MULTI-MATERIAL MODEL AND SHAPE OPTIMIZATION
FOR BENDING AND TORSION OF INEXTENSIBLE RODS

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ABSTRACT. We derive a model for the optimization of bending and torsional rigidity of non-homogeneous elastic rods, by studying a sharp interface shape optimization problem with perimeter penalization for the rod cross section, that treats the resulting torsional and bending rigidities as objectives. We then formulate a phase field approximation to the optimization problem and show Γ-convergence to the aforementioned sharp interface model. This also implies existence of minimizers for the sharp interface optimization problem. Finally, we numerically find minimizers of the phase field problem using a steepest descent approach and relate the resulting optimal shapes to the development of plant morphology.

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1. Introduction

Tailoring resistance of a rod against bending and torsional deformations is a decisive factor in several fields like civil- or bio-engineering as well as in the development of plant morphology, see e.g. [Vog92, KK00, WVLS+19]. In particular, in the construction of building components, it is necessary to optimize certain responses of rods subject to bending and torsional moments. A well known way to accomplish that is to optimize their bending and torsional rigidity, which are suitable measures of resistance against bending and torsional deformations.

If we assume that the rod $\Omega_h$ is described by $\Omega_h = (0,L) \times hS$, where $h \in \mathbb{R}^+$ and the bounded cross-section $S$ is an open and bounded subset of $\mathbb{R}^2$ with Lipschitz boundary, then an optimization of the bending and torsional rigidity of $\Omega_h$ mainly consists in the computation of an optimal shape of the cross-section $S$ or, if the rod is non-homogeneous, in determining optimal distributions of different materials inside $S$, see [KK00, WVLS+19, WVSSD21, WVL+22].

For homogeneous rods a rigorous derivation of these rigidities was conducted in [MM03] by means of De Giorgi and Franzoni \( \Gamma \)-convergence [DGF75]. The authors showed that the nonlinear bending-torsion theory can be obtained as the \( \Gamma \)-limit of a sequence of three-dimensional energies of the form

\[
E^{(h)}(v) := \int_{\Omega_h} W(\nabla v(z)) \, dz
\]

where the deformation $v \in W^{1,2}(\Omega_h; \mathbb{R}^3)$ and the stored energy function $W: \mathbb{M}^{3\times3} \rightarrow [0, +\infty]$ satisfies the following classical assumptions:

1. $W \in C^0(\mathbb{M}^{3\times3})$ and $W$ is of class $C^2$ in a neighbourhood of $SO(3)$;
2. $W$ is frame-indifferent, i.e., $W(A) = W(RA)$ for all $A \in \mathbb{M}^{3\times3}$ and for all $R \in SO(3)$;
3. $W(A) = 0$ if $A \in SO(3)$ and there exists a constant $C > 0$ such that $W(A) \geq C \text{dist}^2(A, SO(3))$ for any $A \in \mathbb{M}^{3\times3}$.

As rigorously justified in [ABP91], energies (1) of order $h^2$ correspond to stretching and shearing deformations, leading to a string theory, while energies of order $h^4$ correspond to bending and torsional deformations, leaving the domain unextended, and lead to a rod theory [Ant73, Ant05].

Let us stress that Theorem 3.1 in [MM03], which inspired the mathematical development of section 3, considers just the case of homogeneous cross-sections $S$ containing a single material. The bending-torsion theory for non-homogeneous rods, where the stored energy function $W$ additionally depends on the coordinates $(z_1, z_2, z_3) \in \Omega_h$ is derived in [Neu12] as a special case of non-oscillatory materials in a homogenized bending torsion theory.

In this paper, we consider deformations of elastic rods with multiple materials inside the cross-section $S$, under bending and torsional loads and derive the respective torsional and bending rigidity for non-homogeneous elastic rods. The choice of the material is described by a scalar density function
$u \in L^\infty(S)$, bounded from below by a positive constant $c$, i.e., satisfying
\[ u \geq c > 0 \quad \text{in } S \]
and the energies we consider have the form
\[
E^{(h)}(v) := \int_{\Omega_h} u\left( \frac{z_2}{h}, \frac{z_3}{h} \right) W(\nabla v(z)) \, dz.
\]

To overcome the dependence of the domain $\Omega_h$ on $h$, we introduce the following change of variables:
\[
(z_1, z_2, z_3) \ni (0, L) \times hS \longleftrightarrow (x_1, x_2, x_3) \in (0, L) \times S
\]
\[ z_1 = x_1, \quad z_2 = hx_2, \quad z_3 = hx_3 \]
and we replace both $v$ and $u$ with $y \in W^{1,2}(\Omega; \mathbb{R}^3)$ and a not relabeled $u \in L^\infty(S)$, defined by
\[
y(x) := v(z(x))
\]
\[ u(x_2, x_3) := u(z_2(x), z_3(x)) \]
for any $x \in \Omega := (0, L) \times S$. By this change of variables, energy (2) becomes
\[
E^{(h)}(y) = h^2 \int_{\Omega} u(x_2, x_3) W(\nabla_h y(x)) \, dx
\]
where, with the nonstandard notation $y_{,i}$ and $\nabla_h$, we simply mean
\[
y_{,i} := \frac{\partial y}{\partial x_i} = \frac{\partial v}{\partial z_i} \frac{\partial z_i}{\partial x_i}, \quad i = 1, 2, 3, \text{ and}
\]
\[
\nabla_h y := \begin{pmatrix} y_1 \left| \frac{1}{h} y_2 \right| \frac{1}{h} y_3 \end{pmatrix}.
\]

The paper is organized as follows: In section 3, we study the asymptotic behaviour of energies (3), rescaled by $h^4$, by means of De Giorgi and Franzoni $\Gamma$-convergence [DGF75] and we derive a nonlinear bending-torsion theory for non-homogeneous inextensible rods. We note that this model is a restriction of the model derived in [Neu12], aimed to cover the case of pure bending and pure torsion of non-homogeneous rods for isotropic materials. In section 3.1, we recover the classical Saint-Venant theory of pure torsion and theory of pure bending of isotropic non-homogeneous rods. As in the classical theory, torsion is due to a torsional moment at the top of $\Omega_h$ (see e.g. [Lek71]), while bending is due to an outer normal force on $\Omega_h$ at $x_1 = L$.

In order to determine arrangements of different materials inside a reference cross-section $S$, for which the bending and torsional rigidity of the rod $\Omega_h$ is optimal, in the main section of the paper, namely section 4, we study a shape optimization problem that considers the optimal distribution of two materials (governed by function $u$) inside $S$. Here the objectives in the optimization problem are the bending and torsional rigidity, derived in section 3.1, for isotropic stored energy functions $W$. The curvature and twist of the rod subject to bending and torsional moments are then proportional to the bending and torsional rigidity, respectively. The problem of finding optimal structures in mechanical engineering has a long history. Without aim of completeness, we refer the interested reader to
To study the existence of solutions to the optimization problem, we consider a perimeter penalization on the set \( \{ u = 1 \} \), that is, we add an additional perimeter functional that penalizes the perimeter of the stiffer material inside \( S \). Then, to compute solutions of the optimization problem numerically, we approximate the objective functional by a means of a phase field approach, which consists of replacing the penalization perimeter with Ginzburg-Landau energies.

In Section 5, we provide numerical experiments, by using a steepest descent approach. In particular, we recover the optimal distribution of two materials inside \( S \) for multiple types of optimization problems arising from different relative weightings of the involved objectives and connect the resulting optimal arrangements of materials to the development of different morphologies in plant stems. We conclude the paper by showing in the Appendix the proof of Theorem 3.3 in details.

2. Notation

Through the paper we will use the following standard notation: \( SO(3) \) denotes the group of all rotations about the origin of three-dimensional Euclidean space \( \mathbb{R}^3 \) under the operation of composition, \( M_{3 \times 3} \) denotes the spaces of matrices of dimension 3, while \( M_{3 \times 3}^{\text{sym}} \) and \( M_{3 \times 3}^{\text{skew}} \) denote, respectively, the subspaces of \( M_{3 \times 3} \) of symmetric and skew-symmetric matrices. The entries of a matrix \( G \in M_{3 \times 3}^{\text{sym}} \) are denoted as follows: \( g_1 := g_{11} \), \( g_2 := g_{12} = g_{21} \), \( g_3 := g_{13} = g_{31} \), \( g_4 := g_{22} \), \( g_5 := g_{23} = g_{32} \), \( g_6 := g_{33} \).

From the functional point of view, we will instead use the following non-standard notation: given any function \( y \) belonging the Sobolev space of vector-valued functions of order \( m \geq 1 \), \( W^{m,2}(\Omega; \mathbb{R}^3) \), we denote by \( y, i \) the vector of weak derivatives of \( y \) w.r.t. the \( i \)-th variable \( (\frac{\partial y_1}{\partial x_i}, \frac{\partial y_2}{\partial x_i}, \frac{\partial y_3}{\partial x_i}) \), \( i = 1, 2, 3 \), and by \( \nabla_h y \) the \( 3 \times 3 \) matrix, whose columns are \( (y, 1\mid \frac{1}{h} y, 2\mid \frac{1}{h} y, 3) \), \( h \in \mathbb{R}^+ \).

3. Nonlinear bending-torsion theory of non-homogeneous rods

From now on, we assume that

\[
\int_S u(x_2, x_3)x_2 \, dx_2 dx_3 = \int_S u(x_2, x_3)x_3 \, dx_2 dx_3 = 0,
\]

\[
\int_S u(x_2, x_3)x_2 x_3 \, dx_2 dx_3 = 0.
\]

Let us point out that (4) and (5) are satisfied by a proper choice of the coordinate system. They are, therefore, not restrictive. In the proof of Theorem 4.4, only condition (4) will be required, while (5) is optional, see also Remark 3.4.
The aim of this section is to study the asymptotic behaviour of the sequence of rescaled energies \( \frac{1}{h^2} E^{(h)}_h \), as \( h \) goes to 0. We first define functionals \( I^{(h)} : W^{1,2}(\Omega; \mathbb{R}^3) \to \mathbb{R} \cup \{ +\infty \} \) by

\[
I^{(h)}(y) := \frac{1}{h^2} E^{(h)}_h(y) = \int_{\Omega} u(x_2, x_3) W_h(y(x)) \, dx
\]

for any \( y \in W^{1,2}(\Omega; \mathbb{R}^3) \) and \( h \in \mathbb{N} \).

In analogy with [MM03], we provide a \( \Gamma \)-convergence theorem for non-homogeneous rods, namely Theorem 3.3. Let us first recall the well-known definition of \( \Gamma \)-convergence in such a metric setting and the Fundamental Theorem of \( \Gamma \)-convergence (see e.g. [DM93, DGF75] for details).

**Definition 3.1.** Let \( (X, d) \) be a metric space, and let \( F_h : X \to \overline{\mathbb{R}} \), \( h \in \mathbb{N} \), be a sequence of functionals. We say that \( (F_h) \) \( \Gamma \)-converges to \( F \), and we write \( F = \Gamma \lim h F_h \), if the following conditions are fulfilled:

1. (\( \Gamma \)-lim inf inequality) for any \( x \in X \) and for any sequence \( (x_h) \) converging to \( x \) in \( X \) one has

\[
F(x) \leq \liminf_{h \to \infty} F_h(x_h);
\]

2. (\( \Gamma \)-lim sup inequality) for any \( x \in X \), there exists a sequence \( (\bar{x}_h) \) converging to \( x \) in \( X \) such that

\[
F(x) \geq \limsup_{h \to \infty} F_h(\bar{x}_h).
\]

**Theorem 3.2** (Fundamental Theorem of \( \Gamma \)-convergence). Let \( F : X \to \overline{\mathbb{R}} \) satisfy \( F = \Gamma \lim_h F_h \) and let a compact set \( K \subset X \) exist such that

\[
\inf_X F_h = \inf_K F_h \quad \text{for any } h \in \mathbb{N}.
\]

Then \( F \) admits a minimum in \( X \) and

\[
\min_X F = \lim_{h \to \infty} \inf_X F_h.
\]

Moreover, if the sequence \( (F_h) \) is equicoercive (on \( X \)), that is, for each \( t \in \mathbb{R} \) there exists a closed countably compact set \( K_t \subset X \) such that

\[
\{ x \in X : F_h(x) \leq t \} \subset K_t \quad \text{for each } h \in \mathbb{N},
\]

then \( F \) is coercive (and lower semicontinuous, by definition of the \( \Gamma \)-limit) and any sequence of minimizers for \( (F_h) \), \( (x_h) \), that is satisfying

\[
F_h(x_h) = \inf_X F_h,
\]

admits a limit in \( X \), i.e., there exists \( x \in X \) such that

\[
x_h \to x \text{ in } X \text{ and } F(x) = \min_X F.
\]

**Theorem 3.3.** Assume that the stored energy \( W \) satisfies hypotheses 1–3, given in the Introduction, let \( Q_3 \) be twice the quadratic form of linearized elasticity

\[
Q_3(G) := \frac{\partial^2 W}{\partial F^2}(Id)(G, G) \quad \text{for any } G \in M_{3 \times 3}^{3 \times 3}
\]
and denote $Q_2 : M^3_{\text{skew}} \to [0, +\infty)$ the quadratic form defined through the minimization problem

$$
Q_2(A) := \min_{\alpha \in W^{1,2}(S;\mathbb{R}^3)} \int_S u(x_2, x_3) Q_3 \left( A \begin{pmatrix} 0 & x_2 \\ x_2 & x_3 \end{pmatrix} \begin{pmatrix} \alpha_2 \\ \alpha_3 \end{pmatrix} \right) \, dx_2 \, dx_3
$$

for any $A \in M^3_{\text{skew}}$, with $u \in L^\infty(S)$, $u \geq c > 0$ for some constant $c$.

Then, there exists $I : W^{2,2}(\Omega; \mathbb{R}^3) \times W^{1,2}(\Omega; \mathbb{R}^3) \times W^{1,2}(\Omega; \mathbb{R}^3) \to \mathbb{R} \cup \{ +\infty \}$ such that, up to subsequences,

$$
\frac{1}{h^2} I^{(h)} \Gamma\text{-converges to } I \quad \text{(as } h \to 0) \}
$$

in the strong and weak topologies of $W^{1,2}(\Omega; \mathbb{R}^3)$. Moreover, defined the set

$$
\mathcal{A} := \{ (y, d_2, d_3) \in W^{2,2}(\Omega; \mathbb{R}^3) \times W^{1,2}(\Omega; \mathbb{R}^3) \times W^{1,2}(\Omega; \mathbb{R}^3) : y, d_2, d_3 \text{ do not depend on } x_2, x_3, \\
[y_1] = [d_2] = [d_3] = 1, \\
y_1 \cdot d_2 = y_1 \cdot d_3 = d_2 \cdot d_3 = 0 \},
$$

and the matrix-valued function

$$
R := (y_1 | d_2 | d_3) \in W^{2,2}(0, L; M^3_{\text{skew}}),
$$

($R$ is independent of $x_2, x_3$, and satisfies $R^T R_1 \in M^3_{\text{skew}}$), then the $\Gamma$-limit $I$ can be represented by

$$
I(y, d_2, d_3) = \begin{cases} 
\frac{1}{2} \int_0^L Q_2(R^T R_1) \, dx_1 & \text{if } (y, d_2, d_3) \in \mathcal{A} \\
+\infty & \text{else}
\end{cases}
$$

for any $(y, d_2, d_3) \in W^{2,2}(\Omega; \mathbb{R}^3) \times W^{1,2}(\Omega; \mathbb{R}^3) \times W^{1,2}(\Omega; \mathbb{R}^3)$.

For a proof of Theorem 3.3 we refer the interested reader to the Appendix, since the proof is a direct adaptation of [MM03, Theorem 3.1] and the result itself is a special case of [Neu12, Theorem 3.1].

The limit energy is therefore finite only on isometric deformations of the center line $(0, L)$. Then, the energy is a quadratic form in the entries of the matrix $R^T R_1$ where for $y \in \mathcal{A}$ the matrix $R^T R_1$ is skew-symmetric.

If $k = 2, 3$, it follows that

$$
y_1 = d_{k,1} = -(R^T R_1)_{k1} = (R^T R_1)_{1k},
$$

which is related to curvature that is caused by bending moments, while the relation

$$
(R^T R_1)_{23} = -(R^T R_1)_{32} = d_2 \cdot d_{3,1}
$$

is related to torsion of the rod caused by torsional moments, see also [MM03].

In our framework, minimum problem (7) has a unique solution (module a constant), which can be equivalently computed on the class of functions

$$
V := \{ \alpha \in W^{1,2}(S; \mathbb{R}^3) : \int_S u(x_2, x_3) \alpha \, dx_2 \, dx_3 = \int_S u(x_2, x_3) \nabla \alpha \, dx_2 \, dx_3 = 0 \}.
$$
The uniqueness of the minimizer is guaranteed by the convexity of $Q_3$ on symmetric matrices. In the sequel, $Q_3$ is identified through

$$Q_3(G) = \sum_{i,j \in \{1,4,6\}} \frac{1}{2} q_{ij} q_{ij} + \sum_{i,j \in \{2,3,5\}} 2 q_{ij} q_{ij} + \sum_{i \in \{1,4,6\}} \sum_{j \in \{2,3,5\}} 2 q_{ij} g_i g_j,$$

where $Q := (q_{ij})_{i,j=1,...,6}$ is a positive definite matrix and $G \in M_{3 \times 3}^{\text{sym}}$ is, for simplicity, denoted by

$$G = \begin{pmatrix} g_1 & g_2 & g_3 \\ g_2 & g_4 & g_5 \\ g_3 & g_5 & g_6 \end{pmatrix}.$$

3.1. **The mathematical model of isotropic materials.** In this section we derive the bending and torsional rigidity of non-homogeneous elastic rods in the case of isotropic materials. Assume that the stored energy $W$ satisfies the following additional hypothesis:

4. $W(A) = W(AR)$ for every $R \in SO(3)$

and denote $Q_{i_1,j_2}^{i_3,j_4}$ the $(2 \times 2)$-submatrix of $Q$, obtained from the $i_1,i_2$-th rows and $j_1,j_2$-th columns of $Q$. Let further $\alpha \in V$ be the unique minimizer of (7) for fixed $A := (a_{ij})_{i,j} \in M_{3 \times 3}^{\text{sym}}$.

Then the minimizer $\alpha$ satisfies the following system of Euler-Lagrange equations in the distributional sense (for simplicity, we denote $u(x_2,x_3)$ by $u$)

$$\begin{aligned}
&\text{div}(u(Q_{23}^{23} \nabla \alpha_1 + Q_{23}^{45} \nabla \alpha_2 + Q_{23}^{56} \nabla \alpha_3)) = -u(a_{12} q_{12} - a_{13} q_{13}) \\
&\text{div}(u(Q_{25}^{25} \nabla \alpha_1 + Q_{25}^{45} \nabla \alpha_2 + Q_{25}^{56} \nabla \alpha_3)) = -u(a_{14} q_{14} - a_{15} q_{15} + a_{23}(q_{34} - q_{25})) \\
&\text{div}(u(Q_{56}^{56} \nabla \alpha_1 + Q_{56}^{45} \nabla \alpha_2 + Q_{56}^{56} \nabla \alpha_3)) = -u(a_{12} q_{15} - a_{16} q_{15} + a_{23}(q_{35} - q_{26}))
\end{aligned}$$

in $S$ with the following boundary conditions on $\partial S$

$$\begin{aligned}
&(Q_{23}^{23} \nabla \alpha_1 + Q_{23}^{45} \nabla \alpha_2 + Q_{23}^{56} \nabla \alpha_3) \cdot \theta = -q_{23} \cdot \theta \\
&(Q_{25}^{25} \nabla \alpha_1 + Q_{25}^{45} \nabla \alpha_2 + Q_{25}^{56} \nabla \alpha_3) \cdot \theta = -q_{45} \cdot \theta \\
&(Q_{56}^{56} \nabla \alpha_1 + Q_{56}^{45} \nabla \alpha_2 + Q_{56}^{56} \nabla \alpha_3) \cdot \theta = -q_{56} \cdot \theta
\end{aligned}$$

with outer unit normal $\theta$ on $\partial S$ and

$$\eta_j(x_2,x_3) := (a_{12} x_2 + a_{13} x_3)(q_{11},q_{1j}) + a_{23} Q_{23}^{23}(x_3,-x_2).$$

Since solutions to the system depend linearly on the entries $(a_{ij})$, then $Q_2$, defined in (7), is a quadratic form of $A$.

Assuming that $u(x_2,x_3)$ is piecewise constant on $I_1,\ldots,I_n$, disjoint subsets of $S$ with Lipschitz boundary $\partial I_i$, then, if $W$ is isotropic (see 4.), then on each subset $I_i$ the quadratic form $Q_3$ is given by

$$Q_3(G) = 2\mu u_i \left| \frac{G + G^T}{2} \right|^2 + \lambda u_i (\text{trace}(G))^2 \text{ on } I_i,$$

with Lamé’s constants $\mu$ and $\lambda$ and $u_i = \chi_{I_i} u(x_2,x_3)$.

Therefore, for any $i = 1,\ldots,n$, the system reads

$$\begin{aligned}
&\Delta \alpha_1 = 0 \quad \text{ in } I_i \\
&\partial_\nu \alpha_1 = -a_{23}(x_3,-x_2) \cdot \theta \quad \text{ on } \partial I_i
\end{aligned}$$
The function solving the Neumann problem for \( \alpha(x_2, x_3) \) of (10)-(12) has components
\[
\begin{align*}
&\alpha_1(x_2, x_3) = a_{23}w(x_2, x_3) \\
&\alpha_2(x_2, x_3) = -\frac{1}{4} \frac{\lambda}{\mu + \lambda} (a_{12}x_2^2 - a_{12}x_3^2 + 2a_{13}x_2x_3) \\
&\alpha_3(x_2, x_3) = -\frac{1}{4} \frac{\lambda}{\mu + \lambda} (-a_{13}x_2^2 + a_{13}x_3^2 + 2a_{12}x_2x_3)
\end{align*}
\]
Computing the value of the functional at these minimum points we find
\[
Q_2(A) = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} \left( a_{12}^2 \int_S u(x_2, x_3)x_2^2 \, dx_2 dx_3 + a_{13}^2 \int_S u(x_2, x_3)x_3^2 \, dx_2 dx_3 \right) + \mu D_T a_{23}^2
\]
with
\[
D_T := \int_S u(x_2, x_3)(x_2^2 + x_3^2 - x_2w_3 + x_3w_2) \, dx_2 dx_3.
\]
The constant \( D_T \) represents the so-called torsional rigidity for non-homogeneous elastic rods and is frequently used in classical theory as, for instance, in [Sad09] or [LKN00]. The first two terms on the right hand side of (14) are referred to the second moments of inertia, whose average determines the mean bending rigidity \( D_{\text{mean}} \) of a non-homogeneous elastic rod, see the following remark.

**Remark 3.4.** Notice that, without assumption (5), the energy \( Q_2(A) \) in (14) reads
\[
Q_2(A) = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} \left( a_{12}^2 \int_S u(x_2, x_3)x_2^2 \, dx_2 dx_3 + a_{13}^2 \int_S u(x_2, x_3)x_3^2 \, dx_2 dx_3 \right) + \mu D_T a_{23}^2
\]
and so we recover the moment curvature relation in classical bending theory, i.e.,
\[
\begin{pmatrix} M_{x_2} \\ M_{x_3} \end{pmatrix} = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} \begin{pmatrix} D_{x_2}^u & D_{x_3}^u \\ D_{x_2x_3}^u & D_{x_3}^u \end{pmatrix} \begin{pmatrix} a_{12} \\ a_{13} \end{pmatrix}.
\]
$M_{x_3}, M_{x_2}$ denote the bending moments applied at the end of the rod ($x_1 = L$) and the $u$-dependent moments of inertia $D^u_{x_2}, D^u_{x_3}$ and the product of inertia $D^u_{x_2x_3}$ are given by

$$D^u_{x_2} = \int_{\Omega} u(x_2, x_3)x_2^2 \, dx_2dx_3, \quad D^u_{x_3} = \int_{\Omega} u(x_2, x_3)x_3^2 \, dx_2dx_3,$$

$$D^u_{x_2x_3} = \int_{\Omega} u(x_2, x_3)x_2x_3 \, dx_2dx_3.$$

The maximal and minimal bending rigidities $D_{\text{min}}$ and $D_{\text{max}}$ along the principal axes are determined by the maximal and minimal eigenvalue of the matrix in (16), leading to

$$(17) \quad D^u_{\text{max/min}} = \left( D^u_{\text{mean}} \pm \sqrt{\frac{(D^u_{x_2} - D^u_{x_3})^2}{4} + (D^u_{x_2x_3})^2} \right),$$

with $D^u_{\text{mean}} = \frac{D^u_{x_2} + D^u_{x_3}}{2}$.

3.2. Stress Function Formulation. With regard to the numerical approximation of (10), we use a different representation of the torsional rigidity (15). We consider Prandtl’s stress function $\Phi$, which is determined by conditions

$$(18) \quad \frac{1}{u} \frac{\partial \Phi}{\partial x_3} = \left( \frac{\partial w}{\partial x_2} - x_3 \right), \quad \text{and} \quad \frac{1}{u} \frac{\partial \Phi}{\partial x_2} = - \left( \frac{\partial w}{\partial x_3} + x_2 \right),$$

where $w$ is the torsion function from above.

Using a parametrization $s \to (x_2(s), x_3(s))$ of connected components $\Gamma_i$ of the boundary curve $\partial S$ the components $\zeta_{x_2}$ and $\zeta_{x_3}$ of the outer unit normal $\zeta$ on the respective boundary curve $\Gamma_i$ can be expressed as

$$\zeta_{x_2} = \frac{dx_3}{ds}, \quad \text{and} \quad \zeta_{x_3} = - \frac{dx_2}{ds},$$

and thus, incorporating (13) and (18), we find

$$\frac{\partial \Phi}{\partial x_2} \frac{dx_2}{ds} + \frac{\partial \Phi}{\partial x_3} \frac{dx_3}{ds} = 0,$$

which can be equivalently written as

$$\frac{d\Phi}{ds} = 0, \quad \text{on} \partial S.$$

Therefore, the stress function $\Phi$ must be a constant on each connected component $\Gamma_i$ of the boundary $\partial S$. By means of (13), $\Phi$ is then determined by the boundary value problem

$$(19) \quad \begin{cases} - \text{div} \left( \frac{1}{u} \nabla \Phi \right) = 2 & \text{in} \ S \\ \Phi = \Phi_i & \text{on} \ \Gamma_i \end{cases} \quad \text{for constants } \Phi_i.$$

We generally assume in the following the $S$ is connected. For simply connected domains $S$ we can assume without loss of generality that $\Phi$ must be zero on $\partial S$, while for multiply connected domains $S$ the value of $\Phi$ can be
set to zero only on the outer boundary $\Gamma_0$ of $S$. On the inner boundaries $\Gamma_i$ the constants $\Phi_i$ are determined by the conditions

\begin{equation}
\int_{\Gamma_i} \frac{1}{u} \frac{\partial \Phi}{\partial \theta} \, ds = 2|A_i|, \quad \text{for } i = 1, \ldots, N, \tag{20}
\end{equation}

where $A_i$ are the sets enclosed by $\Gamma_i$ and using the outer unit normal $\theta$ on $\partial S$. Since $\omega$ must be single-valued, then

\begin{align*}
0 &= \int_{\Gamma_i} \frac{\partial \omega}{\partial x_2} \, dx_2 + \int_{\Gamma_i} \frac{\partial \omega}{\partial x_3} \, dx_3 \\
&= -\int_{\Gamma_i} \frac{\partial \Phi}{\partial \zeta} \, ds - \int_{\Gamma_i} (x_2, x_3) \cdot \zeta \, ds
\end{align*}

and condition (20) follows directly by an application of Green’s theorem to the last integral and the fact that $\theta = -\zeta$.

The torsional rigidity $D_T$ (15) is then given by an integration of Prandtl’s stress function, taking into account the boundary conditions, i.e.,

\begin{equation}
D_T = 2 \int_S \Phi \, dx_2 dx_3 + 2 \sum_{i=1}^N \Phi_i |A_i|. \tag{21}
\end{equation}

4. Optimization of Rigidities

Inspired by the recent phase field approaches to the structural topology optimization [BGHR16, TNK10], we study in this section shape optimization problems for bending and torsion of inextensible and non-homogeneous elastic rods in the case of isotropic materials (9) involving two different materials, a stiffer material and a softer material, inside a fixed cross-section $S$.

In what follows, the distribution of the two materials inside $S$ will be described equivalently by means of functions $\varphi$ belonging to the class

\[ U := \{ \varphi \in BV(S; \{0,1\}) : \int_S \varphi(x_2, x_3) \, dx_2 dx_3 = m_1 \leq |S| \}, \]

and by their 1-1 corresponding functions $u^\varphi \in BV(S; \{c,1\})$, having the same mass constraint and defined by

\begin{equation}
u^\varphi(x_2, x_3) = \varphi(x_2, x_3)(1-c) + c \quad \text{for any } (x_2, x_3) \in S, \tag{22}
\end{equation}

for a fixed positive constant $c$. This second notation is aimed to be more familiar with the topics introduced in section 3.

Then, the set $\{u^\varphi = 1\}$, or equivalently $\{\varphi = 1\}$, describes regions where only the stiffer material is present (up to a set of measure zero), while the set $\{u^\varphi = c\}$ regions containing only the softer material. Note that, if $c = 1$, we are in the special case of a single homogeneous material, i.e.

\[ u^\varphi(x_2, x_3) = 1 \quad \text{for any } (x_2, x_3) \in S. \]
By (9), the material values $\mu, \lambda$ become
\[ \mu(x_2, x_3) = \mu_1 u^2(x_2, x_3) \quad \text{and} \quad \lambda(x_2, x_3) = \lambda_1 u^2(x_2, x_3) \] for any $(x_2, x_3) \in S$.

4.1. **Perimeter penalized shape optimization.** In this section, we look in particular for solutions to the following minimization problem
\[ \min_{\phi \in \mathcal{U}} J_0(\phi), \] where the functional $J_0: \mathcal{U} \to \mathbb{R} \cup \{+\infty\}$ is defined by
\[ J_0(\phi) := \sigma_1 D_{\text{mean}}(\phi) + \sigma_2 \mu_1 D_T(\phi) + \gamma \text{Per}(\{\phi = 1\}). \] Here $\sigma_1, \sigma_2, \gamma \in \mathbb{R}$ are weighing factors and the objectives in the optimization problem are the mean bending rigidity (see (14)), which is defined by
\[ D_{\text{mean}}(\phi) := \frac{\mu_1(3\lambda_1 + 2\mu_1)}{\lambda_1 + \mu_1} \int_S u^2(x_2, x_3)(x_2^2 + x_3^2) \, dx_2 dx_3 \quad \text{for any } \phi \in \mathcal{U}, \] and the torsional rigidity $D_T$ (see (21)) is
\[ D_T(\phi) = 2 \int_{\tilde{S}} \Phi \, dx_2 dx_3 \quad \text{for any } \phi \in \mathcal{U}. \] Here $\tilde{S}$ is the set enclosed by the outer boundary $\Gamma_0$ of the cross-section $S$ (i.e., $S$ with any holes filled in, if $S$ was not simply connected), and $\Phi$ is the Prandtl’s stress function associated with $\phi$, i.e. a weak solution to the boundary value problem (19), in the sense that
\[ \int_{\tilde{S}} \frac{1}{w^\phi} \nabla \Phi \cdot \nabla v \, dx_2 dx_3 = 2 \int_{\tilde{S}} v \, dx_2 dx_3 \] for any $v \in H := \{ w \in H^1_0(\tilde{S}) : w = \text{const.} \text{ in } \tilde{S} \setminus S\}$.

By Riesz’s representation theorem, equation (27) admits a unique solution $\Phi_0$. Moreover, $\Phi_0$ satisfies condition 20 in the distributional sense. Therefore let $v = \chi_{A_i}$ for any hole $A_i$. Then $\nabla v = \delta_{A_i} \theta$ (with the outer unit normal $\theta$ on $\partial S$) and we deduce we get
\[ - \int_{\tilde{S}} \frac{1}{w^\phi} \frac{\partial \Phi}{\partial \theta} \, ds = - \int_{A_i} \frac{1}{w^\phi} \nabla \Phi \cdot \delta_{A_i} \theta \, dx_2 dx_3 = \int_{A_i} \frac{1}{w^\phi} \nabla \Phi \cdot \nabla v \, dx_2 dx_3 \]
\[ = 2 \int_{S} \chi_{A_i} \, dx_2 dx_3 = 2 |A_i|. \]

Let us note that minimizers for problem (23) are equivalent to minimizers for the functional $J_0: L^1(S) \to \mathbb{R}$, defined by
\[ J_0(\phi) := \begin{cases} J_0(\phi) & \text{in } \mathcal{U} \\ +\infty & \text{in } L^1(S) \setminus \mathcal{U}. \end{cases} \]

Moreover, the existence of a minimizer is ensured by the presence of the perimeter term on the cross-sections of the stiffer material, that is the set $\{\phi = 1\}$. From a mathematical point of view, we will recover the existence result as a consequence of Theorem 3.2 (see Corollary 4.5 for details).
4.2. Phase field approach. To solve numerically (23), we use a phase field approach. We first define the Sobolev space
\[ \mathcal{U}_{\text{ad}} := \{ w \in H^1_0(S) : 0 \leq w \leq 1, \int_S w(x_2, x_3) \, dx_2 dx_3 = m_1 \leq |S| \}, \]
which is the admissible set in the phase field approach and, for any \( \varphi \in \mathcal{U}_{\text{ad}} \) and \( \epsilon > 0 \), we approximate the perimeter in \( J_0 \) by means of the Ginzburg-Landau energy \( E_{\epsilon} : \mathcal{U}_{\text{ad}} \to \mathbb{R}_+^+ \cup \{+\infty\} \), defined by
\[
E_{\epsilon}(\varphi) := \int_S \left( \frac{\epsilon}{2} |\nabla \varphi|^2 + \frac{1}{\epsilon} F(\varphi) \right) \, dx_2 dx_3.
\]
Here \( F : \mathcal{U}_{\text{ad}} \to \mathbb{R}_+^+ \cup \{+\infty\} \) is a double obstacle potential, that is a non-convex and continuous function having two local minimizers (up to translations, it is not restrictive to assume the minima both 0). A prototype of \( F \) is the function
\[
F(\varphi) = \frac{1}{4} \varphi^2 (1 - \varphi)^2 \quad \text{for any } \varphi \in \mathcal{U}_{\text{ad}}.
\]
We then denote \((J_{\epsilon})_{\epsilon > 0}\) the approximating sequence of \( J_0 \) where, for any \( \epsilon > 0 \), the functional \( J_{\epsilon} : \mathcal{U}_{\text{ad}} \to \mathbb{R} \cup \{+\infty\} \) is now defined by
\[
J_{\epsilon}(\varphi) := \sigma_1 D_{\text{mean}}(\varphi) + \sigma_2 \mu_1 D_{T}(\varphi) + \frac{\gamma}{c_0} E_{\epsilon}(\varphi),
\]
and we consider the sequence of minimization problems
\[
(30) \quad \min_{\varphi \in \mathcal{U}_{\text{ad}}} J_{\epsilon}(\varphi), \quad \epsilon > 0.
\]

**Remark 4.1.** The presence of the constant \( c_0 \) in the definition of \( J_{\epsilon} \) is a technical requirement. It allows us to recover the normalized perimeter in the limit functional \( J_0 \) (see e.g. [Mod87]).

As in (28), we note that solutions to (30) are equivalent to minimizers in \( L^1(S) \) for the sequence of functionals \( J_{\epsilon} : L^1(S) \to \mathbb{R}, \epsilon > 0 \), defined by
\[
J_{\epsilon}(\varphi) := \left\{ \begin{array}{ll}
J_{\epsilon}(\varphi) & \text{in } \mathcal{U}_{\text{ad}} \\
+\infty & \text{in } L^1(S) \setminus \mathcal{U}_{\text{ad}}.
\end{array} \right.
\]

Our first step in the phase field approach is to show that the continuity of the rigidities \( D_{\text{mean}} \) and \( D_T \), with respect to the strong topology of \( L^1(S) \), ensures the existence of a minimizer to any minimization problem in (30) (see Theorem 4.3).

**Lemma 4.2.** Let \( D_{\text{mean}} \) and \( D_T \) be the mean bending rigidity and the torsional rigidity given in (25) and (26), respectively. Then, the functional
\[
\{ w \in L^1(S) : 0 \leq w \leq 1 \text{ a.e. in } S \} \ni \varphi \mapsto \sigma_1 D_{\text{mean}}(\varphi) + \sigma_2 \mu_1 D_T(\varphi)
\]
is continuous with respect to the strong topology of \( L^1(S) \).

**Proof.** By the boundedness of the cross-section \( S \), one can easily prove the continuity of \( D_{\text{mean}} \). We then just focus on the torsional rigidity term \( D_T \).

Let \( (\varphi_k)_k \) be a sequence strongly convergent to \( \varphi_0 \) in \( L^1(S) \), as \( k \to \infty \), and, for any \( k \in \mathbb{N} \), denote \( \Phi_k \in \mathcal{H} \) the Prandtl’s stress function associated with \( \varphi_k \), in the sense of (27). To conclude we show the existence of a
Prandtl’s stress $\Phi_0$ which is still a solution of (27), with $\varphi = \varphi_0$, and to which the sequence $(\Phi_k)_k$ strongly converges in $L^2(\tilde{S})$.

By Poincaré inequality, the sequence $(\Phi_k)_k$ is bounded in $H^1_0(\tilde{S})$ and, by reflexivity, there exist a subsequence of $(\Phi_k)_k$, $(\Phi_{kj})_k$, and $\Phi_0 \in H^1_0(\tilde{S})$ such that $\Phi_{kj}$ weakly converges to $\Phi_0$ in $H^1_0(\tilde{S})$. Let us first show that $\Phi_0 \in H^1$.

Note that the sequence $\left(\frac{1}{u^\epsilon k_j} \Phi_{kj}\right)$ is also bounded in $H^1_0(\tilde{S})$, and, up to a further (not-relabelled) subsequence, it holds that

$$\left| \int_{\tilde{S}} \frac{1}{u^\epsilon k_j} \nabla \Phi_{kj} \cdot \nabla v \, dx \, dx_3 - \int_{\tilde{S}} \frac{1}{u^\epsilon \varphi_0} \nabla \Phi_0 \cdot \nabla v \, dx \, dx_3 \right|$$

$$\leq \int_{\tilde{S}} \left| \frac{1}{u^\epsilon k_j} - \frac{1}{u^\epsilon \varphi_0} \right| \nabla \Phi_{kj} \cdot \nabla v \, dx \, dx_3$$

$$+ \int_{\tilde{S}} \frac{1}{u^\epsilon \varphi_0} \left| \nabla \Phi_{kj} \cdot \nabla v - \nabla \Phi_0 \cdot \nabla v \right| \, dx \, dx_3 \to 0$$

as $k_j \to \infty$, for any $v \in H$, in virtue of the dominated convergence theorem. Thus, $\Phi_0$ is a weak solution to problem (27), and belongs to the set $\mathcal{H}$.

By applying the previous argument to any subsequence of the starting sequence $(\Phi_k)_k$, we find that every subsequence of $(\Phi_k)_k$ has a subsequence weakly convergent in $\mathcal{H}$ to the unique solution of (27) (with $\varphi = \varphi_0$). Then, by well-known results, we get the weak convergence of the whole sequence $(\Phi_k)_k$ in $\mathcal{H}$ and, by Rellich theorem, the strong convergence in $L^2(\tilde{S})$ and the thesis readily follows. □

**Theorem 4.3.** There exists at least a minimizer for problem (30), for any $\epsilon > 0$.

**Proof.** The existence of a minimizer for any problem (30) is shown by means of the direct method in the calculus of variation.

Fix $\epsilon > 0$, consider the functional

$$J_{\epsilon}(\varphi) = \sigma_1 D_{\text{mean}}(\varphi) + \sigma_2 \mu_1 D_T(\varphi) + \gamma \frac{\epsilon}{c_0} \int_{\tilde{S}} \left( \frac{\epsilon}{2} |\nabla \varphi|^2 + \frac{1}{\epsilon} F(\varphi) \right) \, dx \, dx_3,$$

for any $\varphi \in \mathcal{U}_{\text{ad}}$, and denote $\Phi \in \mathcal{H}$ the Prandtl’s stress function associated with $\varphi$, in the sense of (27), which is bounded on $\mathcal{H}$. By the boundedness of $S$, there exist positive constants $C_1, C_2$, only depending on $S$, such that

$$D_{\text{mean}}(\varphi) > -C_1$$

and

$$D_T(\varphi) > -C_2$$

for any $\varphi \in \mathcal{U}_{\text{ad}}$.

Then, the properties on the double obstacle potential $F$ ensure a control from below on $J_\epsilon$ by means of $\epsilon \|\varphi\|_{H^1_0(S)}$, and so each functional $J_\epsilon$ is coercive in $L^1(S)$, for any $\epsilon > 0$. 13
Let \((\varphi_{\epsilon_k})_k\) be a minimizing sequence of \(J_\epsilon\). Note that \(\sup_{\epsilon_k \in \mathbb{N}} J_\epsilon(\varphi_{\epsilon_k}) < \infty\) implies that
\[
\sup_{k \in \mathbb{N}} \|\nabla \varphi_{\epsilon_k}\|_{L^2(S)} < \infty,
\]
and so \((\varphi_{\epsilon_k})_k\) is bounded in \(H^1_0(S)\).

Then, there exists \(\varphi_0 \in H^1_0(S)\) such that, up to subsequences, \((\varphi_{\epsilon_k})_k\) converges weakly in \(H^1_0(S)\), strongly in \(L^2(S)\) and a.e. in \(S\) to \(\varphi_0\) (this last convergence is actually pointwise, being \((\varphi_{\epsilon_k})_k\) a minimizing sequence). Moreover, it is easy to show that, by the pointwise convergence, \(\varphi_0 \in [0, 1]\) and satisfies the mass constraint \(\int_S \varphi_0(x_2, x_3) \, dx_2 dx_3 \leq |S|\), and hence \(\varphi_0 \in \mathcal{U}_{\text{ad}}\).

To conclude, note that, by the continuity of \(F\) and the lower semicontinuity of \(\|\varphi\|_{H^1_0(S)}\), the Ginzburg-Landau energy \(E_\epsilon\) is sequentially lower semicontinuous. Then, by Lemma 4.2, the functional \(J_\epsilon\) is lower semicontinuous and the thesis follows as a consequence of the Weierstrass Theorem (see e.g. [DM93, Theorem 1.15]).

4.3. Sharp interface limit. We conclude this section by proving a classical Modica-Mortola-type theorem, Theorem 4.4, that provides the \(\Gamma\)-convergence in the strong topology of \(L^1(S)\) of the sequence of functionals \((J_\epsilon)_\epsilon\), defined in (31), to the functional \(J_0\), introduced in (28). As a consequence of Theorem (4.4), we will finally prove in Corollary 4.5 the existence of a solution for the minimization problem (23).

**Theorem 4.4.** Let \(J_\epsilon : L^1(S) \to \mathbb{R}, \epsilon > 0\), and let \(J_0 : L^1(S) \to \mathbb{R}\) be the functionals defined in (31) and in (28), respectively. Then
\[(J_\epsilon)_\epsilon \quad \Gamma\text{-converges to } J_0\]
in the strong topology of \(L^1(S)\), as \(\epsilon\) goes to 0.

**Proof.** The proof of the assertion is carried out similarly as in [BGHR16, Thorem 20].

Denote \(\mathbb{1}_A\) the indicator of any set \(A \subset L^1(S)\), that is,
\[
\mathbb{1}_A(x) := \begin{cases} 0 & \text{if } x \in A \\ +\infty & \text{otherwise} \end{cases}
\]
and, for any \(\epsilon > 0\), rewrite functionals \(J_\epsilon\) as
\[
J_\epsilon(\varphi) = D_r(\varphi) + \frac{\gamma_c}{c_0} E_\epsilon(\varphi) + \mathbb{1}_K \quad \text{for any } \varphi \in L^1(S),
\]
Here \(D_r(\varphi) := \sigma_1 D_{\text{mean}}(\varphi) + \sigma_2 \mu_1 D_T(\varphi)\) for any \(\varphi \in \mathcal{U}_{\text{ad}}\) and
\[
K := \{ \varphi \in L^1(S) : \int_S \varphi(x_2, x_3) \, dx_2 dx_3 = m_1 \leq |S| \}.
\]

By the classical result of Modica and Mortola [Mod87], we know that the sequence of energies \(E_\epsilon : L^1(S) \to \mathbb{R} \cup \{+\infty\}\), defined by
\[
E_\epsilon(\varphi) := E_\epsilon(\varphi) + \mathbb{1}_{H^1(S)}(\varphi) = \begin{cases} E_\epsilon(\varphi) & \text{in } H^1(S) \\ +\infty & \text{in } L^1(S) \setminus H^1(S) \end{cases}
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\(\square\)

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and, for any \(\epsilon > 0\), rewrite functionals \(J_\epsilon\) as
\[
J_\epsilon(\varphi) = D_r(\varphi) + \frac{\gamma_c}{c_0} E_\epsilon(\varphi) + \mathbb{1}_K \quad \text{for any } \varphi \in L^1(S),
\]
Here \(D_r(\varphi) := \sigma_1 D_{\text{mean}}(\varphi) + \sigma_2 \mu_1 D_T(\varphi)\) for any \(\varphi \in \mathcal{U}_{\text{ad}}\) and
\[
K := \{ \varphi \in L^1(S) : \int_S \varphi(x_2, x_3) \, dx_2 dx_3 = m_1 \leq |S| \}.
\]

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\[
E_\epsilon(\varphi) := E_\epsilon(\varphi) + \mathbb{1}_{H^1(S)}(\varphi) = \begin{cases} E_\epsilon(\varphi) & \text{in } H^1(S) \\ +\infty & \text{in } L^1(S) \setminus H^1(S) \end{cases}
\]

\(\square\)
\[ \Gamma\text{-converges in the strong topology of } L^1(S), \text{ as } \epsilon \to 0, \text{ to the limit functional } E_0 : L^1(S) \to \mathbb{R} \cup \{+\infty\}, \text{ which can be represented by} \]
\[ E_0(\phi) := \begin{cases} 
  c_0 \text{Per}(\{\phi = 1\}) & \text{in } BV(\{0,1\}) \\
  +\infty & \text{in } L^1(S) \setminus BV(\{0,1\}).
\end{cases} \]
Moreover, by using the same construction of Modica [Mod87], one can also show that
\[ \frac{\gamma}{c_0} E_\epsilon(\phi) + 1_K \epsilon \] \[ \Gamma\text{-converges to } \gamma E_0 + 1_K, \text{ as } \epsilon \to 0 \]
and the assertion then follows by Lemma 4.2 and [DM93, Proposition 6.21].

As a consequence of the previous result, we finally show that any sequence of minimizers of functionals \( J_\epsilon, \epsilon > 0 \), strongly converges in \( L^1(S) \) to a solution of the sharp interface problem (23).  

**Corollary 4.5.** Let \( \phi_\epsilon \) be a minimizer of \( J_\epsilon \), for any \( \epsilon > 0 \). Then, there exists a minimizer of \( J_0, \phi \in \mathcal{U} \), such that, up to subsequences
\[ \lim_{\epsilon \to 0} \| \phi_\epsilon - \phi \|_{L^1(S)} = 0 \] \[ \text{and } \lim_{\epsilon \to 0} J_\epsilon(\phi_\epsilon) = J_0(\phi). \]

**Proof.** Since the sequence \( (\phi_\epsilon)_\epsilon \) is a sequence of minimizers, then
\[ \sup_{\epsilon > 0} J_\epsilon(\phi_\epsilon) < \infty \] \[ \text{and } \sup_{\epsilon > 0} E_\epsilon(\phi_\epsilon) < \infty. \]
Then, arguing as in the proof of [Mod87, Proposition 3], the sequence of Ginzburg-Landau energies \( (E_\epsilon)_\epsilon \) is equicoercive in \( L^1(S) \).

The thesis then follows as an application of Theorem 3.2 and Theorem 4.4.

\[ \square \]

5. Numerical experiments

To compute solutions of (30) numerically we use a steepest descent approach. That is we compute a time-discrete \( L^2 \)-gradient flow of \( J_\epsilon \) until a stationary state has been reached. For this we use a discretization of the domain \( S \) by P1 triangular finite elements and a forward discretization in time for time step \( \tau \) and integer iteration steps \( n \geq 1 \). This leads to an artificial time variable \( t = \tau \cdot n \), also called pseudo time. A stationary state of the gradient flow is usually a local solution of our minimization problem. Further we can decouple equation (27) from the gradient flow and calculate it separately using again by P1 finite elements. The mass constraint is finally imposed using a Lagrange multiplier. We then use a semi-implicit first order Euler scheme treating only the linear highest gradient term implicitly for an initial condition \( \varphi^0 \) of the phase field variable. For more details on the implementation of the finite element method we refer to our previous work [WVLS+19].

Inspired by multi-material composites found in the morphology of plant stems [RIS04, SSS20, WVSSD21] we study the optimal distribution of two
materials inside a cross-section $S$ where the ratio between the Lamé parameters of the two materials is of order $O(10^{-1})$. In the following this ratio is modeled within the density function $u^\varphi$ using the phase field variable $\varphi$ and setting

$$u^\varphi(x_2, x_3) = \varphi(x_2, x_3)(1 - c) + c$$

with $c = 0.1$. Further Lamé parameters $\mu_1, \lambda_1$ in (30) are set to $\mu_1 = 26$ and $\lambda_1 = 70.57$.

We consider different values of the weighting factors $\sigma_1, \sigma_2$ and $\gamma$ corresponding to different terms of optimization, i.e., maximization or minimization of torsional and bending rigidity. The results of the numerical simulations are depicted in Fig. 1, 2 and Tab. 1. The reference cross-section $S$ is chosen as a circle with radius $r = 0.7$ and the initial condition $\varphi^0$ is also a circle with radius $r = 0.5$. Starting with a circular initial condition is justified by observations from the morphology of plant stems where circular domains are typically observed in young ontogenetic states, see for instance [RIS04, WVLS+19]. Depending on the weighting factors we observe different stationary states of the gradient flow. In the case of a maximization of rigidities ($\sigma_1 = -1, \sigma_2 = -3$) and a sole minimization of torsional rigidity ($\sigma_2 = 3$) we obtain a symmetric circular tube and an I-beam like structure, see (a) and (b) in Fig. 1, which are well known rigidity optimizers in the case of homogeneous rods, see, for instance, [KK00].

Concerning the morphology of plant stems it must be mentioned that plants are not inclined by a maximization of rigidity but more by an optimization of both strength and flexibility, see, for instance, [Nik92, Vog07]. In general one observes a high twist-to-bend ratio

$$\frac{D_{\text{mean}}(u^\varphi)}{D_T(u^\varphi)}$$

that implies high bending rigidity on the one hand and a comparatively low torsional rigidity on the other. In our model this can be achieved by a maximization of bending and a minimization of torsional rigidity ($\sigma_1 = -3, \sigma_2 = 3$) and leads to a reinforcement by “fibre strands”. These “fibre strands” are formed by the stiffer material and are uniformly distributed along the boundary of $S$, see (d) and (e) in Fig. 1. For a smaller weighting factor $\gamma$ of the perimeter a higher number of “fibre strands” occurs, see (e) in Fig. 1. This leads to a slight increase of the twist-to-bend ratio which is mainly driven by a decrease of the torsional rigidity, see (c) in Fig. 2 and Tab. 1.

Finally we consider the minimization of both bending and torsional rigidity ($\sigma_1 = 1.5, \sigma_2 = 3$) that treats the case of achieving maximum flexibility. This is of special interest in the investigation of vines, like liana plants, with a growth habit of trailing or scandent where flexibility in both bending and torsion is crucial. Minimizing both torsional and bending rigidity leads to structures with deep-grooves, see (f) and (g) in Fig 1. As in the experiments (d) and (e) a lower weighting of the perimeter functional has an influence on the shape of the minimizers where in this case a lower weighting of the perimeter term causes the stiffer material to form a deep-grooved shape with additional branched fingers, see (g) in Fig. 1.
The study in Fig. 1 is crucial as it provides an approach for the analysis of material distribution inside plant stems cross-sections. The results in Fig. 1 (d) and (e) can be compared to the arrangement of fibre strands in several plant stems cross-sections. For instance, “fibre-reinforced” structures as in (d) and (e) are found in the morphology of Carex Pendula and Caladium Bicolor where reinforcing by sclerenchymatous and collenchymatous stiffening tissues, respectively, causes a particularly high twist-to-bend ratio, see, for instance, [SSS20, WVSSD21, WVSL+22].

The results in Fig. 1 (f) on the other hand can be compared to the arrangement of a non-dense flexible secondary xylem with wide-diameter vessels and broad wood rays, as well as a flexible cortex during the ontogeny of a liana plant of the species Condylocarpon Guianense, see Fig. 3. During its ontogeny the plant is inclined by increasing its flexibility by a rearrangement of the main load bearing element, the secondary xylem. This is achieved by decreasing the bending and torsional rigidity of its plant stem by the secondary xylem forming a structure with deep grooves and branched fingers. For a detailed description of the evolution of the secondary xylem during the ontogeny of Condylocarpon Guianense we refer to [WVLS+19, RIS04].
Figure 1. Local solutions of (30) for different weighting factors $\sigma_1, \sigma_2, \gamma$ corresponding to a maximization of rigidities in (b), a sole minimization of torsional rigidity in (c), a minimization of torsional and a maximization of bending rigidity in (d) and (e) and a minimization of both bending and torsional rigidity in (e) and (f). In experiments (b), (c) and (f) the weighting factor $\gamma$ for the perimeter penalization is set to $\gamma = 0.5$, where in (e) and (g) the weighting factor is $\gamma = 0.25$. In experiment (d) the weighting factor is set to $\gamma = 1.0$. The stiffer material ($u = 1$) is depicted in red where the softer material ($u = 0.1$) is depicted in blue.
Figure 2. Convergence history of the rigidities $D_T$ and $D_{\text{mean}}$ with respect to pseudo-time $t$ during a gradient descent.

| Experiment | $D_{\text{mean}}(u)$ | $D_T(u)$ | $D_{\text{mean}}(u)/D_T(u)$ |
|------------|----------------------|----------|----------------------------|
| (a)        | 3.54                 | 2.75     | 1.29                       |
| (b)        | 10.71                | 7.9      | 1.35                       |
| (c)        | 4.71                 | 2.08     | 2.26                       |
| (d)        | 8.96                 | 2.86     | 3.13                       |
| (e)        | 8.88                 | 2.74     | 3.24                       |
| (f)        | 3.79                 | 2.31     | 1.64                       |
| (g)        | 3.69                 | 2.17     | 1.7                        |

Table 1. Values of torsional and bending rigidities and the twist-to-bend ratio for stationary states in experiments (b)-(g) and initial condition (a).
Conclusions

Inspired by the bending-torsion theory of non-homogeneous elastic rods, we derived a new model for the optimization of the rod’s bending and torsional rigidity. It was done by studying a sharp interface shape optimization problem with perimeter penalization, that treats the torsional and bending rigidity as objectives. We have then incorporated a diffuse interface approach, for which we have proven existence of solutions to the optimization problem. As a consequence of a Γ-convergence result, we showed that, as the thickness of the interface tends to zero, the sequence of minimizers of the diffuse interface approach convergences to the minimizer of the sharp interface problem in $L^1(S)$.

In the last part of the paper, we employed a numerical approximation of solutions to the phase field problem using a steepest descent approach. To this aim, we studied four different cases of optimization: a maximization of both rigidities, a sole minimization of the torsional rigidity, a minimization of torsional and a maximization of bending rigidity, and, finally, the minimization of both rigidities. The two latter cases were inspired by observations in plant morphology that implied that plants are more inclined to produce a high flexibility, especially in torsion, instead of high stiffness of their stems.

A numerical approximation of minimizers in these two cases resulted in characteristic shapes and distributions of two materials inside a circular cross-section $S$. The appearing distributions of the materials then coincided with the tissue arrangements in the morphology of different plant stems and thus revealed the optimization of bending and torsional rigidity as a driving force in the development of plant stems.
Appendix - Proof of Theorem 3.3

We conclude the paper with a rigorous proof of Theorem 3.3. Let us recall
two preliminary results: a geometric rigidity theorem, by Friesecke, James
and Müller [FJM02], and a compactness theorem by Mora and Müller [MM03].

Theorem 5.1. [FJM02, Theorem 3.1] Let $U$ be a bounded Lipschitz domain
in $\mathbb{R}^n$, $n \geq 2$. Then, there exists a positive constant $C$, only dependent on
$U$, such that the following statement holds true:
For any $v \in W^{1,2}(U; \mathbb{R}^3)$ there is an associated rotation $R \in SO(3)$ such
that
$$\|\nabla v - R\|_{L^2(U)} \leq C \| \text{dist}(\nabla v, SO(3)) \|_{L^2(U)}.$$  

Theorem 5.2. [MM03, Theorem 2.1] Let $(y(h))$ be a sequence in $W^{1,2}(\Omega; \mathbb{R}^3)$
satisfying
\begin{equation}
\limsup_{h \to 0} \frac{1}{h^2} \int_\Omega \text{dist}^2(\nabla y(h), SO(3)) \, dx < +\infty.
\end{equation}

Then, there exist $y \in W^{2,2}(\Omega; \mathbb{R}^3)$ and $d_2, d_3 \in W^{1,2}(\Omega; \mathbb{R}^3)$ such that, up
to subsequences,
$$\nabla_h y(h) \to (y_1|d_2|d_3) \quad \text{strongly in } L^2(\Omega; M_3^{3 \times 3}), \text{ as } h \to 0;$$
$$(y_1|d_2|d_3) \in SO(3) \quad \text{a.e. in } \Omega;$$
$$(y_1|d_2|d_3) \text{ is independent of } x_2 \text{ and } x_3.$$

Remark 5.3. In the following proof of Theorem 3.3, we are going to study
the $\Gamma$-limit of $(1/h^2 I(h))$ only in the weak topology of $W^{1,2}(\Omega; \mathbb{R}^3)$. The proof in
the strong topology can be easily achieved by similar arguments, by checking
that conditions (1) and (2), given in Definition 3.1, are satisfied. To this
aim, one should replace the weak convergences in the spaces $L^2(\Omega; \mathbb{R}^3)$ and
$W^{1,2}(\Omega; \mathbb{R}^3)$, given in (33), with the strong ones.

Proof of the Theorem 3.3. By hypothesis 3. on the stored energy $W$, there
exists a functional $\Psi : W^{1,2}(\Omega; \mathbb{R}^3) \to \mathbb{R}$ such that
$$\Psi(y) \leq \frac{1}{h^2} f(h)(y)$$
for any $y \in W^{1,2}(\Omega; \mathbb{R}^3)$ and for any $h \in \mathbb{N}$. Moreover,
$$\lim_{\|y\|_{W^{1,2}(\Omega; \mathbb{R}^3)} \to \infty} \Psi(y) = +\infty.$$

Then, since the space $W^{1,2}(\Omega; \mathbb{R}^3)$ compactly embeds in $L^2(\Omega; \mathbb{R}^3)$, we can
characterize the $\Gamma$-limit of $(1/h^2 I(h))$ (in the weak topology of $W^{1,2}(\Omega; \mathbb{R}^3)$) in
terms of sequences, in virtue of [DM93, Proposition 8.10], that is, by
studying the $\Gamma$-lim inf and the $\Gamma$-lim sup inequalities, stated in Definition
3.1, where we replace the strong convergences in the space with the weak
ones. The proof in then divided into two parts.

Part 1: $\Gamma$-lim inf inequality
Let \((h_j)\) be a sequence of positive real numbers converging to 0 as \(j \to \infty\) and let \((y^{(h_j)})\) be a sequence in \(W^{1,2}(\Omega, \mathbb{R}^3)\) satisfying
\[
\liminf_{j \to \infty} \frac{1}{h_j^2} I^{(h_j)}(y^{(h_j)}) < +\infty.
\]

Then, there exists a not relabelled subsequence of \((y^{(h_j)})\) such that
\[
\lim_{j \to \infty} \frac{1}{h_j^2} I^{(h_j)}(y^{(h_j)}) = \liminf_{j \to \infty} \frac{1}{h_j^2} I^{(h_j)}(y^{(h_j)})
\]
and assumption (32) is fulfilled, by the hypotheses on \(W\).

Therefore, by Theorem 5.2, there exist vector-valued functions \(y \in W^{2,2}(\Omega; \mathbb{R}^3)\) and \(d_2, d_3 \in W^{1,2}(\Omega; \mathbb{R}^3)\) such that
\[
y^{(h_j)} \to y \quad \text{weakly in } W^{1,2}(\Omega; \mathbb{R}^3),
\]
(33)
\[
\left( \frac{1}{h_j} y_1^{(h_j)}, \frac{1}{h_j} y_3^{(h_j)} \right) \to (d_2, d_3) \quad \text{weakly in } L^2(\Omega; \mathbb{R}^3).
\]

Fix \(h_j \in \mathbb{R}^+\). If we apply Theorem 5.1 to
\[
u^{(h_j)}(z_1, z_2, z_3) := y^{(h_j)}(z_1, \frac{z_2}{h_j}, \frac{z_3}{h_j}),
\]
we also recover, by (32), the existence of a piecewise constant mapping \(R^{(h_j)}: [0, L] \to SO(3)\) and of a positive constant \(\overline{C}\) satisfying
\[
\int_{\Omega} |\nabla_{h_j} y^{(h_j)} - R^{(h_j)}|^2 \, dx \leq C^2 \int_{\Omega} \text{dist}^2(\nabla_{h_j} y^{(h_j)}, SO(3)) \, dx \leq \overline{C} h_j^2.
\]
(34)

To measure the deviation of \(\nabla_{h_j} y^{(h_j)}\) from \(SO(3)\), we also define the matrix-valued function \(G^{(h_j)}: \Omega \to M^{3 \times 3}\) as follows
\[
G^{(h_j)}(x) := \frac{R^{(h_j)}(x)}{h_j} \nabla_{h_j} y^{(h_j)}(x) - \text{Id}
\]
for any \(x \in \Omega\),
(35)

and we notice that, by (34), the sequence \((G^{(h_j)})\) is bounded in \(L^2(\Omega; M^{3 \times 3})\).

Then, by the reflexivity of the space, there exists \(G \in L^2(\Omega; M^{3 \times 3})\) such that (up to a subsequence)
\[
G^{(h_j)} \to G \quad \text{weakly in } L^2(\Omega; M^{3 \times 3}).
\]
(36)

By (6), we expand \(W\) in a neighbourhood of the identity
\[
W(Id + F) = \frac{1}{2} Q_3(F) + \eta(F),
\]
(37)

for any \(F \in M^{3 \times 3}\) such that \(\frac{\eta(F)}{|F|} \to 0\) as \(|F| \to 0\).

Denote \(\omega(t) := \sup_{|F| \leq t} |\eta(F)|, t \in \mathbb{R}^+\). Then, by (37)
\[
W(Id + h_j F) \geq \frac{1}{2} Q_3(h_j F) - \omega(|h_j F|)
\]
(38)
and \( \omega(t) \to 0 \) as \( t \to 0 \). Moreover, by the frame-indifference of \( W \), by (6), (35) and (38), we get
\[
\frac{1}{h^2_j} \int_{\Omega} u(x_2, x_3)W(\nabla_{h_j} y^{(h_j)})
= \frac{1}{h^2_j} \int_{\Omega} u(x_2, x_3)W(R^{(h_j)}(x_1)^T \nabla_{h_j} y^{(h_j)})
dx
= \frac{1}{h^2_j} \int_{\Omega} u(x_2, x_3)W(Id + h_j G^{(h_j)}(x))
dx
\geq \int_\Omega u(x_2, x_3)(\frac{1}{2}Q_3(G^{(h_j)}) - \frac{1}{h^2_j} \omega(h_j|G^{(h_j)}|))dx.
\]
Moreover, since \( Q_3 \) is nonnegative definite (by the hypotheses on \( W \)) and, therefore, lower-semicontinuous w.r.t. the convergence in (36), we get
\[
\liminf_{j \to \infty} \frac{1}{h^2_j} \int_{\Omega} u(x_2, x_3)W(\nabla_{h_j} y^{(h_j)})
dx \geq \frac{1}{2} \int_{\Omega} u(x_2, x_3)Q_3(G)
dx.
\]
We conclude the first part of the proof by showing that
\[
\liminf_{j \to \infty} \frac{1}{h^2_j} \int_{\Omega} u(x_2, x_3)W(\nabla_{h_j} y^{(h_j)})dx \geq \frac{1}{2} \int_{0}^{L} Q_2(R^3 R_{1,1},x_1)dx_1,
\]
where \( R := (y_1, d_2, d_3) \).

Let \( G^{(h_j)}_1 \) and \( G_1 \) denote the first columns of \( G^h \) and \( G \), respectively, consider the finite difference quotient of \( G^{(h_j)}_1 \) in the \( x_k \)-directions \( k = 2, 3 \)
\[
H^{(h_j)}_k(x) := \frac{G^{(h_j)}_1(x + te_k) - G^{(h_j)}_1(x)}{t}
= R^{(h_j)}(x_1)^T y^{(h_j)}_1(x + te_k) - y^{(h_j)}_1(x), \quad x \in \Omega, \; t \in \mathbb{R},
\]
let \( S' \) be a compact subset of \( S \), let \( |t| < \text{dist}(S', \partial S) \) and let \( \Omega' := (0, L) \times S' \). By (36), it holds that
\[
H^{(h_j)}_k(x) \to H_k \quad \text{weakly in } L^2(\Omega'; \mathbb{R}^3),
\]
with
\[
H_k(x) := \frac{G_1(x + te_k) - G_1(x)}{t}.
\]
Moreover, by Theorem 5.2 and (34),
\[
R^{(h_j)} \to R \quad \text{strongly in } L^2(\Omega; M^{3 \times 3})
\]
and so
\[
\frac{y^{(h_j)}_1(x + te_k) - y^{(h_j)}_1(x)}{th_j} = R^{(h_j)}H^{(h_j)}_k \to RH_k \quad \text{weakly in } L^2(\Omega'; \mathbb{R}^3).
\]
To find a representation of the limit \( H_k \), note that the left-hand side of (43) equals the transverse average

\[
\frac{y_1^{(h_j)}(x + te_k) - y_1^{(h_j)}(x)}{th_j} = \partial_{x_1} \left( \frac{1}{t} \int_0^t \frac{1}{h_j} y_k^{(h_j)}(x + se_k) \, ds \right)
\]

and that

\[
\frac{1}{t} \int_0^t \frac{1}{h_j} y_k^{(h_j)}(\cdot + se_k) \, ds \to \frac{1}{t} \int_0^t d_k(\cdot + se_k) \, ds = d_k \quad \text{strongly in } L^2(\Omega'; \mathbb{R}^3).
\]

This last convergence follows since, by Theorem 5.2,

\[
\frac{1}{h_j} y_k^{(h_j)} \to d_k \quad \text{strongly in } L^2(\Omega; \mathbb{R}^3)
\]

and \( d_k \) does not depend on \( x_k \), for any \( k = 2, 3 \).

By (44), we then get

\[
\frac{y_1^{(h_j)}(x + te_k) - y_1^{(h_j)}(x)}{th_j} \to d_{k,1} \quad \text{weakly in } W^{-1,2}(\Omega'; \mathbb{R}^3)
\]

and, by (43),

\[
H_k = R^T d_{k,1} \quad \text{for any } k = 2, 3
\]

and \( H_k \) is independent of \( x_2, x_3 \).

Fix \( x = (x_1, x_2, x_3) \in \mathbb{R}^3 \) and apply (41) with \( t = -x_3, k = 3 \). Then

\[
G_1(x) = G_1(x_1, x_2, 0) + x_3 H_3(x_1).
\]

In a similar way, applying again (41) with \( t = -x_2, k = 2 \), we get

\[
G_1(x) = G_1(x_1, x_2, 0) + x_3 H_3(x_1) = G_1(x_1, 0, 0) + x_2 H_2(x_1) + x_3 H_3(x_1),
\]

and, defining \( A(x_1) = R^T R, \) we finally have

\[
G_1(x) = G_1(x_1, 0, 0) + A(x_1) \begin{pmatrix} 0 \\ x_2 \\ x_3 \end{pmatrix}.
\]

We then need to identify the remaining columns of \( G \), namely \( G_2 \) and \( G_3 \). Define

\[
\alpha^{(h_j)}(x) := \frac{R^{(h_j)}(x_1)T}{h_j} \frac{1}{h_j} y_j^{(h_j)} - x_2 e_2 - x_3 e_3
\]

and note that

\[
\alpha_k^{(h_j)} = G_k^{(h_j)} \quad \text{for } k = 2, 3,
\]

where \( G_k^{(h_j)} \) denotes the \( k \)-th column of \( G^{(h_j)} \). Moreover, denote

\[
\alpha_0^{(h_j)}(x_1) := \int_S \alpha^{(h_j)}(x) \, dx_2 dx_3.
\]
Then, by the Poincaré inequality, there exists a positive constant \( C_S \), only dependent on \( S \), such that
\[
\int_S |\alpha^{(h_j)}(x) - \alpha_0^{(h_j)}(x)|^2 \, dx_2 dx_3 \leq C_S \int_S \left( |\alpha_{1,2}^{(h_j)}(x)|^2 + |\alpha_{3,3}^{(h_j)}(x)|^2 \right) \, dx_2 dx_3
\]
for a.e. \( x_1 \in (0, L) \) and, by integrating with respect to \( x_1 \), we get
\[
\|\alpha^{(h_j)} - \alpha_0^{(h_j)}\|_{L^2(\Omega)}^2 \leq C_S \left( \|\alpha_{1,2}^{(h_j)}\|_{L^2(\Omega)}^2 + \|\alpha_{3,3}^{(h_j)}\|_{L^2(\Omega)}^2 \right).
\]
Since \((G^{(h_j)})\) is bounded in \( L^2(\Omega; \mathbb{M}^{3 \times 3})\), then, by reflexivity, there exists a limit \( \alpha \in L^2(\Omega) \) such that
\[
(\alpha^{(h_j)} - \alpha_0^{(h_j)}) \rightharpoonup \alpha \quad \text{weakly in } L^2(\Omega; \mathbb{R}^3)
\]
and, by (36) and (46),
\[
\alpha_{,k} = G_k \quad \text{for } k = 2, 3.
\]
Therefore, \( \alpha_{,k} \in L^2(\Omega; \mathbb{R}^3) \) for \( k = 2, 3 \).

Define
\[
m := \int_S u(x_2, x_3) \, dx_2 dx_3
\]
and
\[
\tilde{\alpha} := \alpha(x_2, x_3) - \frac{x_2}{m} \int_S u(x_2, x_3) \alpha_{,2} \, dx_2 dx_3 - \frac{x_3}{m} \int_S u(x_2, x_3) \alpha_{,3} \, dx_2 dx_3.
\]
Then, \( \tilde{\alpha} \in W^{1,2}(S; \mathbb{R}^3) \) and, by construction
\[
\int_S u(x_2, x_3) \tilde{\alpha}_{,k} \, dx_2 dx_3 = 0 \quad \text{for any } k = 2, 3.
\]
Moreover, by (47)
\[
G_k(x) = \frac{1}{m} \int_S u(x_2, x_3) \alpha_{,k} \, dx_2 dx_3 + \tilde{\alpha}_{,k}, \quad \text{for any } k = 2, 3
\]
and so, by (45), we can decompose \( G \) as
\[
G = \left( G_1(x_1, 0, 0) \right| \frac{1}{m} \int_S u \, \alpha_{,2} \bigg| \frac{1}{m} \int_S u \, \alpha_{,3} \right) + \left( A(x_1) \left( \begin{array}{c} 0 \\ x_2 \\ x_3 \end{array} \right) \right| \tilde{\alpha}_{,2} \tilde{\alpha}_{,3},
\]
where the first part of the decomposition is independent of \( x_2 \) and \( x_3 \).
Therefore, by expanding the quadratic form $Q_3$ and by (4) and (48), we get
\[
\int_S u(x_2, x_3)Q_3(G(x)) \, dx_2 dx_3 =
\]
\[
= \int_S u(x_2, x_3)Q_3 \left( G_1(x_1, 0, 0) \left| \frac{1}{m} \int_S u_{\alpha, 2} \right| \frac{1}{m} \int_S u_{\alpha, 3} \right) \, dx_2 dx_3
\]
\[
+ \int_S u(x_2, x_3)Q_3 \left( A(x_1) \begin{pmatrix} 0 \\ x_2 \\ x_3 \end{pmatrix} | \tilde{\alpha}_2 | \tilde{\alpha}_3 \right) \, dx_2 dx_3.
\]

Finally, dropping the nonnegative first term on the right hand side and recalling the definition of $Q_2$ (7), we find

\[
\int_\Omega u(x_2, x_3)Q_3(G(x)) \, dx \geq \int_\Omega u(x_2, x_3)Q_3 \left( A(x_1) \begin{pmatrix} 0 \\ x_2 \\ x_3 \end{pmatrix} | \tilde{\alpha}_2 | \tilde{\alpha}_3 \right) \, dx
\]
\[
\geq \int_0^L Q_2(A(x_1)) \, dx_1 = \int_0^L Q_2(R^T R_1) \, dx_1.
\]

Then, (40) follows by (39).

**Part 2:** $\Gamma$-lim sup inequality

Fix $(y, d_2, d_3) \in A$ such that
\[
y \in C^2([0, L]; \mathbb{R}^3), \quad d_2, d_3 \in C^1([0, L]; \mathbb{R}^3),
\]
and for $x \in \Omega$ define
\[
y^{(h)}(x) := y(x_1) + hx_2d_2(x_1) + hx_3d_3(x_1) + h^2 \beta(x)
\]
for any $h > 0$, for a given $\beta \in C^1(\Omega; \mathbb{R}^3)$. By construction,
\[
\nabla_h y^{(h)} = \begin{pmatrix} y^{(h)}_1 \\ h \frac{1}{h} y^{(h)}_2 \\ \frac{1}{h} y^{(h)}_3 \end{pmatrix}
\]
\[
= \left( y_1 + h(x_2d_{2,1} + x_3d_{3,1}) + h^2 \beta_1 |d_2 + h\beta_2|d_3 + h\beta_3 \right)
\]
\[
= R + h (x_2d_{2,1} + x_3d_{3,1} |\beta_2| \beta_3) + h^2 (\beta_1 |0| 0),
\]
with $R = (y_1 |d_2| d_3) \in SO(3)$. Set
\[
B^{(h)}(x) = \frac{R^T \nabla_h y^{(h)} - Id}{h}
\]
\[
= R^T (x_2d_{2,1} + x_3d_{3,1} |\beta_2| \beta_3) + hR^T (\beta_1 |0| 0)
\]
and fix $h$ sufficiently small, such that $Id + hB^{(h)}(x)$ belongs to the neighbourhood of $Id$ for a.e. $x \in \Omega$ (the one in which the stored energy function $W$ is of class $C^2$). By Taylor expansion (37), if $F = Id + hB^{(h)}$, then, by (37) and (49)
\[
\lim_{h \to 0} \frac{1}{h^2} W(Id + hB^{(h)}(x)) = \frac{1}{2} Q_3(R^T (x_2d_{2,1} + x_3d_{3,1} |\beta_2| \beta_3)) \quad \text{a.e. } x \in \Omega
\]
and, for any $u \in L^\infty(S)$ there exists a positive constant $C$ such that
\[
\frac{1}{h^2} u(x_2, x_3) W(I d + h B^{(k)}) \leq C |B^{(k)}|^2 \leq C(|d_{2,1}|^2 + |d_{3,1}|^2 + |\nabla \beta|^2) \in L^1(\Omega) .
\]
Then, by the frame-indifference of $W$, the dominated convergence theorem, and since $I d + h B^{(k)} = R^T \nabla_h y^{(k)}$ by (49), we get
\[
\lim_{h \to 0} \frac{1}{h^2} \int_{\Omega} u(x_2, x_3) W(\nabla_h y^{(k)}) \, dx = \lim_{h \to 0} \frac{1}{h^2} \int_{\Omega} u(x_2, x_3) W(R^T \nabla_h y^{(k)}) \, dx = \frac{1}{2} \int_{\Omega} u(x_2, x_3) Q_3(R^T (x_2 d_{2,1} + x_3 d_{3,1} |\beta_2, \beta_3)) \, dx .
\]

In the general case, let $(y, d_2, d_3) \in \mathcal{A}$ and denote $R = (y_1 |d_2| d_3)$. By classical arguments, if $(\rho_j)_j$ is a sequence of mollifiers, then the sequence $\tilde{R}^{(j)} := \rho_j * R \in C^1([0, L]; \mathbb{M}^{3 \times 3})$ satisfies
\[
\tilde{R}^{(j)} \to R \quad \text{in} \quad W^{1,2}((0, L); \mathbb{M}^{3 \times 3}) ;
\]
\[
\tilde{R}^{(j)} \to R \quad \text{uniformly in} \quad [0, L] \quad \text{as} \quad j \to \infty ,
\]
where the last convergence follows by the Sobolev embedding.

Moreover, if $\alpha(x_1, \cdot) \in V$ denotes the minimizer defining $Q_3(R^T R_1)$, then the sequence $\alpha^{(j)} := \rho_j * \alpha \in C^1(\bar{\Omega}; \mathbb{R}^3)$ satisfies the following convergences
\[
\alpha^{(j)} \to \alpha \quad \text{in} \quad L^2(\Omega; \mathbb{R}^3) ;
\]
\[
\alpha^{(j)}_2 \to \alpha_2 \quad \text{in} \quad L^2(\Omega; \mathbb{R}^3) ;
\]
\[
\alpha^{(j)}_3 \to \alpha_3 \quad \text{in} \quad L^2(\Omega; \mathbb{R}^3) \quad \text{as} \quad j \to \infty .
\]
Denote $\Pi : \mathbb{M}^{3 \times 3} \to SO(3)$ the projection from a neighbourhood of $SO(3)$ onto $SO(3)$, define
\[
R^{(j)} := \Pi(\tilde{R}^{(j)}) \quad \text{for any} \quad j \in \mathbb{N}
\]
and set
\[
y^{(j)}(x_1) := \int_0^{x_1} R^{(j)}(s) e_1 \, ds , \quad d_2^{(j)}(x_1) := R^{(j)}(x_1) e_2 , \quad d_3^{(j)}(x_1) := R^{(j)}(x_1) e_3 .
\]
By construction, $(y^{(j)}, d_2^{(j)}, d_3^{(j)}) \in \mathcal{A}$ and, since $\tilde{R}^{(j)} \in C^1([0, L]; \mathbb{M}^{3 \times 3})$, then
\[
y^{(j)} \in C^2([0, L]; \mathbb{R}^3) , \quad d_2^{(j)}, d_3^{(j)} \in C^1([0, L]; \mathbb{R}^3)
\]
and, by (51)
\[
R^{(j)} = (y^{(j)}, d_2^{(j)}, d_3^{(j)}) \to R \quad \text{in} \quad W^{1,2}((0, L); \mathbb{M}^{3 \times 3}) \quad \text{and uniformly on} \quad [0, L] .
\]

For any $j \in \mathbb{N}$, consider the functional $F : \mathcal{A} \to [0, \infty)$
\[
F(y^{(j)}, d_2^{(j)}, d_3^{(j)}) := \int_{\Omega} u(x_2, x_3) Q_3(x_2(R^{(j)})^T d_2^{(j)} + x_3(R^{(j)})^T d_3^{(j)} |\alpha^{(j)}_2, \alpha^{(j)}_3) \, dx .
\]
Then, by (51) and (52) and by continuity of the functional on the left-hand side with respect to the kind of convergence in (51) and (52), we can assume (up to subsequences) that

\[(53)\]
\[
\frac{1}{2} F(y^{(j)}, d^{(j)}_2, d^{(j)}_3) \leq \frac{1}{2} \int_{\Omega} u(x_2, x_3) Q_3(x_2 R^T d_{2,1} + x_3 R^T d_{3,1} |\alpha_2| \alpha_3)) \, dx + \frac{1}{j} 
= I(y, d_2, d_3) + \frac{1}{j} \quad \text{for any } j \in \mathbb{N}.
\]

Finally, fix \((h_j)_j\) convergent to 0 as \(j \to \infty\), and considered the sequence

\[
y^{(h_j)}(x) := y^{(j)}(x_1) + h_j x_2 d^{(j)}_2(x_1) + h_j x_3 d^{(j)}_3(x_1) + h^2 R^{(j)} \alpha^{(j)},
\]
then, by (51) and (52), (up to subsequences)

\[
y^{(h_j)} \to y \quad \text{in } W^{1,2}(\Omega; \mathbb{R}^3),
\]

\[
\left(\frac{1}{h_j} y^{(h_j)}_2, \frac{1}{h_j} y^{(h_j)}_3\right) \to (d_2, d_3) \quad \text{in } L^2(\Omega; \mathbb{R}^3) \times L^2(\Omega; \mathbb{R}^3)
\]

and, by (50) and (53) (up to subsequences)

\[
\limsup_{h \to 0} \frac{1}{h^2} I^{(h_j)}(y^{(h_j)}) \, dx = I(y, d_2, d_3).
\]

\[\square\]

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