e}^i} &= \frac{1}{2\|\mathbf{e}^{i-1}\|\|\mathbf{e}^i\|}\left[\frac{2[\mathbf{t}^{i-1}]_\times}{\chi} - (\kappa \mathbf{b})_i \otimes \left(\frac{\mathbf{t}^{i-1} + \mathbf{t}^i}{\chi}\right)\right]
\end{aligned}$$

$$\frac{\partial^2 m_i}{\partial \mathbf{e}^{i-1}\partial \mathbf{e}^{i-1}} = \frac{1}{2\|\mathbf{e}^{i-1}\|^2}\left[-\frac{2[\mathbf{t}^i]_\times}{\chi} - (\kappa\mathbf{b})_i \otimes \left(\frac{\mathbf{t}^{i-1}+\mathbf{t}^i}{\chi} + \mathbf{t}^{i-1}\right)\right].$$

Note that this Hessian is actually *not* symmetric. This asymmetry is due to the path-dependence caused by the internal state stored in material frame vectors $\mathbf{d}_2$. The appendix of [Bergou et al., 2010] incorrectly symmetrizes these terms.

4.5 Gradient and Hessian of Twisting Energy (Infinitesimal Transport)

The twisting energy is defined as:

$$E_t = \frac{1}{2}\sum_{i=1}^{\mathtt{nv}-2} \frac{\beta_i}{\bar{l}_i}(m_i - \overline{m}_i)^2, \tag{A2}$$

and its gradient is:

$$\nabla E_t = \sum_{i=1}^{\mathtt{nv}-2} \frac{\beta_i}{\bar{l}_i}(m_i - \overline{m}_i)\nabla m_i.$$

Here ∇m_i collects the partial derivatives with respect to centerline position degrees of freedom and θ (material axis) degrees of freedom. These are given by:

$$\frac{\partial m_i}{\partial \mathbf{x}_a} = \frac{(\kappa\mathbf{b})_i}{2\|\mathbf{e}^i\|}(\delta_{a(i+1)} - \delta_{ai}) + \frac{(\kappa\mathbf{b})_i}{2\|\mathbf{e}^{i-1}\|}(\delta_{ai} - \delta_{a(i-1)}), \quad \frac{\partial m_i}{\partial \theta^a} = \delta_{ai} - \delta_{a(i-1)}.$$

The Hessian is:

$$HE_t = \sum_{i=1}^{\mathtt{nv}-2} \frac{\beta_i}{\bar{l}_i}\Big(\nabla m_i \otimes \nabla m_i + (m_i - \overline{m}_i)Hm_i\Big).$$

This full Hessian can be built by assembling per-vertex Hessian contributions that involve only the $\mathbf{x}$ and θ degrees of freedom for the vertex and its two neighbors. The "θ, θ part" of this Hessian is:

$$\frac{\partial^2 E_t}{\partial \theta^a \partial \theta^b} = \sum_{i=1}^{\mathtt{nv}-2} \frac{\beta_i}{\bar{l}_i}(\delta_{ai} - \delta_{a(i-1)})(\delta_{bi} - \delta_{b(i-1)}),$$

where the Hm_i term vanished because m_i is linear with respect to the θ variables.

The "$\theta, \mathbf{x}$ part" is:

$$\begin{aligned}\frac{\partial^2 E_t}{\partial \theta^a \partial \mathbf{x}_b} &= \sum_{i=1}^{\mathtt{nv}-2} \frac{\beta_i}{\bar{l}_i}(\delta_{ai} - \delta_{a(i-1)})\left(\frac{(\kappa\mathbf{b})_i}{2\|\mathbf{e}^i\|}(\delta_{b(i+1)} - \delta_{bi}) + \frac{(\kappa\mathbf{b})_i}{2\|\mathbf{e}^{i-1}\|}(\delta_{bi} - \delta_{b(i-1)})\right) \\ &= \sum_{i=1}^{\mathtt{nv}-2} \frac{\beta_i}{2\bar{l}_i}(\kappa\mathbf{b})_i(\delta_{ai} - \delta_{a(i-1)})\left(\frac{\delta_{b(i+1)} - \delta_{bi}}{\|\mathbf{e}^i\|} + \frac{\delta_{bi} - \delta_{b(i-1)}}{\|\mathbf{e}^{i-1}\|}\right),\end{aligned}$$

where again the Hm_i term vanished because no term of m_i contains both θ and $\mathbf{x}$ variables.

Finally, the "$\mathbf{x}, \mathbf{x}$ part is:

$$\begin{aligned}\frac{\partial^2 E_t}{\partial \mathbf{x}_a \partial \mathbf{x}_b} = \sum_{i=1}^{\mathtt{nv}-2} &\frac{\beta_i}{4\bar{l}_i}[(\kappa\mathbf{b})_i \otimes (\kappa\mathbf{b})_i]\left(\frac{\delta_{a(i+1)} - \delta_{ai}}{\|\mathbf{e}^i\|} + \frac{\delta_{ai} - \delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right)\left(\frac{\delta_{b(i+1)} - \delta_{bi}}{\|\mathbf{e}^i\|} + \frac{\delta_{bi} - \delta_{b(i-1)}}{\|\mathbf{e}^{i-1}\|}\right) \\ &+ \frac{\beta_i}{\bar{l}_i}(m_i - \overline{m}_i)\frac{\partial^2 m_i}{\partial \mathbf{x}_a \partial \mathbf{x}_b}.\end{aligned}$$

4.6 Gradient and Hessian of Bending Energy (Infinitesimal Transport)

The bending energy from [Bergou et al., 2010] is defined as:

$$E_b = \frac{1}{2}\sum_{i=1}^{\texttt{nv}-2} \frac{1}{\bar{l}_i}\Big(B_{11}(\kappa_{1i}-\overline{\kappa_{1i}})^2 + B_{22}(\kappa_{2i}-\overline{\kappa_{2i}})^2\Big), \tag{A3}$$

where κ_{1i} and κ_{2i} are the curvature normal's components in the (averaged) material frame at vertex i:

$$\kappa_{1i} = (\kappa\mathbf{b})_i \cdot \frac{1}{2}\big(\mathbf{d}_2^{i-1} + \mathbf{d}_2^{i}\big), \quad \kappa_{2i} = -(\kappa\mathbf{b})_i \cdot \frac{1}{2}\big(\mathbf{d}_1^{i-1} + \mathbf{d}_1^{i}\big).$$

The gradient of the bending energy is:

$$\nabla E_b = \sum_{i=1}^{\texttt{nv}-2} \frac{1}{\bar{l}_i}\Big(B_{11}(\kappa_{1i}-\overline{\kappa_{1i}})\nabla\kappa_{1i} + B_{22}(\kappa_{2i}-\overline{\kappa_{2i}})\nabla\kappa_{2i}\Big),$$

where $\nabla\kappa_{1i}$ and $\nabla\kappa_{2i}$ collect partial derivatives with respect to the $\mathbf{x}$ and θ variables:

$$\frac{\partial\kappa_{1i}}{\partial\theta^a} = (\kappa\mathbf{b})_i \cdot \frac{1}{2}\left(\frac{\partial\mathbf{d}_2^{i-1}}{\partial\theta^a} + \frac{\partial\mathbf{d}_2^{i}}{\partial\theta^a}\right) = -(\kappa\mathbf{b})_i \cdot \frac{1}{2}\Big(\mathbf{d}_1^{i-1}\delta_{a(i-1)} + \mathbf{d}_1^{i}\delta_{ai}\Big)$$

$$\frac{\partial\kappa_{2i}}{\partial\theta^a} = -(\kappa\mathbf{b})_i \cdot \frac{1}{2}\left(\frac{\partial\mathbf{d}_1^{i-1}}{\partial\theta^a} + \frac{\partial\mathbf{d}_1^{i}}{\partial\theta^a}\right) = -(\kappa\mathbf{b})_i \cdot \frac{1}{2}\Big(\mathbf{d}_2^{i-1}\delta_{a(i-1)} + \mathbf{d}_2^{i}\delta_{ai}\Big)$$

$$\left(\frac{\partial\kappa_{1i}}{\partial\mathbf{x}_a}\right)^T = \frac{1}{2}\left(\mathbf{d}_2^{i-1} + \mathbf{d}_2^{i}\right) \cdot \frac{\partial(\kappa\mathbf{b})_i}{\partial\mathbf{x}_a} + \cancelto{0}{(\kappa\mathbf{b})_i \cdot \frac{1}{2}\left(\frac{\partial\mathbf{d}_2^{i-1}}{\partial\mathbf{x}_a} + \frac{\partial\mathbf{d}_2^{i}}{\partial\mathbf{x}_a}\right)}$$

$$\left(\frac{\partial\kappa_{2i}}{\partial\mathbf{x}_a}\right)^T = -\frac{1}{2}\left(\mathbf{d}_1^{i-1} + \mathbf{d}_1^{i}\right) \cdot \frac{\partial(\kappa\mathbf{b})_i}{\partial\mathbf{x}_a} - \cancelto{0}{(\kappa\mathbf{b})_i \cdot \frac{1}{2}\left(\frac{\partial\mathbf{d}_1^{i-1}}{\partial\mathbf{x}_a} + \frac{\partial\mathbf{d}_1^{i}}{\partial\mathbf{x}_a}\right)}$$

The second terms of the partial derivatives with respect to $\mathbf{x}_a$ vanish because parallel transporting the material frame from a given edge to its perturbed configuration varies the frame vectors only in the edge's tangential direction (which is orthogonal to $(\kappa\mathbf{b})_i$). Now we evaluate the first term for κ_1, working instead with derivatives with respect to edge vectors for simplicity:

$$\begin{aligned}
\frac{\partial\kappa_{1i}}{\partial\mathbf{e}^a} &= \frac{1}{2}\left(\frac{\delta_{ai}}{\|\mathbf{e}^i\|}\left[\frac{2[\mathbf{t}^{i-1}]_\times}{\chi} - \frac{(\kappa\mathbf{b})_i}{\chi}\otimes(\mathbf{t}^{i-1}+\mathbf{t}^i)\right] + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\left[-\frac{2[\mathbf{t}^{i}]_\times}{\chi} - \frac{(\kappa\mathbf{b})_i}{\chi}\otimes(\mathbf{t}^{i-1}+\mathbf{t}^i)\right]\right)^T\left(\mathbf{d}_2^{i-1}+\mathbf{d}_2^i\right)\\
&= \frac{\delta_{ai}}{\|\mathbf{e}^i\|}\Big(-\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\Big) + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\Big(\mathbf{t}^{i}\times\tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\Big) = \tilde{\mathbf{d}}_2\times\left(\frac{\mathbf{t}^{i-1}\delta_{ai}}{\|\mathbf{e}^i\|} - \frac{\mathbf{t}^{i}\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right) - \kappa_{1i}\tilde{\mathbf{t}}\left(\frac{\delta_{ai}}{\|\mathbf{e}^i\|} + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right)\\
\frac{\partial\kappa_{2i}}{\partial\mathbf{e}^a} &= \frac{\delta_{ai}}{\|\mathbf{e}^i\|}\Big(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1 - \kappa_{2i}\tilde{\mathbf{t}}\Big) + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\Big(-\mathbf{t}^{i}\times\tilde{\mathbf{d}}_1 - \kappa_{2i}\tilde{\mathbf{t}}\Big) = \tilde{\mathbf{d}}_1\times\left(\frac{\mathbf{t}^{i}\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|} - \frac{\mathbf{t}^{i-1}\delta_{ai}}{\|\mathbf{e}^{i}\|}\right) - \kappa_{2i}\tilde{\mathbf{t}}\left(\frac{\delta_{ai}}{\|\mathbf{e}^i\|} + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right)
\end{aligned}$$

The Hessian of the bending energy is:

$$HE_b = \sum_{i=1}^{\texttt{nv}-2} \frac{1}{\bar{l}_i}\left[B_{11}\Big(\nabla\kappa_{1i}\otimes\nabla\kappa_{1i} + (\kappa_{1i}-\overline{\kappa_{1i}})H\kappa_{1i}\Big) + B_{22}\Big(\nabla\kappa_{2i}\otimes\nabla\kappa_{2i} + (\kappa_{2i}-\overline{\kappa_{2i}})H\kappa_{2i}\Big)\right]$$

We evaluate the second partial derivatives making up the Hessians of κ_{1i} and κ_{2i} beginning with the simpler terms involving the θ variables:

$$\frac{\partial^2\kappa_{1i}}{\partial\theta^a\partial\theta^b} = -(\kappa\mathbf{b})_i \cdot \frac{1}{2}\Big(\mathbf{d}_2^{i-1}\delta_{a(i-1)}\delta_{b(i-1)} + \mathbf{d}_2^{i}\delta_{ai}\delta_{bi}\Big), \quad \frac{\partial^2\kappa_{2i}}{\partial\theta^a\partial\theta^b} = (\kappa\mathbf{b})_i \cdot \frac{1}{2}\Big(\mathbf{d}_1^{i-1}\delta_{a(i-1)}\delta_{b(i-1)} - \mathbf{d}_1^{i}\delta_{ai}\delta_{bi}\Big)$$

$$\frac{\partial^2 \kappa_{1i}}{\partial \mathbf{e}^a \partial \theta^b} = \frac{1}{\chi}\left(\frac{\mathbf{t}^{i-1}\delta_{ai}}{\|\mathbf{e}^i\|} - \frac{\mathbf{t}^i \delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right) \times \left(\mathbf{d}_1^{i-1}\delta_{b(i-1)} + \mathbf{d}_1^i \delta_{bi}\right) + \tilde{\mathbf{t}}\left(\frac{\delta_{ai}}{\|\mathbf{e}^i\|} + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right)\left[(\kappa\mathbf{b})_i \cdot \frac{1}{2}\left(\mathbf{d}_1^{i-1}\delta_{b(i-1)} + \mathbf{d}_1^i \delta_{bi}\right)\right]$$

$$\frac{\partial^2 \kappa_{2i}}{\partial \mathbf{e}^a \partial \theta^b} = \frac{1}{\chi}\left(\frac{\mathbf{t}^{i-1}\delta_{ai}}{\|\mathbf{e}^i\|} - \frac{\mathbf{t}^i \delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right) \times \left(\mathbf{d}_2^{i-1}\delta_{b(i-1)} + \mathbf{d}_2^i \delta_{bi}\right) + \tilde{\mathbf{t}}\left(\frac{\delta_{ai}}{\|\mathbf{e}^i\|} + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right)\left[(\kappa\mathbf{b})_i \cdot \frac{1}{2}\left(\mathbf{d}_2^{i-1}\delta_{b(i-1)} + \mathbf{d}_2^i \delta_{bi}\right)\right]$$

Next, we compute the Hessian of κ_{1i} with respect to the edge vectors $\mathbf{e}$:

$$\begin{aligned}
\frac{\partial^2 \kappa_{1i}}{\partial \mathbf{e}^a \partial \mathbf{e}^b} = &-\frac{\delta_{ai}\delta_{bi}}{\|\mathbf{e}^i\|^2}\left(-\mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes \mathbf{t}^i - \frac{\delta_{a(i-1)}\delta_{b(i-1)}}{\|\mathbf{e}^{i-1}\|^2}\left(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes \mathbf{t}^{i-1} \\
&+ \left[\frac{\delta_{ai}}{\|\mathbf{e}^i\|}\left(-\mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\left(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right)\right] \otimes \frac{\partial(1/\chi)}{\partial \mathbf{e}^b} \\
&+ \frac{1}{\chi}\frac{\partial(\mathbf{d}_2^{i-1} + \mathbf{d}_2^i)}{\partial \mathbf{e}^b} \times \left(\frac{\mathbf{t}^{i-1}\delta_{ai}}{\|\mathbf{e}^i\|} - \frac{\mathbf{t}^i\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right) - \tilde{\mathbf{t}} \otimes \frac{\partial \kappa_{1i}}{\partial \mathbf{e}^b}\left(\frac{\delta_{ai}}{\|\mathbf{e}^i\|} + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right) \\
&+ [\tilde{\mathbf{d}}_2]_\times \left(\delta_{ai}\delta_{b(i-1)}\frac{I - \mathbf{t}^{i-1} \otimes \mathbf{t}^{i-1}}{\|\mathbf{e}^i\|\|\mathbf{e}^{i-1}\|} - \delta_{a(i-1)}\delta_{bi}\frac{I - \mathbf{t}^i \otimes \mathbf{t}^i}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^i\|}\right) - \frac{\kappa_{1i}}{\chi}\frac{\partial(\mathbf{t}^{i-1} + \mathbf{t}^i)}{\partial \mathbf{e}^b}\left(\frac{\delta_{ai}}{\|\mathbf{e}^i\|} + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right)
\end{aligned}$$

To evaluate this, we'll need to compute $\frac{\partial \mathbf{d}_2^k}{\partial \mathbf{e}^b}$ and $\frac{\partial(1/\chi)}{\partial \mathbf{e}^b}$. The material frame derivative term requires determining how the parallel-transported frame vector changes as the edge vector is perturbed. Parallel transport from tangent vector $\mathbf{t}$ to $\mathbf{t}+\delta\mathbf{t}$ simply rotates around axis $\mathbf{t}\times(\mathbf{t}+\delta\mathbf{t}) = \mathbf{t}\times\delta\mathbf{t}$ by angle $\|\mathbf{t}\times\delta\mathbf{t}\|$ (small angle approximation). Thus, the infinitesimal rotation amounts to perturbing $\mathbf{d}_2$ by $(\mathbf{t}\times\delta\mathbf{t})\times\mathbf{d}_2 = -\mathbf{t}(\delta\mathbf{t}\cdot\mathbf{d}_2)+\delta\mathbf{t}(\cancel{\mathbf{t}\cdot\mathbf{d}_2})$. Hence,

$$\frac{\partial \mathbf{d}_2^k}{\partial \mathbf{e}^b} = -\mathbf{t}^k\left(\mathbf{d}_2^k \cdot \frac{I - \cancel{\mathbf{t}^k \otimes \mathbf{t}^k}}{\|\mathbf{e}^k\|}\right)\delta_{kb} = -\delta_{kb}\frac{\mathbf{t}^k \otimes \mathbf{d}_2^k}{\|\mathbf{e}^k\|}.$$

Next, we compute:

$$\frac{\partial(1/\chi)}{\partial \mathbf{e}^b} = -\frac{1}{\chi^2}\left(\frac{(I - \mathbf{t}^{i-1} \otimes \mathbf{t}^{i-1})\mathbf{t}^i}{\|\mathbf{e}^{i-1}\|}\delta_{b(i-1)} + \frac{(I - \mathbf{t}^i \otimes \mathbf{t}^i)\mathbf{t}^{i-1}}{\|\mathbf{e}^i\|}\delta_{bi}\right).$$

Substituting these expressions into the Hessian above:

$$\begin{aligned}
\frac{\partial^2 \kappa_{1i}}{\partial \mathbf{e}^a \partial \mathbf{e}^b} = &-\frac{\delta_{ai}\delta_{bi}}{\|\mathbf{e}^i\|^2}\left(-\mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes \mathbf{t}^i - \frac{\delta_{a(i-1)}\delta_{b(i-1)}}{\|\mathbf{e}^{i-1}\|^2}\left(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes \mathbf{t}^{i-1} \\
&- \frac{1}{\chi}\left[\frac{\delta_{ai}}{\|\mathbf{e}^i\|}\left(-\mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\left(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right)\right] \otimes \left(\frac{(I - \mathbf{t}^{i-1} \otimes \mathbf{t}^{i-1})\mathbf{t}^i}{\|\mathbf{e}^{i-1}\|}\delta_{b(i-1)} + \frac{(I - \mathbf{t}^i \otimes \mathbf{t}^i)\mathbf{t}^{i-1}}{\|\mathbf{e}^i\|}\delta_{bi}\right) \\
&- \frac{1}{\chi}\left(\left[\frac{\delta_{b(i-1)}\mathbf{t}^{i-1}}{\|\mathbf{e}^{i-1}\|} \times \left(\cancel{\frac{\delta_{ai}\mathbf{t}^{i-1}}{\|\mathbf{e}^i\|}} - \frac{\delta_{a(i-1)}\mathbf{t}^i}{\|\mathbf{e}^{i-1}\|}\right)\right] \otimes \mathbf{d}_2^{i-1} + \left[\frac{\delta_{bi}\mathbf{t}^i}{\|\mathbf{e}^i\|} \times \left(\frac{\delta_{ai}\mathbf{t}^{i-1}}{\|\mathbf{e}^i\|} - \cancel{\frac{\delta_{a(i-1)}\mathbf{t}^i}{\|\mathbf{e}^{i-1}\|}}\right)\right] \otimes \mathbf{d}_2^i\right) \\
&- \tilde{\mathbf{t}} \otimes \frac{\partial \kappa_{1i}}{\partial \mathbf{e}^b}\left(\frac{\delta_{ai}}{\|\mathbf{e}^i\|} + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right) \\
&+ [\tilde{\mathbf{d}}_2]_\times \left(\delta_{ai}\delta_{b(i-1)}\frac{I - \mathbf{t}^{i-1} \otimes \mathbf{t}^{i-1}}{\|\mathbf{e}^i\|\|\mathbf{e}^{i-1}\|} - \delta_{a(i-1)}\delta_{bi}\frac{I - \mathbf{t}^i \otimes \mathbf{t}^i}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^i\|}\right) \\
&- \frac{\kappa_{1i}}{\chi}\left(\delta_{b(i-1)}\frac{I - \mathbf{t}^{i-1} \otimes \mathbf{t}^{i-1}}{\|\mathbf{e}^{i-1}\|} + \delta_{bi}\frac{I - \mathbf{t}^i \otimes \mathbf{t}^i}{\|\mathbf{e}^i\|}\right)\left(\frac{\delta_{ai}}{\|\mathbf{e}^i\|} + \frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right).
\end{aligned}$$

Next, we simplify the individual blocks of this Hessian starting with:

$$\begin{aligned}
\frac{\partial^2 \kappa_{1i}}{\partial \mathbf{e}^{i-1} \partial \mathbf{e}^{i-1}} = &-\frac{1}{\|\mathbf{e}^{i-1}\|^2}\left(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes \mathbf{t}^{i-1} \\
&- \frac{1}{\chi\|\mathbf{e}^{i-1}\|}\left(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes \frac{(I - \mathbf{t}^{i-1} \otimes \mathbf{t}^{i-1})\mathbf{t}^i}{\|\mathbf{e}^{i-1}\|}
\end{aligned}$$

$$
\begin{aligned}
&+ \frac{1}{\chi}\left[\frac{\mathbf{t}^{i-1}}{\|\mathbf{e}^{i-1}\|} \times \frac{\mathbf{t}^{i}}{\|\mathbf{e}^{i-1}\|}\right] \otimes \mathbf{d}_2^{i-1} \\
&- \tilde{\mathbf{t}} \otimes \frac{1}{\|\mathbf{e}^{i-1}\|^2}\left(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) - \frac{\kappa_{1i}}{\chi}\frac{I - \mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}}{\|\mathbf{e}^{i-1}\|^2} \\
= &\frac{1}{\|\mathbf{e}^{i-1}\|^2}\Bigg[- \left(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes \left(\mathbf{t}^{i-1} + \frac{\mathbf{t}^i - (\mathbf{t}^i\cdot\mathbf{t}^{i-1})\mathbf{t}^{i-1}}{\chi}\right) \\
&\quad + \frac{(\kappa\mathbf{b})_i}{2} \otimes \mathbf{d}_2^{i-1} - \tilde{\mathbf{t}} \otimes \left(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) - \frac{\kappa_{1i}}{\chi}(I - \mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1})\Bigg]
\end{aligned}
$$

Noticing that

$$
\mathbf{t}^{i-1} + \frac{\mathbf{t}^i - (\mathbf{t}^i\cdot\mathbf{t}^{i-1})\mathbf{t}^{i-1}}{\chi} = \frac{\chi\mathbf{t}^{i-1} + \mathbf{t}^i - (\chi-1)\mathbf{t}^{i-1}}{\chi} = \tilde{\mathbf{t}},
$$

we further simplify:

$$
\begin{aligned}
\frac{\partial^2\kappa_{1i}}{\partial\mathbf{e}^{i-1}\partial\mathbf{e}^{i-1}} &= \frac{1}{\|\mathbf{e}^{i-1}\|^2}\left[-(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}) \otimes \tilde{\mathbf{t}} - \tilde{\mathbf{t}} \otimes (\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}) + \frac{(\kappa\mathbf{b})_i \otimes \mathbf{d}_2^{i-1}}{2} - \frac{\kappa_{1i}}{\chi}(I - \mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1})\right] \\
&= \boxed{\frac{1}{\|\mathbf{e}^{i-1}\|^2}\left[2\kappa_{1i}\tilde{\mathbf{t}}\otimes\tilde{\mathbf{t}} - (\mathbf{t}^i \times \tilde{\mathbf{d}}_2)\otimes\tilde{\mathbf{t}} - \tilde{\mathbf{t}}\otimes(\mathbf{t}^i \times \tilde{\mathbf{d}}_2) + \frac{(\kappa\mathbf{b})_i \otimes \mathbf{d}_2^{i-1}}{2} - \frac{\kappa_{1i}}{\chi}(I - \mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1})\right]}
\end{aligned}
$$

Now we consider:

$$
\begin{aligned}
\frac{\partial^2\kappa_{1i}}{\partial\mathbf{e}^{i}\partial\mathbf{e}^{i}} = &-\frac{1}{\|\mathbf{e}^i\|^2}\left(- \mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes \mathbf{t}^i \\
&- \frac{1}{\chi\|\mathbf{e}^i\|}\left(- \mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes \frac{(I - \mathbf{t}^i\otimes\mathbf{t}^i)\mathbf{t}^{i-1}}{\|\mathbf{e}^i\|} \\
&- \frac{1}{\chi}\left[\frac{\mathbf{t}^i}{\|\mathbf{e}^i\|} \times \frac{\mathbf{t}^{i-1}}{\|\mathbf{e}^i\|}\right] \otimes \mathbf{d}_2^i \\
&- \tilde{\mathbf{t}} \otimes \frac{1}{\|\mathbf{e}^i\|^2}\left(-\mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) - \frac{\kappa_{1i}}{\chi}\frac{I - \mathbf{t}^i\otimes\mathbf{t}^i}{\|\mathbf{e}^i\|^2} \\
= &\frac{1}{\|\mathbf{e}^i\|^2}\Bigg[- \left(-\mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes \left(\mathbf{t}^i + \frac{\mathbf{t}^{i-1} - (\mathbf{t}^{i-1}\cdot\mathbf{t}^i)\mathbf{t}^i}{\chi}\right) \\
&\quad + \frac{(\kappa\mathbf{b})_i}{2} \otimes \mathbf{d}_2^i - \tilde{\mathbf{t}} \otimes \left(- \mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) - \frac{\kappa_{1i}}{\chi}(I - \mathbf{t}^i\otimes\mathbf{t}^i)\Bigg] \\
= &\frac{1}{\|\mathbf{e}^i\|^2}\left[(\mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 + \kappa_{1i}\tilde{\mathbf{t}}) \otimes \tilde{\mathbf{t}} + \tilde{\mathbf{t}} \otimes (\mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 + \kappa_{1i}\tilde{\mathbf{t}}) + \frac{(\kappa\mathbf{b})_i \otimes \mathbf{d}_2^i}{2} - \frac{\kappa_{1i}}{\chi}(I - \mathbf{t}^i\otimes\mathbf{t}^i)\right] \\
= &\boxed{\frac{1}{\|\mathbf{e}^i\|^2}\left[2\kappa_{1i}\tilde{\mathbf{t}}\otimes\tilde{\mathbf{t}} + (\mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2)\otimes\tilde{\mathbf{t}} + \tilde{\mathbf{t}}\otimes(\mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2) + \frac{(\kappa\mathbf{b})_i \otimes \mathbf{d}_2^i}{2} - \frac{\kappa_{1i}}{\chi}(I - \mathbf{t}^i\otimes\mathbf{t}^i)\right].}
\end{aligned}
$$

Finally:

$$
\begin{aligned}
\frac{\partial^2\kappa_{1i}}{\partial\mathbf{e}^{i-1}\partial\mathbf{e}^{i}} = &-\frac{1}{\chi\|\mathbf{e}^{i-1}\|\|\mathbf{e}^i\|}\left(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes (I - \mathbf{t}^i\otimes\mathbf{t}^i)\mathbf{t}^{i-1} \\
&- \frac{1}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^i\|}\tilde{\mathbf{t}} \otimes \left(- \mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) - [\tilde{\mathbf{d}}_2]_\times \frac{I - \mathbf{t}^i\otimes\mathbf{t}^i}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^i\|} - \frac{\kappa_{1i}}{\chi}\frac{I - \mathbf{t}^i\otimes\mathbf{t}^i}{\|\mathbf{e}^i\|\|\mathbf{e}^{i-1}\|}. \\
= &\frac{1}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^i\|}\Bigg[\left(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) \otimes (\mathbf{t}^i - \tilde{\mathbf{t}}) - \tilde{\mathbf{t}} \otimes \left(- \mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_{1i}\tilde{\mathbf{t}}\right) - [\tilde{\mathbf{d}}_2]_\times + (\tilde{\mathbf{d}}_2 \times \mathbf{t}^i)\otimes\mathbf{t}^i \\
&\quad - \frac{\kappa_{1i}}{\chi}(I - \mathbf{t}^i\otimes\mathbf{t}^i)\Bigg]
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{1}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^{i}\|}\Bigg[-\Big(\mathbf{t}^{i}\times\tilde{\mathbf{d}}_2-\kappa_{1i}\tilde{\mathbf{t}}\Big)\otimes\tilde{\mathbf{t}}-\tilde{\mathbf{t}}\otimes\Big(-\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_2-\kappa_{1i}\tilde{\mathbf{t}}\Big)-[\tilde{\mathbf{d}}_2]_\times \\
&\qquad -\frac{\kappa_{1i}}{\chi}\Big((\mathbf{t}^{i-1}+\mathbf{t}^{i})\otimes\mathbf{t}^{i}+I-\mathbf{t}^{i}\otimes\mathbf{t}^{i}\Big)\Bigg] \\
&= \frac{1}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^{i}\|}\Bigg[-\Big(\mathbf{t}^{i}\times\tilde{\mathbf{d}}_2-\kappa_{1i}\tilde{\mathbf{t}}\Big)\otimes\tilde{\mathbf{t}}-\tilde{\mathbf{t}}\otimes\Big(-\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_2-\kappa_{1i}\tilde{\mathbf{t}}\Big)-[\tilde{\mathbf{d}}_2]_\times-\frac{\kappa_{1i}}{\chi}(I+\mathbf{t}^{i-1}\otimes\mathbf{t}^{i})\Bigg] \\
&= \boxed{\frac{1}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^{i}\|}\Bigg[2\kappa_{1i}\tilde{\mathbf{t}}\otimes\tilde{\mathbf{t}}-(\mathbf{t}^{i}\times\tilde{\mathbf{d}}_2)\otimes\tilde{\mathbf{t}}+\tilde{\mathbf{t}}\otimes(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_2)-[\tilde{\mathbf{d}}_2]_\times-\frac{\kappa_{1i}}{\chi}(I+\mathbf{t}^{i-1}\otimes\mathbf{t}^{i})\Bigg].}
\end{aligned}
$$

Notice that $\frac{\partial^2\kappa_{1i}}{\partial\mathbf{e}^{i-1}\partial\mathbf{e}^{i-1}}$ and $\frac{\partial^2\kappa_{1i}}{\partial\mathbf{e}^{i}\partial\mathbf{e}^{i}}$ are actually *not* symmetric. This asymmetry is due to the path-dependence caused by the internal state stored in material frame vectors $\mathbf{d}_2$. The appendix of [Bergou et al., 2010] incorrectly symmetrizes these terms, replacing e.g. $\frac{(\kappa\mathbf{b})_i\otimes\mathbf{d}_2^{i-1}}{2}$ with $\frac{(\kappa\mathbf{b})_i\otimes\mathbf{d}_2^{i-1}+\mathbf{d}_2^{i-1}\otimes(\kappa\mathbf{b})_i}{4}$.

Now we compute the Hessian of κ_{2i} with respect to the edge vectors.

$$
\begin{aligned}
\frac{\partial^2\kappa_{2i}}{\partial\mathbf{e}^{a}\partial\mathbf{e}^{b}} &= -\frac{\delta_{ai}\delta_{bi}}{\|\mathbf{e}^{i}\|^2}\Big(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)\otimes\mathbf{t}^{i}-\frac{\delta_{a(i-1)}\delta_{b(i-1)}}{\|\mathbf{e}^{i-1}\|^2}\Big(-\mathbf{t}^{i}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)\otimes\mathbf{t}^{i-1} \\
&\quad -\frac{1}{\chi}\left[\frac{\delta_{ai}}{\|\mathbf{e}^{i}\|}\Big(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)+\frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\Big(-\mathbf{t}^{i}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)\right]\otimes\left(\frac{I-\mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}}{\|\mathbf{e}^{i-1}\|}\mathbf{t}^{i}\delta_{b(i-1)}+\frac{I-\mathbf{t}^{i}\otimes\mathbf{t}^{i}}{\|\mathbf{e}^{i}\|}\mathbf{t}^{i-1}\delta_{bi}\right) \\
&\quad -\frac{1}{\chi}\left(\left[\delta_{b(i-1)}\frac{\mathbf{t}^{i-1}}{\|\mathbf{e}^{i-1}\|}\times\left(\frac{\mathbf{t}^{i}\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}-\cancel{\frac{\mathbf{t}^{i-1}\delta_{ai}}{\|\mathbf{e}^{i}\|}}\right)\right]\otimes\mathbf{d}_1^{i-1}+\left[\delta_{bi}\frac{\mathbf{t}^{i}}{\|\mathbf{e}^{i}\|}\times\left(\cancel{\frac{\mathbf{t}^{i}\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}}-\frac{\mathbf{t}^{i-1}\delta_{ai}}{\|\mathbf{e}^{i}\|}\right)\right]\otimes\mathbf{d}_1^{i}\right) \\
&\quad -\tilde{\mathbf{t}}\otimes\left[\frac{\delta_{bi}}{\|\mathbf{e}^{i}\|}\Big(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)+\frac{\delta_{b(i-1)}}{\|\mathbf{e}^{i-1}\|}\Big(-\mathbf{t}^{i}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)\right]\left(\frac{\delta_{ai}}{\|\mathbf{e}^{i}\|}+\frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right) \\
&\quad +[\tilde{\mathbf{d}}_1]_\times\left(\delta_{a(i-1)}\delta_{bi}\frac{I-\mathbf{t}^{i}\otimes\mathbf{t}^{i}}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^{i}\|}-\delta_{ai}\delta_{b(i-1)}\frac{I-\mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}}{\|\mathbf{e}^{i}\|\|\mathbf{e}^{i-1}\|}\right) \\
&\quad -\frac{\kappa_{2i}}{\chi}\left(\frac{I-\mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}}{\|\mathbf{e}^{i-1}\|}\delta_{b(i-1)}+\frac{I-\mathbf{t}^{i}\otimes\mathbf{t}^{i}}{\|\mathbf{e}^{i}\|}\delta_{bi}\right)\left(\frac{\delta_{ai}}{\|\mathbf{e}^{i}\|}+\frac{\delta_{a(i-1)}}{\|\mathbf{e}^{i-1}\|}\right)
\end{aligned}
$$

And, simplifying the individual Hessian blocks:

$$
\begin{aligned}
\frac{\partial^2\kappa_{2i}}{\partial\mathbf{e}^{i-1}\partial\mathbf{e}^{i-1}} &= \frac{1}{\|\mathbf{e}^{i-1}\|^2}\Bigg[-\Big(-\mathbf{t}^{i}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)\otimes\Big(\mathbf{t}^{i-1}+\frac{I-\mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}}{\chi}\mathbf{t}^{i}\Big)-\frac{(\kappa\mathbf{b})_i}{2}\otimes\mathbf{d}_1^{i-1} \\
&\qquad -\tilde{\mathbf{t}}\otimes\Big(-\mathbf{t}^{i}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)-\frac{\kappa_{2i}}{\chi}\left(I-\mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}\right)\Bigg] \\
&= \boxed{\frac{1}{\|\mathbf{e}^{i-1}\|^2}\Bigg[2\kappa_{2i}\tilde{\mathbf{t}}\otimes\tilde{\mathbf{t}}+(\mathbf{t}^{i}\times\tilde{\mathbf{d}}_1)\otimes\tilde{\mathbf{t}}+\tilde{\mathbf{t}}\otimes(\mathbf{t}^{i}\times\tilde{\mathbf{d}}_1)-\frac{(\kappa\mathbf{b})_i}{2}\otimes\mathbf{d}_1^{i-1}-\frac{\kappa_{2i}}{\chi}(I-\mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1})\Bigg]} \\
\frac{\partial^2\kappa_{2i}}{\partial\mathbf{e}^{i}\partial\mathbf{e}^{i}} &= \frac{1}{\|\mathbf{e}^{i}\|^2}\Bigg[-\Big(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)\otimes\Big(\mathbf{t}^{i}+\frac{I-\mathbf{t}^{i}\otimes\mathbf{t}^{i}}{\chi}\mathbf{t}^{i-1}\Big)-\frac{(\kappa\mathbf{b})_i}{2}\otimes\mathbf{d}_1^{i} \\
&\qquad -\tilde{\mathbf{t}}\otimes\Big(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)-\frac{\kappa_{2i}}{\chi}\left(I-\mathbf{t}^{i}\otimes\mathbf{t}^{i}\right)\Bigg] \\
&= \boxed{\frac{1}{\|\mathbf{e}^{i}\|^2}\Bigg[2\kappa_{2i}\tilde{\mathbf{t}}\otimes\tilde{\mathbf{t}}-(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1)\otimes\tilde{\mathbf{t}}-\tilde{\mathbf{t}}\otimes(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1)-\frac{(\kappa\mathbf{b})_i}{2}\otimes\mathbf{d}_1^{i}-\frac{\kappa_{2i}}{\chi}(I-\mathbf{t}^{i}\otimes\mathbf{t}^{i})\Bigg]} \\
\frac{\partial^2\kappa_{2i}}{\partial\mathbf{e}^{i-1}\partial\mathbf{e}^{i}} &= \frac{1}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^{i}\|}\Bigg[-\Big(-\mathbf{t}^{i}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)\otimes\left(\tilde{\mathbf{t}}-\mathbf{t}^{i}\right) \\
&\qquad -\tilde{\mathbf{t}}\otimes\Big(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1-\kappa_{2i}\tilde{\mathbf{t}}\Big)+[\mathbf{d}_1]_\times-(\mathbf{d}_1\times\mathbf{t}^{i})\otimes\mathbf{t}^{i}-\frac{\kappa_{2i}}{\chi}\left(I-\mathbf{t}^{i}\otimes\mathbf{t}^{i}\right)\Bigg]
\end{aligned}
$$

$$= \frac{1}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^{i}\|}\left[2\kappa_{2i}\tilde{\mathbf{t}}\otimes\tilde{\mathbf{t}} + (\mathbf{t}^i\times\tilde{\mathbf{d}}_1)\otimes\tilde{\mathbf{t}} - \tilde{\mathbf{t}}\otimes(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1) + [\mathbf{d}_1]_\times - \frac{\kappa_{2i}}{\chi}\left(I - \mathbf{t}^i\otimes\mathbf{t}^i + \chi\tilde{\mathbf{t}}\otimes\mathbf{t}^i\right)\right]$$

$$= \boxed{\frac{1}{\|\mathbf{e}^{i-1}\|\|\mathbf{e}^{i}\|}\Big[2\kappa_{2i}\tilde{\mathbf{t}}\otimes\tilde{\mathbf{t}} + (\mathbf{t}^i\times\tilde{\mathbf{d}}_1)\otimes\tilde{\mathbf{t}} - \tilde{\mathbf{t}}\otimes(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1) + [\mathbf{d}_1]_\times - \frac{\kappa_{2i}}{\chi}(I + \mathbf{t}^{i-1}\otimes\mathbf{t}^i)\Big].}$$

5 Hessians of Material Curvatures for Finite Transport

The Hessian and gradient formulas we derived above assumed that the reference frame is continuously transported from the previous instant in time. However, an optimization or simulation algorithm will always take finite steps, transporting the frame from the previous iteration with a finite rotation. The asymmetric Hessians we computed are inaccurate for these discrete steps; to accurately model the change in energy and forces made by a discrete step, we need to compute the Hessian for the energy defined by transporting from a fixed "source" reference frame (which will then be updated at the start of the next iteration). To simplify the Hessian, we evaluate it only at the configuration from which the source reference frame was set (i.e., we assume the source reference frame is updated before we compute the Hessian). However, to compute this Hessian, we will need a formula for the gradient that is accurate any any configuration.

In the following differentiations, we will distinguish the (constant) source frame quantities with hats. For example: $\widehat{\mathbf{t}^{i-1}}, \underline{\widehat{\mathbf{d}_1^{i-1}}}, \underline{\widehat{\mathbf{d}_1^{i}}}$. With this notation, first material curvature is written as:

$$\kappa_1 = (\kappa\mathbf{b})_i\cdot\frac{1}{2}\left(\mathbf{d}_2^{i-1} + \mathbf{d}_2^{i}\right) = (\kappa\mathbf{b})_i\cdot\frac{1}{2}\left(P_{\widehat{\mathbf{t}^{i-1}}}^{\mathbf{t}^{i-1}}\widehat{\mathbf{d}_2^{i-1}} + P_{\widehat{\mathbf{t}^{i}}}^{\mathbf{t}^{i}}\widehat{\mathbf{d}_2^{i}}\right).$$

Notice, parallel transport is linear, so we can directly transport the material frame itself instead of the two reference directors.

Now we compute the derivative with respect to the edge vectors:

$$\begin{aligned}
\frac{\partial\kappa_{1i}}{\partial\mathbf{e}^{i-1}} &= \frac{1}{2}\left(\frac{\partial(\kappa\mathbf{b})_i}{\partial\mathbf{e}^{i-1}}\right)^T\left(\mathbf{d}_2^{i-1} + \mathbf{d}_2^{i}\right) + \frac{1}{2}\left(\frac{\partial P_{\widehat{\mathbf{t}^{i-1}}}^{\mathbf{t}^{i-1}}\widehat{\mathbf{d}_2^{i-1}}}{\partial\mathbf{e}^{i-1}}\right)^T(\kappa\mathbf{b})_i \\
&= -\frac{1}{2\chi\|\mathbf{e}^{i-1}\|}\left(2[\mathbf{t}^i]_\times + (\kappa\mathbf{b})_i\otimes(\mathbf{t}^{i-1} + \mathbf{t}^i)\right)^T\left(\mathbf{d}_2^{i-1} + \mathbf{d}_2^{i}\right) \\
&\quad + \frac{1}{2\|\mathbf{e}^{i-1}\|}\left(\frac{\partial P_{\widehat{\mathbf{t}^{i-1}}}^{\mathbf{t}^{i-1}}\widehat{\mathbf{d}_2^{i-1}}}{\partial\mathbf{t}^{i-1}}\left(I - \mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}\right)\right)^T(\kappa\mathbf{b})_i \\
&= -\frac{1}{2\chi\|\mathbf{e}^{i-1}\|}\left(2[\mathbf{t}^i]_\times + (\kappa\mathbf{b})_i\otimes(\mathbf{t}^{i-1} + \mathbf{t}^i)\right)^T\left(\mathbf{d}_2^{i-1} + \mathbf{d}_2^{i}\right) \\
&\quad + \frac{I - \mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}}{2\|\mathbf{e}^{i-1}\|}\Bigg(\frac{\big[(\widehat{\mathbf{t}^{i-1}}\times\mathbf{t}^{i-1})\cdot\widehat{\mathbf{d}_2^{i-1}}\big][\widehat{\mathbf{t}^{i-1}}]_\times^T + (\widehat{\mathbf{d}_2^{i-1}}\times\widehat{\mathbf{t}^{i-1}})\otimes(\widehat{\mathbf{t}^{i-1}}\times\mathbf{t}^{i-1})}{1 + \widehat{\mathbf{t}^{i-1}}\cdot\mathbf{t}^{i-1}} \\
&\qquad - \frac{(\widehat{\mathbf{t}^{i-1}}\times\mathbf{t}^{i-1})\cdot\widehat{\mathbf{d}_2^{i-1}}}{(1 + \widehat{\mathbf{t}^{i-1}}\cdot\mathbf{t}^{i-1})^2}\widehat{\mathbf{t}^{i-1}}\otimes(\widehat{\mathbf{t}^{i-1}}\times\mathbf{t}^{i-1}) + \cancel{(\widehat{\mathbf{t}^{i-1}}\cdot\widehat{\mathbf{d}_2^{i-1}})}I - \widehat{\mathbf{d}_2^{i-1}}\otimes\widehat{\mathbf{t}^{i-1}} + \widehat{\mathbf{t}^{i-1}}\otimes\widehat{\mathbf{d}_2^{i-1}}\Bigg)(\kappa\mathbf{b})_i \\
&= \frac{1}{\|\mathbf{e}^{i-1}\|}\left(\mathbf{t}^i\times\tilde{\mathbf{d}}_2 - \kappa_1\tilde{\mathbf{t}}\right) + \\
&\quad \frac{I - \mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}}{2\|\mathbf{e}^{i-1}\|}\Bigg(\frac{\big[(\widehat{\mathbf{d}_2^{i-1}}\times\widehat{\mathbf{t}^{i-1}})\cdot\mathbf{t}^{i-1}\big][\widehat{\mathbf{t}^{i-1}}]_\times^T + \widehat{\mathbf{d}_1^{i-1}}\otimes(\widehat{\mathbf{t}^{i-1}}\times\mathbf{t}^{i-1})}{1 + \widehat{\mathbf{t}^{i-1}}\cdot\mathbf{t}^{i-1}} \\
&\qquad - \frac{(\widehat{\mathbf{d}_2^{i-1}}\times\widehat{\mathbf{t}^{i-1}})\cdot\mathbf{t}^{i-1}}{(1 + \widehat{\mathbf{t}^{i-1}}\cdot\mathbf{t}^{i-1})^2}\widehat{\mathbf{t}^{i-1}}\otimes(\widehat{\mathbf{t}^{i-1}}\times\mathbf{t}^{i-1}) - \widehat{\mathbf{d}_2^{i-1}}\otimes\widehat{\mathbf{t}^{i-1}} + \widehat{\mathbf{t}^{i-1}}\otimes\widehat{\mathbf{d}_2^{i-1}}\Bigg)(\kappa\mathbf{b})_i
\end{aligned}$$

$$
= \frac{1}{\|\mathbf{e}^{i-1}\|}\Big(\mathbf{t}^i \times \tilde{\mathbf{d}}_2 - \kappa_1 \tilde{\mathbf{t}}\Big) +
$$

$$
(A)\left\{ \frac{I - \mathbf{t}^{i-1}\otimes \mathbf{t}^{i-1}}{2\|\mathbf{e}^{i-1}\|}\Bigg(\frac{\big(\widehat{\mathbf{d}_1^{i-1}}\cdot \mathbf{t}^{i-1}\big)[\widehat{\mathbf{t}^{i-1}}]_\times^T + \widehat{\mathbf{d}_1^{i-1}} \otimes (\widehat{\mathbf{t}^{i-1}} \times \mathbf{t}^{i-1})}{1+\widehat{\mathbf{t}^{i-1}}\cdot \mathbf{t}^{i-1}} - \frac{\widehat{\mathbf{d}_1^{i-1}}\cdot \mathbf{t}^{i-1}}{(1+\widehat{\mathbf{t}^{i-1}}\cdot \mathbf{t}^{i-1})^2}\widehat{\mathbf{t}^{i-1}} \otimes (\widehat{\mathbf{t}^{i-1}} \times \mathbf{t}^{i-1}) - \widehat{\mathbf{d}_2^{i-1}} \otimes \widehat{\mathbf{t}^{i-1}} + \widehat{\mathbf{t}^{i-1}} \otimes \widehat{\mathbf{d}_2^{i-1}}\Bigg)(\kappa \mathbf{b})_i \right.
$$

$$
\frac{\partial \kappa_{1i}}{\partial \mathbf{e}^i} = \frac{1}{\|\mathbf{e}^i\|}\Big(- \mathbf{t}^{i-1} \times \tilde{\mathbf{d}}_2 - \kappa_1 \tilde{\mathbf{t}}\Big) +
$$

$$
(B)\left\{ \frac{I - \mathbf{t}^i \otimes \mathbf{t}^i}{2\|\mathbf{e}^i\|}\Bigg(\frac{\big(\widehat{\mathbf{d}_1^i}\cdot \mathbf{t}^i\big)[\widehat{\mathbf{t}^i}]_\times^T + \widehat{\mathbf{d}_1^i}\otimes(\widehat{\mathbf{t}^i}\times \mathbf{t}^i)}{1+\widehat{\mathbf{t}^i}\cdot \mathbf{t}^i} - \frac{\widehat{\mathbf{d}_1^i}\cdot \mathbf{t}^i}{(1+\widehat{\mathbf{t}^i}\cdot \mathbf{t}^i)^2}\widehat{\mathbf{t}^i}\otimes(\widehat{\mathbf{t}^i}\times \mathbf{t}^i) - \widehat{\mathbf{d}_2^i}\otimes \widehat{\mathbf{t}^i} + \widehat{\mathbf{t}^i}\otimes \widehat{\mathbf{d}_2^i}\Bigg)(\kappa \mathbf{b})_i. \right.
$$

Notice that the second term of each of these gradients vanishes when we evaluate at $\mathbf{t}^{i-1} = \widehat{\mathbf{t}^{i-1}}, \mathbf{t}^i = \widehat{\mathbf{t}^i}$, matching the gradient we reported in the continuous, infinitesimal transport setting.

Now we compute the Hessian evaluated at $\mathbf{t}^{i-1} = \widehat{\mathbf{t}^{i-1}}, \mathbf{t}^i = \widehat{\mathbf{t}^i}$ for simplicity. In fact, the Hessian we computed in the infinitesimal transport setting corresponds to the derivatives of the first terms, and we need only to differentiate the additional second terms now, which we labeled "A" and "B". Notice that, since we are evaluating the Hessian at the source reference frame, we can pretend $\|\mathbf{e}^{i-1}\|$, denominator $1+\widehat{\mathbf{t}^{i-1}}\cdot \mathbf{t}^{i-1}$, and the entire term containing $\frac{1}{(1+\widehat{\mathbf{t}^{i-1}}\cdot \mathbf{t}^{i-1})^2}$ are constant (after substituting in the source frame, the derivatives with respect to these terms vanish). Furthermore, the cross terms $\frac{\partial A}{\partial \mathbf{e}^i}$ and $\frac{\partial B}{\partial \mathbf{e}^{i-1}}$ are clearly zero, so the Hessian blocks $\frac{\partial^2 \kappa_1}{\partial \mathbf{e}^{i-1}\partial \mathbf{e}^i}$ and $\frac{\partial^2 \kappa_1}{\partial \mathbf{e}^i \partial \mathbf{e}^{i-1}}$ will remain the same as in the infinitesimal transport setting.

$$
\begin{aligned}
\frac{\partial A}{\partial \mathbf{e}^{i-1}}\bigg|_{\mathbf{t}^{i-1}=\widehat{\mathbf{t}^{i-1}}} &= -\frac{1}{2\|\mathbf{e}^{i-1}\|}\Bigg[\frac{\partial \mathbf{t}^{i-1}}{\partial \mathbf{e}^{i-1}}\Big(\widehat{\mathbf{d}_2^{i-1}}\cdot(\kappa \mathbf{b})_i\Big) + \mathbf{t}^{i-1}\otimes\Bigg(\cancelto{\perp}{\Big(\frac{\partial \mathbf{t}^{i-1}}{\partial \mathbf{e}^{i-1}}\Big)^T\bigg|_{\mathbf{t}^{i-1}=\widehat{\mathbf{t}^{i-1}}}\widehat{\mathbf{t}^{i-1}}}\Big(\widehat{\mathbf{d}_2^{i-1}}\cdot(\kappa \mathbf{b})_i\Big)\Bigg)\Bigg] \\
&\quad + \frac{I-\widehat{\mathbf{t}^{i-1}}\otimes\widehat{\mathbf{t}^{i-1}}}{2\|\mathbf{e}^{i-1}\|}\Bigg[\frac{(\kappa \mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}}{1+\widehat{\mathbf{t}^{i-1}}\cdot\widehat{\mathbf{t}^{i-1}}}\otimes\Bigg(\frac{\partial \mathbf{t}^{i-1}}{\partial \mathbf{e}^{i-1}}^T\widehat{\mathbf{d}_1^{i-1}}\Bigg) + \frac{\widehat{\mathbf{d}_1^{i-1}}\otimes\Big(\frac{\partial \mathbf{t}^{i-1}}{\partial \mathbf{e}^{i-1}}^T\Big((\kappa \mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}\Big)\Big)}{1+\widehat{\mathbf{t}^{i-1}}\cdot\widehat{\mathbf{t}^{i-1}}}\Bigg] \\
&\quad + \frac{I-\widehat{\mathbf{t}^{i-1}}\otimes\widehat{\mathbf{t}^{i-1}}}{2\|\mathbf{e}^{i-1}\|}\Big[-\widehat{\mathbf{d}_2^{i-1}}\otimes\widehat{\mathbf{t}^{i-1}} + \cancel{\widehat{\mathbf{t}^{i-1}}\otimes\widehat{\mathbf{d}_2^{i-1}}}\Big]\frac{\partial(\kappa \mathbf{b})_i}{\partial \mathbf{e}^{i-1}}\bigg|_{\mathbf{t}^{i-1}=\widehat{\mathbf{t}^{i-1}}} \\
&= \frac{I-\widehat{\mathbf{t}^{i-1}}\otimes\widehat{\mathbf{t}^{i-1}}}{2\|\mathbf{e}^{i-1}\|^2}\Bigg[-\Big(\widehat{\mathbf{d}_2^{i-1}}\cdot(\kappa \mathbf{b})_i\Big)I + \frac{\big((\kappa \mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}\big)\otimes\widehat{\mathbf{d}_1^{i-1}} + \widehat{\mathbf{d}_1^{i-1}}\otimes\big((\kappa \mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}\big)}{2} \\
&\qquad - \Big(\widehat{\mathbf{d}_2^{i-1}}\otimes\widehat{\mathbf{t}^{i-1}}\Big)\Big(-\frac{2[\widehat{\mathbf{t}^i}]_\times}{\chi} - \frac{\cancelto{\perp}{(\kappa \mathbf{b})_i}}{\chi}\otimes(\widehat{\mathbf{t}^{i-1}}+\widehat{\mathbf{t}^i})\Big)\Bigg] \\
&= \frac{1}{2\|\mathbf{e}^{i-1}\|^2}\Bigg[\frac{\big((\kappa \mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}\big)\otimes\widehat{\mathbf{d}_1^{i-1}} + \widehat{\mathbf{d}_1^{i-1}}\otimes\big((\kappa \mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}\big)}{2} - \Big(\widehat{\mathbf{d}_2^{i-1}}\cdot(\kappa \mathbf{b})_i\Big)(I-\widehat{\mathbf{t}^{i-1}}\otimes\widehat{\mathbf{t}^{i-1}}) \\
&\qquad + \widehat{\mathbf{d}_2^{i-1}}\otimes\underbrace{\frac{2\widehat{\mathbf{t}^{i-1}}\times\widehat{\mathbf{t}^i}}{\chi}}_{(\kappa \mathbf{b})_i}\Bigg].
\end{aligned}
$$

Likewise:

$$
\frac{\partial B}{\partial \mathbf{e}^i}\bigg|_{\mathbf{t}^i=\widehat{\mathbf{t}^i}} = \frac{1}{2\|\mathbf{e}^i\|^2}\Bigg[\frac{\big((\kappa \mathbf{b})_i\times\widehat{\mathbf{t}^i}\big)\otimes\widehat{\mathbf{d}_1^i} + \widehat{\mathbf{d}_1^i}\otimes\big((\kappa \mathbf{b})_i\times\widehat{\mathbf{t}^i}\big)}{2} - \Big(\widehat{\mathbf{d}_2^i}\cdot(\kappa \mathbf{b})_i\Big)(I-\widehat{\mathbf{t}^i}\otimes\widehat{\mathbf{t}^i}) + \widehat{\mathbf{d}_2^i}\otimes(\kappa \mathbf{b})_i\Bigg].
$$

Thus, the diagonal Hessian blocks of κ_1 *to be evaluated only at the source frame* are given by:

$$
\boxed{
\begin{aligned}
\frac{\partial^2 \kappa_{1i}}{\partial \mathbf{e}^{i-1}\partial \mathbf{e}^{i-1}} = \frac{1}{\|\mathbf{e}^{i-1}\|^2}\Bigg[&2\kappa_{1i}\tilde{\mathbf{t}}\otimes\tilde{\mathbf{t}} - (\mathbf{t}^i\times\tilde{\mathbf{d}}_2)\otimes\tilde{\mathbf{t}} - \tilde{\mathbf{t}}\otimes(\mathbf{t}^i\times\tilde{\mathbf{d}}_2) + \frac{(\kappa\mathbf{b})_i\otimes\mathbf{d}_2^{i-1}+\mathbf{d}_2^{i-1}\otimes(\kappa\mathbf{b})_i}{2} \\
&- \left(\frac{\kappa_{1i}}{\chi} + \frac{\mathbf{d}_2^{i-1}\cdot(\kappa\mathbf{b})_i}{2}\right)(I-\mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}) + \frac{\big((\kappa\mathbf{b})_i\times\mathbf{t}^{i-1}\big)\otimes\mathbf{d}_1^{i-1}+\mathbf{d}_1^{i-1}\otimes\big((\kappa\mathbf{b})_i\times\mathbf{t}^{i-1}\big)}{4}\Bigg] \\
\frac{\partial^2 \kappa_{1i}}{\partial \mathbf{e}^{i}\partial \mathbf{e}^{i}} = \frac{1}{\|\mathbf{e}^{i}\|^2}\Bigg[&2\kappa_{1i}\tilde{\mathbf{t}}\otimes\tilde{\mathbf{t}} + (\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_2)\otimes\tilde{\mathbf{t}} + \tilde{\mathbf{t}}\otimes(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_2) + \frac{(\kappa\mathbf{b})_i\otimes\mathbf{d}_2^{i}+\mathbf{d}_2^{i}\otimes(\kappa\mathbf{b})_i}{2} \\
&- \left(\frac{\kappa_{1i}}{\chi} + \frac{\mathbf{d}_2^{i}\cdot(\kappa\mathbf{b})_i}{2}\right)(I-\mathbf{t}^{i}\otimes\mathbf{t}^{i}) + \frac{\big((\kappa\mathbf{b})_i\times\mathbf{t}^{i}\big)\otimes\mathbf{d}_1^{i}+\mathbf{d}_1^{i}\otimes\big((\kappa\mathbf{b})_i\times\mathbf{t}^{i}\big)}{4}\Bigg],
\end{aligned}
}
$$

where we highlighted in red the differences from the formulas in the appendix of [Bergou et al., 2010]. The off-diagonal blocks are the same as the infinitesimal transport versions.

We can also slightly simplify the gradient of κ_1 (*to be evaluated anywhere*):

$$
\boxed{
\begin{aligned}
\frac{\partial \kappa_{1i}}{\partial \mathbf{e}^{i-1}} &= \frac{1}{\|\mathbf{e}^{i-1}\|}\left(\mathbf{t}^i\times\tilde{\mathbf{d}}_2 - \kappa_1\tilde{\mathbf{t}}\right) + \\
&\frac{I-\mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}}{2\|\mathbf{e}^{i-1}\|}\Bigg(\frac{(\widehat{\mathbf{d}_1^{i-1}}\cdot\mathbf{t}^{i-1})[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}]+\widehat{\mathbf{d}_1^{i-1}}(\mathbf{t}^{i-1}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}])}{1+\widehat{\mathbf{t}^{i-1}}\cdot\mathbf{t}^{i-1}} \\
&\qquad - \frac{\widehat{\mathbf{d}_1^{i-1}}\cdot\mathbf{t}^{i-1}}{(1+\widehat{\mathbf{t}^{i-1}}\cdot\mathbf{t}^{i-1})^2}\widehat{\mathbf{t}^{i-1}}(\mathbf{t}^{i-1}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}]) + \widehat{\mathbf{d}_1^{i-1}}\times(\kappa\mathbf{b})_i\Bigg) \\
\frac{\partial \kappa_{1i}}{\partial \mathbf{e}^{i}} &= \frac{1}{\|\mathbf{e}^{i}\|}\left(-\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_2 - \kappa_1\tilde{\mathbf{t}}\right) + \\
&\frac{I-\mathbf{t}^{i}\otimes\mathbf{t}^{i}}{2\|\mathbf{e}^{i}\|}\Bigg(\frac{(\widehat{\mathbf{d}_1^{i}}\cdot\mathbf{t}^{i})[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i}}]+\widehat{\mathbf{d}_1^{i}}(\mathbf{t}^{i}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i}}])}{1+\widehat{\mathbf{t}^{i}}\cdot\mathbf{t}^{i}} \\
&\qquad - \frac{\widehat{\mathbf{d}_1^{i}}\cdot\mathbf{t}^{i}}{(1+\widehat{\mathbf{t}^{i}}\cdot\mathbf{t}^{i})^2}\widehat{\mathbf{t}^{i}}(\mathbf{t}^{i}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i}}]) + \widehat{\mathbf{d}_1^{i}}\times(\kappa\mathbf{b})_i\Bigg),
\end{aligned}
}
$$

where again the terms missing in [Bergou et al., 2010] are highlighted in red.

The gradients and diagonal Hessian blocks for the second material curvatures are:

$$
\boxed{
\begin{aligned}
\frac{\partial \kappa_{2}}{\partial \mathbf{e}^{i-1}} &= \frac{1}{\|\mathbf{e}^{i-1}\|}\left(-\mathbf{t}^i\times\tilde{\mathbf{d}}_1 - \kappa_2\tilde{\mathbf{t}}\right) + \\
&\frac{I-\mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}}{2\|\mathbf{e}^{i-1}\|}\Bigg(\frac{(\widehat{\mathbf{d}_2^{i-1}}\cdot\mathbf{t}^{i-1})[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}]+\widehat{\mathbf{d}_2^{i-1}}(\mathbf{t}^{i-1}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}])}{1+\widehat{\mathbf{t}^{i-1}}\cdot\mathbf{t}^{i-1}} \\
&\qquad - \frac{\widehat{\mathbf{d}_2^{i-1}}\cdot\mathbf{t}^{i-1}}{(1+\widehat{\mathbf{t}^{i-1}}\cdot\mathbf{t}^{i-1})^2}\widehat{\mathbf{t}^{i-1}}(\mathbf{t}^{i-1}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}]) + \widehat{\mathbf{d}_2^{i-1}}\times(\kappa\mathbf{b})_i\Bigg) \\
\frac{\partial \kappa_{2}}{\partial \mathbf{e}^{i}} &= \frac{1}{\|\mathbf{e}^{i}\|}\left(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1 - \kappa_2\tilde{\mathbf{t}}\right) + \\
&\frac{I-\mathbf{t}^{i}\otimes\mathbf{t}^{i}}{2\|\mathbf{e}^{i}\|}\Bigg(\frac{(\widehat{\mathbf{d}_2^{i}}\cdot\mathbf{t}^{i})[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i}}]+\widehat{\mathbf{d}_2^{i}}(\mathbf{t}^{i}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i}}])}{1+\widehat{\mathbf{t}^{i}}\cdot\mathbf{t}^{i}} \\
&\qquad - \frac{\widehat{\mathbf{d}_2^{i}}\cdot\mathbf{t}^{i}}{(1+\widehat{\mathbf{t}^{i}}\cdot\mathbf{t}^{i})^2}\widehat{\mathbf{t}^{i}}(\mathbf{t}^{i}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i}}]) + \widehat{\mathbf{d}_2^{i}}\times(\kappa\mathbf{b})_i\Bigg)
\end{aligned}
}
$$

$$
\begin{aligned}
\frac{\partial^2 \kappa_{2i}}{\partial \mathbf{e}^{i-1}\partial \mathbf{e}^{i-1}} &= \frac{1}{\|\mathbf{e}^{i-1}\|^2}\Bigg[2\kappa_{2i}\tilde{\mathbf{t}}\otimes\tilde{\mathbf{t}} + (\mathbf{t}^i\times\tilde{\mathbf{d}}_1)\otimes\tilde{\mathbf{t}} + \tilde{\mathbf{t}}\otimes(\mathbf{t}^i\times\tilde{\mathbf{d}}_1) - \frac{(\kappa\mathbf{b})_i\otimes\mathbf{d}_1^{i-1} + \mathbf{d}_1^{i-1}\otimes(\kappa\mathbf{b})_i}{2} \\
&\qquad - \left(\frac{\kappa_{2i}}{\chi} - \frac{\mathbf{d}_1^{i-1}\cdot(\kappa\mathbf{b})_i}{2}\right)(I - \mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}) + \frac{\left((\kappa\mathbf{b})_i\times\mathbf{t}^{i-1}\right)\otimes\mathbf{d}_2^{i-1} + \mathbf{d}_2^{i-1}\otimes\left((\kappa\mathbf{b})_i\times\mathbf{t}^{i-1}\right)}{4}\Bigg] \\
\frac{\partial^2 \kappa_{2i}}{\partial \mathbf{e}^{i}\partial \mathbf{e}^{i}} &= \frac{1}{\|\mathbf{e}^{i}\|^2}\Bigg[2\kappa_{2i}\tilde{\mathbf{t}}\otimes\tilde{\mathbf{t}} - (\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1)\otimes\tilde{\mathbf{t}} - \tilde{\mathbf{t}}\otimes(\mathbf{t}^{i-1}\times\tilde{\mathbf{d}}_1) - \frac{(\kappa\mathbf{b})_i\otimes\mathbf{d}_1^{i} + \mathbf{d}_1^{i}\otimes(\kappa\mathbf{b})_i}{2} \\
&\qquad - \left(\frac{\kappa_{2i}}{\chi} - \frac{\mathbf{d}_1^{i}\cdot(\kappa\mathbf{b})_i}{2}\right)(I - \mathbf{t}^{i}\otimes\mathbf{t}^{i}) + \frac{\left((\kappa\mathbf{b})_i\times\mathbf{t}^{i}\right)\otimes\mathbf{d}_2^{i} + \mathbf{d}_2^{i}\otimes\left((\kappa\mathbf{b})_i\times\mathbf{t}^{i}\right)}{4}\Bigg].
\end{aligned}
$$

5.1 Gradients and Hessians of Twist for Finite Transport

The derivatives of twist also become more complicated in the finite transport setting. Recall,

$$
m_i = \theta^i - \theta^{i-1} + \underline{m}_i
$$

where $\overline{m}_i$ is the constant *rest twist*, and $\underline{m}_i$ is the *reference twist*:

$$
\underline{m}_i = \angle\left(P_{\mathbf{t}^{i-1}}^{\mathbf{t}^i} P_{\widehat{\mathbf{t}^{i-1}}}^{\mathbf{t}^{i-1}} \widehat{\mathbf{d}_2^{i-1}}, P_{\widehat{\mathbf{t}^i}}^{\mathbf{t}^i}\widehat{\mathbf{d}_2^i}\right).
$$

We begin with the derivative of the angle between two *unit* vectors:

$$
\frac{\partial}{\partial \mathbf{a}}\angle(\mathbf{a},\mathbf{b}) = -\frac{\mathbf{b}}{\sin(\angle(\mathbf{a},\mathbf{b}))}, \quad \frac{\partial}{\partial \mathbf{b}}\angle(\mathbf{a},\mathbf{b}) = -\frac{\mathbf{a}}{\sin(\angle(\mathbf{a},\mathbf{b}))}.
$$

So:

$$
\left(\frac{\partial \underline{m}_i}{\partial \mathbf{e}^i}\right)^T = -\frac{1}{\sin(\underline{m}_i)}\Bigg(\underbrace{\mathbf{d}_2^i\cdot\frac{\partial}{\partial \mathbf{e}^i}\left(P_{\mathbf{t}^{i-1}}^{\mathbf{t}^i}\mathbf{d}_2^{i-1}\right)}_{(A)} + \underbrace{\left(P_{\mathbf{t}^{i-1}}^{\mathbf{t}^i}\mathbf{d}_2^{i-1}\right)\cdot\frac{\partial}{\partial \mathbf{e}^i}\left(P_{\widehat{\mathbf{t}^i}}^{\mathbf{t}^i}\widehat{\mathbf{d}_2^i}\right)}_{(B)}\Bigg).
$$

Now we evaluate:

$$
\begin{aligned}
(A) = \mathbf{d}_2^i\cdot\Bigg[&\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)[\mathbf{t}^{i-1}]_\times + \frac{(\kappa\mathbf{b})_i}{2}\otimes(\mathbf{d}_2^{i-1}\times\mathbf{t}^{i-1}) - \left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\frac{(\kappa\mathbf{b})_i}{2}\otimes\mathbf{t}^{i-1} \\
&+ \cancelto{\perp}{(\mathbf{t}^{i-1}\cdot\mathbf{d}_2^{i-1})}I - \mathbf{t}^{i-1}\otimes\mathbf{d}_2^{i-1} + \mathbf{d}_2^{i-1}\otimes\mathbf{t}^{i-1}\Bigg]\frac{I - \mathbf{t}^i\otimes\mathbf{t}^i}{\|\mathbf{e}^i\|} \\
= \Bigg[&\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\left(\mathbf{d}_2^i\times\mathbf{t}^{i-1}\right)^T + \left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i}\right)\left(\mathbf{d}_1^{i-1}\right)^T \\
&- \left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i}\right)\left(\mathbf{t}^{i-1}\right)^T + \left(\mathbf{d}_1^{i-1}\times\mathbf{d}_2^i\right)^T\Bigg]\frac{\mathbf{d}_1^i\otimes\mathbf{d}_1^i + \mathbf{d}_2^i\otimes\mathbf{d}_2^i}{\|\mathbf{e}^i\|} \\
= \frac{{\mathbf{d}_2^i}^T}{\|\mathbf{e}^i\|}\Bigg[&\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i}\right)\mathbf{d}_1^{i-1}\cdot\mathbf{d}_2^i - \left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i}\right)\underbrace{\mathbf{t}^{i-1}\cdot\mathbf{d}_2^i}_{\mathbf{t}^{i-1}\cdot(\mathbf{t}^i\times\mathbf{d}_1^i)}\Bigg] \\
+ \frac{{\mathbf{d}_1^i}^T}{\|\mathbf{e}^i\|}\Bigg[&\underbrace{\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)}_{\frac{\mathbf{t}^i\cdot\mathbf{d}_1^{i-1}}{\chi}}\underbrace{\mathbf{t}^i\cdot\mathbf{t}^{i-1}}_{\cancel{\chi}-1} + \left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i}\right)\mathbf{d}_1^{i-1}\cdot\mathbf{d}_1^i - \left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i}\right)\underbrace{\mathbf{t}^{i-1}\cdot\mathbf{d}_1^i}_{-\chi\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^i} - \cancel{\mathbf{t}^i\cdot\mathbf{d}_1^{i-1}}\Bigg] \\
= \frac{(\kappa\mathbf{b})_i^T\left(\mathbf{d}_2^i\otimes\mathbf{d}_2\right)}{2\|\mathbf{e}^i\|}\Bigg[&\underbrace{\mathbf{d}_1^{i-1}\cdot\mathbf{d}_2^i - \left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_1^{i}\right)\chi}_{:=\alpha_1}\Bigg]
\end{aligned}
$$

$$+\frac{{\mathbf{d}_1^i}^T}{\|\mathbf{e}^i\|}\left[\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^i\right)\mathbf{d}_1^{i-1}\cdot\mathbf{d}_1^i+\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\left(\left(1-\mathbf{t}^{i-1}\cdot\mathbf{t}^i\right)-\chi\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_1^i\right)^2\right)-\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\right]$$

Where we used the $\sin^2+\cos^2=1$ trig identity in the last step. Now, simplifying only the $\frac{\mathbf{d}_1^i}{\|\mathbf{e}^i\|}$ coefficient:

$$\begin{aligned}
&\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^i\right)\mathbf{d}_1^{i-1}\cdot\mathbf{d}_1^i-\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_1^i\right)^2\chi-\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\mathbf{t}^{i-1}\cdot\mathbf{t}^i\\
&=\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^i\right)\underbrace{(\mathbf{d}_2^{i-1}\times\mathbf{t}^{i-1})\cdot(\mathbf{d}_2^i\times\mathbf{t}^i)}_{\cancel{(\mathbf{d}_2^{i-1}\cdot\mathbf{d}_2^i)(\mathbf{t}^{i-1}\cdot\mathbf{t}^i)}-(\mathbf{d}_2^{i-1}\cdot\mathbf{t}^i)(\mathbf{t}^{i-1}\cdot\mathbf{d}_2^i)}-\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_1^i\right)^2\chi\\
&\qquad-\left[\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_1^i\right)(\mathbf{d}_2^{i-1}\cdot\mathbf{d}_1)+\cancel{\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^i\right)(\mathbf{d}_2^{i-1}\cdot\mathbf{d}_2^i)}\right]\mathbf{t}^{i-1}\cdot\mathbf{t}^i\\
&=-\underbrace{\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^i\right)(\mathbf{d}_2^{i-1}\cdot\mathbf{t}^i)(\mathbf{t}^{i-1}\cdot\mathbf{d}_2^i)}_{(\mathbf{t}^{i-1}\cdot\mathbf{d}_1^i)(\mathbf{d}_2^{i-1}\cdot\mathbf{t}^i)\left(\mathbf{d}_1^i\cdot\frac{(\kappa\mathbf{b})_i}{2}\right)}-\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_1^i\right)^2\chi-\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_1^i\right)(\mathbf{d}_2^{i-1}\cdot\mathbf{d}_1)\mathbf{t}^{i-1}\cdot\mathbf{t}^i\\
&=\left(\mathbf{d}_1^i\cdot\frac{(\kappa\mathbf{b})_i}{2}\right)\left[\underbrace{(\mathbf{t}^{i-1}\cdot\mathbf{d}_1^i)(\mathbf{d}_2^{i-1}\cdot\mathbf{t}^i)-\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_2^{i-1}\right)\left(\frac{(\kappa\mathbf{b})_i}{2}\cdot\mathbf{d}_1^i\right)\chi-(\mathbf{d}_2^{i-1}\cdot\mathbf{d}_1)\mathbf{t}^{i-1}\cdot\mathbf{t}^i}_{:=\alpha_2}\right].
\end{aligned}$$

Finally, we notice that:

$$\begin{aligned}
\sin(\underline{m}_i)=\mathbf{d}_1^i\cdot P_{\mathbf{t}^{i-1}}^{\mathbf{t}^i}\mathbf{d}_2^{i-1}&=\underbrace{\left(\mathbf{d}_1^i\cdot\frac{(\kappa\mathbf{b})_i}{2}\right)\left(\mathbf{d}_2^{i-1}\cdot\frac{(\kappa\mathbf{b})_i}{2}\right)\chi-(\mathbf{d}_1^i\cdot\mathbf{t}^{i-1})(\mathbf{t}^i\cdot\mathbf{d}_2^{i-1})+(\mathbf{t}^{i-1}\cdot\mathbf{t}^i)(\mathbf{d}_1^i\cdot\mathbf{d}_2^{i-1})}_{-\alpha_2}\\
&=\left(\mathbf{d}_1^i\cdot\frac{(\kappa\mathbf{b})_i}{2}\right)\left(\mathbf{d}_2^{i-1}\cdot\frac{(\kappa\mathbf{b})_i}{2}\right)\chi+\mathbf{d}_1^i\cdot\big(\underbrace{(\mathbf{t}^{i-1}\times\mathbf{d}_2^{i-1})}_{-\mathbf{d}_1^{i-1}}\times\mathbf{t}^i\big)\\
&=\left(\mathbf{d}_1^i\cdot\frac{(\kappa\mathbf{b})_i}{2}\right)\left(\mathbf{d}_2^{i-1}\cdot\frac{(\kappa\mathbf{b})_i}{2}\right)\chi-\mathbf{d}_1^{i-1}\cdot(\mathbf{t}^i\times\mathbf{d}_1^i)=\underbrace{\left(\mathbf{d}_1^i\cdot\frac{(\kappa\mathbf{b})_i}{2}\right)\left(\mathbf{d}_2^{i-1}\cdot\frac{(\kappa\mathbf{b})_i}{2}\right)\chi-\mathbf{d}_1^{i-1}\cdot\mathbf{d}_2^i}_{-\alpha_1},
\end{aligned}$$

meaning: $(A)=-\frac{(\kappa\mathbf{b})_i^T(\mathbf{d}_2^i\otimes\mathbf{d}_2)}{2\|\mathbf{e}^i\|}\sin(\underline{m}_i)-\frac{(\kappa\mathbf{b})_i^T(\mathbf{d}_1^i\otimes\mathbf{d}_1)}{2\|\mathbf{e}^i\|}\sin(\underline{m}_i)=\boxed{-\sin(\underline{m}_i)\frac{(\kappa\mathbf{b})_i^T}{2\|\mathbf{e}^i\|}}$. Now, we move on to:

$$\begin{aligned}
(B)&=\left[(\mathbf{d}_1^i\otimes\mathbf{d}_1^i+\mathbf{d}_2^i\otimes\mathbf{d}_2^i)\left(P_{\mathbf{t}^{i-1}}^{\mathbf{t}^i}\mathbf{d}_2^{i-1}\right)\right]\cdot\frac{\partial}{\partial\mathbf{e}^i}\left(P_{\widehat{\mathbf{t}^i}}^{\mathbf{t}^i}\widehat{\mathbf{d}_2^i}\right)=\left(\sin(\underline{m}_i)\mathbf{d}_1^i+\cos(\underline{m}_i)\cancelto{\perp}{\mathbf{d}_2^i}\right)\cdot\frac{\partial}{\partial\mathbf{e}^i}\left(P_{\widehat{\mathbf{t}^i}}^{\mathbf{t}^i}\widehat{\mathbf{d}_2^i}\right)\\
&=\sin(\underline{m}_i)\mathbf{d}_1^i\cdot\left(\frac{(\widehat{\mathbf{d}_1^i}\cdot\mathbf{t}^i)[\widehat{\mathbf{t}^i}]_\times+(\widehat{\mathbf{t}^i}\times\mathbf{t}^i)\otimes\widehat{\mathbf{d}_1^i}}{1+\widehat{\mathbf{t}^i}\cdot\mathbf{t}^i}-\frac{\widehat{\mathbf{d}_1^i}\cdot\mathbf{t}^i}{(1+\widehat{\mathbf{t}^i}\cdot\mathbf{t}^i)^2}(\widehat{\mathbf{t}^i}\times\mathbf{t}^i)\otimes\widehat{\mathbf{t}^i}-\widehat{\mathbf{t}^i}\otimes\widehat{\mathbf{d}_2^i}+\widehat{\mathbf{d}_2^i}\otimes\widehat{\mathbf{t}^i}\right)\frac{I-\mathbf{t}^i\otimes\mathbf{t}^i}{\|\mathbf{e}^i\|}\\
&=\sin(\underline{m}_i)\left(\frac{(\widehat{\mathbf{d}_1^i}\cdot\mathbf{t}^i)(\mathbf{d}_1^i\times\widehat{\mathbf{t}^i})^T+(\mathbf{d}_2^i\cdot\widehat{\mathbf{t}^i})\widehat{\mathbf{d}_1^i}^T}{1+\widehat{\mathbf{t}^i}\cdot\mathbf{t}^i}-\frac{(\widehat{\mathbf{d}_1^i}\cdot\mathbf{t}^i)(\mathbf{d}_2^i\cdot\widehat{\mathbf{t}^i})}{(1+\widehat{\mathbf{t}^i}\cdot\mathbf{t}^i)^2}\widehat{\mathbf{t}^i}^T-(\mathbf{d}_1^i\cdot\widehat{\mathbf{t}^i})\widehat{\mathbf{d}_2^i}^T+(\mathbf{d}_1^i\cdot\widehat{\mathbf{d}_2^i})\widehat{\mathbf{t}^i}^T\right)\frac{I-\mathbf{t}^i\otimes\mathbf{t}^i}{\|\mathbf{e}^i\|}\\
&=\sin(\underline{m}_i)\left(\frac{(\widehat{\mathbf{d}_1^i}\cdot\mathbf{t}^i)(\mathbf{d}_1^i\times\widehat{\mathbf{t}^i})^T+(\mathbf{d}_2^i\cdot\widehat{\mathbf{t}^i})\widehat{\mathbf{d}_1^i}^T}{1+\widehat{\mathbf{t}^i}\cdot\mathbf{t}^i}-\frac{(\widehat{\mathbf{d}_1^i}\cdot\mathbf{t}^i)(\mathbf{d}_2^i\cdot\widehat{\mathbf{t}^i})}{(1+\widehat{\mathbf{t}^i}\cdot\mathbf{t}^i)^2}\widehat{\mathbf{t}^i}^T+\left[(\widehat{\mathbf{d}_2^i}\times\widehat{\mathbf{t}^i})\times\mathbf{d}_1^i\right]^T\right)\frac{I-\mathbf{t}^i\otimes\mathbf{t}^i}{\|\mathbf{e}^i\|}
\end{aligned}$$

Notice that in the infinitesimal transport setting ($\mathbf{t}^i = \widehat{\mathbf{t}^i}, \mathbf{d}_2^i = \widehat{\mathbf{d}_2^i}$), term (A) is unchanged, while (B) actually vanishes, reducing our gradient formula to $\frac{\partial \underline{m}_i}{\partial \mathbf{e}^i} = \frac{(\kappa \mathbf{b})_i}{2\|\mathbf{e}^i\|}$ as reported in the appendix of [Bergou et al., 2010]. However, in the finite transport setting, we have the gradient:

$$\boxed{\frac{\partial \underline{m}_i}{\partial \mathbf{e}^i} = \frac{(\kappa \mathbf{b})_i}{2\|\mathbf{e}^i\|} - \frac{I - \mathbf{t}^i \otimes \mathbf{t}^i}{\|\mathbf{e}^i\|}\left(\frac{(\widehat{\mathbf{d}_1^i} \cdot \mathbf{t}^i)(\mathbf{d}_1^i \times \widehat{\mathbf{t}^i}) + (\mathbf{d}_2^i \cdot \widehat{\mathbf{t}^i})\widehat{\mathbf{d}_1^i}}{1 + \widehat{\mathbf{t}^i} \cdot \mathbf{t}^i} - \frac{(\widehat{\mathbf{d}_1^i} \cdot \mathbf{t}^i)(\mathbf{d}_2^i \cdot \widehat{\mathbf{t}^i})}{(1 + \widehat{\mathbf{t}^i} \cdot \mathbf{t}^i)^2}\widehat{\mathbf{t}^i} + \widehat{\mathbf{d}_1^i} \times \mathbf{d}_1^i\right),}$$

where the term in red is missing from [Bergou et al., 2010]. Similarly:

$$\boxed{\begin{aligned}\frac{\partial \underline{m}_i}{\partial \mathbf{e}^{i-1}} = \frac{(\kappa \mathbf{b})_i}{2\|\mathbf{e}^{i-1}\|} + \frac{I - \mathbf{t}^{i-1} \otimes \mathbf{t}^{i-1}}{\|\mathbf{e}^{i-1}\|}\Bigg(&\frac{(\widehat{\mathbf{d}_1^{i-1}} \cdot \mathbf{t}^{i-1})(\mathbf{d}_1^{i-1} \times \widehat{\mathbf{t}^{i-1}}) + (\mathbf{d}_2^{i-1} \cdot \widehat{\mathbf{t}^{i-1}})\widehat{\mathbf{d}_1^{i-1}}}{1 + \widehat{\mathbf{t}^{i-1}} \cdot \mathbf{t}^{i-1}} \\ &- \frac{(\widehat{\mathbf{d}_1^{i-1}} \cdot \mathbf{t}^{i-1})(\mathbf{d}_2^{i-1} \cdot \widehat{\mathbf{t}^{i-1}})}{(1 + \widehat{\mathbf{t}^{i-1}} \cdot \mathbf{t}^{i-1})^2}\widehat{\mathbf{t}^{i-1}} + \widehat{\mathbf{d}_1^{i-1}} \times \mathbf{d}_1^{i-1}\Bigg).\end{aligned}}$$

Notice that the new term is *added* here, not subtracted. This second formula follows from the relationship:

$$\underline{m}_i = \angle\left(P_{\mathbf{t}^{i-1}}^{\mathbf{t}^i} P_{\widehat{\mathbf{t}^{i-1}}}^{\mathbf{t}^{i-1}} \widehat{\mathbf{d}_2^{i-1}}, P_{\widehat{\mathbf{t}^i}}^{\mathbf{t}^i} \widehat{\mathbf{d}_2^i}\right) = \angle\left(P_{\widehat{\mathbf{t}^{i-1}}}^{\mathbf{t}^{i-1}} \widehat{\mathbf{d}_2^{i-1}}, P_{\mathbf{t}^i}^{\mathbf{t}^{i-1}} P_{\widehat{\mathbf{t}^i}}^{\mathbf{t}^i} \widehat{\mathbf{d}_2^i}\right) = -\angle\left(P_{\mathbf{t}^i}^{\mathbf{t}^{i-1}} P_{\widehat{\mathbf{t}^i}}^{\mathbf{t}^i} \widehat{\mathbf{d}_2^i}, P_{\widehat{\mathbf{t}^{i-1}}}^{\mathbf{t}^{i-1}} \widehat{\mathbf{d}_2^{i-1}}\right),$$

which swaps the role of indices i and $i-1$.

Like in the material curvature case, we evaluate the Hessian only at the source frame to simplify the expression. This means, when differentiating the new red terms in, e.g. $\frac{\partial \underline{m}_i}{\partial \mathbf{e}^i}$, we can pretend that $\|\mathbf{e}^i\|$, $1 + \widehat{\mathbf{t}^i} \cdot \mathbf{t}^i$, and the entire term containing $(1 + \widehat{\mathbf{t}^i} \cdot \mathbf{t}^i)^2$ are constant when differentiating.

First we rewrite the red term in $\frac{\partial \underline{m}_i}{\partial \mathbf{e}^i}$ in a form that's remarkably similar to the new term added to the material curvature gradient:

$$(A) := \frac{I - \mathbf{t}^i \otimes \mathbf{t}^i}{\|\mathbf{e}^i\|}\left(\frac{(\widehat{\mathbf{d}_1^i} \cdot \mathbf{t}^i)[\widehat{\mathbf{t}^i}]_\times^T + \widehat{\mathbf{d}_1^i} \otimes (\widehat{\mathbf{t}^i} \times \mathbf{t}^i)}{1 + \widehat{\mathbf{t}^i} \cdot \mathbf{t}^i} - \frac{(\widehat{\mathbf{d}_1^i} \cdot \mathbf{t}^i)}{(1 + \widehat{\mathbf{t}^i} \cdot \mathbf{t}^i)^2}\widehat{\mathbf{t}^i} \otimes (\widehat{\mathbf{t}^i} \times \mathbf{t}^i) + [\widehat{\mathbf{d}_1^i}]_\times\right)\mathbf{d}_1^i.$$

In fact, this term is identical to the material curvature term apart from the factor of $1/2$ and the presence of $\mathbf{d}_1^i$ at the end instead of $(\kappa \mathbf{b})_i$. The derivative of this term is:

$$\begin{aligned}\frac{\partial (A)}{\partial \mathbf{e}^i} :=& \frac{I - \mathbf{t}^i \otimes \mathbf{t}^i}{\|\mathbf{e}^i\|^2}\left(\frac{(\widehat{\mathbf{d}_1^i} \times \widehat{\mathbf{t}^i}) \otimes \widehat{\mathbf{d}_1^i} + \widehat{\mathbf{d}_1^i} \otimes (\widehat{\mathbf{d}_1^i} \times \widehat{\mathbf{t}^i})}{1 + \widehat{\mathbf{t}^i} \cdot \mathbf{t}^i} - [\widehat{\mathbf{d}_1^i}]_\times (\widehat{\mathbf{t}^i} \otimes \mathbf{d}_1^i)\right) \\ =& \frac{1}{\|\mathbf{e}^i\|^2}\left(\frac{\widehat{\mathbf{d}_2^i} \otimes \widehat{\mathbf{d}_1^i} - \widehat{\mathbf{d}_1^i} \otimes \widehat{\mathbf{d}_2^i}}{2}\right) = \frac{[\widehat{\mathbf{t}^i}]_\times}{2\|\mathbf{e}^i\|^2}.\end{aligned}$$

Similarly, the additional Hessian term from the red part of $\frac{\partial \underline{m}_i}{\partial \mathbf{e}^{i-1}}$ is:

$$\frac{[\widehat{\mathbf{t}^{i-1}}]_\times}{2\|\mathbf{e}^{i-1}\|^2}.$$

Surprisingly, these purely skew-symmetric terms cancel out the skew-symmetric parts of the infinitesimal transport twisting Hessian, leaving exactly the symmetric part. So, for twisting, the symmetrized Hessian formulas given in [Bergou et al., 2010]'s appendix are actually correct for finite transport.

5.2 Bergou 2008 Bending

The original discrete bending energy proposed in [Bergou et al., 2008] differs from the one in [Bergou et al., 2010]: instead of averaging the material frames for each adjacent edge to compute the material curvature, [Bergou et al., 2008] averages the bending energy computed with each edge's frame. Averaging the energy is more physically meaningful: averaging the material frame vectors at a vertex with nonzero twist yields frame vectors that are neither unit length nor orthogonal. While our implementation supports both bending energies, we prefer the original expression. This section derives gradients and Hessians for this energy in the finite transport setting and discusses how both energies can be implemented efficiently in a common framework.

Specifically, the bending energy from [Bergou et al., 2008] is (after diagonalizing the stiffness tensor):

$$E_b^{2008} = \frac{1}{2}\sum_{i=1}^{\texttt{nv}-2}\sum_{j=i-1}^{i}\frac{\overline{l}^j}{2\overline{l}_i^2}\left(B_{11}({\kappa_1}_i^j - \overline{\kappa_1}_i)^2 + B_{22}({\kappa_2}_i^j - \overline{\kappa_2}_i)^2\right), \tag{A4}$$

where ${\kappa_1}_i^j = \kappa\mathbf{b}_i \cdot \mathbf{d}_2^j$, ${\kappa_2}_i^j = -\kappa\mathbf{b}_i \cdot \mathbf{d}_1^j$ and we made the slight change of integrating edge j's energy contribution over $\overline{l}^j/2$ instead of $\overline{l}_i/2$. This should be compared with the energy from [Bergou et al., 2010], which we relabel as:

$$E_b^{2010} = \frac{1}{2}\sum_{i=1}^{\texttt{nv}-2}\frac{1}{\overline{l}_i}\left(B_{11}({\kappa_1}_i - \overline{\kappa_1}_i)^2 + B_{22}({\kappa_2}_i - \overline{\kappa_2}_i)^2\right),$$

To simultaneously support both bending energies with the same code, it will be helpful to calculate derivatives of $(\kappa\mathbf{b})_i \cdot \mathbf{d}_1^j$ and $(\kappa\mathbf{b})_i \cdot \mathbf{d}_2^j$, and then use the relationship ${\kappa_1}_i = \frac{1}{2}\left({\kappa_1}_i^{i-1} + {\kappa_1}_i^i\right)$ to differentiate E_b^{2010}.

We now compute the finite transport gradient and Hessian of these quantities, starting with the gradient:

$$\begin{aligned}
\frac{\partial(\kappa_1)_i^{i-1}}{\partial\mathbf{e}^{i-1}} &= \left[\mathbf{d}_2^{i-1}\cdot\frac{\partial(\kappa\mathbf{b})_i}{\partial\mathbf{e}^{i-1}} + (\kappa\mathbf{b})_i\cdot\frac{\partial\mathbf{d}_2^{i-1}}{\partial\mathbf{e}^{i-1}}\right]^T \\
&= \frac{1}{\|\mathbf{e}^{i-1}\|}\left[2\frac{\mathbf{t}^i\times\mathbf{d}_2^{i-1}}{\chi} - (\kappa_1)_i^{i-1}\tilde{\mathbf{t}}\right] \\
&+ \frac{I - \mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}}{\|\mathbf{e}^{i-1}\|}\Bigg(\frac{\left(\widehat{\mathbf{d}_1^{i-1}}\cdot\mathbf{t}^{i-1}\right)[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}] + \widehat{\mathbf{d}_1^{i-1}}(\mathbf{t}^{i-1}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}])}{1+\widehat{\mathbf{t}^{i-1}}\cdot\mathbf{t}^{i-1}} \\
&\qquad - \frac{\widehat{\mathbf{d}_1^{i-1}}\cdot\mathbf{t}^{i-1}}{(1+\widehat{\mathbf{t}^{i-1}}\cdot\mathbf{t}^{i-1})^2}\widehat{\mathbf{t}^{i-1}}(\mathbf{t}^{i-1}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}]) + \widehat{\mathbf{d}_1^{i-1}}\times(\kappa\mathbf{b})_i\Bigg) \\
\frac{\partial(\kappa_1)_i^{i-1}}{\partial\mathbf{e}^{i}} &= \frac{1}{\|\mathbf{e}^{i}\|}\left[-2\frac{\mathbf{t}^{i-1}\times\mathbf{d}_2^{i-1}}{\chi} - (\kappa_1)_i^{i-1}\tilde{\mathbf{t}}\right] \\
\frac{\partial(\kappa_1)_i^{i}}{\partial\mathbf{e}^{i-1}} &= \frac{1}{\|\mathbf{e}^{i-1}\|}\left[2\frac{\mathbf{t}^i\times\mathbf{d}_2^{i}}{\chi} - (\kappa_1)_i^{i}\tilde{\mathbf{t}}\right] \\
\frac{\partial(\kappa_1)_i^{i}}{\partial\mathbf{e}^{i}} &= \frac{1}{\|\mathbf{e}^{i}\|}\left[-2\frac{\mathbf{t}^{i-1}\times\mathbf{d}_2^{i}}{\chi} - (\kappa_1)_i^{i}\tilde{\mathbf{t}}\right] \\
&+ \frac{I - \mathbf{t}^{i}\otimes\mathbf{t}^{i}}{\|\mathbf{e}^{i}\|}\Bigg(\frac{\left(\widehat{\mathbf{d}_1^{i}}\cdot\mathbf{t}^{i}\right)[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i}}] + \widehat{\mathbf{d}_1^{i}}(\mathbf{t}^{i}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i}}])}{1+\widehat{\mathbf{t}^{i}}\cdot\mathbf{t}^{i}} \\
&\qquad - \frac{\widehat{\mathbf{d}_1^{i}}\cdot\mathbf{t}^{i}}{(1+\widehat{\mathbf{t}^{i}}\cdot\mathbf{t}^{i})^2}\widehat{\mathbf{t}^{i}}(\mathbf{t}^{i}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i}}]) + \widehat{\mathbf{d}_1^{i}}\times(\kappa\mathbf{b})_i\Bigg) \\
\frac{\partial(\kappa_2)_i^{i-1}}{\partial\mathbf{e}^{i-1}} &= \left[-\mathbf{d}_1^{i-1}\cdot\frac{\partial(\kappa\mathbf{b})_i}{\partial\mathbf{e}^{i-1}} - (\kappa\mathbf{b})_i\cdot\frac{\partial\mathbf{d}_1^{i-1}}{\partial\mathbf{e}^{i-1}}\right]^T \\
&= \frac{1}{\|\mathbf{e}^{i-1}\|}\left[-2\frac{\mathbf{t}^i\times\mathbf{d}_1^{i-1}}{\chi} - (\kappa_2)_i^{i-1}\tilde{\mathbf{t}}\right] \\
&+ \frac{I - \mathbf{t}^{i-1}\otimes\mathbf{t}^{i-1}}{\|\mathbf{e}^{i-1}\|}\Bigg(\frac{\left(\widehat{\mathbf{d}_2^{i-1}}\cdot\mathbf{t}^{i-1}\right)[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}] + \widehat{\mathbf{d}_2^{i-1}}(\mathbf{t}^{i-1}\cdot[(\kappa\mathbf{b})_i\times\widehat{\mathbf{t}^{i-1}}])}{1+\widehat{\mathbf{t}^{i-1}}\cdot\mathbf{t}^{i-1}}
\end{aligned}$$

$$- \frac{\widehat{\mathbf{d}_2^{i-1}} \cdot \mathbf{t}^{i-1}}{(1+\widehat{\mathbf{t}^{i-1}} \cdot \mathbf{t}^{i-1})^2} \widehat{\mathbf{t}^{i-1}} (\mathbf{t}^{i-1} \cdot [(\kappa \mathbf{b})_i \times \widehat{\mathbf{t}^{i-1}}]) + \widehat{\mathbf{d}_2^{i-1}} \times (\kappa \mathbf{b})_i \Bigg)$$

$$\frac{\partial (\kappa_2)_i^{i-1}}{\partial \mathbf{e}^i} = \frac{1}{\|\mathbf{e}^i\|} \left[2 \frac{\mathbf{t}^{i-1} \times \mathbf{d}_1^{i-1}}{\chi} - (\kappa_2)_i^{i-1} \tilde{\mathbf{t}} \right]$$

$$\frac{\partial (\kappa_2)_i^{i}}{\partial \mathbf{e}^{i-1}} = \frac{1}{\|\mathbf{e}^{i-1}\|} \left[-2 \frac{\mathbf{t}^{i} \times \mathbf{d}_1^{i}}{\chi} - (\kappa_2)_i^{i} \tilde{\mathbf{t}} \right]$$

$$\frac{\partial (\kappa_2)_i^{i}}{\partial \mathbf{e}^i} = \frac{1}{\|\mathbf{e}^i\|} \left[2 \frac{\mathbf{t}^{i-1} \times \mathbf{d}_1^{i}}{\chi} - (\kappa_2)_i^{i} \tilde{\mathbf{t}} \right]$$

$$+ \frac{I - \mathbf{t}^i \otimes \mathbf{t}^i}{\|\mathbf{e}^i\|} \Bigg(\frac{(\widehat{\mathbf{d}_2^i} \cdot \mathbf{t}^i)[(\kappa \mathbf{b})_i \times \widehat{\mathbf{t}^i}] + \widehat{\mathbf{d}_2^i}(\mathbf{t}^i \cdot [(\kappa \mathbf{b})_i \times \widehat{\mathbf{t}^i}])}{1 + \widehat{\mathbf{t}^i} \cdot \mathbf{t}^i}$$

$$- \frac{\widehat{\mathbf{d}_2^i} \cdot \mathbf{t}^i}{(1+\widehat{\mathbf{t}^i} \cdot \mathbf{t}^i)^2} \widehat{\mathbf{t}^i} (\mathbf{t}^i \cdot [(\kappa \mathbf{b})_i \times \widehat{\mathbf{t}^i}]) + \widehat{\mathbf{d}_2^i} \times (\kappa \mathbf{b})_i \Bigg).$$

First, we compute the diagonal Hessian blocks for $\kappa 1$:

$$\frac{\partial^2 (\kappa_1)_i^{i-1}}{\partial \mathbf{e}^i \partial \mathbf{e}^i} = \frac{1}{\|\mathbf{e}^i\|^2} \left[2(\kappa_1)_i^{i-1} \tilde{\mathbf{t}} \otimes \tilde{\mathbf{t}} + \frac{2}{\chi} \Big((\mathbf{t}^{i-1} \times \mathbf{d}_2^{i-1}) \otimes \tilde{\mathbf{t}} + \tilde{\mathbf{t}} \otimes (\mathbf{t}^{i-1} \times \mathbf{d}_2^{i-1}) \Big) - \left(\frac{(\kappa_1)_i^{i-1}}{\chi} \right) (I - \mathbf{t}^i \otimes \mathbf{t}^i) \right]$$

$$\frac{\partial^2 (\kappa_1)_i^{i}}{\partial \mathbf{e}^i \partial \mathbf{e}^i} = \frac{1}{\|\mathbf{e}^i\|^2} \Bigg[2(\kappa_1)_i^{i} \tilde{\mathbf{t}} \otimes \tilde{\mathbf{t}} + \frac{2}{\chi} \Big((\mathbf{t}^{i-1} \times \mathbf{d}_2^{i}) \otimes \tilde{\mathbf{t}} + \tilde{\mathbf{t}} \otimes (\mathbf{t}^{i-1} \times \mathbf{d}_2^{i}) \Big) + (\kappa \mathbf{b})_i \otimes \mathbf{d}_2^i + \mathbf{d}_2^i \otimes (\kappa \mathbf{b})_i$$

$$- \left(\frac{(\kappa_1)_i^{i}}{\chi} + (\kappa_1)_i^{i} \right) (I - \mathbf{t}^i \otimes \mathbf{t}^i) + \frac{\big((\kappa \mathbf{b})_i \times \mathbf{t}^i\big) \otimes \mathbf{d}_1^i + \mathbf{d}_1^i \otimes \big((\kappa \mathbf{b})_i \times \mathbf{t}^i\big)}{2} \Bigg]$$

$$\frac{\partial^2 (\kappa_1)_i^{i-1}}{\partial \mathbf{e}^{i-1} \partial \mathbf{e}^{i-1}} = \frac{1}{\|\mathbf{e}^{i-1}\|^2} \Bigg[2(\kappa_1)_i^{i-1} \tilde{\mathbf{t}} \otimes \tilde{\mathbf{t}} - \frac{2}{\chi} \Big((\mathbf{t}^{i} \times \mathbf{d}_2^{i-1}) \otimes \tilde{\mathbf{t}} + \tilde{\mathbf{t}} \otimes (\mathbf{t}^{i} \times \mathbf{d}_2^{i-1}) \Big) + (\kappa \mathbf{b})_i \otimes \mathbf{d}_2^{i-1} + \mathbf{d}_2^{i-1} \otimes (\kappa \mathbf{b})_i$$

$$- \left(\frac{(\kappa_1)_i^{i-1}}{\chi} + (\kappa_1)_i^{i-1} \right) (I - \mathbf{t}^{i-1} \otimes \mathbf{t}^{i-1}) + \frac{\big((\kappa \mathbf{b})_i \times \mathbf{t}^{i-1}\big) \otimes \mathbf{d}_1^{i-1} + \mathbf{d}_1^{i-1} \otimes \big((\kappa \mathbf{b})_i \times \mathbf{t}^{i-1}\big)}{2} \Bigg]$$

$$\frac{\partial^2 (\kappa_1)_i^{i}}{\partial \mathbf{e}^{i-1} \partial \mathbf{e}^{i-1}} = \frac{1}{\|\mathbf{e}^{i-1}\|^2} \left[2(\kappa_1)_i^{i} \tilde{\mathbf{t}} \otimes \tilde{\mathbf{t}} - \frac{2}{\chi} \Big((\mathbf{t}^{i} \times \mathbf{d}_2^{i}) \otimes \tilde{\mathbf{t}} + \tilde{\mathbf{t}} \otimes (\mathbf{t}^{i} \times \mathbf{d}_2^{i}) \Big) - \left(\frac{(\kappa_1)_i^{i}}{\chi} \right) (I - \mathbf{t}^{i-1} \otimes \mathbf{t}^{i-1}) \right]$$

It's easy to check that these indeed average to the finite transport Hessians $\frac{\partial^2 k_{1i}}{\partial \mathbf{e}^i \partial \mathbf{e}^i}$ and $\frac{\partial^2 k_{1i}}{\partial \mathbf{e}^{i-1} \partial \mathbf{e}^{i-1}}$ we computed in Section 5.

Now we look at a mixed term:

$$\frac{\partial^2 (\kappa_1)_i^{i-1}}{\partial \mathbf{e}^{i-1} \partial \mathbf{e}^i} = \frac{1}{\|\mathbf{e}^{i-1}\| \|\mathbf{e}^i\|} \left[2(\kappa_1)_i^{i-1} \tilde{\mathbf{t}} \otimes \tilde{\mathbf{t}} - \frac{2}{\chi} \Big((\mathbf{t}^{i} \times \mathbf{d}_2^{i-1}) \otimes \tilde{\mathbf{t}} + \tilde{\mathbf{t}} \otimes \mathbf{d}_1^{i-1} + [\mathbf{d}_2^{i-1}]_\times \Big) - \frac{(\kappa_1)_i^{i-1}}{\chi} (I + \mathbf{t}^{i-1} \otimes \mathbf{t}^i) \right]$$

$$\frac{\partial^2 (\kappa_1)_i^{i}}{\partial \mathbf{e}^{i-1} \partial \mathbf{e}^i} = \frac{1}{\|\mathbf{e}^{i-1}\| \|\mathbf{e}^i\|} \left[2(\kappa_1)_i^{i} \tilde{\mathbf{t}} \otimes \tilde{\mathbf{t}} + \frac{2}{\chi} \Big(\mathbf{d}_1^{i} \otimes \tilde{\mathbf{t}} + \tilde{\mathbf{t}} \otimes (\mathbf{t}^{i-1} \times \mathbf{d}_2^{i}) - [\mathbf{d}_2^{i}]_\times \Big) - \frac{(\kappa_1)_i^{i}}{\chi} (I + \mathbf{t}^{i-1} \otimes \mathbf{t}^i) \right],$$

which again average to the infinitesimal transport Hessian $\frac{\partial^2 k_{1i}}{\partial \mathbf{e}^{i-1} \partial \mathbf{e}^i}$ computed in Section 4.6 (which happens to be correct in the finite transport setting too).

The expressions for κ_2 and derivatives with respect to $\mathbf{e}^{i-1}$ are analogous.

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