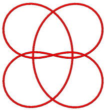

Approximating gradient flow evolutions of self-avoiding inextensible curves and elastic knots

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Motivation: Bilayer bending

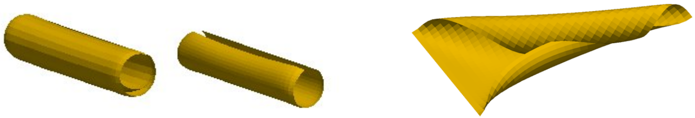
Energy for large bending deformations of thin elastic sheets (e.g., paper):

$$I_{\mathrm{bend}}(y) = \frac{1}{2}\int_\Omega |II|^2 \,\mathrm{d}x - \int_\Omega f \cdot y \,\mathrm{d}x, \quad I = \mathrm{id}$$

with fundamental forms $I, II : \Omega \to \mathbb{R}^{2\times 2}$ associated with $y : \Omega \to \mathbb{R}^3$

- Flat isometries: angle/length relations preserved
- Nonlinear constraint implies linearity: $|II|^2 = |D^2 y|^2$
- Kirchhoff's bending model derived by [Friesecke, James & Müller '02]

Nanotechnology application [B., Bonito & Nochetto '15]: bilayer bending



Challenge: Large deformations ok but injectivity not guaranteed

Overview

Energy as sum of bending and self-avoidance effects for arclength curves:

$$E(u) = \frac{\varkappa}{2} \int_I |u''(s)|^2 \, \mathrm{d}s + \varrho \, \mathrm{TP}(u), \quad |u'|^2 = 1$$

Reduce energy via gradient flow $\partial_t u = -\nabla_X E(u) + \big(\lambda u'\big)'$, discretized:

$$(d_t u_h^k, v_h)_X + \varkappa([u_h^k]'', v_h'') = -\varrho \, \mathrm{TP}(u_h^{k-1}), \quad [d_t u_h^k]', [v_h]' \perp [u_h^{k-1}]'$$

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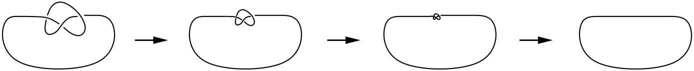
- Stability and convergence (energy law and consistency) ?
- Characterization of representatives (e.g., elastic knots always flat) ?

Modeling curves

Nonlinear bending

Aim: Detect low-energy configurations within isotopy class of u_0, i.e., prevent curves from self-intersecting and pulling tight

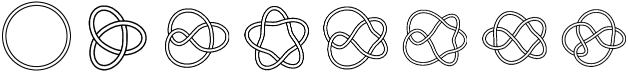


Curvature of arc-length curve $u : \mathbb{R}/\mathbb{Z} \to \mathbb{R}^3$ given by $k(s) = |u''(s)|$

Bending energy **[Bernoulli, 1738]**

$$u \mapsto \frac{1}{2} \int_{\mathbb{R}/\mathbb{Z}} k(s)^2 \, \mathrm{d}s$$

- Applications: cell filaments, DNA molecules, nanotechnology, ...
- Gradient flow [Dziuk, Kuwert, Schätzle; Barrett, Garcke, Nürnberg; Dall'Acqua, Lin, Pozzi; ...] – global constraints, no injectivity

Examples:  ...

Minimization problem

Let $\mathscr{C} = \left\{ u \in H^2(\mathbb{R}/\mathbb{Z}, \mathbb{R}^3) \,\middle|\, |u'| = 1, u \in \mathcal{K} \right\}$ for some isotopy class $\mathcal{K}$

Variational problem

$$E(u) = \frac{\varkappa}{2} \int_{\mathbb{R}/\mathbb{Z}} |u''(s)|^2 \, \mathrm{d}s + \varrho \, \mathrm{TP}(u) \to \min! \qquad \text{on } \mathscr{C}$$

- $\varkappa > 0$, $\varrho \geq 0$, in particular $\varkappa \gg \varrho$ (physical knots)
- Tangent-point functional TP is potential that prevents curves from leaving the isotopy class
- Simple model ignoring twist
- Computational challenge: strong forces related to bending have to be compensated by repulsive forces to avoid self-intersections
- Existence of minimizers for $\varkappa > 0$

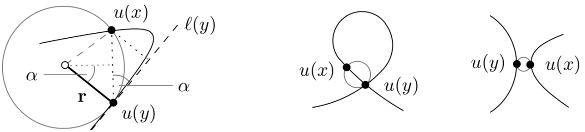
Tangent-point energies

Tangent-point energies

Modeling "thickness" by a smooth functional [Gonzalez & Maddocks '99]

$$\mathrm{TP}(u) = \frac{1}{2^q q} \iint_{[\mathbb{R}/\mathbb{Z}]^2} \frac{\mathrm{d}x\,\mathrm{d}y}{r_u(x,y)^q}, \qquad q > 2,$$

$r_u(x,y)$ is radius of circle tangential at $u(y)$ intersecting in $u(x)$:



- TP is nonlocal and nonlinear with $\frac{1}{r_u(x,y)} \xrightarrow{x \to y} k(y)$
- Self-avoiding property [Strzelecki & von der Mosel '10]
- Characterization of energy spaces [Blatt '13] $\rightsquigarrow$ $W^{2-1/q,q}$
- Smooth, two-dimensional domain, integrand of first variation in L^1

$$r_u(x,y) = \frac{|u(x)-u(y)|^2}{2\,\mathrm{dist}(u(x),\ell(y))} = \frac{|u(x)-u(y)|^2}{2\,|u'(y)\wedge(u(x)-u(y))|}$$

- Generalization to plates available

Bi-Lipschitz bounds

Bi-Lipschitz constant of embedded arclength parametrized curve u

$$\mathrm{biL}(u) = \sup_{x,y\in\mathbb{R}/\mathbb{Z},\, x\neq y} \frac{|x-y|}{|u(x)-u(y)|} \qquad (\geq 1)\,.$$

Lemma (Uniform bi-Lipschitz estimate) [Blatt & Reiter '15]

There is a uniform bound $C_{M,q} < \infty$ such that if $\mathrm{TP}(u) \leq M$ then

$$|x-y|_{\mathbb{R}/\mathbb{Z}} \leq C_{M,q}\,|u(x)-u(y)| \qquad \text{for all } x,y\in\mathbb{R}/\mathbb{Z}.$$

Note: Cannot expect to control $\mathrm{TP}(u)$ by Sobolev norms of u

Corollary (Self-avoidance)

Let $u_k \to u_\infty \in C^0(\mathbb{R}/\mathbb{Z},\mathbb{R}^3)$ pointwise with self-intersection, i.e., $u_\infty(x) = u_\infty(y)$ for $x \neq y$. Then $\mathrm{TP}(u_k) \to \infty$ as $k \to \infty$.

Proof. Assuming the contrary, we infer the existence of a constant $C < \infty$ with $0 < |x-y|_{\mathbb{R}/\mathbb{Z}} \leq C\,|u_k(x)-u_k(y)| \xrightarrow{k\to\infty} 0$. $\square$

Fractional Sobolev spaces

TP finite for bi-Lipschitz curves $u \in W^{1+s,q}(\mathbb{R}/\mathbb{Z};\mathbb{R}^3)$ with $s = 1 - 1/q$:

$$
\begin{aligned}
q\,\mathrm{TP}(u) &= \int_{\mathbb{R}/\mathbb{Z}} \int_{-1/2}^{1/2} \frac{|u'(y) \wedge (u(y+z) - u(y) - zu'(y))|^q}{|u(y+z) - u(y)|^{2q}}\,\mathrm{d}z\,\mathrm{d}y \\
&\le \mathrm{biL}(u)^{2q} \int_{\mathbb{R}/\mathbb{Z}} \int_{-1/2}^{1/2} \frac{\left|\int_0^1 (u'(y+\vartheta z) - u'(y))\,\mathrm{d}\vartheta\right|^q |z|^q}{|z|^{2q}}\,\mathrm{d}z\,\mathrm{d}y \\
&\le \mathrm{biL}(u)^{2q} \int_{\mathbb{R}/\mathbb{Z}} \int_{-1/2}^{1/2} \int_0^1 \frac{|u'(y+\vartheta z) - u'(y)|^q}{|z|^q}\,\mathrm{d}\vartheta\,\mathrm{d}z\,\mathrm{d}y \\
&\le \mathrm{biL}(u)^{2q} \int_0^1 \int_{\mathbb{R}/\mathbb{Z}} \int_{-\vartheta/2}^{\vartheta/2} \vartheta^{q-1} \frac{|u'(y+\tilde{z}) - u'(y)|^q}{|z|^q}\,\mathrm{d}\tilde{z}\,\mathrm{d}y\,\mathrm{d}\vartheta \\
&\le \mathrm{biL}(u)^{2q} \int_{\mathbb{R}/\mathbb{Z}} \int_{-1/2}^{1/2} \frac{|u'(y+z) - u'(y)|^q}{|z|^q}\,\mathrm{d}z\,\mathrm{d}y = \mathrm{biL}(u)^{2q} |u'|^q_{W^{s,q}}.
\end{aligned}
$$

- Use of Sobolev-Slobodeckii seminorm
- Argument transfers to various other estimates

Bounds on variations of TP

Lemma (B)

There are $c_1, c_2, R > 0$ depending on $0 < \lambda \leq \Lambda$, $M > 0$, n, and q such that any embedded and regular curve $u \in W^{2-1/q,q}(\mathbb{R}/\mathbb{Z}, \mathbb{R}^3)$ with

$$\lambda \leq |u'| \leq \Lambda \qquad \textit{and} \qquad \mathrm{TP}(u) \leq M$$

satisfies

$$|\delta\, \mathrm{TP}(u)[w]| \leq c_1 \, \|u'\|^q_{W^{1-1/q,q}} \, \|w'\|_{W^{1-1/q,q}}$$

and, for any $z \in W^{2-1/q,q}$ with $\|z'\|_{W^{1-1/q,q}} \leq R$,

$$\left|\delta^2\, \mathrm{TP}(u+z)[v,w]\right| \leq c_2 \left(\|u'\|^{2q+2}_{W^{1-1/q,q}} + 1 \right) \|v'\|_{W^{1-1/q,q}} \, \|w'\|_{W^{1-1/q,q}} \, .$$

- Use explicit formula for the second derivative of TP
- Employ uniform bi-Lipschitz estimate
- Extends results from [Blatt & Reiter '15]

The gradient flow

The H^2 flow

Recall energy functional

$$E(u) = \frac{\varkappa}{2} \int_{\mathbb{R}/\mathbb{Z}} |u''(s)|^2 \, \mathrm{d}s + \varrho \mathrm{TP}(u) \to \min! \qquad \text{on } \mathscr{C}$$

H^2 gradient flow in $\mathscr{C}$

Compute family $u : [0, T] \to H^2(\mathbb{R}/\mathbb{Z}; \mathbb{R}^3)$ with $u(0) = u_0$ and

$$(u_t, \phi)_{H^2} = -\varkappa(u'', \phi'') - \varrho\delta\, \mathrm{TP}(u)[\phi]$$

for all $\phi \in H^2$ subject to $\phi' \cdot u' = 0$ and $u'_t \cdot u' = 0$.

Semi-implicit discretization defined by linearly constrained system

$$(d_t u^k, \phi)_{H^2} + \varkappa([u^k]'', \phi'') = -\varrho\delta\, \mathrm{TP}(u^{k-1})[\phi]$$
$$\text{s.t. } [d_t u^k]' \cdot [u^{k-1}]' = 0, \quad \phi' \cdot [u^{k-1}]' = 0$$

where $d_t u^k = (u^k - u^{k-1})/\tau$ is backward difference quotient.

- Explicit treatment of TP: parallelization of assembly, sparse matrices

Stability result [B., Reiter '18]

For $\varkappa > 0$, $\varrho \geq 0$, and $q \in (2,4]$, let $(u^k)_{k=0,\dots,K} \subset H^2(\mathbb{R}/\mathbb{Z}, \mathbb{R}^3)$ be unique sequence defined for u^0 with $|[u^0]'|^2 = 1$ via

$$(d_t u^k, \phi)_{H^2} + \varkappa([u^k]'', \phi'')_{L^2} = -\varrho\delta\,\mathrm{TP}(u^{k-1})[\phi],$$

subject to the linearized arclength conditions

$$[d_t u^k]' \cdot [u^{k-1}]' = 0, \qquad \phi' \cdot [u^{k-1}]' = 0.$$

There exists $c' = c'(\varkappa, \varrho, e_0, q) > 0$ with $e_0 = E(u^0)$ which is independent of $\tau > 0$ such that if $\tau c' \leq 1$ then we have the energy stability property

$$E(u^L) + (1 - c'\tau)\tau \sum_{\ell=1}^{L} \|d_t u^\ell\|_{H^2}^2 \leq E(u^0)$$

for all $0 \leq L \leq K$. Moreover, arclength parametrization is preserved:

$$\max_{k=0,\dots,L} \big\| |[u^k]'|^2 - 1 \big\|_{L^\infty} \leq 4\tau c_\infty^2 e_0.$$

Proof of stability property

Want to obtain discrete energy law:

$$E(u^L) + (1 - c'\tau)\tau \sum_{\ell=1}^{L} \|d_t u^\ell\|_{H^2}^2 \le E(u^0)$$

- existence of iterates due to Lax–Milgram
- induction over $L = 1, \ldots, K$

$(*)$ choose $\phi = d_t u_k$ in $(d_t u^k, \phi)_{H^2} + \varkappa([u^k]'', \phi'')_{L^2} = -\varrho\delta\,\mathrm{TP}(u^{k-1})[\phi]$

- applying Lemma (B) and Poincaré inequalities yields

$$\|d_t u^k\|_{H^2}^2 + \varkappa d_t \|[u^k]''\|_{L^2}^2 \le c_a = c_a(\varkappa, \varrho, q, e_0)$$

- $\tau c_a \le e_0$ gives $\tau \sum_{\ell=1}^{k} \|d_t u^\ell\|_{H^2}^2 + \varkappa \|[u^k]''\|_{L^2}^2 \le e_0$
- $|[u^k]'|^2 = |[u^{k-1}]'|^2 + \tau^2 |[d_t u^k]'|^2 = \cdots = |[u^0]'|^2 + \tau^2 \sum_{\ell=1}^{k} |[d_t u^\ell]'|^2$
  $\rightsquigarrow$ arc-length preservation
- apply second part of Lemma (B) to expand the TP-term in $(*)$
  $\rightsquigarrow (1 - c_b\tau)\|d_t u^k\|_{H^2}^2 + d_t E(u^k) \le 0$ for $\tau \ll 1$

Spatial discretization

Choice of FE space

Subspaces $\mathbb{V}_h \subset H^2_{\mathrm{BC}}(I, \mathbb{R}^3)$ subordinated to a partition $\mathcal{T}_h$ of $I = [0,1]$ given by nodes $z_0 < z_1 < \cdots < z_M$

- $\mathbb{V}_h \subset \mathcal{S}^{1,3}(\mathcal{T}_h, \mathbb{R}^3)$ cubic C^1 splines; dof's are positions and tangents
- given $\widetilde{u}_h \in \mathcal{S}^{1,3}(\mathcal{T}_h, \mathbb{R}^3)$ include linearized arc-length condition via

$$\mathbb{F}_h[\widetilde{u}_h] = \{v_h \in \mathbb{V}_h \,|\, v_h'(z_i) \cdot \widetilde{u}_h'(z_i) = 0 \text{ for all } i = 0, \ldots, M\}$$

- Start with initial curve $u_h^0 \in \mathbb{V}_h$ with $\left|(u_h^0)'(z_i)\right| = 1$ for $i = 0, \ldots, M$

Algorithm. (i) Given $u_h^k \in \mathbb{V}_h$ compute velocity $v_h^k \in \mathbb{F}_h[u_h^k]$ such that

$$(v_h^k, \phi_h)_{H^2} = -\varkappa([u_h^k + \tau v_h^k]'', \phi_h'') - \varrho\, \delta\, \mathrm{TP}(u_h^k)[\phi_h] \qquad \forall \phi_h \in \mathbb{F}_h[u_h^k]$$

(ii) Update $u_h^{k+1} = u_h^k + \tau v_h^k$ and repeat.

Scheme requires solving linearly constrained quadratic problems

Removing the diagonal

If the integration domain in TP is replaced by $\mathcal{R}_\varepsilon$,

$$\mathrm{TP}_\varepsilon(u) = \tfrac{1}{q} \iint_{\mathcal{R}_\varepsilon} \frac{|u'(y) \wedge (u(x) - u(y))|^q}{|u(x) - u(y)|^{2q}} \,\mathrm{d}x \,\mathrm{d}y,$$

Here $\mathcal{R}_\varepsilon$ is any measurable set with

$$\widetilde{\mathcal{R}}_\varepsilon = \left\{(x, y) \in \mathbb{R}/\mathbb{Z} \times \mathbb{R}/\mathbb{Z} : |x - y|_{\mathbb{R}/\mathbb{Z}} \geq \varepsilon\right\} \subset \mathcal{R}_\varepsilon \subset \widetilde{\mathcal{R}}_{\varepsilon/2}.$$

Lemma **[B., Reiter, Riege '17]**

We have $\mathrm{TP}_\varepsilon(u) \nearrow \mathrm{TP}(u)$ as $\varepsilon \searrow 0$ for any $u \in \mathscr{C}$ and $q \in [2, \infty)$.
If $u \in \mathscr{C} \cap H^2(\mathbb{R}/\mathbb{Z}, \mathbb{R}^3)$ and $q \in [2, 4)$ we have

$$|\mathrm{TP}_\varepsilon(u) - \mathrm{TP}(u)| \leq C_{\delta,q} \varepsilon^{2-q/2-\delta} \,\mathrm{biL}(u)^{2q} \,\|u'\|_{H^1}^q .$$

- Linear convergence if $u \in \mathscr{C} \cap W^{3,q}(\mathbb{R}/\mathbb{Z}, \mathbb{R}^3)$ and $q \in [2, \infty)$

Approximation result

Define $\mathcal{Q}_h$ via nodal averages on rectangles $I_j \times I_k \subset \mathcal{R}$

$$\mathrm{TP}_{\varepsilon,h}(u) = \frac{1}{q} \iint_{\mathcal{R}_{\varepsilon,h}} \mathcal{Q}_h \left[\frac{|u'(y) \wedge (u(x) - u(y))|^q}{|u(x) - u(y)|^{2q}} \right] \mathrm{d}x \, \mathrm{d}y,$$

Proposition [B., Reiter, Riege '17]

For $0 < 2h \leq \varepsilon$, $q \in [2, \infty)$, and $u \in \mathscr{C} \cap H^2$ we have

$$|\mathrm{TP}_{\varepsilon,h}(u) - \mathrm{TP}_{\varepsilon}(u)| \leq C_q \sqrt{h} \left(\frac{\mathrm{biL}(u)}{\varepsilon} \right)^{q+1} \left(\|u''\|_{L^2} + 1 \right),$$

where integration domain of $\mathrm{TP}_{\varepsilon}$ is chosen to be $\mathcal{R}_{\varepsilon} = \mathcal{R}_{\varepsilon,h}$.

Proof. Show that $f \in C^{0,1/2}$ on $\mathcal{R}_{\varepsilon,h}$ for

$$f(x,y) = \frac{|u'(y) \wedge (u(x) - u(y))|^q}{|u(x) - u(y)|^{2q}} \qquad \square$$

- Linear convergence assuming higher regularity
- Related estimate for first variation

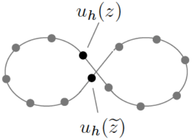
Discrete energy barrier

Discretized tangent-point functional

$$\mathrm{TP}_{\varepsilon,h}(u) = \frac{1}{q} \sum_{\substack{i,j=0,\dots,M \\ |z_i - z_j| \geq \varepsilon}} h_i h_j \beta_i \beta_j \frac{\left| u'(z_i) \wedge \left(u(z_i) - u(z_j) \right) \right|^q}{\left| u(z_i) - u(z_j) \right|^{2q}}$$

Consider discrete self-contact

$$|u_h(z) - u_h(\tilde{z})| \sim h$$



for non-neighboring nodes z and $\tilde{z}$.

If $u_h'(z)$ and $u_h(z) - u_h(\tilde{z})$ are non-parallel then $\mathrm{TP}_{\varepsilon,h}(u_h) \geq ch^{2-q}$

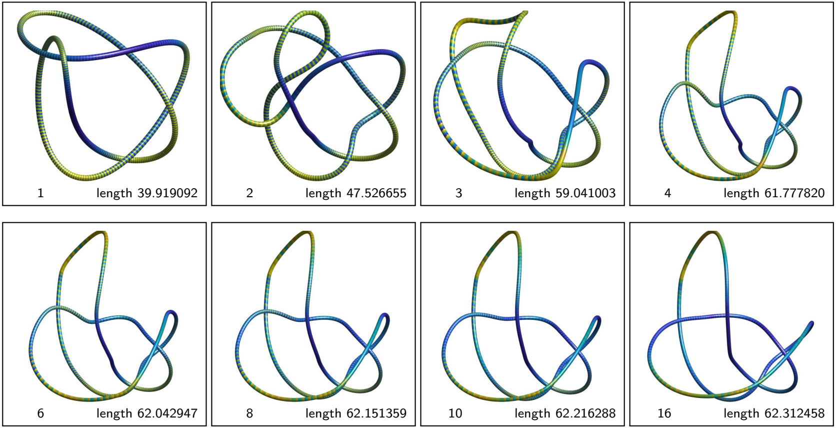
- Exponent $q = 2$ insufficient to avoid self-intersections
- For discrete energy barrier choose $\varrho \geq ch^{q-2-\sigma}$ with $\sigma > 0$; allows for $\sigma \to 0$ as $h \to 0$
- Need h sufficiently small to dominate initial total energy

Stability and isotopy preservation

Preasymptotic instability

Using an initial curve from the 5_2 isotopy class with length ≈ 39.9.

$\varkappa = \frac{1}{10}$, $\varrho = 1$, 400 nodes, $\tau = \frac{1}{5}\sqrt{h_{\max}}$ — note critical $\varrho/\varkappa \gg 1$



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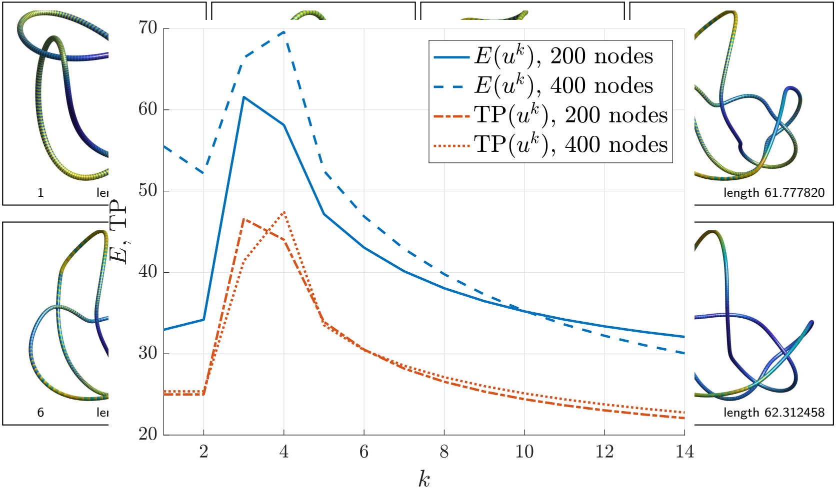
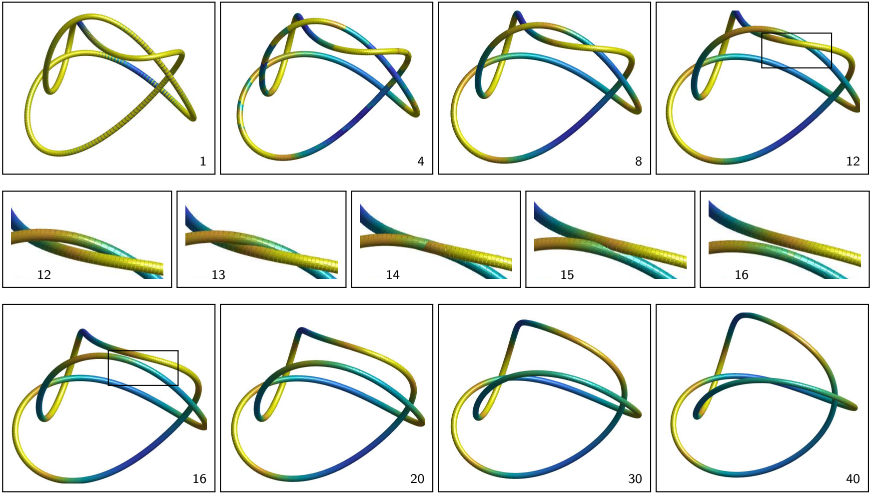


Change of isotopy class

Same curve; $\varkappa = 1$, $\varrho = \frac{1}{100}$, 50 nodes, $\tau \approx \frac{1}{5}$ — note critical $0 < \varrho \ll 1$



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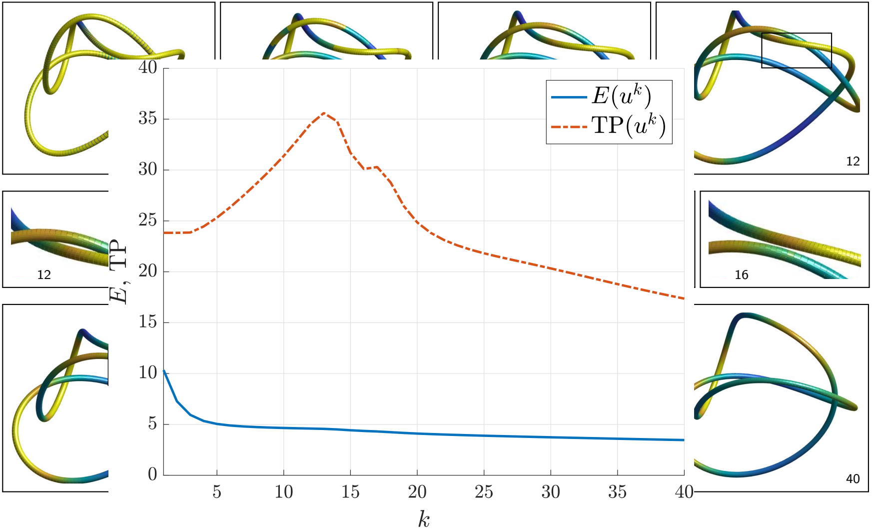


Observations

Numerical scheme is . . .

. . . energy stable if the time-step size τ satisfies $\tau \leq F(\varkappa, \varrho)$

- $F(\varkappa, \varrho) = \mathcal{O}(1)$ if $\varkappa \gg \varrho$
- $F(\varkappa, \varrho) \to 0$ as $\varkappa/\varrho \to 0$
- mesh dependence if $\varrho \gg \varkappa$, possibly related to quadrature errors for TP

. . . preserving the isotopy class if *energy stable* and if for fixed $\varkappa > 0$ the spacial mesh size $h > 0$ satisfies $h \leq G(e_0, \varrho)$

- initial energy $e_0 = E(u_0)$
- $G(e_0, \varrho) \to 0$ as $e_0 \to \infty$ or $\varrho \to 0$

... i.e., bending term gives stability and self-avoidance potential requires sufficient resolution

Simulations

How do minimizers look like?

Expect points of self-intersection for $\varrho \to 0$

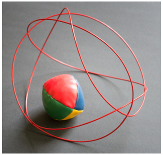
- Extract a weakly converging subsequence of minimizers as $\varrho \to 0$
- If the limit is embedded, there is a C^1 neighborhood of admissible comparison curves

$\rightsquigarrow$ limit curve is a local minimizer of the bending energy

Theorem [Langer & Singer '85]

The circle is the only (local) minimizer of the bending energy in $\mathbb{R}^3$.

- the bending energy cannot be minimized within an isotopy class except for the trivial class
- self-contact is present also in physical models



Unknot class

A non-global minimizer in the unknot class, evolution gets stuck

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nodes: 376, $h_{\text{max}} = 0.1255$

Trefoil evolution

Evolution towards a symmetric possibly unstable configuration

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nodes: 401, $h_{\mathrm{max}} = 0.1312$

Trefoil with perturbation

Avoid unstable symmetric configuration via perturbations

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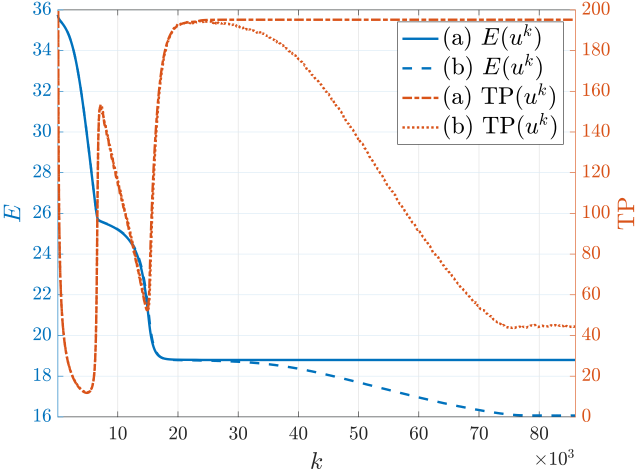
nodes: 401, $h_{\max} = 0.1312$

Trefoil with and without perturbation

Comparison of energies for unperturbed and perturbed evolutions



Minimizer close to doubly covered circle [Gerlach, Reiter, von der Mosel '17]

Figure-eight – first experiment

Initial curve equivalent to figure-eight knot

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nodes 400, $h_{\max} = 0.1370$

Figure-eight – second experiment

Different initial curve equivalent to figure-eight knot

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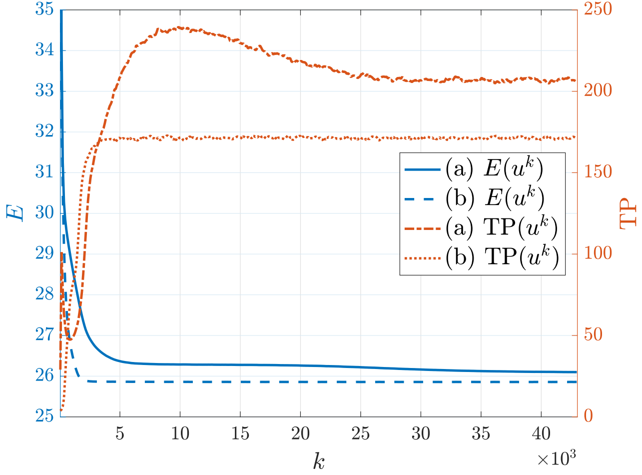
nodes 415, $h_{\max} = 0.1306$

Figure-eight – comparison

Comparison of energies for different initial curves



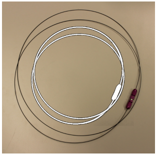
Spherical [Gallotti & Pierre-Louis '07 ; Gerlach et al. '17] and planar [Avvakumov & Sossinsky '14] stationary configurations

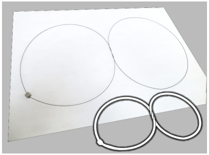
Summary

Summary

- numerical scheme for self-avoiding inextensible curves
- stability result for the semi-discrete setting
  - energy decay and arclength preservation (imply convergence)
  - preservation of isotopy class (for sufficient resolution)
- fast, simple scheme (minutes to compute evolutions)

- future aspects
  - include other physical quantities, e.g., twist
  - extension to self-avoiding flat plates
  - elastic knots always flat ?





Thank you!