

Supplementary Information: Simple deformation measures for Discrete elastic rods and ribbons

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References to equations and sections from the main text are prepended with an asterisk.

1 Plot of function ψ

The function $\psi(t)$ from equation (*2.15) is plotted in figure 1.

2 Detailed derivation of the strain gradients

In this appendix, we provide a detailed derivation of the first and second gradients of the strain appearing in section *2.

To derive the first gradient, we continue to use the conventions of section *2: we use a perturbation $\delta\mathbf{X}$ of the degrees of freedom, and we denote by $\delta\mathbf{y} = \mathbf{f}'(\mathbf{x}) \cdot \delta\mathbf{x}$ the first variation of a generic quantity $\mathbf{y} = \mathbf{f}(\mathbf{x})$ entering in the reconstruction of the discrete strain, where \mathbf{x} depends indirectly on the degrees of freedom \mathbf{X} .

For the second variation, however, we work here in a slightly more general setting than in the main text, as we consider two *independent* perturbations $\delta_1\mathbf{X}$ and $\delta_2\mathbf{X}$ of the degrees of freedom. We denote by $\delta_1\mathbf{x}$ and $\delta_2\mathbf{x}$ the corresponding perturbations to the variable \mathbf{x} , and by $\delta_1\mathbf{y}$ and $\delta_2\mathbf{y}$ the first-order variations of the functions: $\delta_1\mathbf{y} = \mathbf{f}'(\mathbf{x}) \cdot \delta_1\mathbf{x}$ and $\delta_2\mathbf{y} = \mathbf{f}'(\mathbf{x}) \cdot \delta_2\mathbf{x}$ are simply obtained by replacing the generic increment $\delta\mathbf{x}$ appearing in the first order variation $\delta\mathbf{y}$ with $\delta_1\mathbf{x}$ and $\delta_2\mathbf{x}$, respectively. To obtain the second variation, we perturb the argument \mathbf{x} appearing in $\delta_1\mathbf{y} = \mathbf{f}'(\mathbf{x}) \cdot \delta_1\mathbf{x}$ as $\mathbf{x} + \delta_2\mathbf{x}$, leaving $\delta_1\mathbf{x}$ untouched, and we expand the result to first order in $\delta_2\mathbf{x}$. This yields a quantity denoted as $\delta_{12}\mathbf{y}$, which we can write

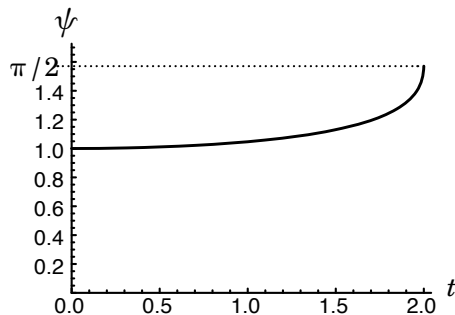


Figure 1: Function $\psi(t)$ from equation (*2.15) used to adjust the norm of the strain κ_i with $t = |\kappa_i|$, see equation (*2.16).

formally as $\delta_{12}\mathbf{y} = \mathbf{f}''(\mathbf{x}) : (\delta_1\mathbf{x} \otimes \delta_2\mathbf{x})$, where $\mathbf{f}''(\mathbf{x})$ is the Hessian. By a classical result in the calculus of variations, the quantity $\delta_{12}\mathbf{y}$ is bilinear and symmetric with respect to $\delta_1\mathbf{x}$ and $\delta_2\mathbf{x}$. The second variation $\delta^2\mathbf{y}$ given in the main text is the quadratic form obtained by ultimately condensing the variations $\delta_1\mathbf{x}$ and $\delta_2\mathbf{x}$ appearing in $\delta_{12}\mathbf{y}$ into a single perturbation $\delta\mathbf{x} = \delta_1\mathbf{x} = \delta_2\mathbf{x}$.

2.1 Infinitesimal rotation vectors

As an important preliminary result, we show that the first variation of a rotation represented by a unit quaternion s can be characterized by means of first-order *vector-valued* increment $\delta\hat{\mathbf{s}} \in \mathbb{R}^3$, and that the second variation of s can be represented by means of a second-order *vector-valued* increment $\delta_{12}\hat{\mathbf{s}} \in \mathbb{R}^3$. These vectors will be referred as the *infinitesimal rotation vectors*. They are connected to the variations δs and $\delta_{12}s$ of the quaternion by

$$\begin{aligned}\delta s &= \frac{1}{2} \delta\hat{\mathbf{s}} s \\ \delta_{12}s &= \left(\frac{1}{2} \delta_{12}\hat{\mathbf{s}} - \frac{1}{4} \delta_1\hat{\mathbf{s}} \cdot \delta_2\hat{\mathbf{s}} \right) s.\end{aligned}\tag{1}$$

The increment $\delta\hat{\mathbf{s}}$ is linear with respect to the variation $\delta\mathbf{X}$ of the degrees of freedom, and the increment $\delta_{12}\hat{\mathbf{s}}$ is bilinear with respect to the independent variations $\delta_1\mathbf{X}$ and $\delta_2\mathbf{X}$ of the degrees of freedom. As usual in our notation, $\delta_1\hat{\mathbf{s}}$ and $\delta_2\hat{\mathbf{s}}$ denote the first-order variation $\delta\hat{\mathbf{s}}$, evaluated on the increment $\delta_1\mathbf{X}$ and $\delta_2\mathbf{X}$, respectively. This representation of the first and second variations of a parameterized quaternion is equivalent to that proposed by [1].

The proof is as follows. By taking the first variation of the condition $2(s\bar{s} - 1) = 0$ that s is a unit quaternion, we have $0 = 2\delta s\bar{s} + 2s\delta\bar{s} = 2\delta s\bar{s} + \overline{2\delta s\bar{s}}$. This shows that the quaternion $2\delta s\bar{s}$ is a pure vector: this is the vector $\delta\hat{\mathbf{s}}$ introduced in equation (1) above. Now, by inserting the increment $\delta_1\mathbf{X}$ in the relation just derived, we have $2\delta_1s\bar{s} \in \mathbb{R}^3$; perturbing this expression as $s \leftarrow s + \delta_2s$, one shows that the following quaternion is a pure vector: $2\delta_{12}s\bar{s} + 2\delta_1s\overline{\delta_2s} = 2\delta_{12}s\bar{s} + \frac{1}{2}(\delta_1\hat{\mathbf{s}}s)(\overline{\delta_2\hat{\mathbf{s}}s}) = 2\delta_{12}s\bar{s} - \frac{1}{2}\delta_1\hat{\mathbf{s}}\delta_2\hat{\mathbf{s}} = 2\delta_{12}s\bar{s} + \frac{1}{2}\delta_1\hat{\mathbf{s}} \cdot \delta_2\hat{\mathbf{s}} - \frac{1}{2}\delta_1\hat{\mathbf{s}} \times \delta_2\hat{\mathbf{s}}$; here, the quaternion product $\delta_1\hat{\mathbf{s}}\delta_2\hat{\mathbf{s}}$ has been evaluated using the definition (*2.1). Adding the vector quantity $\frac{1}{2}\delta_1\hat{\mathbf{s}} \times \delta_2\hat{\mathbf{s}}$, the quantity $2\delta_{12}s\bar{s} + \frac{1}{2}\delta_1\hat{\mathbf{s}} \cdot \delta_2\hat{\mathbf{s}}$ appears to be another pure vector: this is the vector $\delta_{12}\hat{\mathbf{s}}$ introduced in equation (1).

The second-order infinitesimal rotation vector $\delta_{12}\hat{\mathbf{s}}$ can be calculated directly from the first-order one $\delta\hat{\mathbf{s}}$ as

$$\delta_{12}\hat{\mathbf{s}} = \frac{\delta_1(\delta_2\hat{\mathbf{s}}) + \delta_2(\delta_1\hat{\mathbf{s}})}{2}.\tag{2}$$

Here, $\delta_1(\delta_2\hat{\mathbf{s}})$ denotes the first-order variation of $\delta_2\hat{\mathbf{s}}$ when s is perturbed into $s + \delta_1s$; this quantity is *not* symmetric with respect to the perturbations δ_1s and δ_2s . Similarly, $\delta_2(\delta_1\hat{\mathbf{s}})$ denotes the first-order variation of $\delta_1\hat{\mathbf{s}}$ when s is perturbed into $s + \delta_2s$.

The proof of equation (2) is as follows. Take the second variation of $\delta_1s = \frac{1}{2}\delta_1\hat{\mathbf{s}}s$ from equation (1) as $\delta_{12}s = \frac{1}{2}\delta_2(\delta_1\hat{\mathbf{s}})s + \frac{1}{4}\delta_1\hat{\mathbf{s}}\delta_2\hat{\mathbf{s}}s = \left(\frac{1}{2}\delta_2(\delta_1\hat{\mathbf{s}}) - \frac{1}{4}\delta_1\hat{\mathbf{s}} \cdot \delta_2\hat{\mathbf{s}} + \frac{1}{4}\delta_1\hat{\mathbf{s}} \times \delta_2\hat{\mathbf{s}}\right)s$. The left-hand side is symmetric with respect to the perturbations δ_1s and δ_2s , by definition of the second variation. Symmetrizing the right-hand side, we obtain $\delta_{12}s = \left(\frac{\delta_1(\delta_2\hat{\mathbf{s}}) + \delta_2(\delta_1\hat{\mathbf{s}})}{4} - \frac{\delta_1\hat{\mathbf{s}} \cdot \delta_2\hat{\mathbf{s}}}{4}\right)s$. The infinitesimal rotation vector $\delta_{12}\hat{\mathbf{s}}$ can then be identified from equation (1), which yields the result stated in equation (2).

In the following sections, the first and second variations of the rotations that enter into the Discrete elastic rod model, such as the parallel transport p^i and the director rotation d^i , will be systematically represented using the corresponding infinitesimal rotation vectors, such as $\delta\hat{\mathbf{p}}^i$, $\delta_{12}\hat{\mathbf{p}}^i$, $\delta\hat{\mathbf{d}}^i$ and $\delta_{12}\hat{\mathbf{d}}^i$.

2.2 Variation of parallel transport

We start by deriving the variations of the parallel transport p_a^b from the unit vector \mathbf{a} to the unit vector \mathbf{b} defined in equation (*2.3), assuming $\mathbf{b} \neq -\mathbf{a}$. As \mathbf{a} represents the fixed unit tangent \mathbf{T}^i in reference configuration, it remains unperturbed,

$$\delta\mathbf{a} = \mathbf{0} \quad \delta_{12}\mathbf{a} = \mathbf{0}.$$

Since \mathbf{b} remains a unit vector during the perturbation, we have $\frac{1}{2}(|\mathbf{b}|^2 - 1) = 0$. Taking the first and second variation of this constraint, we have

$$\mathbf{b} \cdot \delta\mathbf{b} = 0 \quad \mathbf{b} \cdot \delta_{12}\mathbf{b} + \delta_1\mathbf{b} \cdot \delta_2\mathbf{b} = 0.$$

2.2.1 First variation of parallel transport

As a preliminary step, we consider the case of parallel transport from \mathbf{b} to its perturbation $\mathbf{b} + \delta\mathbf{b}$. Using $\mathbf{b} \cdot \delta\mathbf{b} = 0$, we find from equation (*2.3),

$$p_{\mathbf{b}}^{\mathbf{b}+\delta\mathbf{b}} = 1 + \frac{\mathbf{b} \times \delta\mathbf{b}}{2} + \mathcal{O}(|\delta\mathbf{b}|^2).$$

We now return to the calculation of $p_{\mathbf{a}}^{\mathbf{b}+\delta\mathbf{b}}$. Following the work of [2], as well as equations [3.7] and [A.2] from [3], one can use a holonomy reasoning to shows that, to first order in $\delta\mathbf{b}$,

$$p_{\mathbf{a}}^{\mathbf{b}+\delta\mathbf{b}} = p_{\mathbf{b}}^{\mathbf{b}+\delta\mathbf{b}} p_{\mathbf{a}}^{\mathbf{b}} r_{\mathbf{a}} \left(-\frac{\mathbf{a} \times \mathbf{b}}{1 + \mathbf{a} \cdot \mathbf{b}} \cdot \delta\mathbf{b} \right) + \mathcal{O}(|\delta\mathbf{b}|^2).$$

We rewrite this as

$$p_{\mathbf{a}}^{\mathbf{b}+\delta\mathbf{b}} = p_{\mathbf{b}}^{\mathbf{b}+\delta\mathbf{b}} p_{\mathbf{a}}^{\mathbf{b}} r_{\mathbf{a}}(\delta\theta) + \mathcal{O}(|\delta\mathbf{b}|^2), \quad (3)$$

where $\delta\theta = -\frac{\mathbf{k}}{2} \cdot \delta\mathbf{b}$ and \mathbf{k} is the scaled binormal that characterizes the holonomy (see [2]),

$$\mathbf{k} = \frac{2\mathbf{a} \times \mathbf{b}}{1 + \mathbf{a} \cdot \mathbf{b}}. \quad (4)$$

The infinitesimal rotation $r_{\mathbf{a}}(\delta\theta)$ from equation (3) can be found from equation (*2.2) as

$$\begin{aligned} r_{\mathbf{a}}(\delta\theta) &= 1 + \mathbf{a} \frac{\delta\theta}{2} + \mathcal{O}(\delta\theta^2) \\ &= 1 - \frac{\mathbf{k} \cdot \delta\mathbf{b}}{4} \mathbf{a} + \mathcal{O}(\delta\theta^2) \\ &= 1 - \frac{\mathbf{a} \otimes \mathbf{k}}{4} \cdot \delta\mathbf{b} + \mathcal{O}(\delta\theta^2). \end{aligned} \quad (5)$$

Equation (3) is then rewritten with the help of the operator \mathbf{b}_{\times} from equation (*3.3) as

$$\begin{aligned} p_{\mathbf{a}}^{\mathbf{b}+\delta\mathbf{b}} &= \left(1 + \frac{\mathbf{b}_{\times}}{2} \cdot \delta\mathbf{b} \right) p_{\mathbf{a}}^{\mathbf{b}} \left(1 - \frac{\mathbf{a} \otimes \mathbf{k}}{4} \cdot \delta\mathbf{b} \right) + \mathcal{O}(|\delta\mathbf{b}|^2) \\ &= \left(1 + \frac{\mathbf{b}_{\times}}{2} \cdot \delta\mathbf{b} - \frac{(p_{\mathbf{a}}^{\mathbf{b}} \mathbf{a}) \otimes \mathbf{k}}{4} \cdot \delta\mathbf{b} \right) p_{\mathbf{a}}^{\mathbf{b}} + \mathcal{O}(|\delta\mathbf{b}|^2) \\ &= \left(1 + \frac{2\mathbf{b}_{\times} - \mathbf{b} \otimes \mathbf{k}}{4} \cdot \delta\mathbf{b} \right) p_{\mathbf{a}}^{\mathbf{b}} + \mathcal{O}(|\delta\mathbf{b}|^2). \end{aligned}$$

In view of this, the first order variation of parallel transport writes as

$$\delta p_{\mathbf{a}}^{\mathbf{b}} = \frac{1}{2} \left(\left(\mathbf{b}_{\times} - \frac{\mathbf{b} \otimes \mathbf{k}}{2} \right) \cdot \delta\mathbf{b} \right) p_{\mathbf{a}}^{\mathbf{b}}.$$

Identifying with equation (1), we find that it is captured by the infinitesimal rotation vector

$$\delta \hat{p}_{\mathbf{a}}^{\mathbf{b}} = \left(\mathbf{b}_{\times} - \frac{\mathbf{b} \otimes \mathbf{k}}{2} \right) \cdot \delta\mathbf{b}. \quad (6)$$

2.2.2 Second variation of parallel transport

From equation (6), we have

$$\begin{aligned} \delta_2(\delta_1 \hat{p}_{\mathbf{a}}^{\mathbf{b}}) &= \left((\delta_2 \mathbf{b})_{\times} - \frac{\delta_2 \mathbf{b} \otimes \mathbf{k} + \mathbf{b} \otimes \delta_2 \mathbf{k}}{2} \right) \cdot \delta_1 \mathbf{b} + \left(\mathbf{b}_{\times} - \frac{\mathbf{b} \otimes \mathbf{k}}{2} \right) \cdot \delta_{12} \mathbf{b} \\ &= \delta_2 \mathbf{b} \times \delta_1 \mathbf{b} - \frac{1}{2} \delta_2 \mathbf{b} (\mathbf{k} \cdot \delta_1 \mathbf{b}) - \frac{\mathbf{b}}{2} \delta_2 \mathbf{k} \cdot \delta_1 \mathbf{b} + \left(\mathbf{b}_{\times} - \frac{\mathbf{b} \otimes \mathbf{k}}{2} \right) \cdot \delta_{12} \mathbf{b} \end{aligned} \quad (7)$$

Using equation (4), the variation of the binormal is found as

$$\begin{aligned}\delta_2 \mathbf{k} &= \frac{2\mathbf{a} \times \delta_2 \mathbf{b}}{1+\mathbf{a} \cdot \mathbf{b}} - \frac{2\mathbf{a} \times \mathbf{b}}{(1+\mathbf{a} \cdot \mathbf{b})^2} \mathbf{a} \cdot \delta_2 \mathbf{b} \\ &= \frac{2}{1+\mathbf{a} \cdot \mathbf{b}} \left(\mathbf{a} \times \delta_2 \mathbf{b} - \frac{\mathbf{k}}{2} (\mathbf{a} \cdot \delta_2 \mathbf{b}) \right) \\ &= \frac{2}{1+\mathbf{a} \cdot \mathbf{b}} \left(\mathbf{a} \times - \frac{\mathbf{k} \otimes \mathbf{a}}{2} \right) \cdot \delta_2 \mathbf{b}\end{aligned}$$

Inserting into equation (7) and reordering the terms, we find

$$\delta_2(\delta_1 \hat{\mathbf{p}}_a^b) = \delta_2 \mathbf{b} \times \delta_1 \mathbf{b} + \left(\mathbf{b}_\times - \frac{\mathbf{b} \otimes \mathbf{k}}{2} \right) \cdot \delta_{12} \mathbf{b} - \frac{\mathbf{b}}{(1+\mathbf{a} \cdot \mathbf{b})} \left(\delta_1 \mathbf{b} \cdot \left(\mathbf{a}_\times - \frac{\mathbf{k} \otimes \mathbf{a}}{2} \right) \cdot \delta_2 \mathbf{b} \right) - \frac{\delta_2 \mathbf{b} \otimes \delta_1 \mathbf{b}}{2} \cdot \mathbf{k}$$

In view of equation (2), we can obtain the second-order infinitesimal rotation vector by symmetrizing this with respect to the increments $\delta_1 \mathbf{b}$ and $\delta_2 \mathbf{b}$:

$$\begin{aligned}\delta_{12} \hat{\mathbf{p}}_a^b &= \frac{\delta_2(\delta_1 \hat{\mathbf{p}}_a^b) + \delta_1(\delta_2 \hat{\mathbf{p}}_a^b)}{2} \\ &= \left(\mathbf{b}_\times - \frac{\mathbf{b} \otimes \mathbf{k}}{2} \right) \cdot \delta_{12} \mathbf{b} + \left(\delta_1 \mathbf{b} \cdot \frac{\mathbf{k} \otimes \mathbf{a} + \mathbf{a} \otimes \mathbf{k}}{4(1+\mathbf{a} \cdot \mathbf{b})} \cdot \delta_2 \mathbf{b} \right) \mathbf{b} - \frac{(\delta_1 \mathbf{b} \otimes \delta_2 \mathbf{b} + \delta_2 \mathbf{b} \otimes \delta_1 \mathbf{b})}{2} \cdot \frac{\mathbf{k}}{2}.\end{aligned}\quad (8)$$

2.2.3 Application to a Discrete elastic rod

In a Discrete elastic rod, the transport is from the undeformed tangent $\mathbf{a} = \mathbf{T}^i$ to the deformed tangent $\mathbf{b} = \mathbf{t}^i$, see equation (*2.9). Equation (4) then yields the definition of the binormal \mathbf{k}^i announced in equation (*3.4), and equation (6) yields the expression for $\delta \hat{\mathbf{p}}^i$ announced in equation (*3.2). In equation (8), condensing the independent variations as $\delta_1 \mathbf{b} = \delta_2 \mathbf{b} = \delta \mathbf{t}^i$ and identifying $\delta_{12} \hat{\mathbf{p}}_a^b = \delta^2 \hat{\mathbf{p}}^i$ and $\delta_{12} \mathbf{b} = \delta^2 \mathbf{t}^i$ yields the expression of $\delta^2 \hat{\mathbf{p}}^i$ announced in equation (*3.2).

2.3 Variation of unit tangents

With $\mathbf{E}^i = \mathbf{x}_{i+1} - \mathbf{x}_i$ as the segment vector, the variation of the unit tangent $\mathbf{t}^i = \mathbf{E}^i / |\mathbf{E}^i|$ from equation (*2.6) writes

$$\begin{aligned}\delta \mathbf{t}^i &= \frac{\delta \mathbf{E}^i}{|\mathbf{E}^i|} - \mathbf{E}^i \frac{\delta(|\mathbf{E}^i|)}{|\mathbf{E}^i|^2} \\ &= \frac{\delta \mathbf{E}^i}{|\mathbf{E}^i|} - \mathbf{E}^i \frac{(\mathbf{E}^i \cdot \delta \mathbf{E}^i)}{|\mathbf{E}^i|^3} \\ &= \frac{\mathbf{I} - \mathbf{t}^i \otimes \mathbf{t}^i}{|\mathbf{E}^i|} \cdot \delta_1 \mathbf{E}^i\end{aligned}$$

With $\delta \mathbf{E}^i = \delta \mathbf{x}_{i+1} - \delta \mathbf{x}_i$, this is the expression of the first variation announced in equation (*3.1).

Next, the second variation is calculated as

$$\delta_{12} \mathbf{t}^i = \left(-\frac{\delta_2 \mathbf{t}^i \otimes \mathbf{t}^i + \mathbf{t}^i \otimes \delta_2 \mathbf{t}^i}{|\mathbf{E}^i|} - \frac{(\mathbf{I} - \mathbf{t}^i \otimes \mathbf{t}^i) \mathbf{E}^i \cdot \delta_2 \mathbf{E}^i}{|\mathbf{E}^i|^2 |\mathbf{E}^i|} \right) \cdot \delta_1 \mathbf{E}^i.$$

Here, we have used $\delta_{12} \mathbf{E}^i = \mathbf{0}$ since $\mathbf{E}^i = \mathbf{x}_{i+1} - \mathbf{x}_i$ depends linearly on the degrees of freedom. Inserting the expression of the first variations from equation (*3.1), the second variation $\delta_{12} \mathbf{t}^i$ can be rewritten as

$$\begin{aligned}\delta_{12} \mathbf{t}^i &= \left(-\frac{((\mathbf{I} - \mathbf{t}^i \otimes \mathbf{t}^i) \cdot \delta_2 \mathbf{E}^i) \otimes \mathbf{t}^i + \mathbf{t}^i \otimes ((\mathbf{I} - \mathbf{t}^i \otimes \mathbf{t}^i) \cdot \delta_2 \mathbf{E}^i)}{|\mathbf{E}^i|^2} - \frac{(\mathbf{I} - \mathbf{t}^i \otimes \mathbf{t}^i) \mathbf{t}^i \cdot \delta_2 \mathbf{E}^i}{|\mathbf{E}^i|^2} \right) \cdot \delta_1 \mathbf{E}^i \\ &= -\frac{\tau_{iKJ}^i + \tau_{jKI}^i + \tau_{iJK}^i}{|\mathbf{E}^i|^2} (\delta_1 \mathbf{E}^i)_J (\delta_2 \mathbf{E}^i)_K \mathbf{e}_I \\ &= -\frac{((\boldsymbol{\tau}^i)^T(132) + (\boldsymbol{\tau}^i)^T(231) + \boldsymbol{\tau}^i)_{IJK}}{|\mathbf{E}^i|^2} (\delta_1 \mathbf{E}^i)_J (\delta_2 \mathbf{E}^i)_K \mathbf{e}_I \\ &= -\frac{\boldsymbol{\tau}^i + (\boldsymbol{\tau}^i)^T(132) + (\boldsymbol{\tau}^i)^T(231)}{|\mathbf{E}^i|^2} : ((\delta_1 \mathbf{x}_{i+1} - \delta_1 \mathbf{x}_i) \otimes (\delta_2 \mathbf{x}_{i+1} - \delta_2 \mathbf{x}_i)),\end{aligned}$$

where the third-order tensor $\boldsymbol{\tau}^i = (\mathbf{I} - \mathbf{t}^i \otimes \mathbf{t}^i) \otimes \mathbf{t}^i$ and its generalized transpose are defined below equation (*3.1). The expression of $\delta^2 \mathbf{t}^i$ announced in equation (*3.1) is obtained by condensing $\delta_1 \mathbf{x}_i = \delta_2 \mathbf{x}_i = \delta \mathbf{x}_i$ and identifying $\delta^2 \mathbf{t}^i = \delta_{12} \mathbf{t}^i$.

2.4 Variation of directors rotation

In view of equation (1), the infinitesimal rotation vector $\delta \hat{\mathbf{d}}^i$ associated with the directors rotation d^i is

$$\delta \hat{\mathbf{d}}^i = 2 \delta d^i \bar{d}^i.$$

Differentiating the expression of d^i from equation (*2.8), we have $\delta d^i = \delta (p^i r_{\mathbf{T}^i}(\varphi^i) D^i) = \delta p^i r_{\mathbf{T}^i}(\varphi^i) D^i + p^i \delta (r_{\mathbf{T}^i}(\varphi^i)) D^i$. Equation (*2.2) shows that, with a fixed unit vector \mathbf{T}^i , $\delta (r_{\mathbf{T}^i}(\varphi^i)) = \frac{1}{2} [\delta \varphi^i \mathbf{T}^i] r_{\mathbf{T}^i}(\varphi^i)$ — here, the vector in square bracket is an infinitesimal rotation vector, see equation (1). This yields $\delta d^i = \delta p^i r_{\mathbf{T}^i}(\varphi^i) D^i + \frac{1}{2} p^i \delta \varphi^i \mathbf{T}^i r_{\mathbf{T}^i}(\varphi^i) D^i$. Inserting into the equation above, and using $\bar{d}^i = \bar{D}^i r_{\mathbf{T}^i}(-\varphi^i) \bar{p}^i$ from equation (*2.8), we find

$$\begin{aligned} \delta \hat{\mathbf{d}}^i &= \delta \varphi^i p^i \mathbf{T}^i r_{\mathbf{T}^i}(\varphi^i) D^i \bar{d}^i + 2 \delta p^i r_{\mathbf{T}^i}(\varphi^i) D^i \bar{d}^i \\ &= \delta \varphi^i p^i \mathbf{T}^i \bar{p}^i + 2 \delta p^i \bar{p}^i \\ &= \delta \varphi^i p^i * \mathbf{T}^i + \delta \hat{\mathbf{p}}^i \\ &= \delta \varphi^i \mathbf{t}^i + \delta \hat{\mathbf{p}}^i, \end{aligned}$$

as announced in equation (*3.5).

The second-order infinitesimal rotation vector is then obtained from equation (2) as

$$\begin{aligned} \delta_{12} \hat{\mathbf{d}}^i &= \frac{1}{2} \left(\delta_2 \left(\delta_1 \varphi^i \mathbf{t}^i + \delta_1 \hat{\mathbf{p}}^i \right) + \delta_1 \left(\delta_2 \varphi^i \mathbf{t}^i + \delta_2 \hat{\mathbf{p}}^i \right) \right) \\ &= \frac{\delta_1 \varphi^i \delta_2 \mathbf{t}^i + \delta_2 \varphi^i \delta_1 \mathbf{t}^i}{2} + \delta_{12} \hat{\mathbf{p}}^i. \end{aligned}$$

Here, we have used $\delta_{12} \varphi^i = 0$ as φ^i is a degree of freedom and the variations $\delta_1 \varphi^i$ and $\delta_2 \varphi^i$ are independent.

Upon condensation of the two variations, the equation leads to the expression of $\delta^2 \hat{\mathbf{d}}^i$ announced in equation (*3.5).

2.5 Rotation gradient

In view of equation (1), the infinitesimal rotation vector $\delta \hat{\mathbf{q}}_i$ associated with the rotation gradient $q_i = \overline{d^{i-1}} d^i$ from equation (*2.11) writes

$$\begin{aligned} \delta \hat{\mathbf{q}}_i &= 2 \delta q_i \bar{q}_i \\ &= \left(2 \delta \overline{d^{i-1}} d^i + \overline{d^{i-1}} 2 \delta d^i \right) \bar{q}_i \\ &= \overline{d^{i-1}} (-\delta \hat{\mathbf{d}}^{i-1} + \delta \hat{\mathbf{d}}^i) d^{i-1} \end{aligned}$$

as announced in equation (*3.6).

The following identity yields the variation of the vector $\bar{s} * \mathbf{u}$ obtained by applying the inverse \bar{s} of a rotation s to a vector \mathbf{u} ,

$$\begin{aligned} \delta(\bar{s} * \mathbf{u}) &= \delta(\bar{s} \mathbf{u} s) \\ &= \bar{\delta s} \mathbf{u} s + \bar{s} \mathbf{u} \delta s + \bar{s} \delta \mathbf{u} s \\ &= \frac{-\bar{s} \delta \hat{\mathbf{s}} \mathbf{u} \bar{s} + \bar{s} \mathbf{u} \delta \hat{\mathbf{s}} s}{2} + \bar{s} * \delta \mathbf{u} \\ &= \frac{-(\bar{s} * \delta \hat{\mathbf{s}}) (\bar{s} * \mathbf{u}) + (\bar{s} * \mathbf{u}) (\bar{s} * \delta \hat{\mathbf{s}})}{2} + \bar{s} * \delta \mathbf{u} \\ &= -(\bar{s} * \delta \hat{\mathbf{s}}) \times (\bar{s} * \mathbf{u}) + \bar{s} * \delta \mathbf{u}. \end{aligned}$$

With $\delta = \delta_1$, $s = d^{i-1}$ and $\mathbf{u} = \delta_2 \hat{\mathbf{d}}^i - \delta_2 \hat{\mathbf{d}}^{i-1}$, we have $\bar{s} * \mathbf{u} = \overline{d^{i-1}} * (\delta_2 \hat{\mathbf{d}}^i - \delta_2 \hat{\mathbf{d}}^{i-1}) = \delta_2 \hat{\mathbf{q}}_i$, see equation (*3.6), and the identity above yields

$$\begin{aligned} \delta_1(\delta_2 \hat{\mathbf{q}}_i) &= -(\overline{d^{i-1}} * \delta_1 \hat{\mathbf{d}}^{i-1}) \times \delta_2 \hat{\mathbf{q}}_i + \overline{d^{i-1}} * (\delta_1(\delta_2 \hat{\mathbf{d}}^i) - \delta_1(\delta_2 \hat{\mathbf{d}}^{i-1})) \\ &= \overline{d^{i-1}} * (\delta_1(\delta_2 \hat{\mathbf{d}}^i) - \delta_1(\delta_2 \hat{\mathbf{d}}^{i-1})) + \delta_2 \hat{\mathbf{q}}_i \times (\overline{d^{i-1}} * \delta_1 \hat{\mathbf{d}}^{i-1}). \end{aligned}$$

Symmetrizing with respect to the independent variations δ_1 and δ_2 and using equation (2), we obtain the second infinitesimal vector as

$$\delta_{12}\hat{\mathbf{q}}_i = \overline{d^{i-1}} * \left(\delta_{12}\hat{\mathbf{d}}^i - \delta_{12}\hat{\mathbf{d}}^{i-1} \right) + \frac{\delta_1\hat{\mathbf{q}}_i \times (\overline{d^{i-1}} * \delta_2\hat{\mathbf{d}}^{i-1}) + \delta_2\hat{\mathbf{q}}_i \times (\overline{d^{i-1}} * \delta_1\hat{\mathbf{d}}^{i-1})}{2}.$$

Upon condensation of the two variations, the equation leads to the expression of $\delta^2\hat{\mathbf{q}}_i$ announced in equation (*3.6).

2.6 Strain vector

Equation (*2.13) can be rewritten as $\boldsymbol{\kappa}_i = 2\mathcal{I}(q_i)$, where $\mathcal{I}(q) = \frac{q-\bar{q}}{2}$ denotes the vector part of a quaternion. The operator \mathcal{I} being linear, we have

$$\begin{aligned} \delta\boldsymbol{\kappa}_i &= 2\mathcal{I}(\delta q_i) \\ &= \mathcal{I}(\delta\hat{\mathbf{q}}_i q_i) \end{aligned}$$

as well as

$$\begin{aligned} \delta_{12}\boldsymbol{\kappa}_i &= 2\mathcal{I}(\delta_{12}q_i) \\ &= \mathcal{I}\left(\left(\delta_{12}\hat{\mathbf{q}}_i - \frac{\delta_1\hat{\mathbf{q}}_i \cdot \delta_2\hat{\mathbf{q}}_i}{2}\right) q_i\right), \end{aligned}$$

as announced in equation (*3.7). In the equation above, the second variation of the unit quaternion $\delta_{12}q_i$ has been expressed using equation (1).

2.7 Numerical verification

We verify the gradient and Hessian of the elastic energy, by considering a Kirchhoff rod having 80 nodes. Starting from a straight rod, we increment the magnitude of the natural curvature, magnitude of gravity, and a point load applied at the ends over 100 iterations. At each iteration we compute the equilibrium, disabling the update of the reference configuration discussed in Section *2(c). This allows us to verify the gradient in the generic setting where the reference and current configurations differ significantly from each other. The computed equilibrium solution is denoted by the vector \mathbf{X} . We introduce a second configuration vector $\tilde{\mathbf{X}}$ by adding a random perturbation to \mathbf{X} where each perturbation is chosen randomly between $(-0.1, 0.1)$. This magnitude of perturbation ensures that the configuration $\tilde{\mathbf{X}}$ is sufficiently far from an equilibrium. By starting with the different equilibrium solutions \mathbf{X} , we ensure that the variations are taken at different locations in the configuration space.

The gradient of the discrete strain energy $\mathcal{E} = \sum_{i=1}^{N-1} E_i$ is evaluated at the point $\tilde{\mathbf{X}}$ either as $\nabla\mathcal{E}_a$ computed based on the analytical formula given in the main text, or as $\nabla\mathcal{E}_{fd}$ using finite differences as $(\nabla\mathcal{E}_{fd})_i = (\mathcal{E}(\tilde{\mathbf{X}} + h\mathbf{e}_i) - \mathcal{E}(\tilde{\mathbf{X}} - h\mathbf{e}_i))/2h$ where $h = 10^{-7}$ and \mathbf{e}_i is a unit vector where the i^{th} component is 1.

We then calculate the relative gradient error as:

$$\|\nabla\mathcal{E}_{\text{err}}\| = \frac{\|\nabla\mathcal{E}_a - \nabla\mathcal{E}_{fd}\|_{\infty}}{\|\nabla\mathcal{E}_a\|_{\infty}}$$

Similarly for the Hessian, we calculate the hessian $\nabla^2\mathcal{E}$ of the strain energy gradient at the point $\tilde{\mathbf{X}}$, either analytically ($\nabla^2\mathcal{E}_a$) using the methods described in the manuscript or using finite differences ($\nabla^2\mathcal{E}_{fd}$). We calculate $\nabla^2\mathcal{E}_{fd}$ using finite differences on the analytical form of the gradient. The relative hessian error is calculated as:

$$\|\nabla^2\mathcal{E}_{\text{err}}\| = \frac{\|\nabla^2\mathcal{E}_a - \nabla^2\mathcal{E}_{fd}\|_{\infty}}{\|\nabla^2\mathcal{E}_a\|_{\infty}}.$$

At every iteration, we calculate a different random perturbation and calculate the errors $\|\nabla\mathcal{E}_{\text{err}}\|$ and $\|\nabla^2\mathcal{E}_{\text{err}}\|$ at that point. The results are shown in Figure (2).

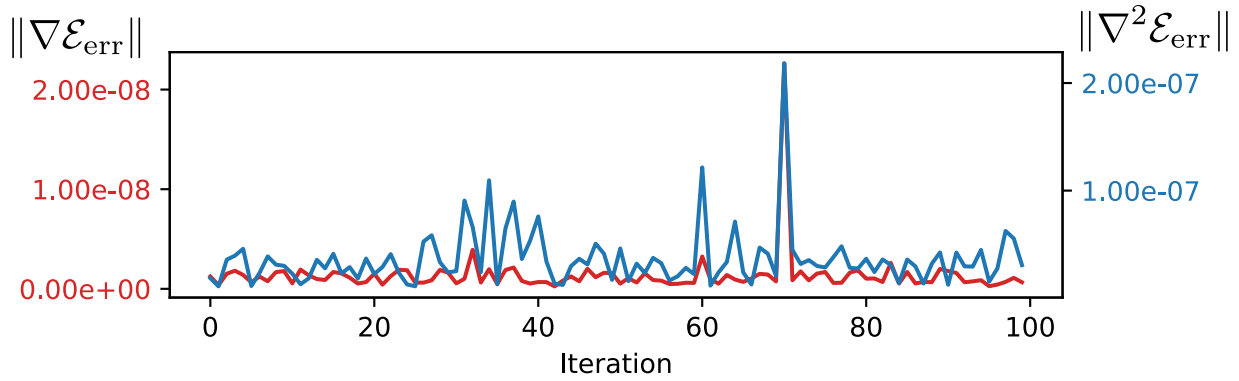


Figure 2: Errors between the analytical and numerical calculations for gradients and Hessians.

References

- [1] Barbič J, Zhao Y. 2011 Real-Time Large-Deformation Substructuring. In *ACM SIGGRAPH 2011 Papers* pp. 1–8 New York, NY, USA. Association for Computing Machinery.
- [2] Bergou M, Wardetzky M, Robinson S, Audoly B, Grinspun E. 2008 Discrete Elastic Rods. *ACM Transactions on Graphics* **27**, 63:1–63:12.
- [3] Lestringant C, Audoly B, Kochmann DM. 2020 A discrete, geometrically exact method for simulating nonlinear, elastic or non-elastic beams. *Computer Methods in Applied Mechanics and Engineering* **361**, 112741.