Approximation of self-avoiding inextensible curves

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Motivation

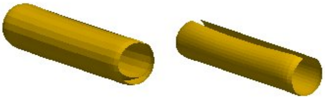
Energy for large bending deformations of thin elastic sheets:

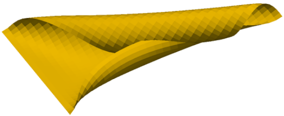
$$I_{\mathrm{bend}}(y) = \frac{1}{2}\int_\omega |II|^2 \,\mathrm{d}x - \int_\omega f \cdot y \,\mathrm{d}x, \qquad I = \mathrm{id}$$

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 simulation (B., Bonito & Nochetto '15): bilayer bending





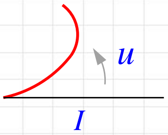
Problem: Large deformations ok but injectivity not guaranteed

Curves

Simpler setting: inextensible curves describing elastic rods

$$I_{\mathrm{bend}}(u) = \frac{1}{2}\int_I |u''(x)|^2 \,\mathrm{d}x, \quad |u'(x)|^2 = 1$$

- curves parametrized by arc-length
- well posed minimization problems on $H^2(I;\mathbb{R}^3)$
- derivation from hyperelasticity: Müller & Mora '04



EL eq's: stationary $u \in H^2(I;\mathbb{R}^3)$ with $|u'(x)|^2 = 1$ characterized by

$$(u'', v'') = \int_I u''(x)\cdot v''(x)\,\mathrm{d}x = 0$$

for admissible $v \in H^2(I;\mathbb{R}^3)$ with

$$u'\cdot v' = 0 \quad \text{in } I.$$

Iteration

B' 12: Practical minimization via gradient flow

$$(\partial_t u, v) + (u'', v'') = 0, \quad u(0) = u_0, \quad |u'(t,x)|^2 = 1$$

for admissible $v \in H^2(I;\mathbb{R}^3)$ with $v' \cdot u'(t,\cdot) = 0$

Observation: relation $\partial_t u' \cdot u' = 0$ implies constraint preservation,

$$|u'(t)|^2 - |u'(0)|^2 = \int_0^t \frac{d}{ds}|u'(s)|^2 \, \mathrm{d}s = 2\int_0^t \partial_t u' \cdot u' \, \mathrm{d}s = 0$$

Algorithm: given u^{n-1} compute $d_t u^n$ with $[d_t u^n]' \cdot [u^{n-1}]' = 0$ and

$$(d_t u^n, v) + ([u^{n-1} + \tau d_t u^n]'', v'') = 0$$

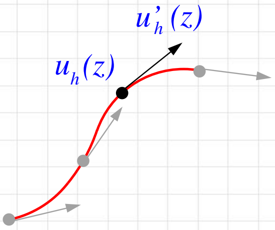
for v with $v' \cdot [u^{n-1}]' = 0$ and update $u^n = u^{n-1} + \tau d_t u^n$

Unconditional stability and controlled constraint violation:

$$|[u^n]'|^2 = |[u^{n-1}]'|^2 + \tau^2 |[d_t u^n]'|^2 = \ldots = |[u^0]'|^2 + \tau^2 \sum_{\ell=1}^{n} |[d_t u^\ell]'|^2 = 1 + \mathcal{O}(\tau)$$

Discretization

Use H^2 conforming piecewise cubic C^1 curves



- DOFs: positions and tangents
- good approximation properties
- flexibility for boundary conditions

Impose constraint/orthogonality at nodes z, i.e.,

$$|u_h'(z)|^2 = 1, \qquad d_t u_h'(z) \cdot u_h'(z) = 0$$

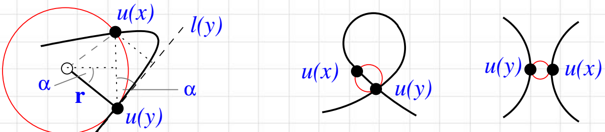
- constraint satisfied in limit $h \to 0$ if H^2 bounds available

Self-avoidance

Maddocks & Gonzales '99: Injectivity enforced via potential

$$\mathrm{TP}(u) = \frac{2^{-q}}{q} \iint_{I\times I} \frac{1}{\mathbf{r}^q(u(y),u(x))}\,\mathrm{d}x\,\mathrm{d}y$$

with $\mathbf{r}$ = radius of circle tangential at $u(y)$ and intersecting in $u(x)$



$\mathbf{r} \longrightarrow 0$ as $u(x) \longrightarrow u(y)$

Using $|u'(y)| = 1$ and $\sin\alpha = |u'(y) \wedge [u(y) - u(x)]|/|u(y) - u(x)|$

$$\mathbf{r}(u(y),u(x)) = \frac{|u(y)-u(x)|^2}{2|u'(y)\wedge[u(y)-u(x)]|}$$

and $1/\mathbf{r} \approx |u''(x)|/2$ for $x \approx y$

Properties

Tangent-point potential

$$\mathrm{TP}(u) = \frac{1}{q} \iint_{I\times I} \frac{|u'(y) \wedge [u(y) - u(x)]|^q}{|u(y) - u(x)|^{2q}} \,\mathrm{d}x\,\mathrm{d}y$$

Sobolev–Slobodeckii spaces defined via seminorm, $0 < s < 1$,

$$[f]_{W^{s,p}(I;\mathbb{R}^3)} = \left(\iint_{I\times I} \frac{|f(x) - f(y)|^p}{|x - y|^{1+sp}} \,\mathrm{d}x\,\mathrm{d}y \right)^{1/p}$$

Class of embedded and arc-length parametrized curves:

$$\mathcal{C}_q = \left\{ u \in W^{2-1/q,q}(I;\mathbb{R}^3) : u \text{ embedded and } |u'(x)| = 1 \right\}$$

Basic properties (Blatt '13, Blatt & Reiter '15) for $q > 2$:

- $u \in \mathcal{C}_q$ implies $1 \le \mathrm{biL}(u) = \mathrm{Lip}(u^{-1}) < \infty$
- TP finite on $\mathcal{C}_q$ and $\mathrm{TP}(u) \le M$ implies $\mathrm{biL}(u) \le C_{M,q}$
- TP is knot energy: $\mathrm{TP}(u_k) \to \infty$ if $\mathrm{pointw.}-\lim u_k \notin \mathcal{C}_q$

Variation

Blatt & Reiter '15: TP is C^1 on embedded $W^{2-1/q,q}$ curves with

$$\delta\mathrm{TP}(u) = \mathcal{M}(u; u, \varphi) + \mathcal{M}(u; \varphi, u) - 2\mathcal{A}(u; u, \varphi)$$

where

$$\mathcal{M}(u; v, w) = \iint_{I\times I} \Phi(x,y) \cdot \big(v'(y) \wedge \big(w(x) - w(y)\big)\big)\,\mathrm{d}x\,\mathrm{d}y$$

$$\mathcal{A}(u; v, w) = \iint_{I\times I} \Psi(x,y)\big(v(x) - v(y)\big) \cdot \big(w(x) - w(y)\big)\,\mathrm{d}x\,\mathrm{d}y$$

with

$$\Phi(x,y) = \frac{|u'(y) \wedge (u(x) - u(y))|^{q-2}}{|u(x) - u(y)|^{2q}} \big(u'(y) \wedge \big(u(x) - u(y)\big)\big),$$

$$\Psi(x,y) = \frac{|u'(y) \wedge \big(u(x) - u(y)\big)|^{q}}{|u(x) - u(y)|^{2q+2}}$$

Note: $\mathcal{A}(u; \cdot, \cdot)$ positive semidefinite and $\mathcal{M}(u; u, u) \geq 0$

Approximation

(A) Removal of singular diagonal

$$\mathrm{TP}_\varepsilon(u) = \iint_{|x-y|\geq\varepsilon} \frac{|u'(y) \wedge [u(y)-u(x)]|^q}{|u(y)-u(x)|^{2q}} \,\mathrm{d}x\,\mathrm{d}y$$

leads to error

$$\left|\mathrm{TP}(u) - \mathrm{TP}_\varepsilon(u)\right| \leq \begin{cases} c_{\delta,q}\, \varepsilon^{2-2/q-\delta}\, \mathrm{biL}(u)^{2q} \|u'\|_{H^1} & u \in H^2 \\ c_q\, \varepsilon\, \mathrm{biL}(u)^{2q} \|u''\|_{L^q}^2 & u \in W^{2,q} \end{cases}$$

(B) Use of quadrature

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

with node average on rectangles $I_j \times I_k$ gives

$$\left|\mathrm{TP}_\varepsilon(u) - \mathrm{TP}_{\varepsilon,h}(u)\right| \leq \begin{cases} c_q\, h^{1/2} \varepsilon^{-(q+1)} \left(\|u''\|_{L^2} + 1\right) & u \in H^2 \\ c_q h\left(\|u\|_{W^{3,\infty}} + 1\right) & u \in W^{3,\infty} \end{cases}$$

Proofs

With $\mathcal{S}_\varepsilon = \{(x,y) \in I \times I : |x-y| < \varepsilon\}$ we have

$$
\begin{aligned}
q\big(\mathrm{TP}(u) - \mathrm{TP}_\varepsilon(u)\big) &\le \iint_{\mathcal{S}_\varepsilon} \frac{\big|u'(y) \wedge \big(u(y+z) - u(y) - zu'(y)\big)\big|^q}{\big|u(y+z)-u(y)\big|^{2q}} \,\mathrm{d}z\,\mathrm{d}y \\
&\le \mathrm{biL}(u)^{2q} \iint_{\mathcal{S}_\varepsilon} \frac{\big|\int_0^1 \big(u'(y+\vartheta z) - u'(y)\big)\,\mathrm{d}\vartheta\big|^q |z|^q}{|z|^{2q}} \,\mathrm{d}z\,\mathrm{d}y \\
&\le \mathrm{biL}(u)^{2q} \iint_{\mathcal{S}_\varepsilon} \int_0^1 \frac{\big|u'(y+\vartheta z) - u'(y)\big|^q}{|z|^q} \,\mathrm{d}\vartheta\,\mathrm{d}z\,\mathrm{d}y \\
&\le \mathrm{biL}(u)^{2q} \int_0^1 \iint_{\mathcal{S}_{\vartheta\varepsilon}} \vartheta^{q-1} \frac{\big|u'(y+z) - u'(y)\big|^q}{|z|^q} \,\mathrm{d}z\,\mathrm{d}y\,\mathrm{d}\vartheta \\
&\le \mathrm{biL}(u)^{2q} \iint_{\mathcal{S}_\varepsilon} \frac{\big|u'(y+z) - u'(y)\big|^q}{|z|^q} \,\mathrm{d}z\,\mathrm{d}y \quad \big(\le \ldots\big)
\end{aligned}
$$

For quadrature estimate show that integrand is in $C^{0,1/2}$

Gradient flow

Weighted sum of bending energy and self-avoidance potential

$$I^{\text{tot}}(u) = I_{\text{bend}}(u) + \varrho \mathrm{TP}_\varepsilon(u)$$

leads to gradient flow dynamics

$$(\partial_t u, v) = -\delta I^{\text{tot}}(u)[v] = -\mathcal{B}(u, v) - 2\varrho \mathcal{M}_\varepsilon^{\text{sym}}(u; u, v) + 2\varrho \mathcal{A}_\varepsilon(u; u, v)$$

with

$$2\mathcal{M}_\varepsilon^{\text{sym}}(u; v, w) = \mathcal{M}_\varepsilon(u; v, w) + \mathcal{M}_\varepsilon(u; w, v)$$

Semi-implicit discretization

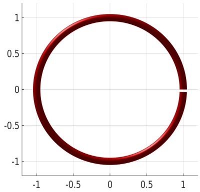
$$(d_t u^n, v) + \mathcal{B}(u^n, v) + 2\varrho \mathcal{M}_\varepsilon^{\text{sym}}(u^{n-1}; u^n, v) = 2\varrho \mathcal{A}_\varepsilon(u^{n-1}; u^{n-1}, v)$$

- constrained linear system of equations
- fully populated system matrices
- parameter ϱ defines length scale

Experiment I

With $I = [0, 2\pi]$ define planar circle

$$u(y) = \begin{bmatrix} \cos(y) \\ \sin(y) \\ 0 \end{bmatrix}.$$



Relative error quantities:

$$\delta^h_{\mathrm{TP}} = \left|\mathrm{TP}_{\varepsilon,h}(I_h u) - \mathrm{TP}(u)\right| / \mathrm{TP}(u),$$
$$\delta^h_{\mathcal{M}} = \left|\mathcal{M}_{\varepsilon,h}(I_h u; I_h u, I_h u) - \mathcal{M}(u; u, u)\right| / \mathcal{M}(u; u, u),$$

Parameters:

$$q = 3, \quad \varepsilon = 2h,$$

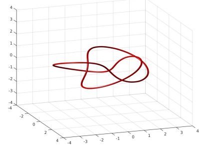
uniform partitions

h_j	δ^j_{TP}	$\delta^j_{\mathcal{M}}$
$2^{-1}/10$	0.049 860	0.039 296
$2^{-2}/10$	0.022 408	0.016 876
$2^{-3}/10$	0.012 522	0.009 712
$2^{-4}/10$	0.005 584	0.004 163
$2^{-5}/10$	0.003 100	0.002 387

Experiment II

With $\widetilde{I} = [0, 1]$ define trefoil knot

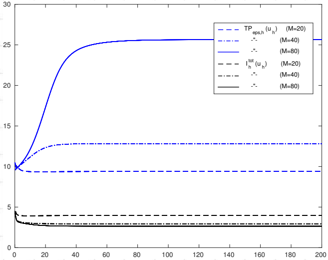
$$\widetilde{u}(\widetilde{y}) = \begin{bmatrix} (2 + \cos(6\pi\widetilde{y}))\cos(4\pi\widetilde{y}) \\ (2 + \cos(6\pi\widetilde{y}))\sin(4\pi\widetilde{y}) \\ \sin(6\pi\widetilde{y}) \end{bmatrix},$$



Movie

and discrete transformation gives

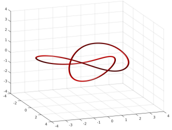
arc-length parametrized $u : I \to \mathbb{R}^3$

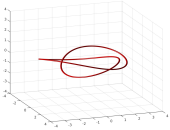


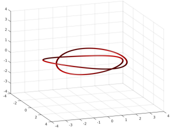
$\tau = h/4$, $\varepsilon = 2h$, $\varrho = h^{1/2}10^{-3}$

Stationary states

$1/h \sim 20, 40, 80$



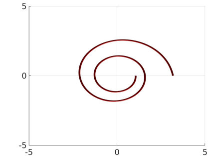




Experiment III

With $\widetilde{I} = [0,1]$ define planar spiral

$$u(\widetilde{y}) = \begin{bmatrix} 20\cos(2\pi(2\widetilde{y}+1))/(2\pi(2\widetilde{y}+1)) \\ 20\sin(2\pi(2\widetilde{y}+1))/(2\pi(2\widetilde{y}+1)) \\ 0 \end{bmatrix}$$



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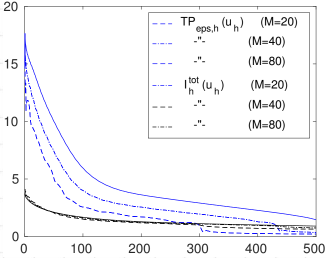
arc-length parametrized $u : I \to \mathbb{R}^3$



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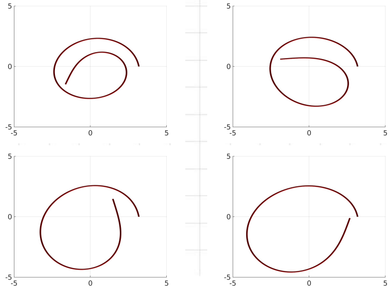

Summary

- Numerical scheme for self-avoiding elastic curves
- Error bounds for approximation and discretization
- Good experimental stability properties

- Future aspects
  - Stability analysis for time-stepping
  - Treatment of surfaces, efficiency

- More information

  http://aam.uni-freiburg.de/bartels