GLOBAL RADII OF CURVATURE, THE BIARC APPROXIMATION OF SPACE CURVES AND IDEAL KNOT SHAPES:

Some Mathematics Arising in Biogeometry

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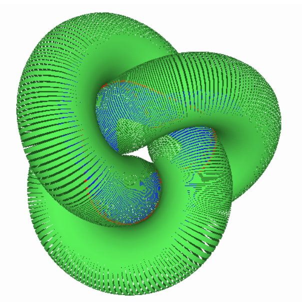
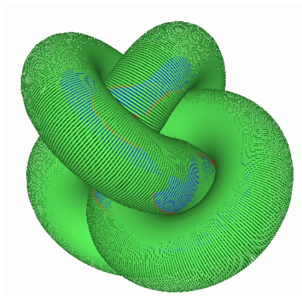




In these three talks I will describe three ideas all pertaining to the analysis and computation of optimal packings of cylindrical tubes centred on arbitrary space curves. While I will not mention the specific applications in any detail, the problem of cylindrical tubes, or fattened lines, arises in a variety of biological contexts, for example packing of DNA into the capsid head of bacteriophages, and the helical form of many bacteria and other simple organisms.

The first idea is that of global radius of curvature, which is a method of characterizing the normal injectivity radius (or informally thickness) of a given space curve.

The second idea is that of biarcs, which are a way of approximating arbitrary space curves with arcs of circles. The biarc discretization combines very well with the approach of global radius of curvature in the computation of thickness.

The third idea is the specific optimal packing problem of ideal knot shapes. Here I will explain the problem, and then show approximately ideal shapes of trefoil and figure-eight knots that were computed via a Monte Carlo code that exploits global radius of curvature and the biarc discretization.

Joint Work:

JHM + Oscar Gonzalez, UT-Austin

JHM + OG + Heiko von der Mosel, Aachen + Friedemann Schuricht, Cologne

JHM + OG + Jana Smutny

JS, PhD Thesis, EPFL 2004 (and the majority of these slides)

JHM + JS + Mathias Carlen, Diplomant, EPFL + Ben Laurie, London

JHM + Andrzej Stasiak, U. of Lausanne

Crucial input from: Remi Langevin, U. of Bourgogne, Arieh Iserles, U. of Cambridge

Plan of Course:

- Lecture 0: Some motivation (and the only biology...)
- Lecture 1: Global radii of curvature, thickness and normal injectivity radius
- Lecture 2: The biarc discretisation of space curves
- Lecture 3: Computations of ideal knot shapes

Lecture 0:

Many problems in biology and elsewhere involve tubular objects, i.e., objects that can be modelled as volumes that can be described as a three dimensional curve with a positive thickness obtained by translating along the curve a constant radius circle in the normal plane.

For example.....

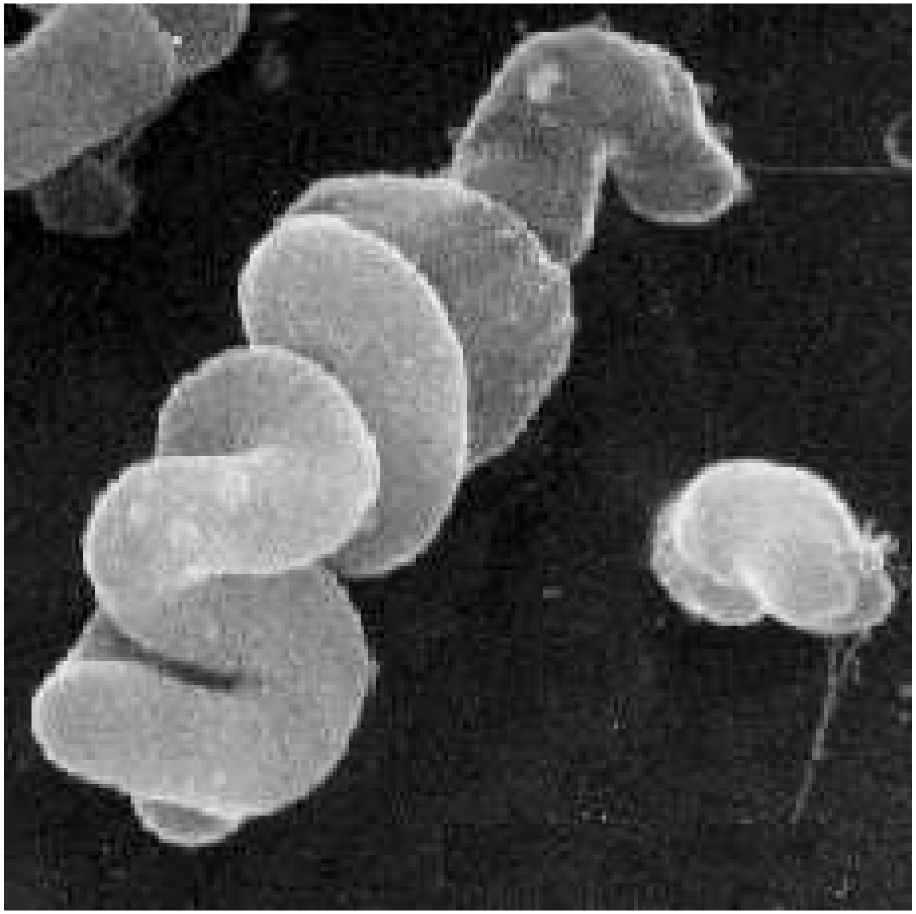
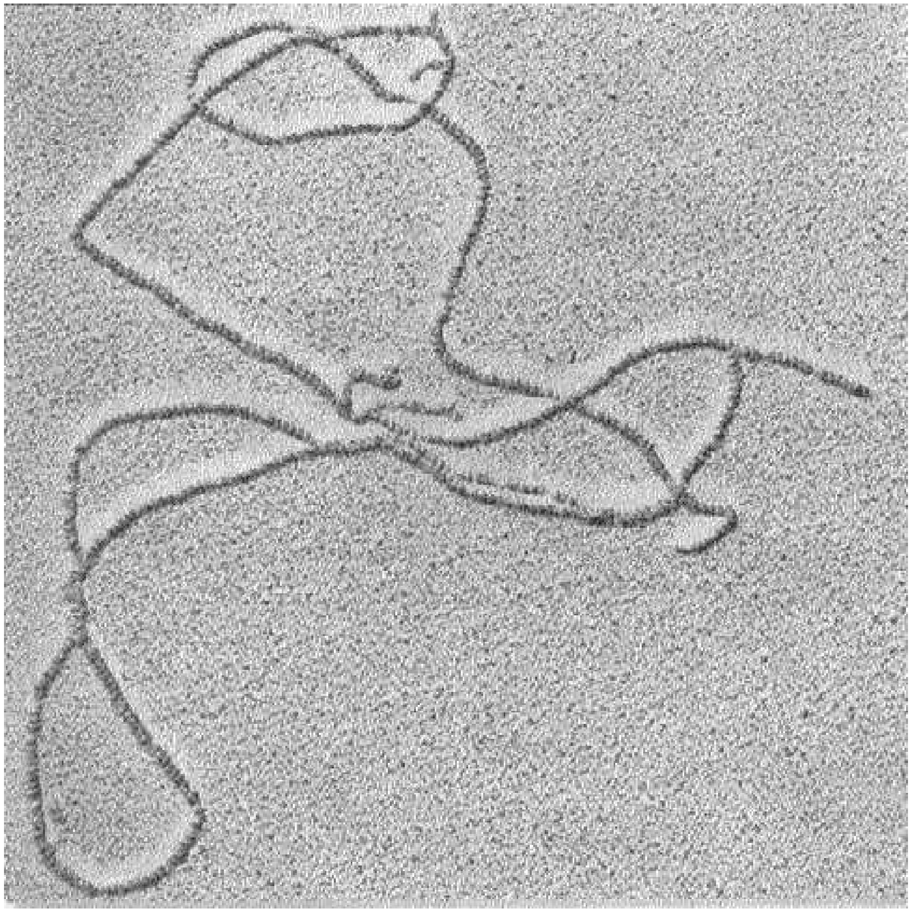
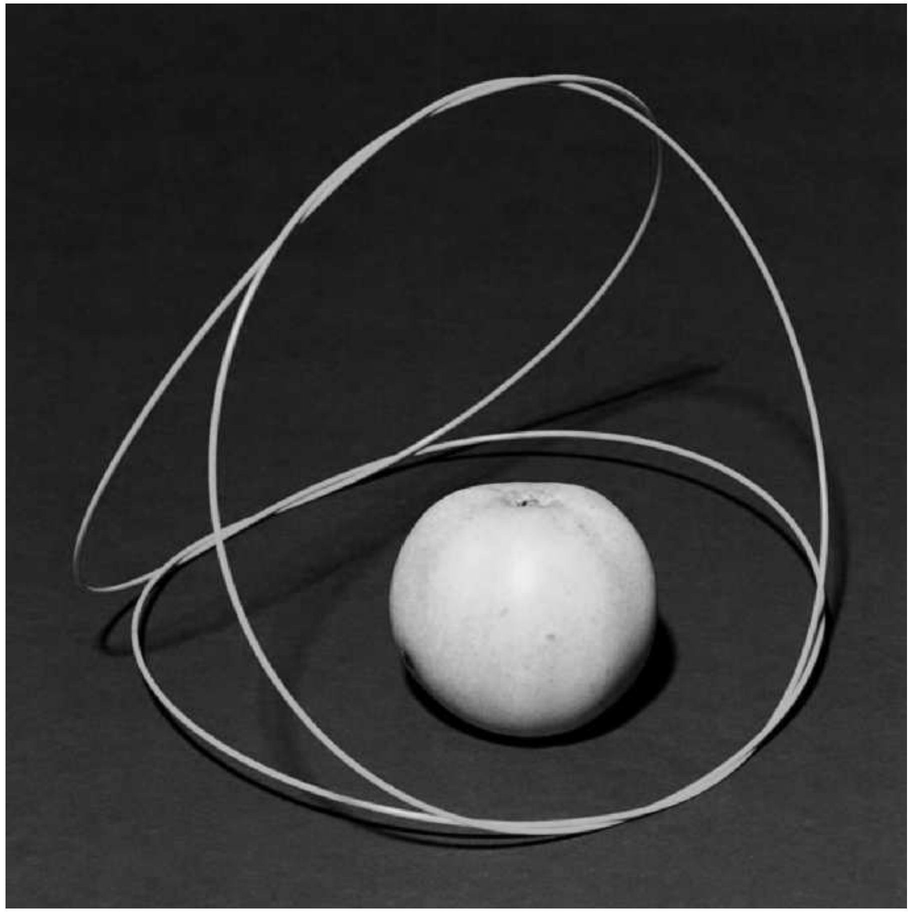


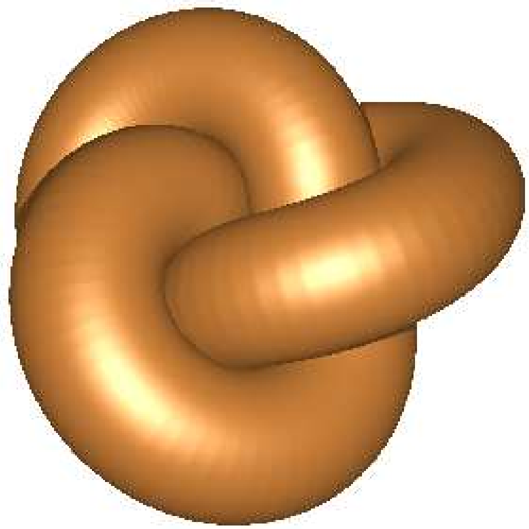
Image of B. Subtilus, image courtesy of M.J. Tilby, or .....



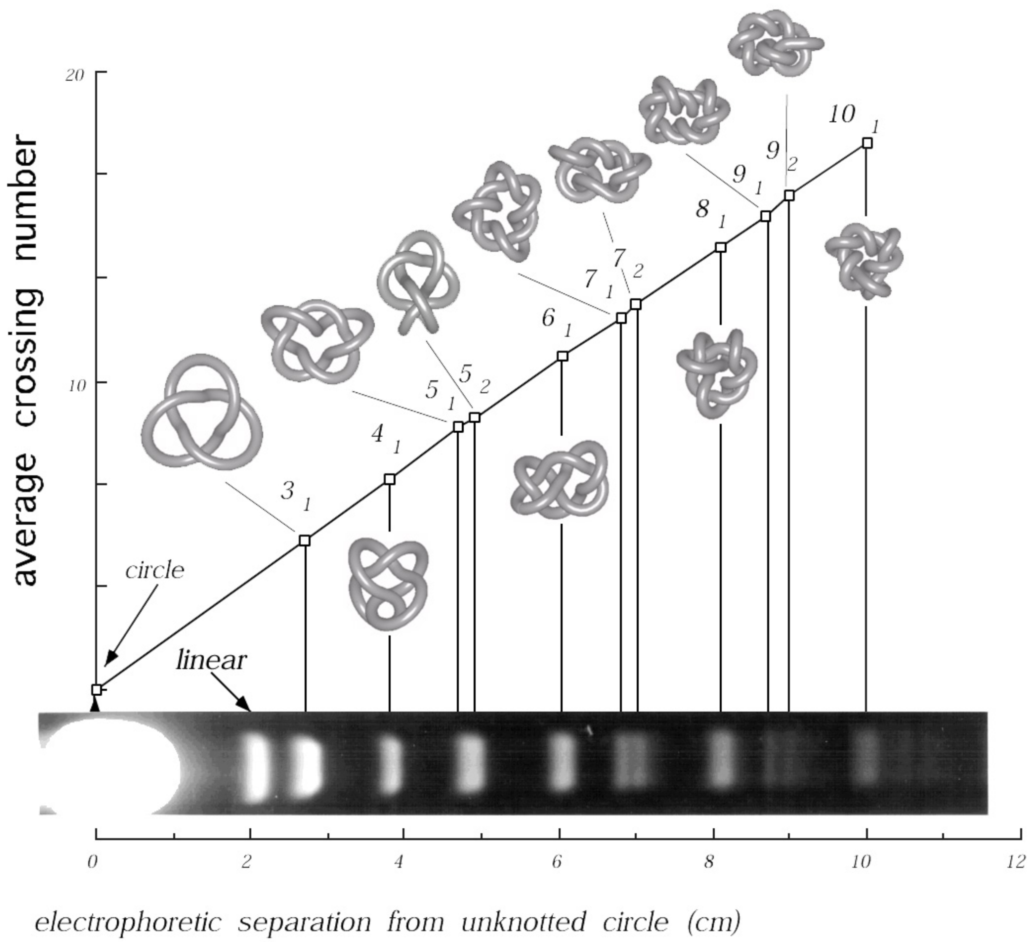
Electron-micrograph of DNA coated with RecA protein with trefoil knot, image courtesy of A. Stasiak, or ....



a jumping knot of J. Langer, which exhibits self-contact but which is far from tight, or ....

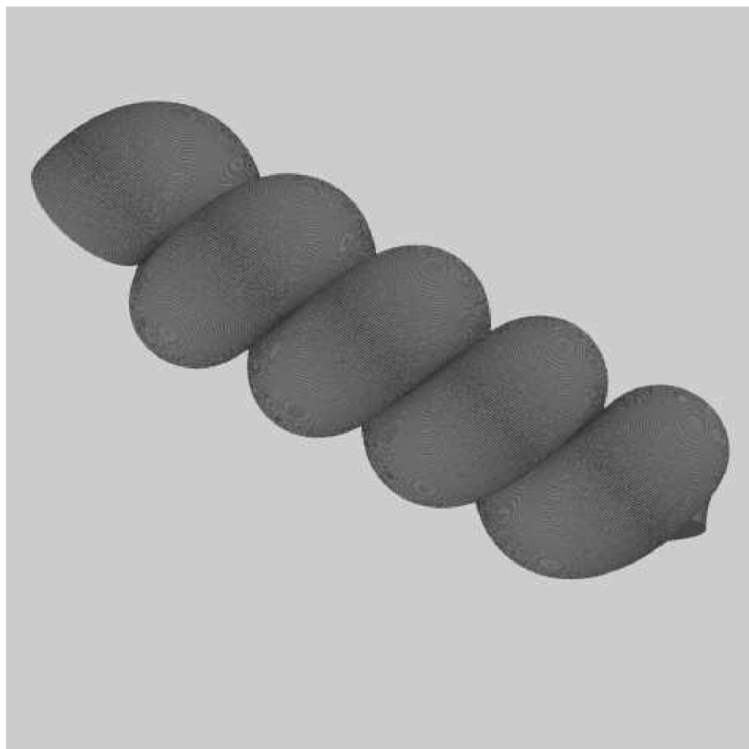


a numerical computation of the tightest or ideal shape of the trefoil knot, i.e., the shape of the usual over-hand knot that can be tied with the shortest amount of rope of given diameter.



Ideal shapes are (still mysteriously) related to gel mobilities of DNA knots (horizontal) vs. Average Crossing Number of the corresponding Knot Shape, image courtesy of A. Stasiak, et al.

Other biological examples including the dense coiling of DNA in bacteriophage capsids, and the observation of Maritan et al Nature **406**(2000) that the C_α carbons of helical proteins of various types all lie on helices with a particular pitch/radius ratio of 2.5126... that also arise in their densest packing numerical simulations



Plan of Lecture 1

Global radii of curvature, thickness and normal injectivity radius

- Self-distance of a curve, what is the big deal?
- Normal Injectivity Radius
- Global radii of curvature
- The case of Helices and optimal packings
- How the global radius of curvature is achieved
- The case of ellipses

What is the problem? For two curves there is no problem

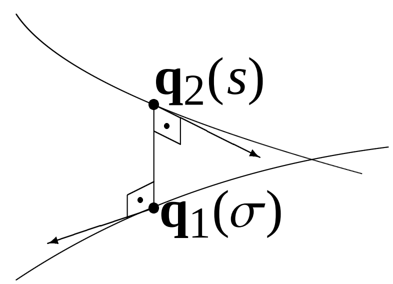
For two non-intersecting (smooth) curves $\mathbf{q}_1$ and $\mathbf{q}_2$ define the distance

$$\mathrm{pp}(s,\sigma) = \frac{1}{2}|\mathbf{q}_1(s) - \mathbf{q}_2(\sigma)|.$$

Here pp is an acronym for point-point and the half is for convenience.

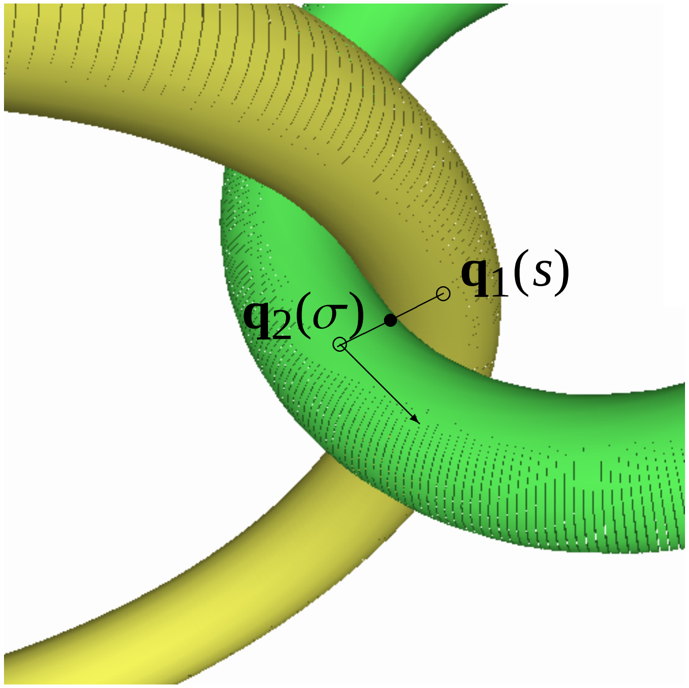
Then the minimum distance $\mathrm{pp}(s,\sigma) > 0$ between the curves is achieved (at ends or) at a doubly critical pair of points, i.e.

$$\mathbf{q}_1'(s) \cdot (\mathbf{q}_1(s) - \mathbf{q}_2(\sigma)) = \mathbf{q}_2'(\sigma) \cdot (\mathbf{q}_1(s) - \mathbf{q}_2(\sigma)) = 0.$$



What is the problem? For two curves there is no problem

And can construct largest possible non-intersecting tubes around the two curves with radius equal to the minimal value of pp(s, σ).



What is the problem? For one curve there is a problem

For one curve $\mathbf{q}$ the minimum of

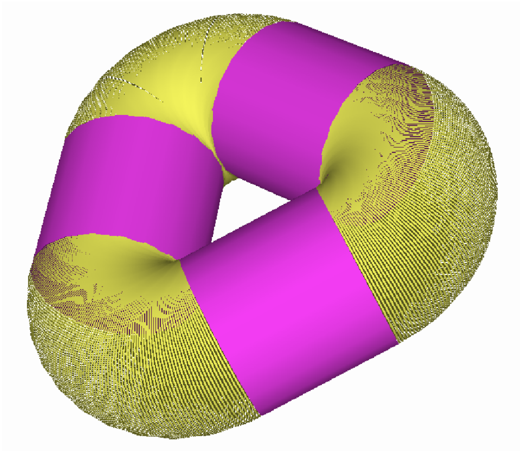
$$\mathrm{pp}(s, \sigma) = \frac{1}{2}|\mathbf{q}(s) - \mathbf{q}(\sigma)|.$$

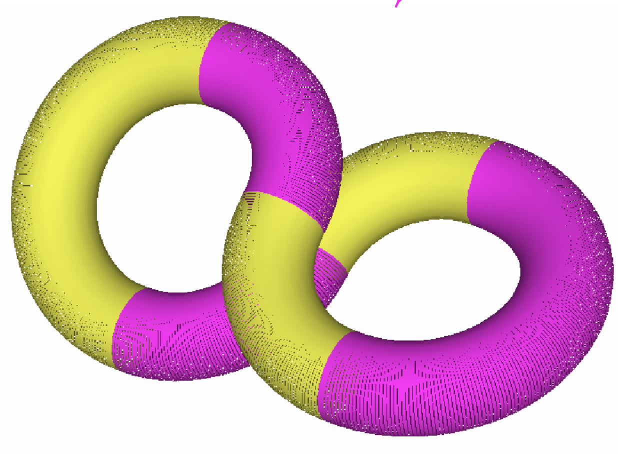
is always zero and is achieved along the diagonal $s = \sigma$.

This gives no useful information. What is the largest non-self-intersecting uniform tube with circular cross-section that can be inflated about a given curve as centreline?

Classic answer is that for a curve that is everywhere C^1 and piecewise C^2, curve thickness or normal injectivity radius NIR is achieved by either:

a local radius of curvature or a double critical distance





These two curves happen to be closed and unknotted.

NIR can be computed various ways, e.g., *thickness* $\Delta[\mathbf{q}]$ of a (simple, closed) curve $\mathbf{q} \in C^2(S^1, \mathbb{R}^3)$ is given by

$$\Delta[\mathbf{q}] = \min\left\{\min_s \rho(s), \frac{1}{2} \min_{(s,\sigma)\in dc} |\mathbf{q}(s) - \mathbf{q}(\sigma)|\right\}$$

where $\rho(s)$ denotes the classic radius of curvature and dc is given by

$$dc = \{(s, \sigma); \mathbf{q}'(s) \cdot (\mathbf{q}(s) - \mathbf{q}(\sigma)) = 0, \mathbf{q}'(\sigma) \cdot (\mathbf{q}(s) - \mathbf{q}(\sigma)) = 0, s \neq \sigma\}$$

More explicit and useful than the geometric notion of NIR, but C^2 is many ways too strong a hypothesis, and the two alternatives are still a little cumbersome.

Different notions of the thickness of a curve

Global radius of curvature

The *thickness* $\Delta_g[\mathbf{q}]$ of a (simple, closed) curve $\mathbf{q} \in C^{0,1}(S^1, \mathbb{R}^3)$ is given by

$$\Delta_g[\mathbf{q}] = \inf_{s \neq \sigma \neq \tau \neq s} r(\mathbf{q}(s), \mathbf{q}(\sigma), \mathbf{q}(\tau))$$

where $r(\mathbf{x}, \mathbf{y}, \mathbf{z})$ denotes the radius of the circle through the points $\mathbf{x}, \mathbf{y}, \mathbf{z}$.

Also for a given curve $\mathbf{q}$ introduce ppp$(s, \sigma, \tau) := r(\mathbf{q}(s), \mathbf{q}(\sigma), \mathbf{q}(\tau))$. In other words we interpret the radius ppp as a ‘distance’ between three points.

Global radius of curvature bounds and regularity

The functional $\Delta_g[\mathbf{q}]$ is well-defined for arc-length parameterised, closed $C^{0,1}$-curves. Such curves having an additional lower bound on thickness $\Delta_g[\mathbf{q}] \geq \theta > 0$, are in fact differentiable and the tangent curve is Lipschitz continuous with Lipschitz constant $K_{\mathbf{q}'} \leq \theta^{-1}$. In other words, closed, arc-length parameterised, Lipschitz continuous curves with positive thickness, are actually $C^{1,1}$-curves, and therefore their curvature exists almost everywhere.

The bound $\Delta_g[\mathbf{q}] \geq \theta > 0$ is weakly closed in $W^{1,p}$ for $p > 1$ which can be exploited in the direct methods of the calculus of variations to prove existence of $C^{1,1}$-minimizers of various energy functionals.

$C^{1,1}$ really seems to be the ‘natural’ smoothness of fattened curves.

Global and local radii of curvature and the DC set

The minimum of $\Delta_g[\mathbf{q}]$ is never achieved only at distinct points. For C^2 curves it is achieved either by a DC pair or by a classic osculating circle.

Proof is elementary geometry. Take the minimizing circle. Construct the associated circumsphere with the given circle as a great-circle. If for example the curve $\mathbf{q}$ enters the interior of this minimal circumsphere a contradiction arises by shrinking the sphere and maintaining three intersections with the curve.

Global Radius of Curvature Functions

A global radius of curvature *function* along a curve $\mathbf{q}$ can be defined via minimisation over all but one argument

$$\rho_g(s) \equiv \rho_{\mathrm{ppp}}(s) := \inf_{\sigma \neq \tau} r(\mathbf{q}(s), \mathbf{q}(\sigma), \mathbf{q}(\tau)) \equiv \inf_{\sigma \neq \tau} \mathrm{ppp}(s, \sigma, \tau).$$

The (original) notation $\rho_g(s)$ was introduced to emphasise that for C^2 curves $\mathbf{q}$ the classic local osculating circle is a competitor in the minimisation, so that the global radius of curvature $\rho_g(s)$ is a non-local generalisation of the limit of the radius of the circle through three points all coalescent at s to the smallest radius of *all* circles intersecting the curve three times.

The second notation $\rho_{\mathrm{ppp}}(s)$ emphasises that the function is defined as an infimum over the radius of a circle through three distinct points.

Global radii of curvature: Coalescence

As a matter of definition

$$\Delta_g[\mathbf{q}] = \Delta_{\text{ppp}}[\mathbf{q}] = \inf_s \rho_{\text{ppp}}(s) = \inf_{s\neq\sigma\neq\tau\neq s} r(\mathbf{q}(s), \mathbf{q}(\sigma), \mathbf{q}(\tau)) = \inf_{s\neq\sigma\neq\tau\neq s} \text{ppp}(s, \sigma, \tau)$$

where the equivalent notations emphasise different points of view.

In point of fact for $C^{1,1}$ curves $\rho_{\text{ppp}}(s)$ is never realised only at three distinct points, so that

$$\rho_{\text{ppp}}(s) = \inf_{s\neq\sigma} \text{pt}(s, \sigma) =: \rho_{\text{pt}}(s)$$

The proof again involves the circumsphere to argue that the curve cannot pierce the circumsphere of the circle realising the infimum.

For computation this simplification is significant.

Global radii of curvature: Pandora's Box

With this point of view, starts to make sense to consider all circular and spherical radii through respectively three and four points along a given curve, coalescent or not in various combinations.

Lots of combinations all of which give rise to a global radius of curvature function.

Note: the different functions require slightly different regularities. But for *all* the functions a pair of doubly critical points is very special.

Global radii of curvature:

Construction of all circular and spherical functions

two points define a line

three points define a circle

four points define a sphere

minimization over all but first argument

	1	2	3	4
line	0	pp		
circle	ρ	pt tp	ppp	
sphere	ρ_{os}	cp* pc* tt	tpp ptp ppt	pppp

$\longrightarrow$

	0	1	2	3
line	0	$\rho_{pp} = 0$		
circle	ρ	ρ_{pt} ρ_{tp}	ρ_{ppp}	
sphere	ρ_{os}	$\rho_{cp}{}^\star$ $\rho_{pc}{}^\star$ ρ_{tt}	ρ_{tpp} ρ_{ptp} ρ_{ppt}	ρ_{pppp}

In fact it possible to define several (actually twelve) global radius of curvature functions based on circular and spherical radii. But fortunately it all simplifies.....

Global radii of curvature: Not so many cases important

Proposition: Under certain hypotheses:

$$\rho_{\text{os}} \geq \left\{ \begin{array}{c} \rho = \rho^{\star}_{\text{cp}} \geq \rho_{\text{tp}} = \rho_{\text{tt}} = \rho_{\text{tpp}} \\ \rho_{\text{pc}} \end{array} \right\} \geq \rho_{\text{pt}} = \rho_{\text{ppp}} = \rho_{\text{ptp}} = \rho_{\text{ppt}} = \rho_{\text{pppp}} \geq 0,$$

and all inequalities are sharp for some curves.

When minimal regularity is of concern consider the functions ppp and pppp and their associated global curvatures ρ_{ppp} and ρ_{pppp}.

Otherwise concentrate on the classic local curvatures ρ and ρ_{os}, and the circular function pt(s, σ) and the two global curvatures it generates namely ρ_{pt} and ρ_{tp} via minimization over respectively its second and first arguments.

$\longrightarrow$ For computations the useful global radius of curvature functions that characterise NIR are ρ_{pt} and ρ_{tp}.

Lemma: Under certain hypotheses:

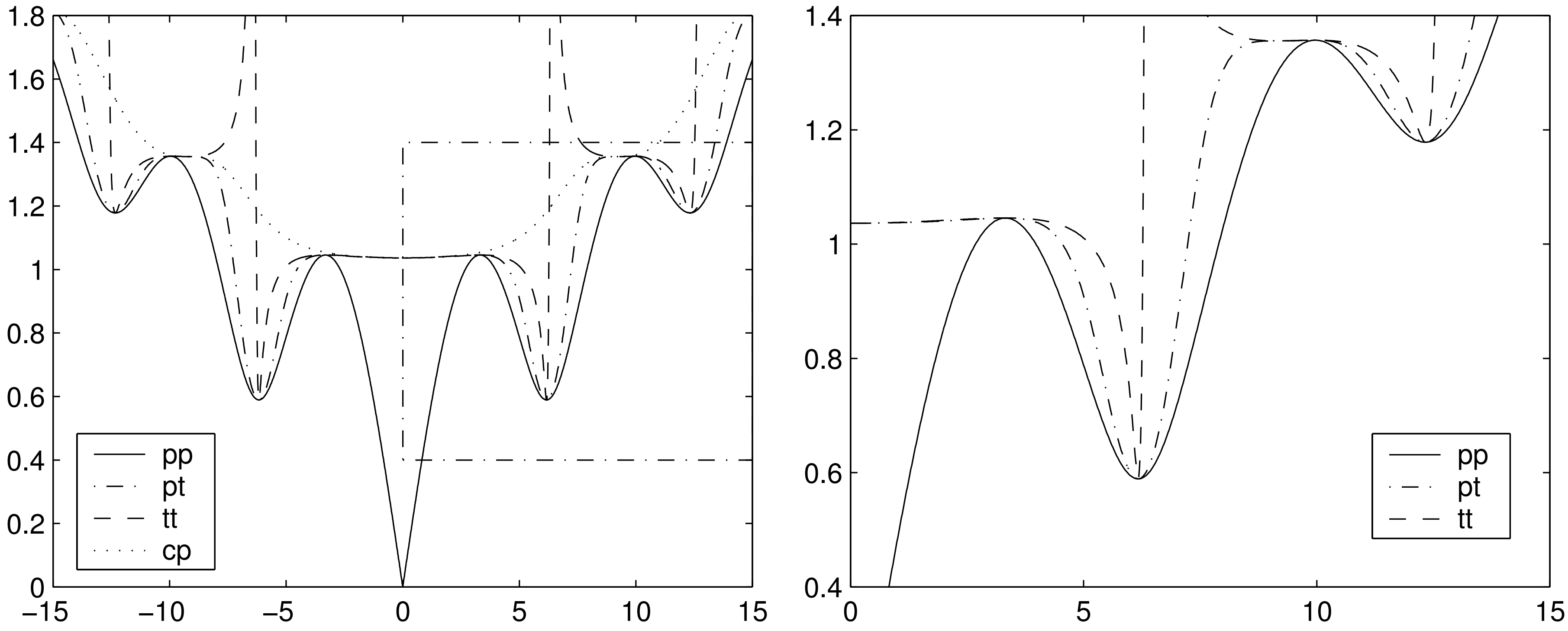
$$\begin{aligned} \Delta[\mathbf{q}] &= \Delta_{\text{pt}}[\mathbf{q}] := \inf_s \rho_{\text{pt}}(s), \\ &= \Delta_{\text{tp}}[\mathbf{q}] := \inf_s \rho_{\text{tp}}(s). \end{aligned}$$

(Circular) Helices are uniform so any curvature function will be constant, and any two argument radius function will depend only on the difference $(s-\sigma) =: \eta$ of the two arc-length arguments.

By dilation can scale so that the radius of the cylinder is 1, and then only remaining free parameter is the pitch.

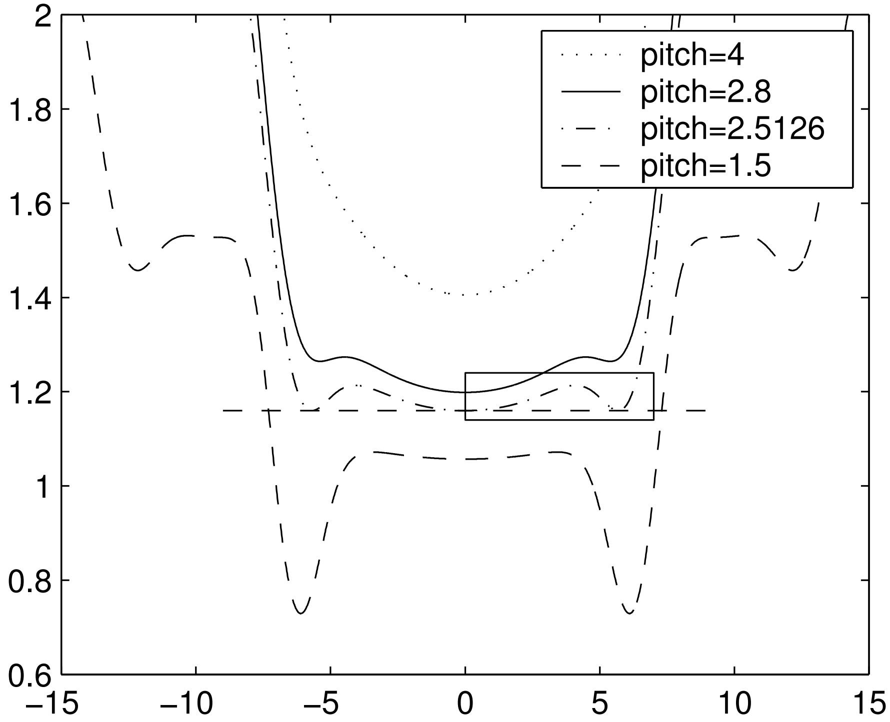
Helices map back to themselves when rotated through π about a principal normal, and this symmetry implies $\mathrm{pt}(s, \sigma) = \mathrm{pt}(\sigma, s)$.

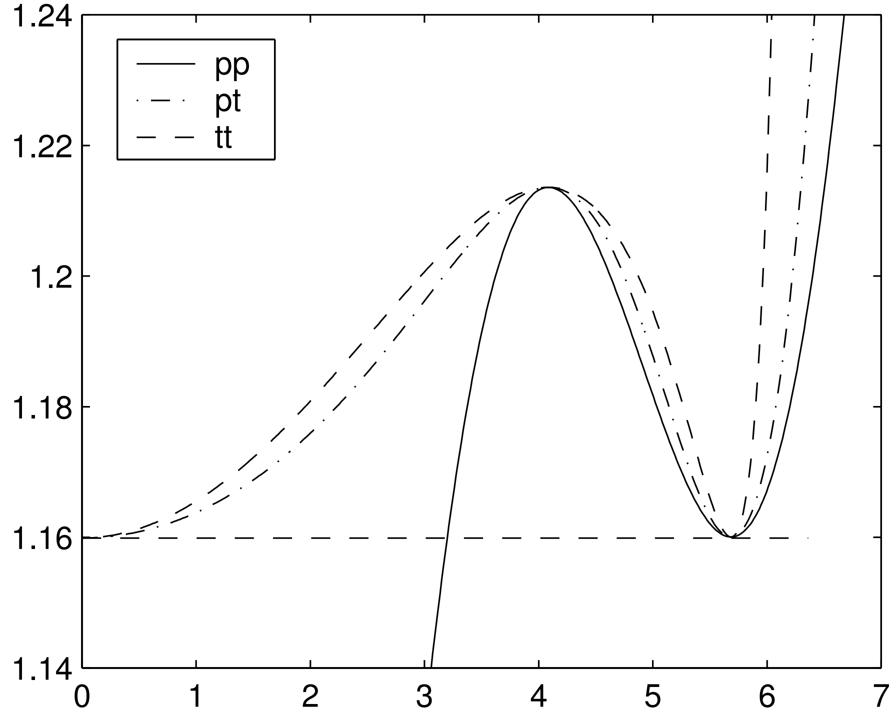
Four radius functions on one helix (pitch 1.2)



Global radii of curvature: Helices

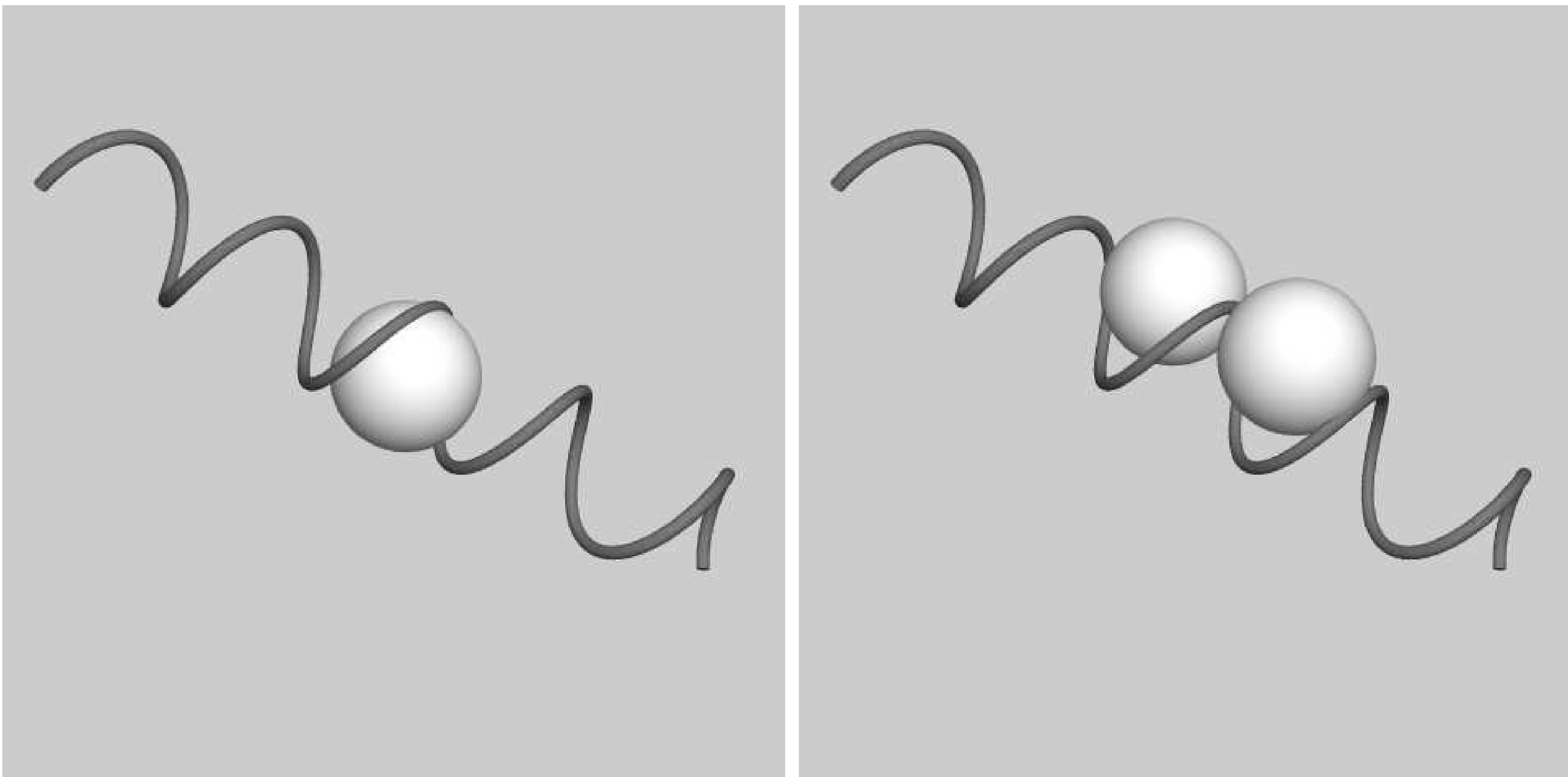
One radius function pt on four helices, and three radius functions on the critical pitch 2.5126 helix of Maritan et al.





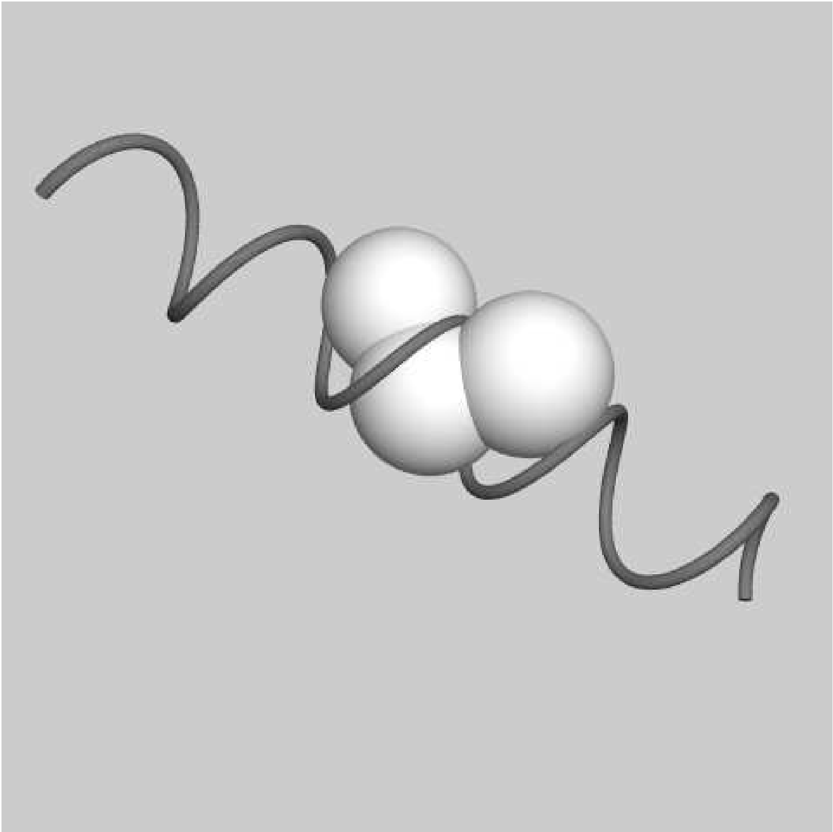
Global radii of curvature: Helices

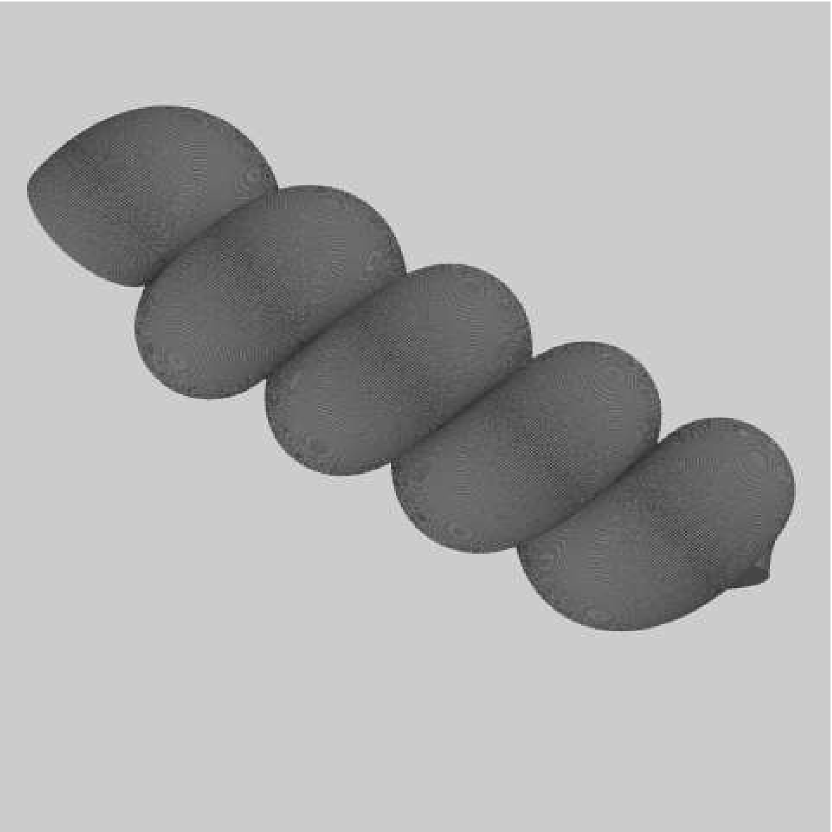
On the critical pitch 2.5126 helix thickness is achieved globally and locally at the same time



Global radii of curvature: Helices

...or....





Maritan et al found these critical helices in Monte Carlo simulations of densest packings of point sets subject to a lower bound on the discrete ppp function.

Plan of Lecture 1

Global radii of curvature, thickness and normal injectivity radius

- Self-distance of a curve, what is the big deal?
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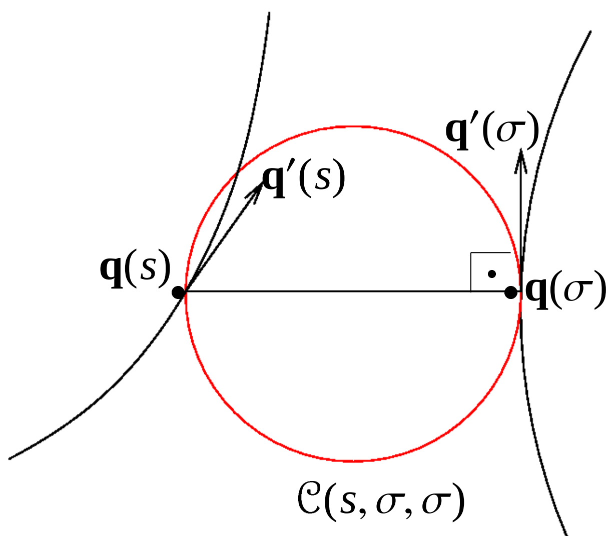
 How ρ_{pt} is achieved in general

Lemma: For $\mathbf{q} \in C^3(I, \mathbb{R}^3)$, $s \in I$, only three non-trivial cases can occur:

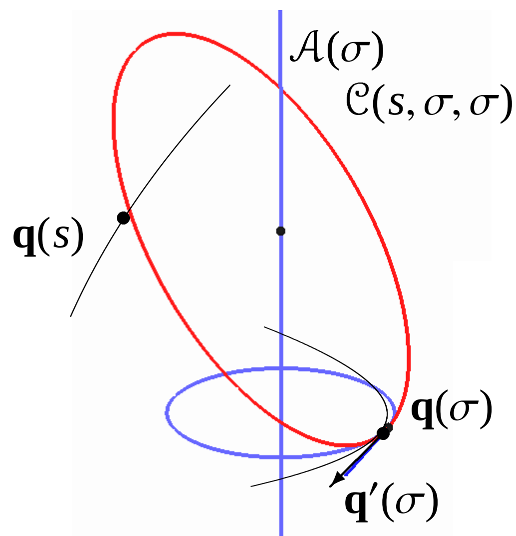
3. $\rho_{\text{pt}}(s) = \rho(s)$, i.e. $\rho_{\text{pt}}(s)$ is achieved locally, in which case $\kappa'(s) = 0$ and $\kappa''(s) \leq \kappa(s)\tau^2(s)$,

4. $\rho_{\text{pt}}(s) = \text{pt}(s, \sigma)$ with $s \neq \sigma$ and $\mathbf{q}'(\sigma) \cdot (\mathbf{q}(\sigma) - \mathbf{q}(s)) = 0$, i.e. $\rho_{\text{pt}}(s)$ is achieved by half of the distance between a pair of single critical points,

5. $\rho_{\text{pt}}(s) = \text{pt}(s, \sigma)$ with $s \neq \sigma$, and $\kappa(\sigma) \neq 0$ and the centre $\mathbf{c}$ of the circle $\mathcal{C}(s, \sigma, \sigma)$ lies on the polar axis $\mathcal{A}(\sigma)$ at σ.

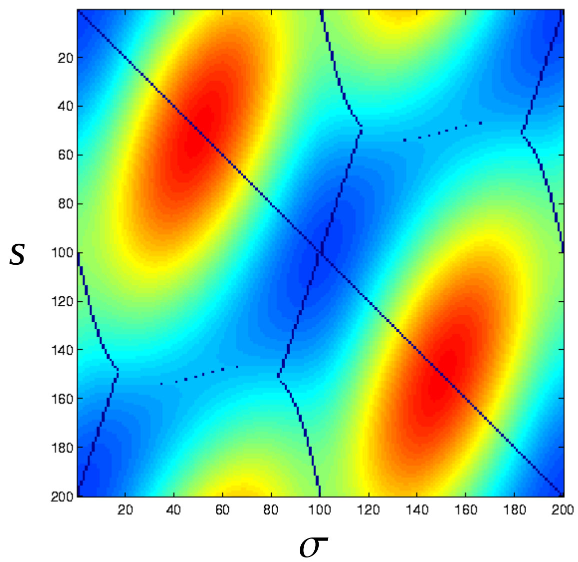


case 4

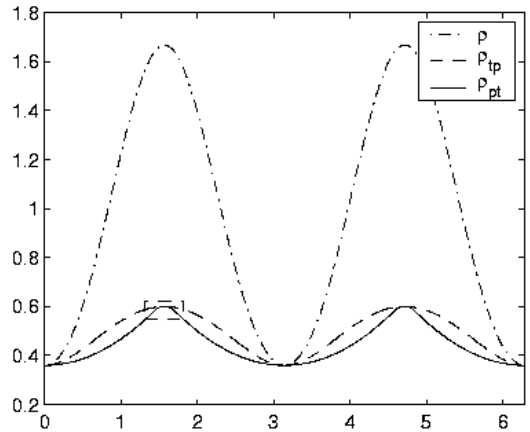


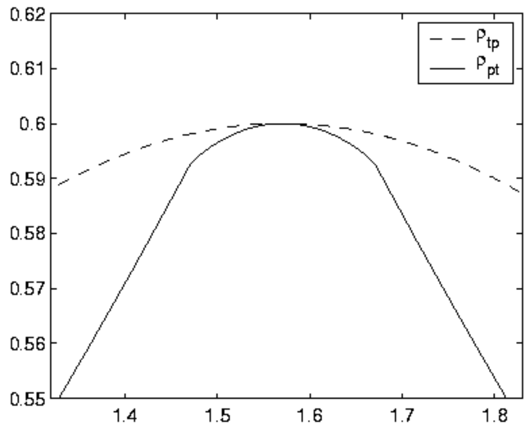
case 5

Global radii of curvature: The example of an ellipse



← The function pt(s, σ):
min of a horizontal cut pt$(s, \cdot)$ is $\rho_{\mathrm{pt}}(s)$
min of a vertical cut pt$(\cdot, \sigma)$ is $\rho_{\mathrm{tp}}(\sigma)$





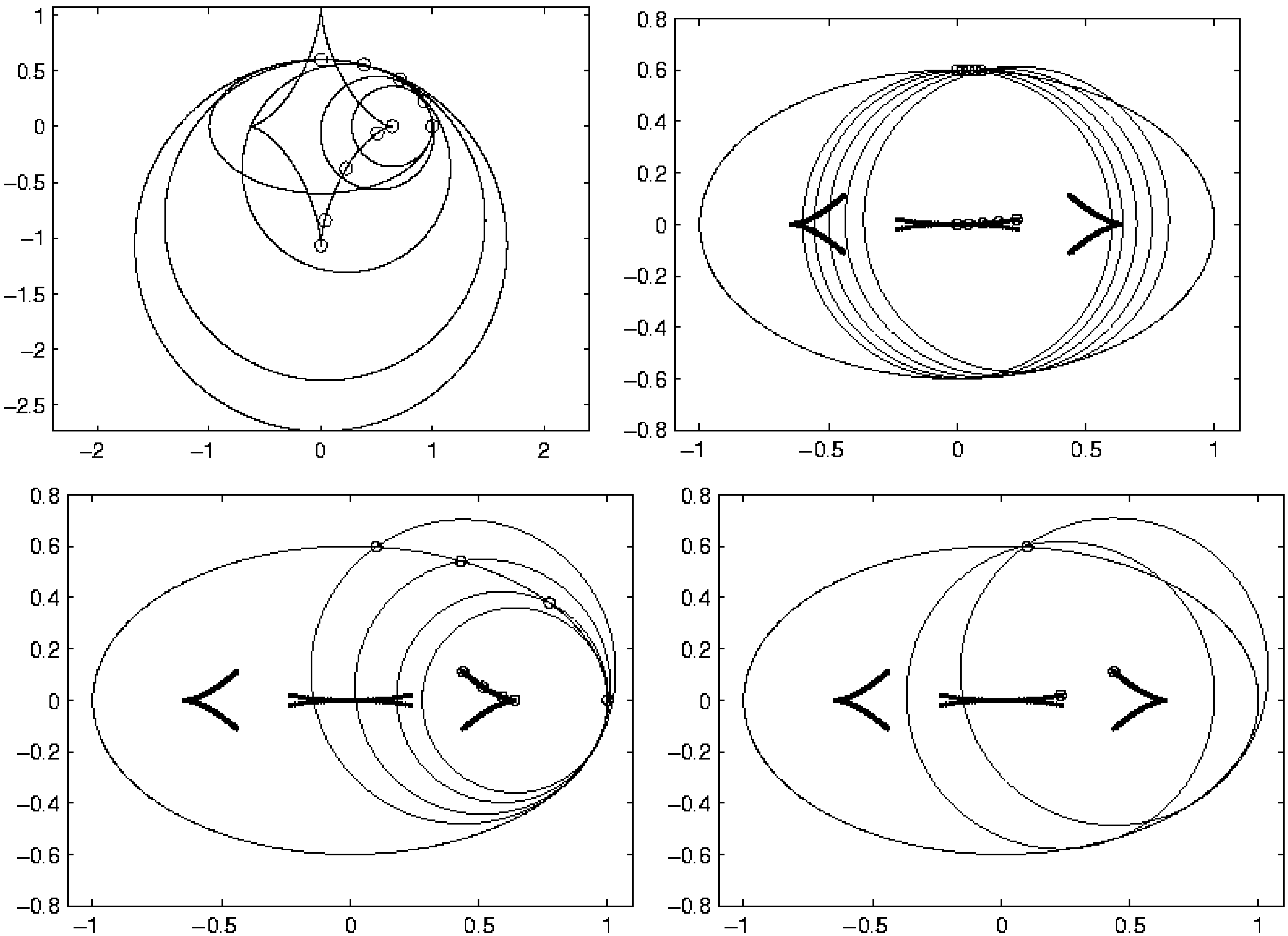
Observations:

– functions ρ, ρ_{pt} and ρ_{tp} are nested,

– at local minimum of ρ all three functions ρ, ρ_{pt} and ρ_{tp} agree,

– ρ_{pt} has a corner, while ρ_{tp} is smooth.

Centres of circles realizing ρ and ρ_{pt}:



Lecture 2

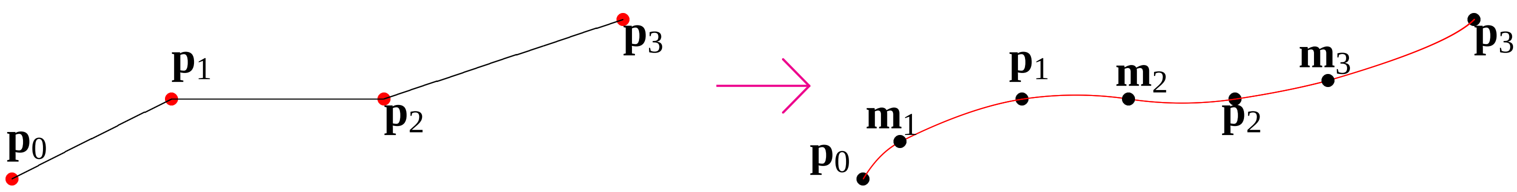
The Biarc discretisation of space curves. How to compute interesting curves with accurate evaluation of global radii of curvature and thickness

Plan of Lecture 2:

- biarcs: construction and convergence results
- evaluation of thickness and ρ_{pt} on arc curves
- biarc approximation of an ellipse and its global radius of curvature functions
- stop early, eat, drink, be merry...

Biarc discretization: Why?

– ideal shapes exist in the space $C^{1,1}$ †‡★
– polygonal discretization has two drawbacks: 1) wrong class, 2) thickness is zero, need to redefine thickness
– cubic spline: no closed form expression for arc length



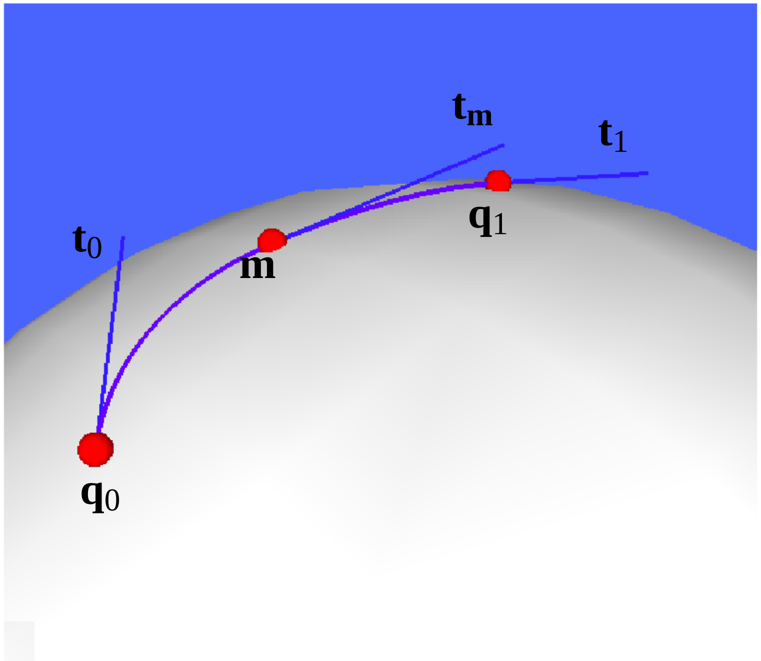
Biarcs:

– arc length and local curvature ρ are easy to compute
– fast algorithm available to evaluate euclidean distance between arcs in space and thickness to specified accuracy
– biarc curves are in $C^{1,1}$, thus competitors for the ideal shape and numerics gives an upper bound for rope length (up to numerical accuracy)
– can evaluate ρ_{pt} precisely

†) Gonzalez, Maddocks, Schuricht, von der Mosel, Calc. Var. 14 (2002), 29–68.
‡) Cantarella, Kusner and Sullivan, Inventiones mathematicae 150(2) (2002), 257-286.
★) Gonzalez and de la Llave, Existence of Ideal Knots, J. Knot Theory and Its Ramifications, 12(1) (2003), 123–133.

Biarc interpolation:

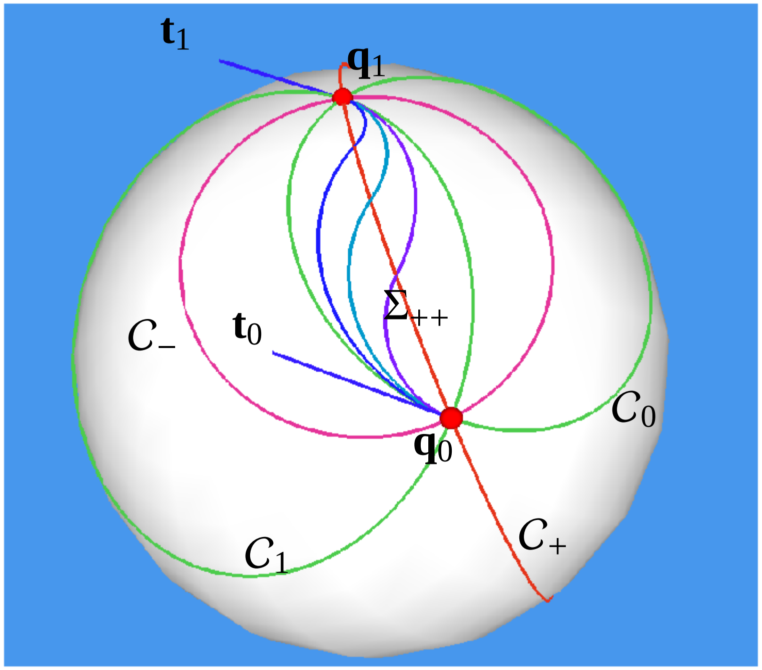
Definition: A *biarc* $(\mathbf{a}, \bar{\mathbf{a}})$ is a pair of circular arcs in $\mathbb{R}^3$, joined continuously and with continuous tangents, that interpolate a point-tangent data pair. The common end point $\mathbf{m}$ of the two arcs $\mathbf{a}$ and $\bar{\mathbf{a}}$ is the *matching point* of the biarc.



Notation: $\mathcal{J} := \mathbb{R}^3 \times S^2$

Biarc interpolation: Existence

Proposition (†): For generic point-tangent data pair $((\mathbf{q}_0, \mathbf{t}_0), (\mathbf{q}_1, \mathbf{t}_1)) \in \mathcal{J} \times \mathcal{J}$, consider the circles C_0, C_1, C_+, and C_-:



Set Σ_+ of matching points of biarcs interpolating $((\mathbf{q}_0, \mathbf{t}_0), (\mathbf{q}_1, \mathbf{t}_1))$ is:

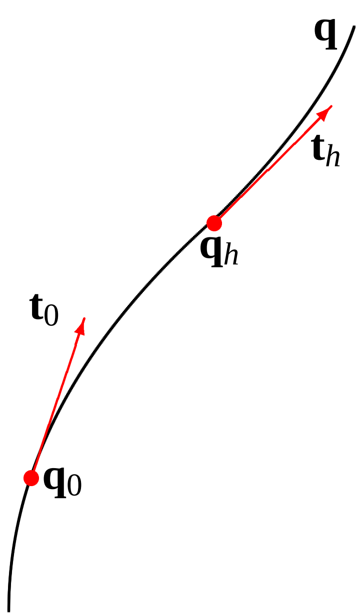
$$\Sigma_+ = C'_+,$$

Set Σ_- of matching points of biarcs interpolating $((\mathbf{q}_0, \mathbf{t}_0), (\mathbf{q}_1, -\mathbf{t}_1))$ is:

$$\Sigma_- = C'_-.$$

Definition of sub arc $\Sigma_{++} \subset \Sigma_+$ for not incompatible cocircular data and of biarc parameter $\Lambda \in (0, 1)$ for proper biarcs.

†) T. J. Sharrock, The Mathematics of Surfaces II (1987).



Hypotheses (H):

1. $\mathbf{q} \in C^{1,1}(I, \mathbb{R}^3)$ is parametrised by arc length, $I = [l_0, l_1] \subset \mathbb{R}$ or $I = [l_0, \infty) \subset \mathbb{R}$.
2. For $s \in I$ and $h \neq 0$ with $s + h \in I$ we denote

$$\mathbf{q}_0 := \mathbf{q}(s),\ \mathbf{t}_0 := \mathbf{q}'(s),\ \mathbf{q}_h := \mathbf{q}(s+h),\ \mathbf{t}_h := \mathbf{q}'(s+h).$$

3. $((\mathbf{q}_0, \mathbf{t}_0), (\mathbf{q}_h, \mathbf{t}_h))$ is interpolated by a biarc $(\mathbf{a}, \overline{\mathbf{a}})_h$ with matching point $\mathbf{m}_h \in \Sigma_{++}$
(that for h sufficiently small corresponds to a biarc parameter $\Lambda_h \in (0,1)$).

constant depends only on $K_{\mathbf{q}'}$

Proposition:

hypotheses:	expansions:
(H)	$\lambda((\mathbf{a}, \overline{\mathbf{a}})_h) - h = O(h^3)$
(H), $\mathbf{q} \in C^2$, $0 < \Lambda_{\min} \leq \Lambda_h$	$\lvert\mathbf{q}''(s) - \mathbf{a}_h''^{+}\rvert = o(1)$

arc $\mathbf{a}$ of biarc $(\mathbf{a}, \overline{\mathbf{a}})_h$ approaches the osculating circle at $\mathbf{q}_0$
speed of convergence independent of s if $\mathbf{q}''$ uniformly continuous

Biarc interpolation: Global convergence

Definition: A *biarc curve* $\boldsymbol{\beta}$ is a space curve assembled from biarcs in a C^1 fashion, where the biarcs interpolate a sequence $\{(\mathbf{q}_i, \mathbf{t}_i)\}$ of point-tangent data.

Notation and Hypothesis (i):

1. Let $I = [l_0, l_1] \subset \mathbb{R}$ and $\mathbf{q} \in C^{1,1}(I, \mathbb{R}^3)$ parametrised by arc length.
2. Consider a sequence of nested meshes $\mathcal{M}_j, \ j \in \mathbb{N}$ on I with mesh size $h_j \to 0$ (wlog h_j monotone decreasing). Denote the members of the mesh $\mathcal{M}_j$ by $s_{j,i}, \ i \in \mathcal{N}_j$.
3. For $j \in \mathbb{N}$ $\boldsymbol{\beta}_{h_j}$ is a biarc curve interpolating the data $(\mathbf{q}(s_{j,i}), \mathbf{q}'(s_{j,i})) \in \mathcal{J}$ with matching points on Σ_{++}.

$\longrightarrow$ In what sense do the biarc curves $\boldsymbol{\beta}_{h_j}$ tend to the base curve $\mathbf{q}$ as $j \to \infty$?

Biarc interpolation: Global convergence of arc length

Corollary: Let Hypotheses (i) hold. Then the arc length of the biarc curve $\boldsymbol{\beta}_{h_j}$ converges to the arc length of the curve $\mathbf{q}$ quadratically:

$$\frac{\lambda(\boldsymbol{\beta}_{h_j})}{\lambda(\mathbf{q})} - 1 = O(h_j^2),$$

and the constant depends only on $K_{\mathbf{q}'}$.

use “natural” reparametrization function φ_j (7 conditions)

$\mathbf{B}_{h_j} := \boldsymbol{\beta}_{h_j} \circ \varphi_j : I \to I_j \to \mathbb{R}^3$

$\Lambda_{\min} \leq \Lambda_{j,i} \leq \Lambda_{\max}$

Theorem: Let Hypotheses (i)-(ii) hold. Then the biarc curves $\mathbf{B}_{h_j}$ converge to the curve $\mathbf{q}$ in the space $C^1(I,\mathbb{R}^3)$ or if additionally $\mathbf{q} \in C^2(I,\mathbb{R}^3)$ in the space $C^{1,1}(I,\mathbb{R}^3)$ as $j \to \infty$. More precisely, for the assumed regularities (left column) and as $j \to \infty$ we have:

	$\Vert\mathbf{q} - \mathbf{B}_{h_j}\Vert_C$	$\Vert(\mathbf{q} - \mathbf{B}_{h_j})'\Vert_C$	$K_{(\mathbf{q}-\mathbf{B}_{h_j})'}$
$\mathbf{q} \in C^{1,1}$	$O(h_j^2)$	$O(h_j)$	-
$\mathbf{q} \in C^2$	$o(h_j^2)$	$o(h_j)$	$o(1)$
$\mathbf{q} \in C^{2,1}$	$O(h_j^3)$	$O(h_j^2)$	$O(h_j)$

Plan of Lecture 2:

- biarcs: construction and convergence results
- evaluation of thickness and ρ_{pt} on arc curves
- biarc approximation of an ellipse and its global radius of curvature functions
- stop early, eat, drink, be merry...

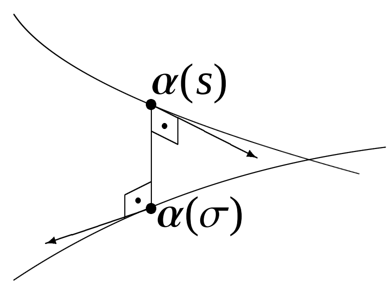
Thickness of arccurves: Algorithm

Proposition: For a non-intersecting arc curve α composed of n arcs $\mathbf{a}_i$ with radii r_i:

$$\Delta[\alpha] = \min\left\{ \min_{1\le i\le n} r_i, \quad \tfrac{1}{2}\min_{(s,t)\in dc} |\alpha(s)-\alpha(t)| \right\},$$

where dc is the set of arguments $(s,\sigma) \in I \times I$ with $s \neq \sigma$ that satisfy

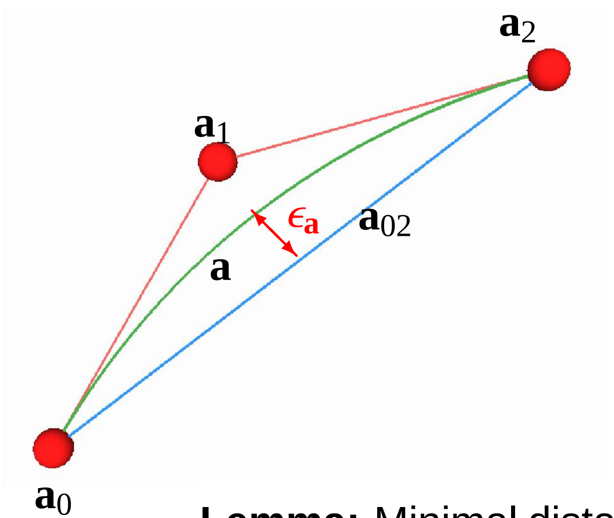
$$\alpha'(s)\cdot(\alpha(s)-\alpha(\sigma)) = \alpha'(\sigma)\cdot(\alpha(s)-\alpha(\sigma)) = 0.$$

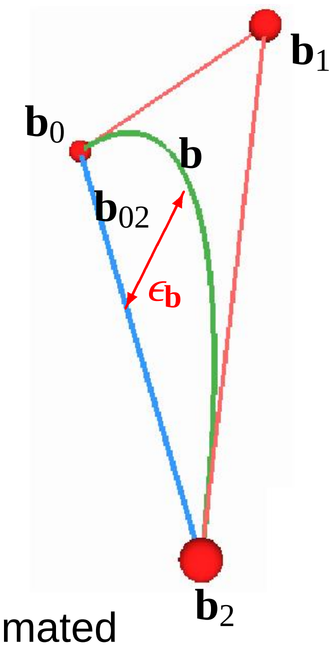


Basic building blocks of the thickness evaluation algorithm:

- linear segment approximation
- bisection
- double critical test

Thickness of arccurves: Linear segment approximation

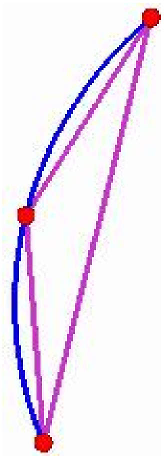




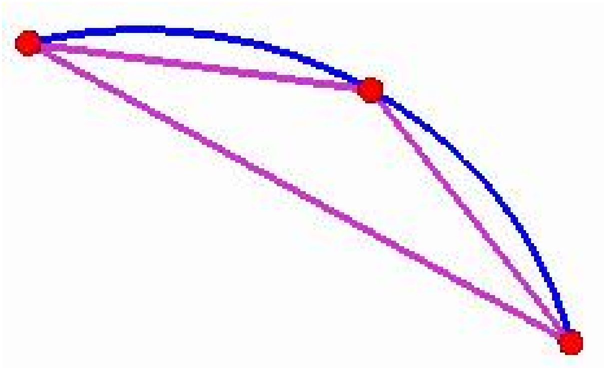
Lemma: Minimal distance between arcs $\mathbf{a}$ and $\mathbf{b}$ can be approximated by minimal distance between straight base line segments $\mathbf{a}_{02}$ and $\mathbf{b}_{02}$:

$$\left| \min_{(\mathbf{x}_1,\mathbf{x}_2)\in\mathbf{a}_{02}\times\mathbf{b}_{02}} |\mathbf{x}_1 - \mathbf{x}_2| - \min_{(\mathbf{y}_1,\mathbf{y}_2)\in\mathbf{a}\times\mathbf{b}} |\mathbf{y}_1 - \mathbf{y}_2| \right| \le \epsilon_{\mathbf{a}} + \epsilon_{\mathbf{b}}.$$

Thickness of arccurves: Linear segment approximation and bisection



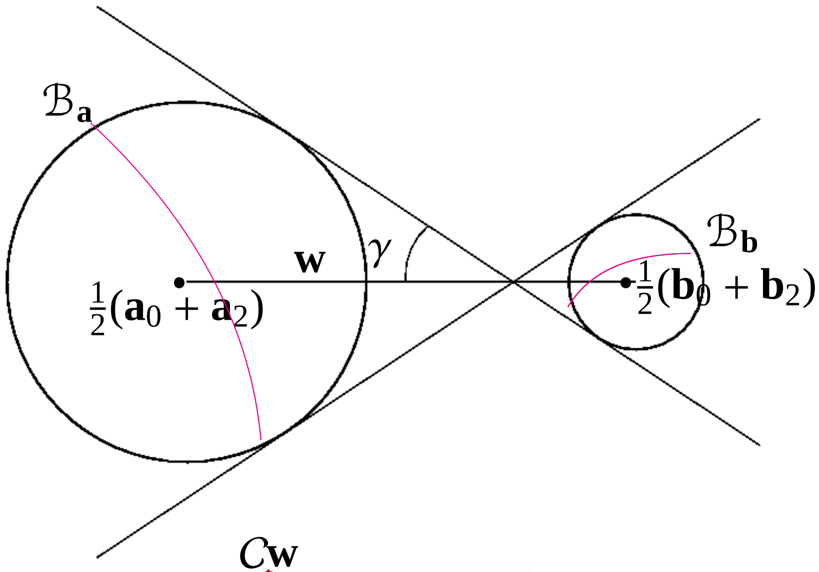
Notation: For an arc $\mathbf{a}$ and $m \in \mathbb{N}$:
$\mathcal{V}_m(\mathbf{a})$ = set of 2^m congruent arcs derived by m successive bisections of $\mathbf{a}$.

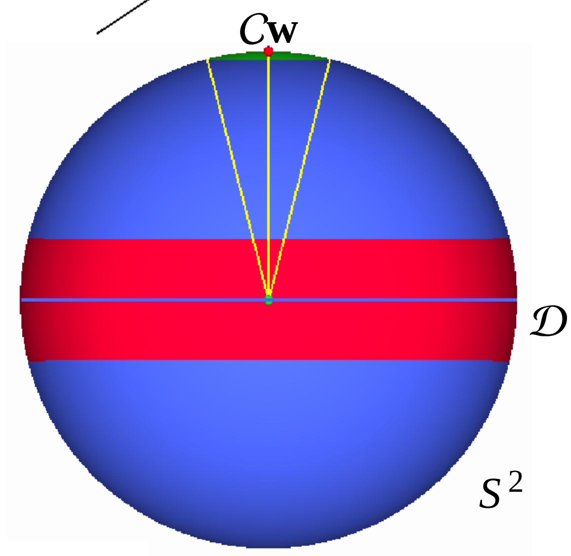


Proposition: For $m \to \infty$, the minima of the minimal distance between the base segments over all sub-arc pairs $(\mathbf{a}^*, \mathbf{b}^*) \in \mathcal{V}_m(\mathbf{a}) \times \mathcal{V}_m(\mathbf{b})$ converges to the minimal distance between the two arcs:

$$\min_{(\mathbf{a}^*,\mathbf{b}^*)\in\mathcal{V}_m(\mathbf{a})\times\mathcal{V}_m(\mathbf{b})} \left(\min_{(\mathbf{x}_1,\mathbf{x}_2)\in\mathbf{a}^*_{02}\times\mathbf{b}^*_{02}} |\mathbf{x}_1 - \mathbf{x}_2| \right) \to \min_{(\mathbf{y}_1,\mathbf{y}_2)\in\mathbf{a}\times\mathbf{b}} |\mathbf{y}_1 - \mathbf{y}_2|, \qquad m \to \infty.$$

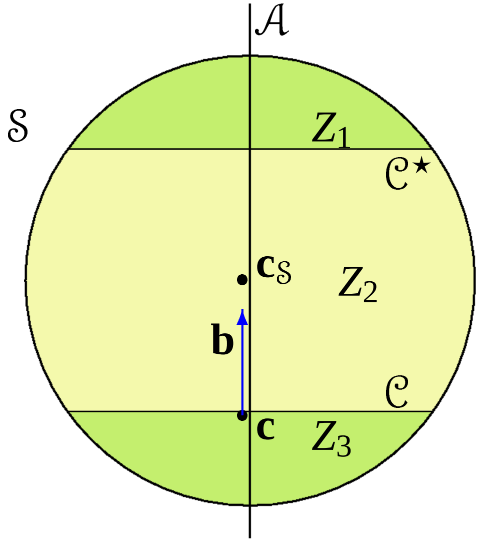
Thickness of arccurves: Double critical test





1. all chords from arc $\mathbf{b}$ to arc $\mathbf{a}$ vary from $\mathbf{w}$ within the angle γ
2. any vector outside “red band” $\mathcal{D}$ is not perpendicular to any chord in the “green region” $\mathcal{C}$
3. tangent indicatrix of an arc is an arc of a great circle
4. suffices to check end tangents

The function ρ_{pt} on arc curves: $\text{pt}(\mathbf{p},\cdot) : \sigma \mapsto \text{pt}(\mathbf{p}, \mathcal{C}(\sigma))$



– want to compute $\rho_{\text{pt}}(s) = \min_{\sigma \in I} \text{pt}(s, \sigma)$ on arc curve

– first study minima of $\text{pt}(\mathbf{p},\cdot) : \sigma \mapsto \text{pt}(\mathbf{p}, \mathcal{C}(\sigma))$ on circle $\mathcal{C}(\cdot)$

– nice geometry: every circle corresponding to $\text{pt}(\mathbf{p}, \mathcal{C}(s))$ lies on sphere defined by $\mathbf{p}$ and $\mathcal{C}(\cdot)$

Lemma: Point $\mathbf{p}$ not contained in the plane of circle $\mathcal{C}$:

$\mathbf{p} \in \mathcal{A}$	$\text{pt}(\mathbf{p},\cdot)$ is constant
$\mathbf{p} \in (Z_1 \cup Z_3 \cup \mathcal{C}^\star) \setminus \mathcal{A}$	2 crit. pts. =1 min, 1 max
$\mathbf{p} \in Z_2$	4 crit. pts. =2 max, 2 min

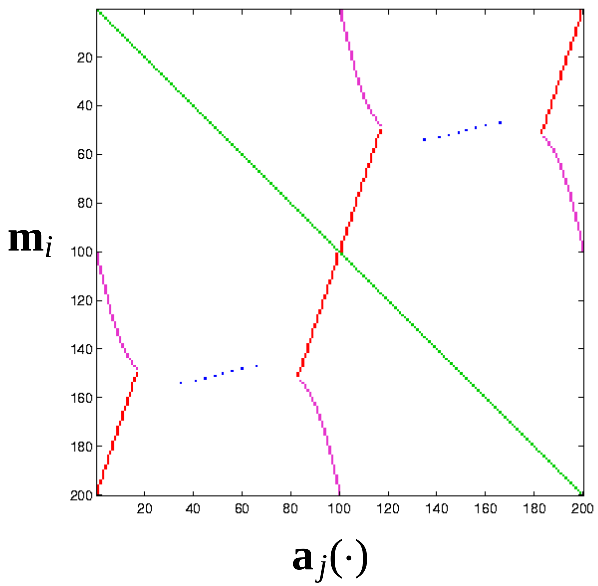
min and max of $\text{pp}(\mathbf{p},\cdot)$

$\longrightarrow$ Can precisely determine the minima and classify how they are achieved!

The function ρ_{pt} on arc curves: $\text{pt}(\mathbf{p},\cdot) : \sigma \mapsto \text{pt}(\mathbf{p}, \mathbf{a}(\sigma))$ The example of a biarc approximation of an ellipse

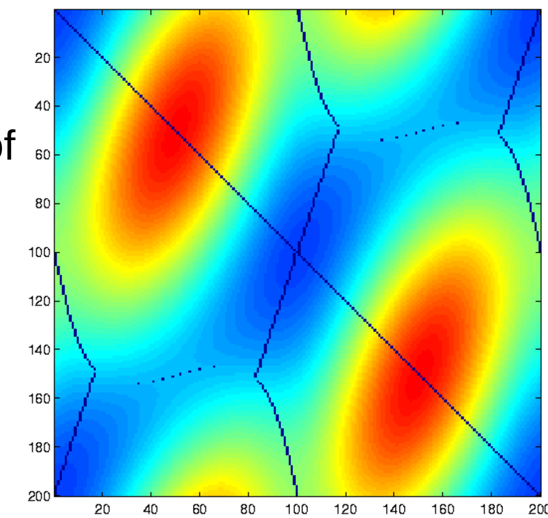
$\longrightarrow$ When we replace the circle $\mathcal{C}(\cdot)$ by an arc $\mathbf{a}(\cdot)$ we have an additional case: a minima can be achieved at an end point!

Approximation of an ellipse with 100 biarcs:



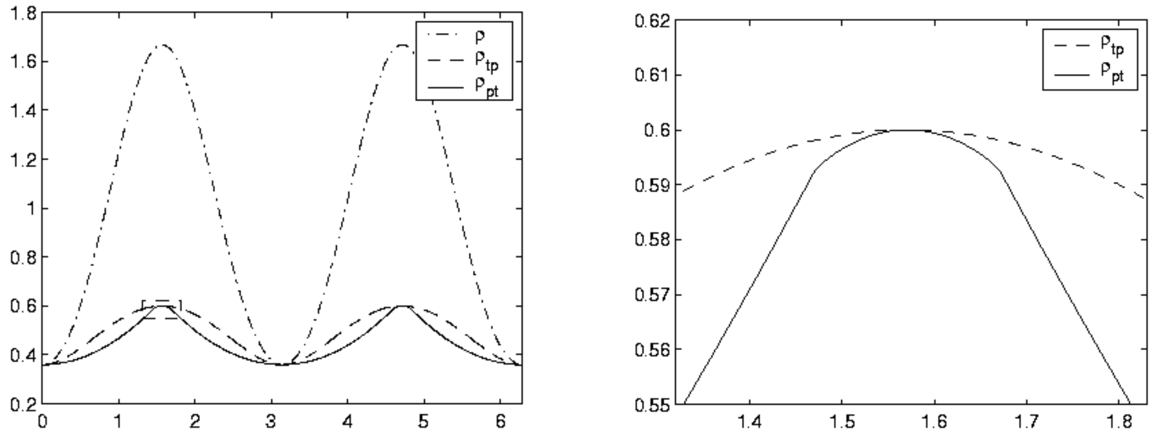
Color at (i, j) if minimum of $\text{pt}(\mathbf{m}_i, \alpha(\cdot))$ achieved inside $\mathbf{a}_j$ by:

- a minimum of pp (blue)
- a maximum of pp (magenta)
- a minimum at end point (red)
- a local radius (green)

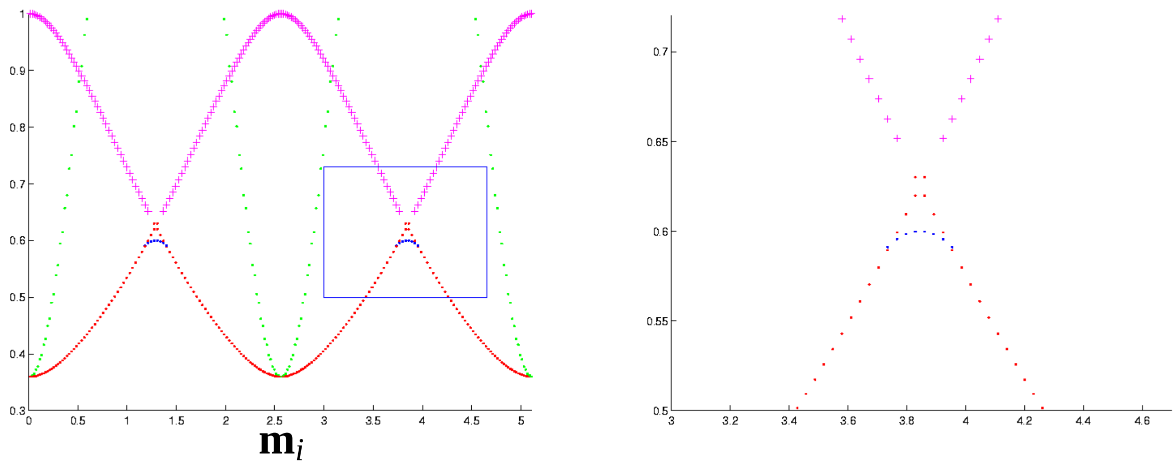


The function ρ_{pt} on arc curves: The example of a biarc approximation of an ellipse

Continuous case:



Biarc approximation:



Plan of Lecture 2:

- biarcs: construction and convergence results
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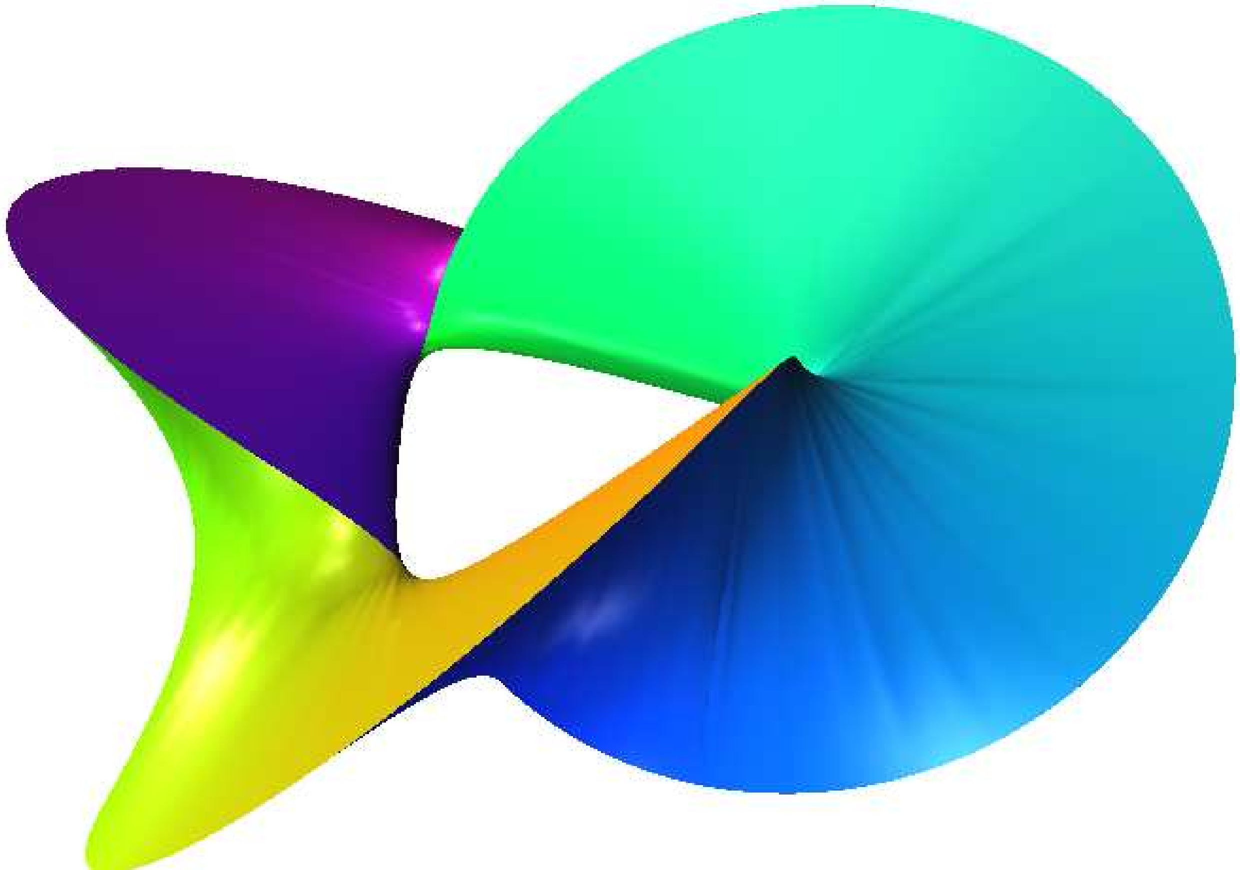
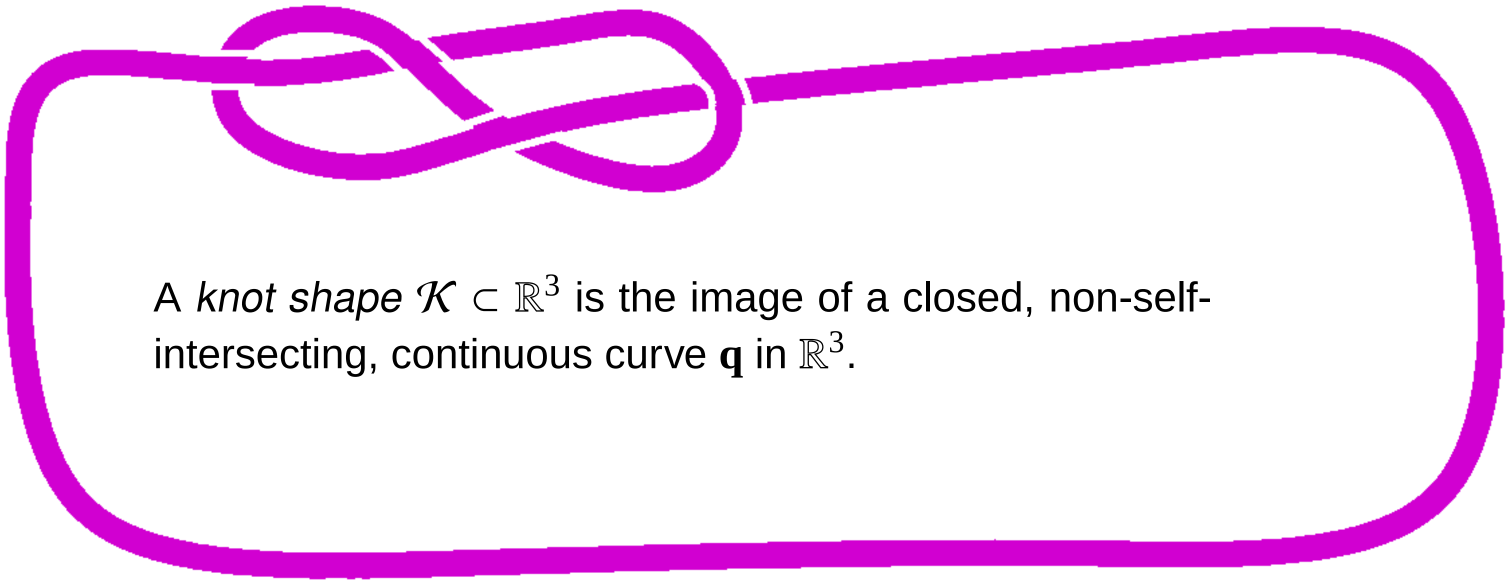
Plan of Lecture 3: Computations of Ideal Shapes

- introduction: knots and ideal shapes of knots
- definition of contact and approximate μ-contact sets
- computations of the ideal 3.1-knot
- computations of the ideal 4.1-knot
- Conclusions

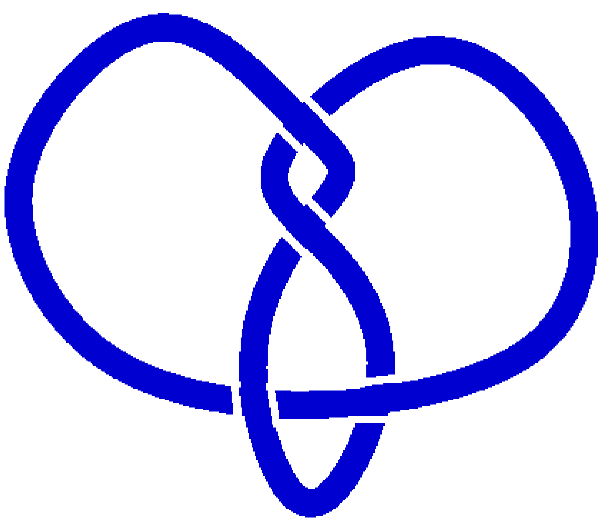
Our objective is to describe how this visualisation of a shaded triangulation of the contact chords of the (approximately) ideal trefoil is computed:



Knots Shapes and Knot types:



A *knot shape* $\mathcal{K} \subset \mathbb{R}^3$ is the image of a closed, non-self-intersecting, continuous curve $\mathbf{q}$ in $\mathbb{R}^3$.



Two knots shapes $\mathcal{K}_1$, $\mathcal{K}_2$ belong to the same *knot (type)* $[\mathcal{K}]$ if one knot can be continuously transformed onto the other.

Ideal shapes of knots:

An *ideal* or *tightest shape* $\mathcal{K}$ of the knot type $[\mathcal{K}^*]$ is a knot shape $\mathcal{K}$ that minimises the functional length/thickness within the knot type $[\mathcal{K}^*]$, i.e. an ideal shape is a solution of

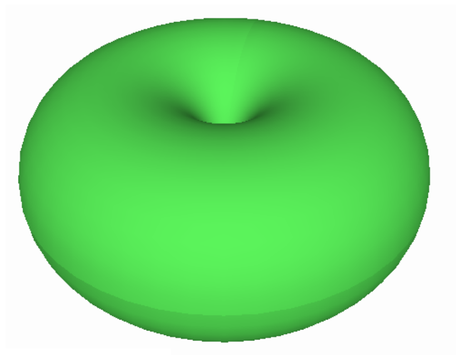
$$\frac{\lambda(\mathcal{K})}{\Delta[\mathcal{K}]} \to \text{min!}$$

subject to $\mathcal{K} \in C(S^1, \mathbb{R}^3), \mathcal{K} \in [\mathcal{K}^*]$.

The positive number $\frac{\lambda(\mathcal{K})}{\Delta[\mathcal{K}]}$ is called the *rope length* of the knot $\mathcal{K}$.

The ideal shape of the trivial knot is a circle. The only known ideal knot shape (also cases of links made from circular arcs and straight line segments, Canterella et al op. cit.)

$\rightarrow$



Ideal knot shapes: Computations

Our approximately ideal shapes were obtained from simulated annealing computations using an upgraded version of a code of Laurie that was originally based on a piece-wise linear discretisation.

The key ingredients in a simulated annealing approach are a) fast and accurate evaluation of rope length, and b) a set of random moves to search configuration space.

Biarc curves are great for both of these. In our computations the thickness was evaluated up to a relative error of 10^{-12}, and to compute contact sets accurately a tolerance of this order of magnitude seems appropriate.

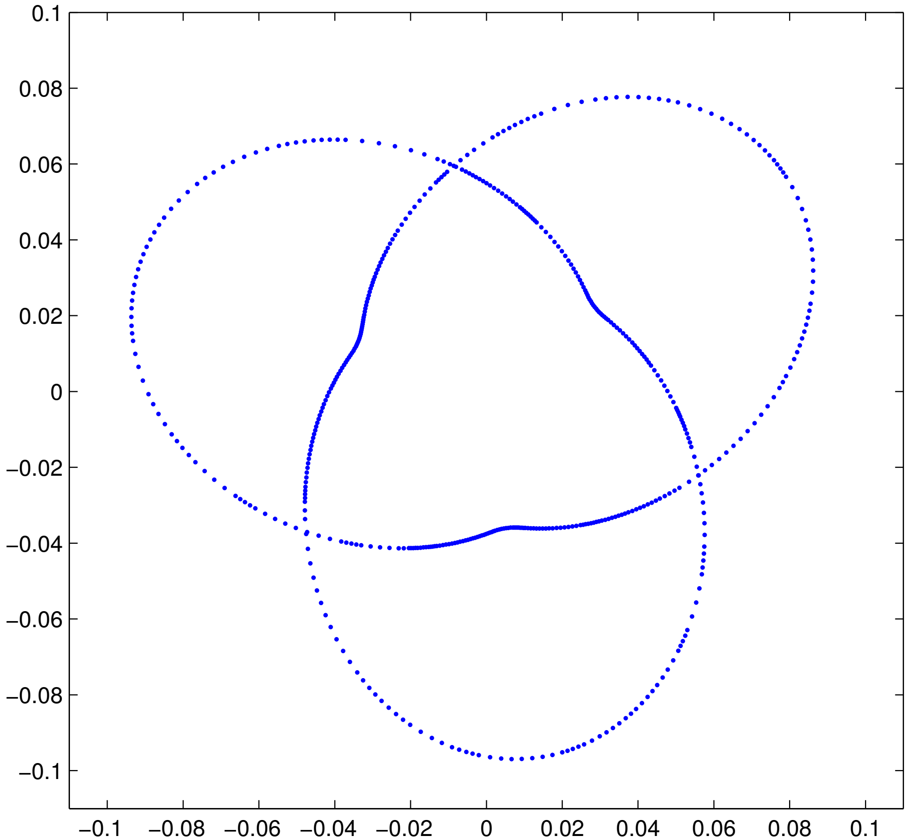
The basic data format is a list of point-tangent data. Then the allowed moves were taken to be random and independent changes in each point and each tangent, but with different, and adaptive, scales for point and tangent moves.

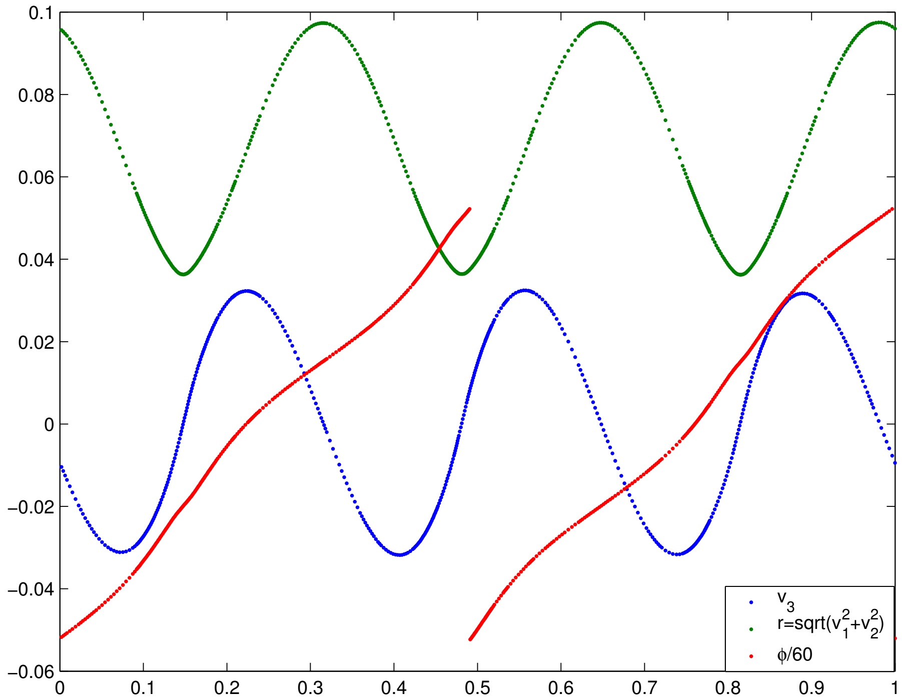
Ideal knot shapes: Numbers for the ideal trefoil

The final bounds of rope length, the length $\lambda(\alpha)$ of the arc curve, the minimal radius $\min_i r_i$, and upper and lower bounds for thickness $\Delta[\alpha]$ on a 528 arc curve are

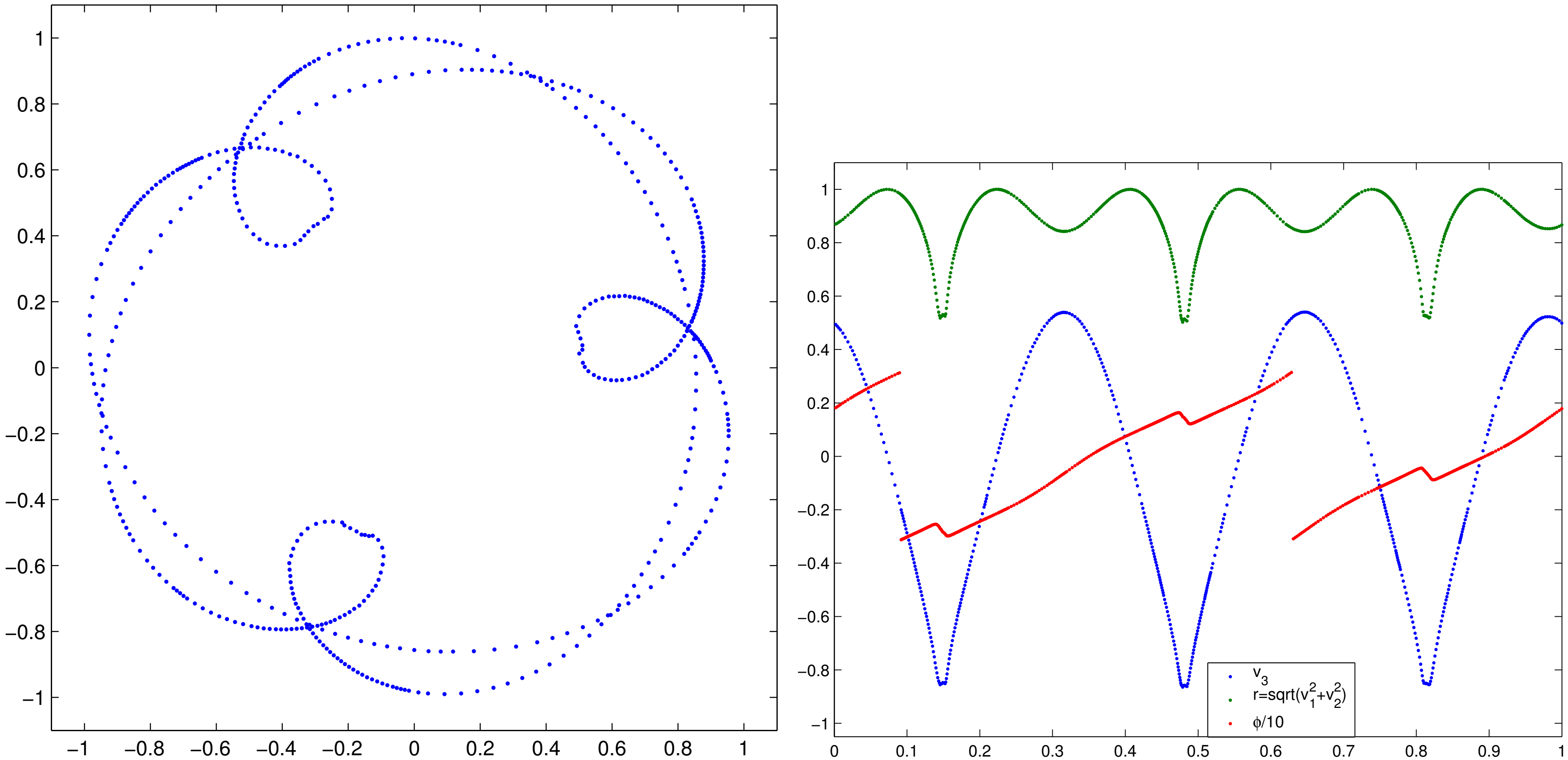
$$\begin{aligned} & \lambda(\alpha) && = 0.99999999997863, \\ & \min_i r_i && = 0.03054053096312, \\ 0.03053951779966 \leq\ & \Delta[\alpha] && \leq 0.03053951779968, \\ 32.74445937679887 \leq\ & \frac{\lambda(\alpha)}{\Delta[\alpha]} && \leq 32.74445937682155. \end{aligned}$$

Ideal knot shapes: Pictures of the ideal trefoil





Ideal knot shapes: Pictures of the ideal trefoil–tangent indicatrix



Very little known about necessary conditions for ideality. On segments where the curve is C^2 have:

1) The segment is either straight or the function $\rho_{\mathrm{pt}}(s)$ is constant and minimal, i.e., equal to the thickness Δ.

2) (A complicated version involving Radon measure of the idea) If local curvature is not active anywhere, and at curved points of the shape, the principal normal of the curve should be in the cone of contact chords, i.e., of doubly critical line segments realising Δ. (vdMosel & Schuricht).

Therefore we need to understand the....

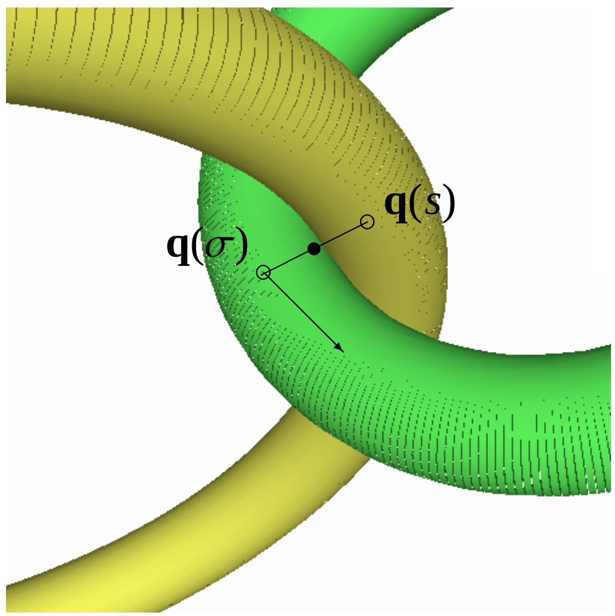
Ideal knot shapes: Contact set χ

Definition: For a closed, non-intersecting curve $\mathbf{q} \in C^1(I, \mathbb{R}^3)$ we define the *contact set* χ to be the set

$$\chi := \{(s, \sigma) \in I \times I; \mathrm{pt}(s, \sigma) = \Delta[\mathbf{q}]\}.$$

That is χ is the set of points in the (s, σ) plane realising the global minimum of $\mathrm{pt}(s, \sigma)$. **Definition:** The *set of contact points* in three dimensional space is the set

$$C := \{\mathbf{c} \in \mathbb{R}^3; \ \mathbf{c} \text{ is the centre of } \mathcal{C}(s, \sigma, \sigma) \ \& \ (s, \sigma) \in \chi\}.$$



For a generic curve the global minimiser of pt will be realised at a single point and both χ and C will be sets containing one point. Such sets are robust.

The ellipse has symmetry, so there are a two points in each set corresponding to the two points of minimal radius of curvature. Already an unstable situation.

And for ideal shapes constancy of ρ_{pt} implies that the exact contact sets should probably be much larger, i.e., at least contain line segments. A very unstable situation under perturbation.

For example the point contact set C for the circle (i.e., the unknot ideal shape) is a single point, namely the centre. But the contact set χ is the entire square $I \times I$, because pt is constant on circles.

→ Thus for approximately ideal shapes, and in particular for numerics we need to introduce a tolerance!

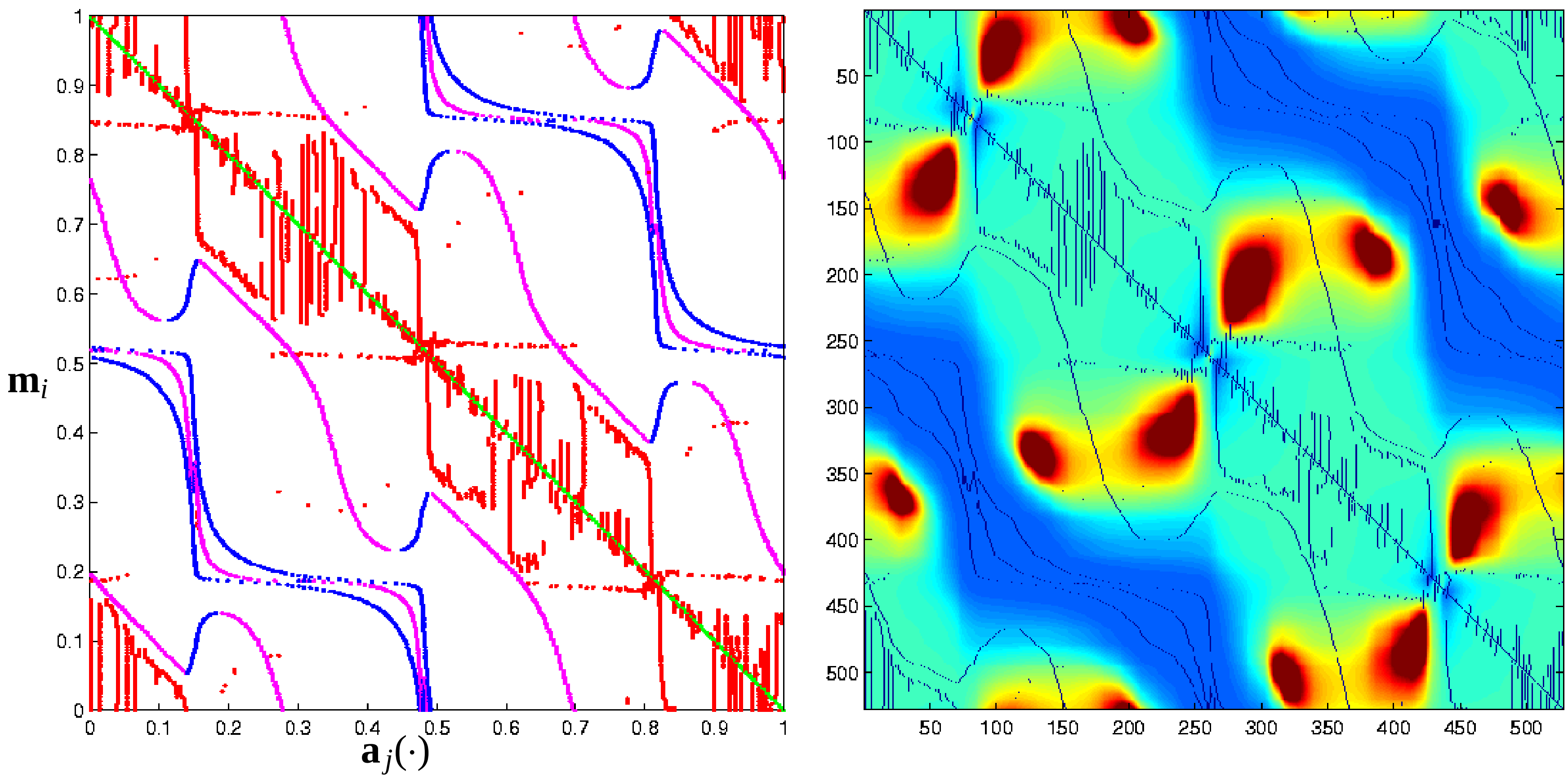
Definition: For each $\mu > 0$ the *μ-contact set* χ_μ is the set

$$\chi_\mu := \{(s,\sigma) \in I \times I;\ \mathrm{pt}(s,\sigma) \le \Delta[\mathbf{q}](1+\mu)\ \ \&\ \ \mathrm{pt}(s,\cdot) \text{ has a local minimum in } \sigma\},$$

and the *set of μ-contact points* in three dimensional space is the set

$$C_\mu := \{\mathbf{c} \in \mathbb{R}^3;\ \mathbf{c} \text{ is the centre of } \mathcal{C}(s,\sigma,\sigma)\ \&\ (s,\sigma) \in \chi_\mu\}.$$

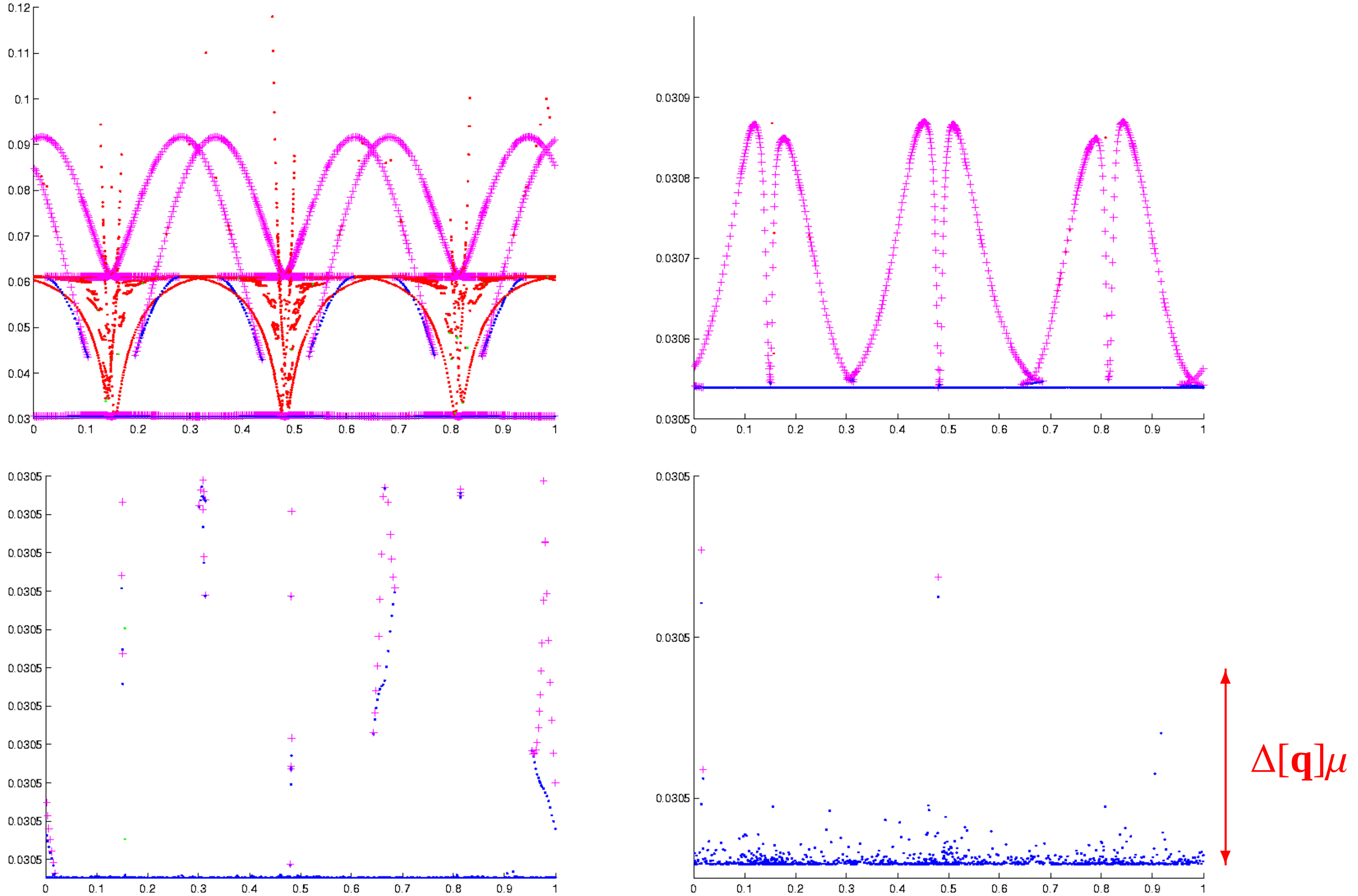
3.1 ideal knot shape: The pt function and μ-contact set χ_μ



Color at (i, j) if minima of pt$(\mathbf{m}_i, \alpha(\cdot))$ achieved inside $\mathbf{a}_j$ by:

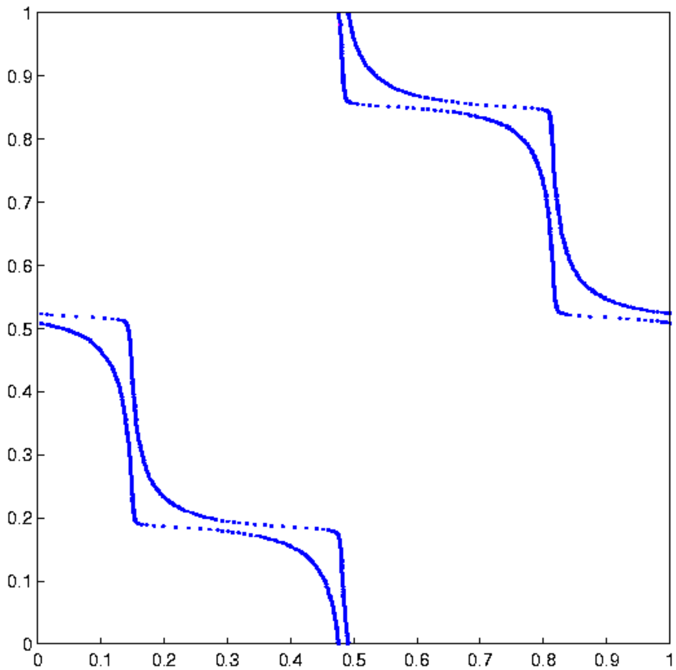
- a minimum of pp (blue)
- a maximum of pp (magenta)
- a minimum at end point (red)
- a local radius (green)

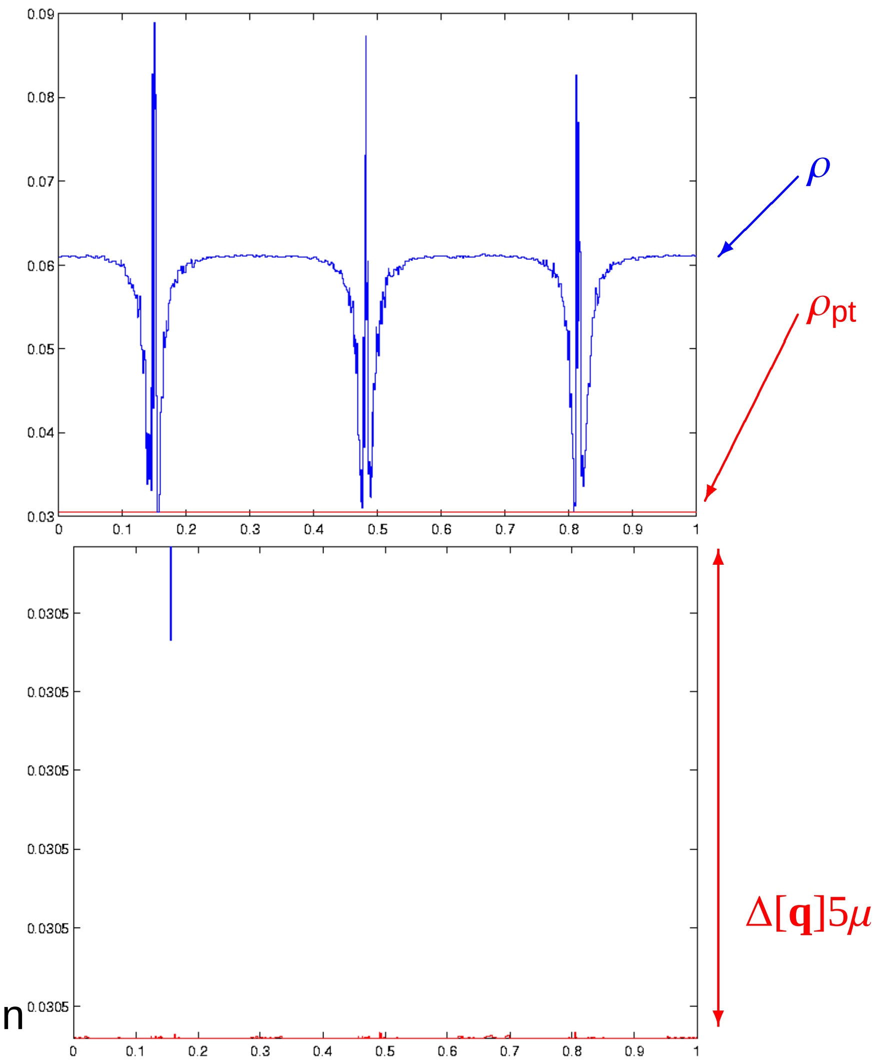
Values of minima of pt($\mathbf{m}_i, \alpha(\cdot)$):



$\mu := 8.1861 \cdot 10^{-6}$ and $\Delta[\mathbf{q}] = 0.0305395$

3.1 ideal knot shape: The μ-contact set χ_μ and ρ_{pt}

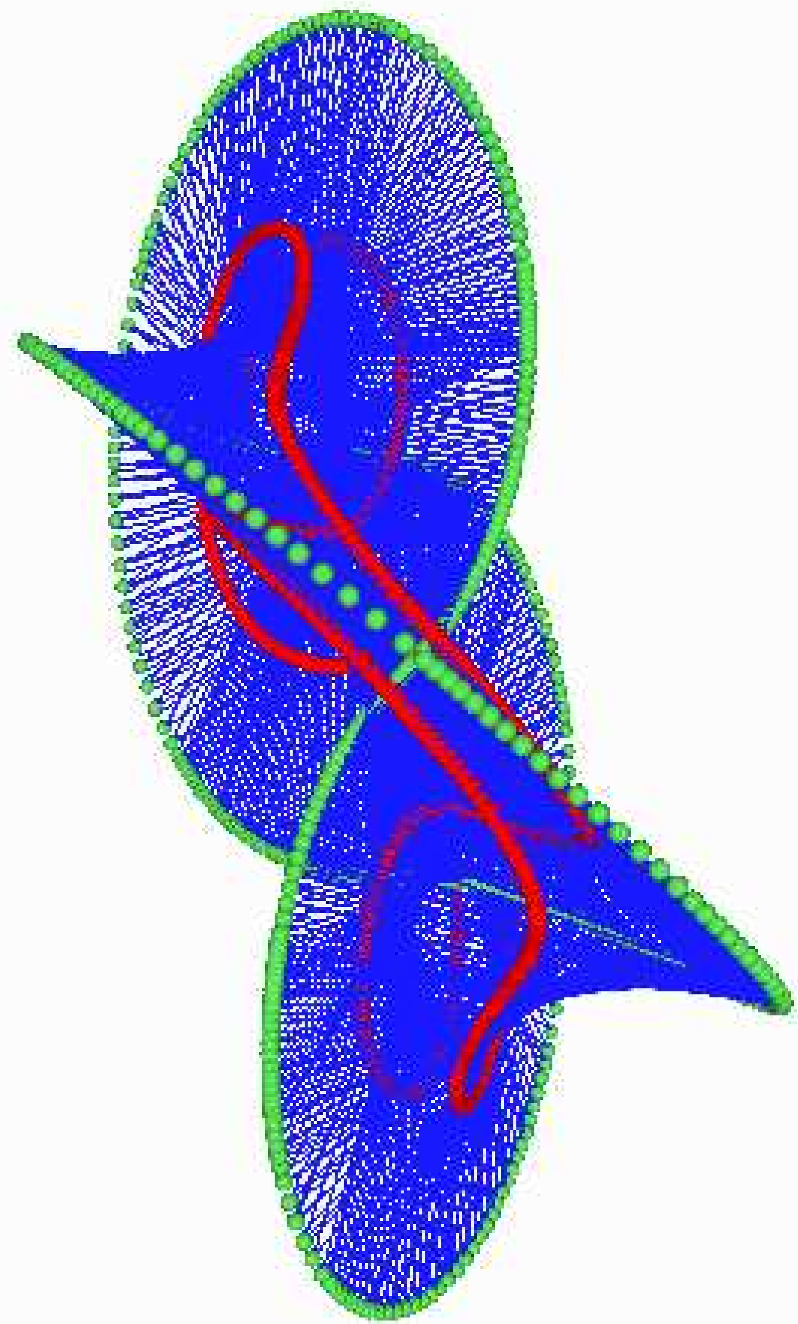


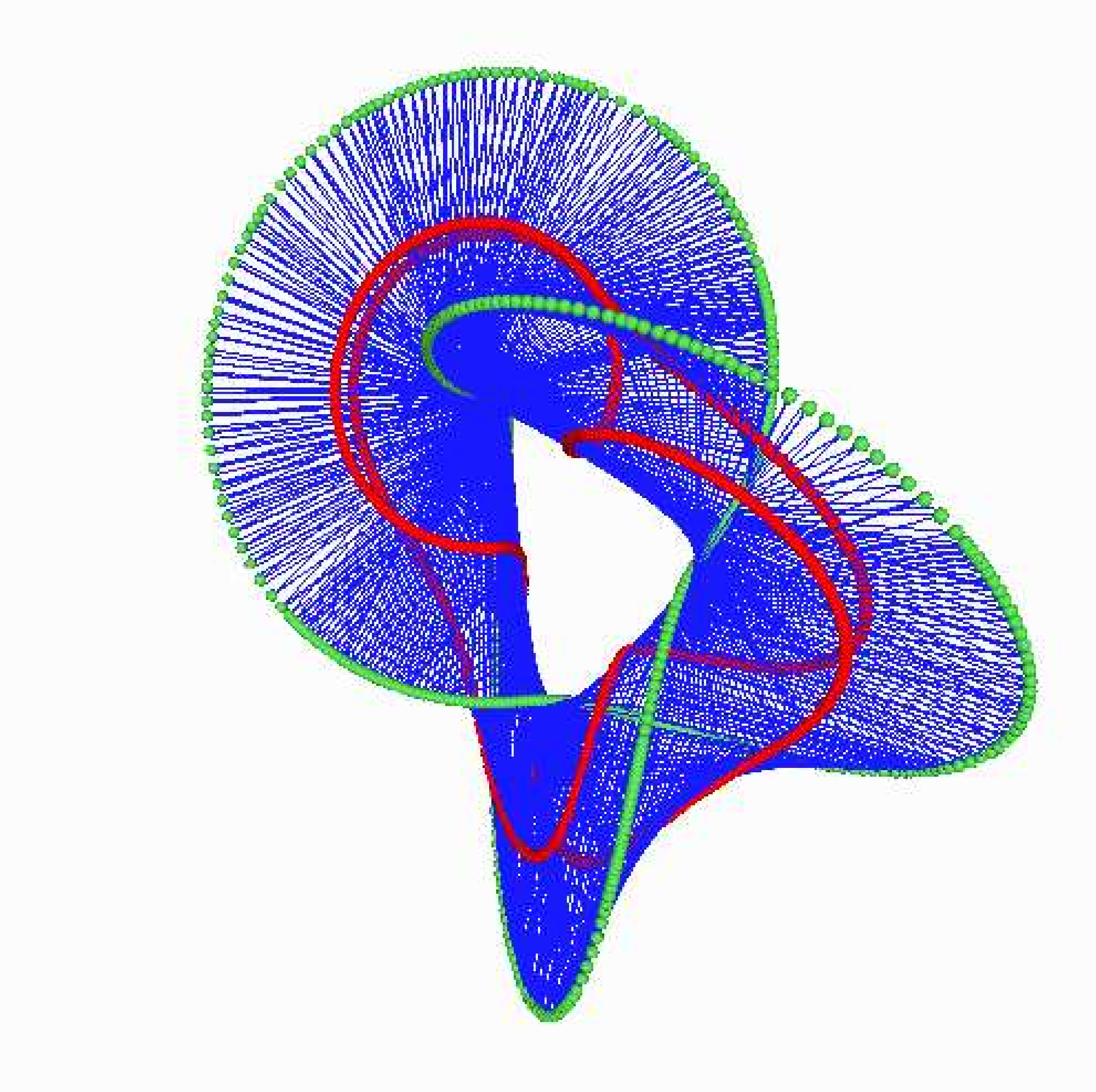


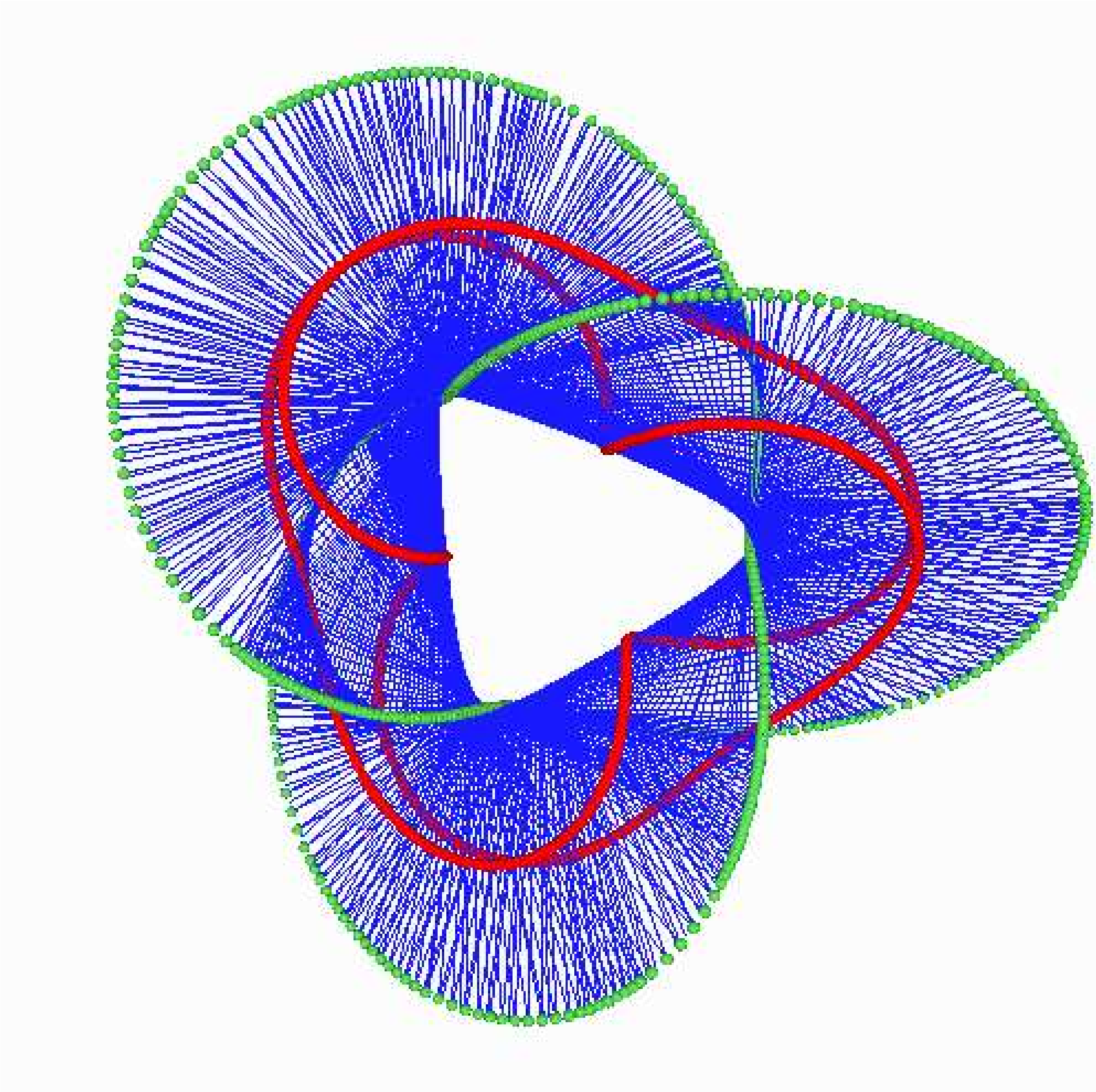
- Can compute ρ_{pt} to test if constant on curved segments
- Can say if local is active in the scale μ

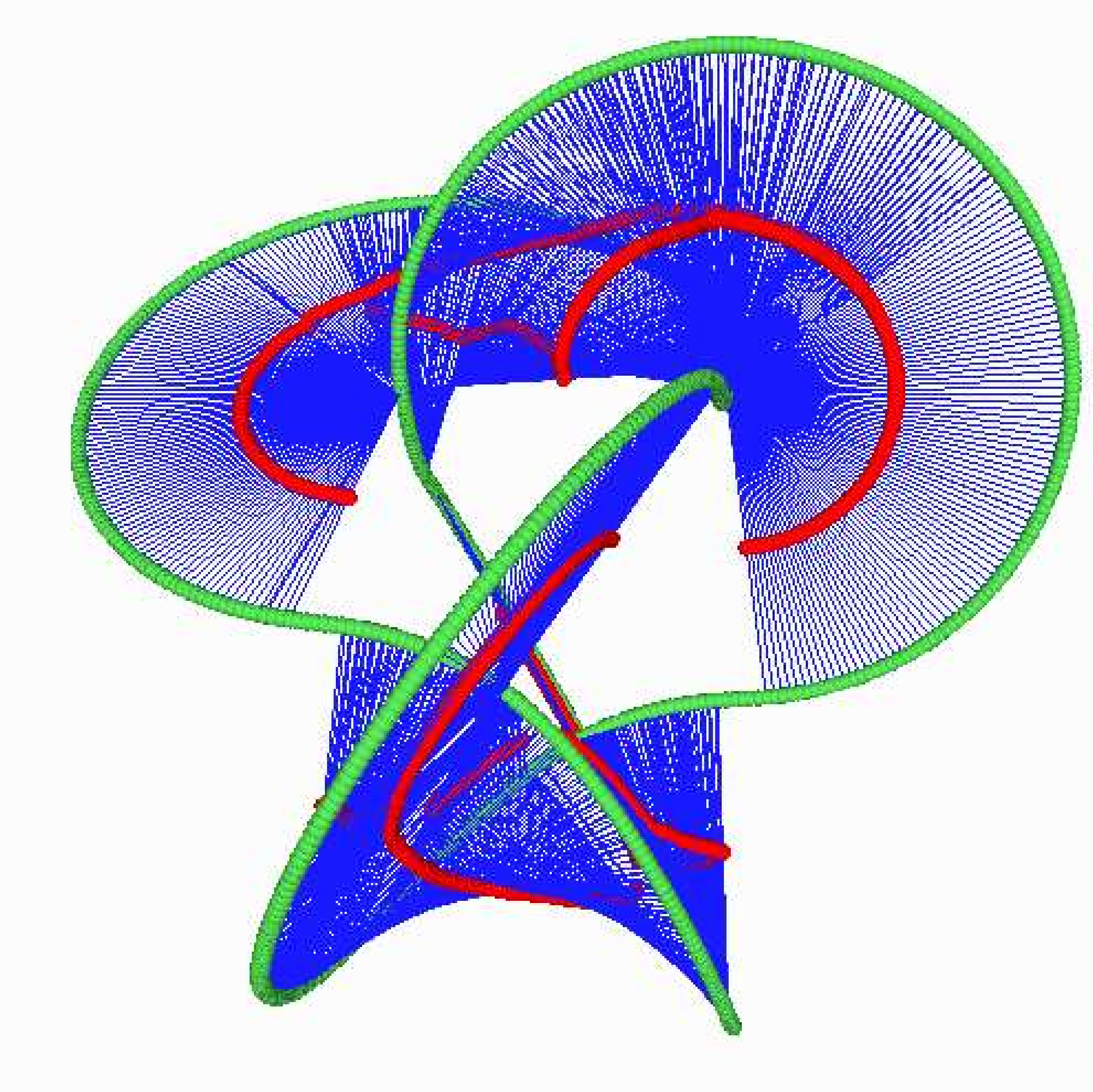
$$\mu := 8.1861 \cdot 10^{-6}$$
$$\Delta[\mathbf{q}] = 0.0305395$$

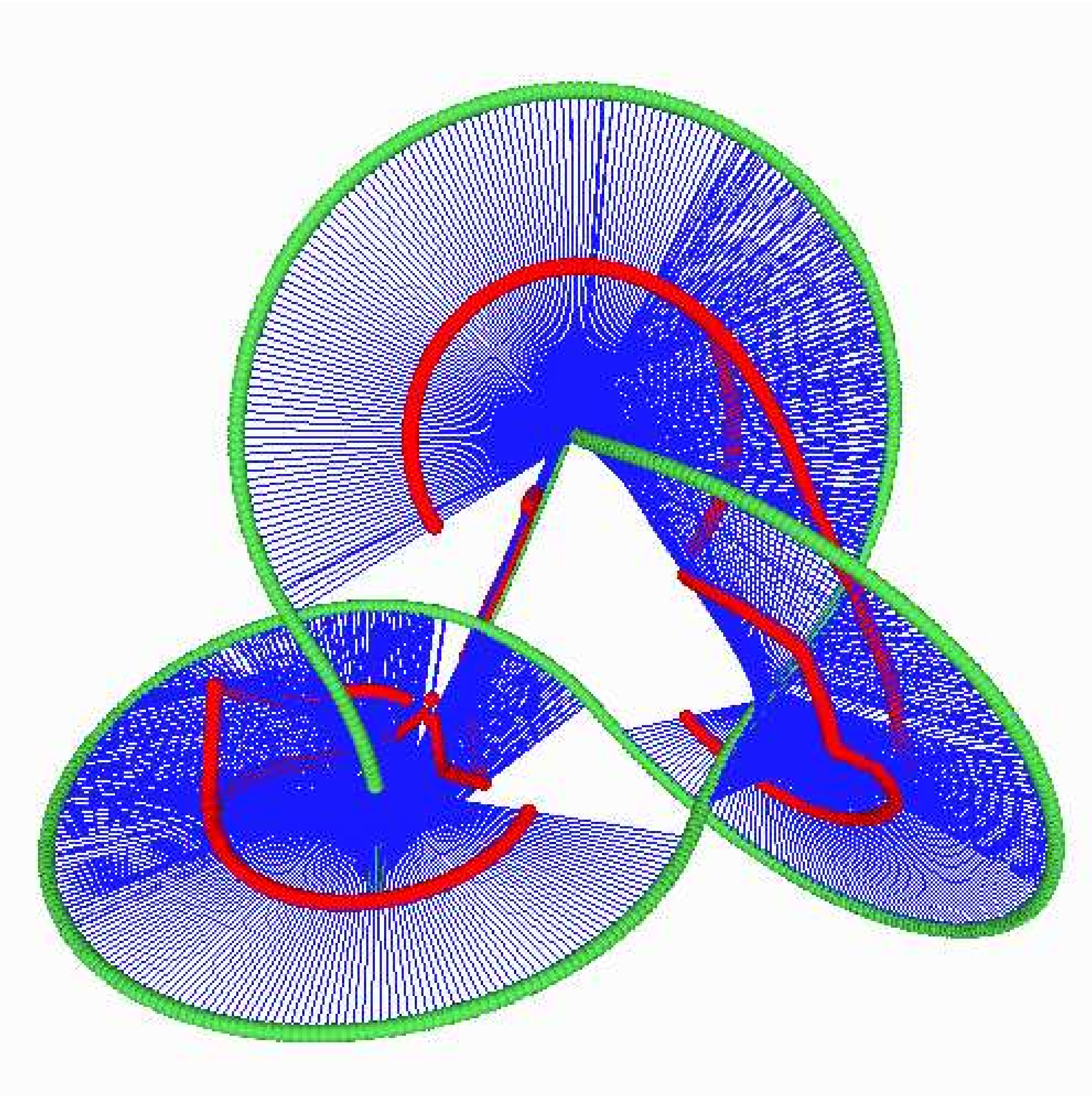
A 3D interactive demonstration of ideal knot shapes has been replaced by three snapshots of each of the approximately ideal 3.1 and 4.1 knot shapes. In all images we have : Green dots are centres of arc curves making up knots. Blue lines are the approximate contact chords, and the red dots are the centres of the approximate contact chords, i.e. the approximate point contact set. For the 3.1 trefoil the red dots overlap to form another trefoil. For the figure-eight 4.1 knot the contact set appears to have two disjoint components.

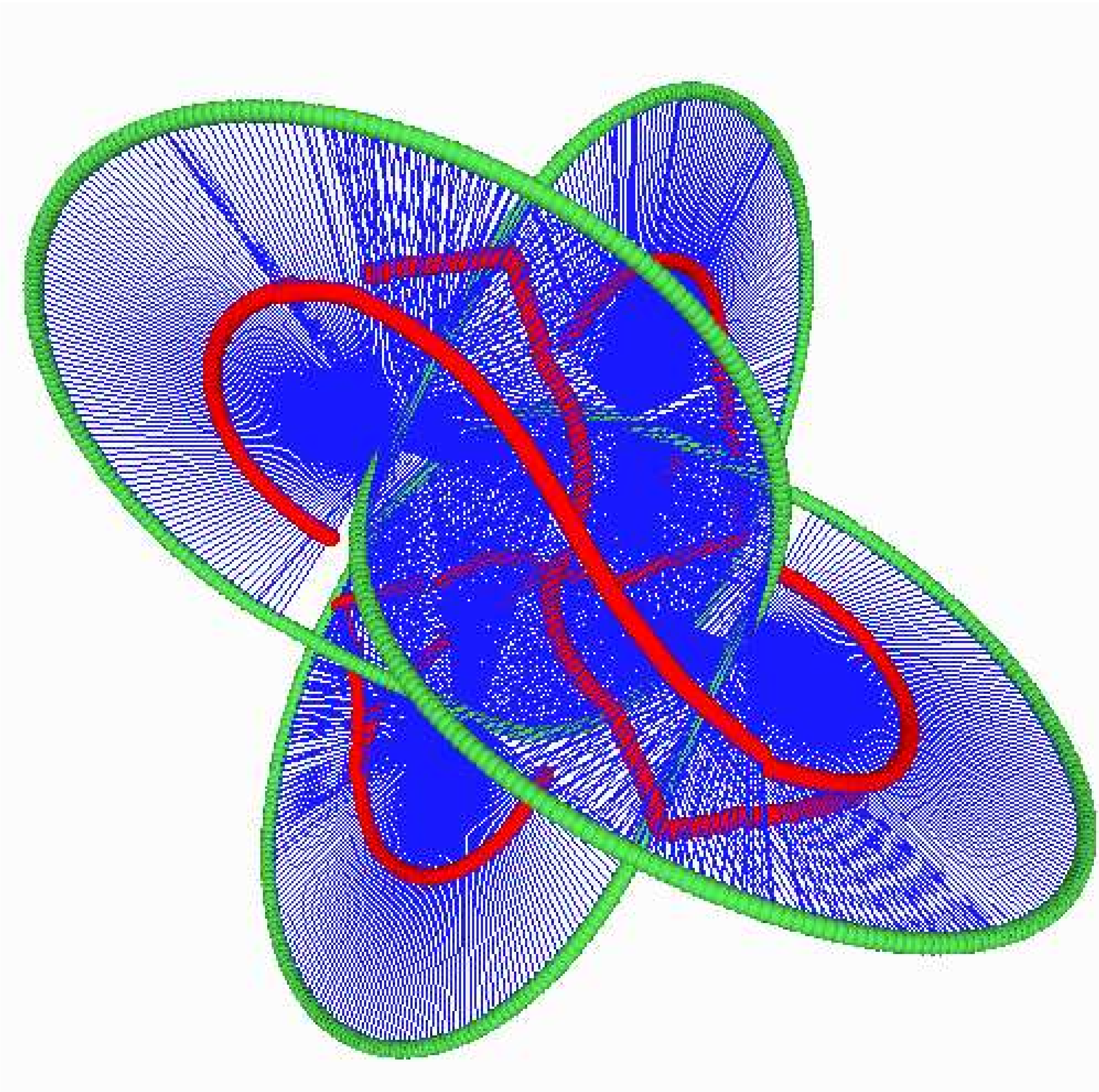












Conclusions:

- global radii of curvature ρ_{pt} and ρ_{tp} are convenient functions to study distance from self-intersection or thickness
- biarcs are a good tool to compute self-avoiding curves
  - right class $C^{1,1}$
  - rigorous upper bound of rope length
  - study of contact set
  - precise evaluation of ρ_{pt}
- computations of ideal knots yield
  - curvature is often (close) to active
  - observe very high torsion (discontinuous serret-frenet frame)
  - best known ideal shapes of 3.1 and 4.1 knot (or they were, Rawdon et al now have slightly lower rope length trefoil....)
  - our ideal knots satisfy necessary condition “ρ_{pt} constant on curved segments”
  - have a scale to judge how close to converged

Thanks:

Merci pour l’invitation....

Merci pour votre attention...

et merci pour le support informatique :-) ....

Joint Work:

JHM + Oscar Gonzalez, UT-Austin

JHM + OG + Heiko von der Mosel, Aachen + Friedemann Schuricht, Cologne

JHM + OG + Jana Smutny

JS, PhD Thesis, EPFL 2004 (and the majority of these slides)

JHM + JS + Mathias Carlen, Diplomant, EPFL + Ben Laurie, London

JHM + Andrzej Stasiak, U. of Lausanne

Crucial input from: Remi Langevin, U. of Bourgogne, Arieh Iserles, U. of Cambridge

The material of the three talks is described at length in the thesis,

Global Radii of Curvature, and the Biarc Approximation of Space Curves: In Pursuit of Ideal Knot Shapes, by Jana Smutny

which is available in pdf as PhD Thesis number [7] on:

http://lcvmwww.epfl.ch/publis.html

and in the five articles (also available electronically from the same page):

[82] M. Carlen, B. Laurie, J.H. Maddocks, J. Smutny, ”Biarcs, Global Radius of Curvature, and the Computation of Ideal Knot Shapes”, Chapter in ”Physical and Numerical Models in Knot Theory and Their Application to the Life Sciences”, Eds. J. Calvo, K. Millett, E. Rawdon, and A. Stasiak, To be published by World Scientific. (A condensed version of Chapters 4, 7 and 8 of the thesis [7])

and

[65] O. Gonzalez, J.H. Maddocks, J. Smutny, ”Curves, circles, and spheres”, Contemporary Mathematics 304 (2002) 195-215. (The original version of Chapter 3 of the thesis [7])

[61] O. Gonzalez, J.H. Maddocks, F. Schuricht, H. von der Mosel, ”Global curvature and self-contact of nonlinearly elastic curves and rods”, Calculus of Variations 14 (2002) 29-68. (A rather technical article showing how global radius of curvature can be used to prove the existence and minimal regularity of various optimal packing problems, including ideal knot shapes.)

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