Using writhing to characterise DNA topology (with a little help from solar physics).

Chris Prior[1] Zachary Sierzega [2] Jeff Wereszczynski [2]

[1]Durham University [2]Illinois Institute of Technology

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Gauss and linking

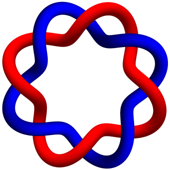
The concept of linking appears to have first arrived with Gauss,

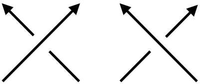
the intertwinings of two closed or infinite curves. Let the coordinates of an undetermined point of the first curve be x, y, z; of the second x', y', z', and let

$$\iint \frac{(x'-x)(\mathrm{d}y\mathrm{d}z'-\mathrm{d}z\mathrm{d}y')+(y'-y)(\mathrm{d}z\mathrm{d}x'-\mathrm{d}x\mathrm{d}z')+(z'-z)(\mathrm{d}x\mathrm{d}y'-\mathrm{d}y\mathrm{d}x')}{[(x'-x)^2+(y'-y)^2+(z'-z)^2]^{3/2}} = V$$

then this integral taken along both curves is $= 4m\pi$ and m the number of intertwinings.[8]

Gauss was interested in the linkng of asteroids and magnetic loops (Epple: Mathematical Intelligencer):



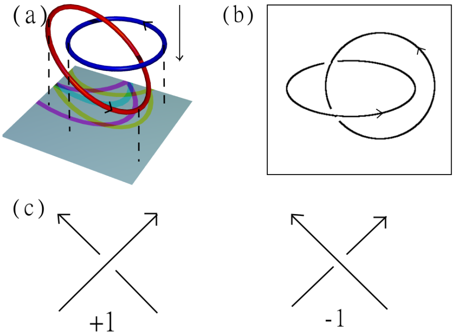


+1 -1

m is half the number of (signed) crossings it is a topological invariant, it only changes if the strands intersect.

Its all a point of view..

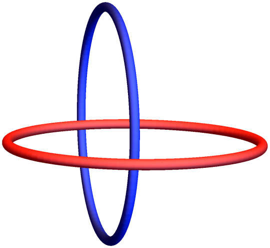
We project a pair of 3-D curves along a fixed direction (a). The link projection is (b).



But which direction to project?

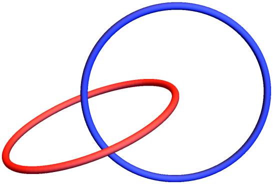
Does it matter?

In fact we will always get the same answer (degree theorem)



The linking integral:

$$Lk = \frac{1}{4\pi}\oint_x \oint_y \mathbf{T}_\mathbf{x}(s) \times \mathbf{T}_\mathbf{y}(t) \cdot \frac{\mathbf{x}(s) - \mathbf{y}(t)}{\|\mathbf{x}(s) - \mathbf{y}(t)\|^3}\,\mathrm{d}s\,\mathrm{d}t,$$



Is the average of the planar link calculated over all projection directions (which can be represented as points on the unit sphere).$\Rightarrow$ Massive redundancy.

Relation to helicity

Moreau and Moffat:

$$H = \int_{\Omega} \mathbf{A} \cdot \mathbf{B}\, \underset{\cdot}{V}, \tag{1}$$

where $\mathbf{B} \cdot \mathbf{n} = 0$ on $\partial\Omega$. Use Biot-Savart gauge for $\mathbf{A}$:

$$\mathbf{A} = \frac{1}{4\pi} \int_{\Omega} \mathbf{B}(\mathbf{y}) \times \frac{\mathbf{x} - \mathbf{y}}{|\mathbf{x} - \mathbf{y}|^3} \mathrm{d}^3 y. \tag{2}$$

Then

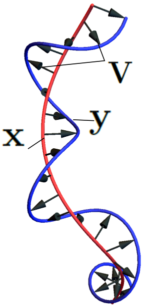
$$H = \frac{1}{4\pi} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \mathbf{B}(\mathbf{x}) \cdot \mathbf{B}(\mathbf{y}) \times \frac{\mathbf{x} - \mathbf{y}}{|\mathbf{x} - \mathbf{y}|^3}\, \mathrm{d}^3 x\, \mathrm{d}^3 y. \tag{3}$$

$\mathbf{B} = |\mathbf{B}|\mathbf{T}$ so the helicity is the flux weighted linking. See David MacTaggart's talk as to why separating topologial and flux information can be important.

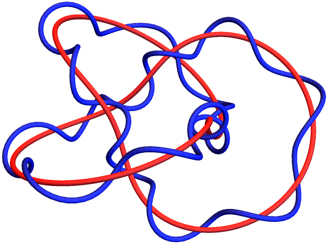
Ribbons and the Călugăreanu theorem 1

A ribbon structure is constructed using a vector field **V** normal to **x** ($\mathbf{V} \cdot \mathbf{T} = 0, \forall s$). This field may rotate around the curve **x** and defines a second curve **y**, the ribbon's edge:

$$\mathbf{y}(s) = \mathbf{x}(s) + \epsilon \mathbf{V}(s), \tag{4}$$



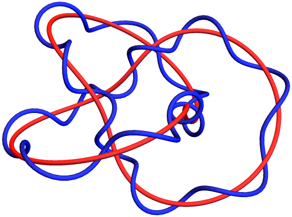
(a)



(b)

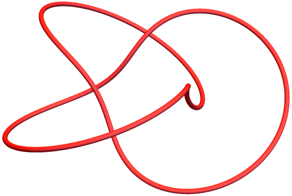
Ribbons and the Călugăreanu theorem 2

The linking topology of the ribbon is a combination of the self-linking (writhe *Wr*) of its axis and the total rotation of the field **V** (*Tw* twist):



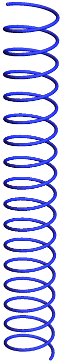
(a) Lk

=



(b) Wr

+



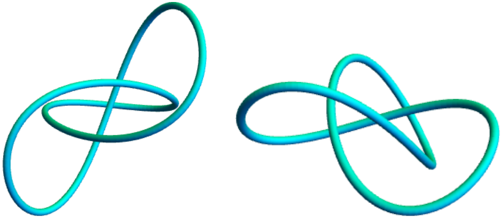
(c) Tw

Writhe and twist, it's still a point of view

$$Wr = \frac{1}{4\pi}\oint_x \oint_x \mathbf{T}_{\mathbf{x}}(s) \times \mathbf{T}_{\mathbf{x}}(t) \cdot \frac{\mathbf{x}(s) - \mathbf{x}(t)}{\|\mathbf{x}(s) - \mathbf{x}(t)\|^3}\, ds\, dt$$

$$Tw = \frac{1}{2\pi}\oint_x \mathbf{T}_x(s) \cdot \mathbf{V}(s) \times \frac{d\mathbf{V}(s)}{ds}\, ds$$

Writhe is just the self linking.



The projection direction **does** matter $\Rightarrow$ Wr is not an integer about 3.2 here. So about 80% see 3 crossings, 20% 4.

Călugăreanu and Fuller a little history

- $Lk = Wr + Tw$ was derived by G Călugăreanu , in a somewhat cumbersome fashion (1959/1962), (see Ricca and Moffatt for a readable perspective)
- It was popularised by F B Fuller (1971), who coined the term writhe. His paper was written on request of Francis Crick with the aim of applying it to DNA. Parts of that work will feature in most modern structural biology textbooks.

Some properties

Lk

- A topological invariant to isotopic motions. Changes by integer values if the curves cross (it detects reconnection!).

Wr

- Changes continually under isotopy. Changes by integer values if the ribbon axis cross itself. Is zero for planar curves.

Tw

- Changes continually under isotopy. Doesn't change by integer values if the ribbon crosses.

The critical point is Lk acts as a fixed anchor. If the axis curve changes shape it tells us how much twist will be lost/gained. Maximise the writhe change you can maximise the twist change. (writhe/kink/Mitchell's instability).

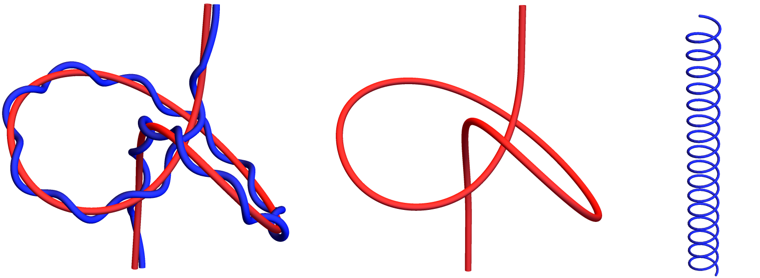
Why this matters

Typically applications include DNA models and elastic rod models (entwined plants/bio-polymers/ropes/Sea-shells!). Mathematical approaches:

- Energy minimization: find energy minimum subject to fixed Lk constraint
- Path integrals: Average over all possible configurations subject to Lk constraint
- Path following: quasi-static evolution of elastic tube under varying parameters (loading), configurations subject to Lk constraint.
- In most models $Tw = Lk - Wr$, Lk is pre-fixed so writhe is the crucial control parameter. If we don't enforce fixed link out model is not physically valid.
- Writhe is probably less important in MHD due to reconnection.

The problem with open ribbons

One can calculate *Lk*, *Wr* and *Tw* for open ribbons, the link is no longer an integer. But *Lk* is not generally a meaningful invariant.

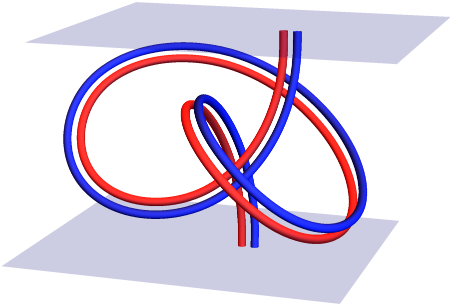


$$Lk \quad = \quad Wr \quad + \quad Tw$$

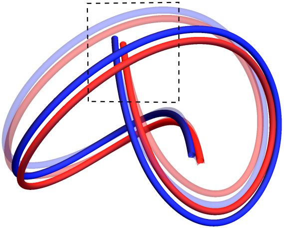
A twisted open ended ribbon. If we fixed its ends from rotating then up to isotopy a meaning full measure of the entanglement should be fixed. But.....

Its still a point of view

Because of the end points some projections see crossings, some don't (hence Lk not being an integer).



(a)

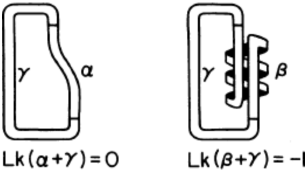


(b) (a) from a particular point of view

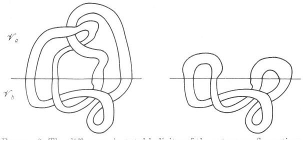
If we deform an interior section of the ribbon (losing no winding) crossings are lost, hence Lk is not invariant. For non normal magnetic fields (fieldlines leaving the domain) the Biot Savart Gauge **A** does not curl to **B**......

Closures

Fuller (1978) had an idea which would have significant consequences in Solar physics: close the ribbon off to get invariant Linking.



(a) Fuller 1978: relative linking

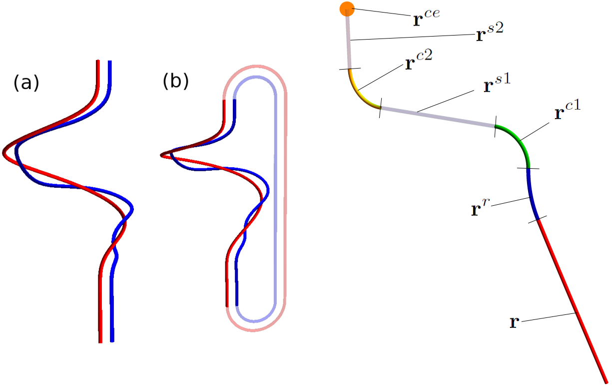


(b) Berger and Field 1984 Relative helicity.

Two significant problems: (a) you always have to construct the closure, (b) the closure/main ribbon contributions are generally significant (even dominant) but this doesn't really exist!!!

Closures-Grrrrrrrrr

Huge amounts of intellectual effort given to constructing closures, even in papers released this year.



But its a complete waste of time...

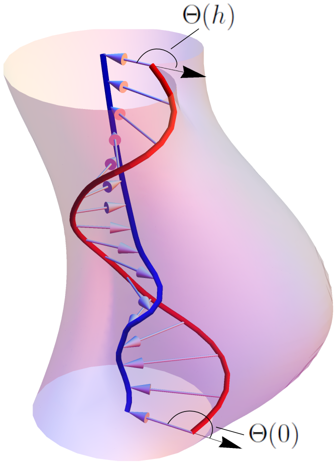
The winding number

See David MacTaggart and Anthony Yeates' excellent talks on the uses of winding in solar physics contexts:

- Split the domain into planes.
- Define $\mathbf{r} = \mathbf{x}(z) - \mathbf{y}(z)$ joining the curves in plane.
- Define an angle Θ, the total rotation of this angle is the *net-winding*,

$$L(\mathbf{x},\mathbf{y}) := \frac{1}{2\pi}\int_0^h \frac{\mathrm{d}}{\mathrm{d}z}\Theta\left(\mathbf{x}(z),\mathbf{y}(z)\right)\mathrm{d}z$$
$$= \frac{1}{2\pi}\Big(\Theta(h)) - \Theta(0)\Big) + N, \qquad (5)$$

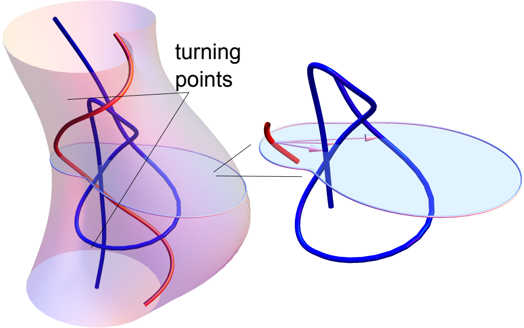
Invariant under isotopy (ideal motion) vanishing at the boundaries.



The winding number extended

For curves whose height function is multivalued we split the curve via its *turning points*. We mark each curve as rising or falling,

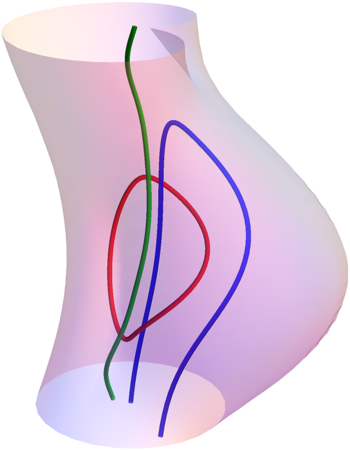
$$\sigma(\mathbf{x}_i) = \begin{cases} 1 & \text{if } \mathrm{d}x_z/\mathrm{d}z > 0, \\ -1 & \text{if } \mathrm{d}x_z/\mathrm{d}z < 0. \end{cases}$$



The following sum is invariant under isotopy [Berger and Prior J.Phys.A 2006].

$$\mathcal{L}(\mathbf{x},\mathbf{y}) := \sum_{i=1}^{n+1}\sum_{j=1}^{m+1} \frac{\sigma(\mathbf{x}_i)\sigma(\mathbf{y}_j)}{2\pi} \int_{z_{ij}^{min}}^{z_{ij}^{max}} \frac{\mathrm{d}\Theta\left(\mathbf{x}_i(z),\mathbf{y}_j(z)\right)}{\mathrm{d}z}\mathrm{d}z. \quad (6)$$

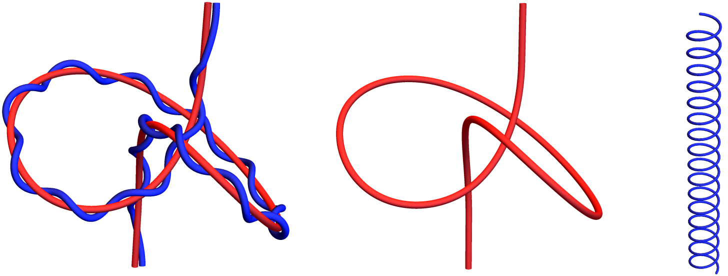
Works for closed curves and loops



The winding is equal to *Lk* for closed curves.

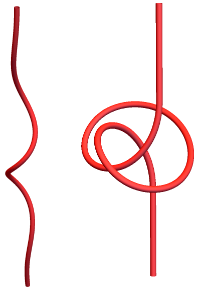
The polar writhe

Mitch Berger, with some help from myself, set out to answer the question: **What is** $Lk - Tw$**?**. We call it the polar writhe W_p. It gives us a more general Călugăreanu type theorem



$$Lk \quad = \quad Wr \quad + \quad Tw$$

Introducing W_p



(a) W_{pl} **(b)** W_{pnl}

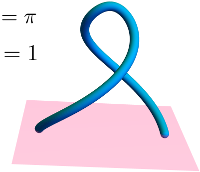
Decomposed into W_{pl} (local helical coiling) and non local components W_{pnl} (knotting). There is no such clear decomposition for Wr.

$$W_p = W_{pl} + W_{pnl} \tag{7}$$

Parabaloids

$\theta = \pi$

$h = 1$

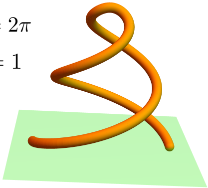


$\mathcal{W}_{pl} = 0.52$

$\mathcal{W}_{pnl} = -1.00$

$\theta = 2\pi$

$h = 1$

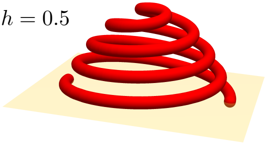


$\mathcal{W}_{pl} = 1.37$

$\mathcal{W}_{pnl} = -2.00$

$\theta = 4\pi$

$h = 0.5$

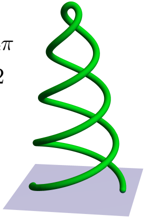


$\mathcal{W}_{pl} = 3.85$

$\mathcal{W}_{pnl} = -4.00$

$\theta = 4\pi$

$h = 2$



$\mathcal{W}_{pl} = 2.37$

$\mathcal{W}_{pnl} = -4.00$

Found linear force free sigmoids writhe sign does not match

Writhe and non-local writhe

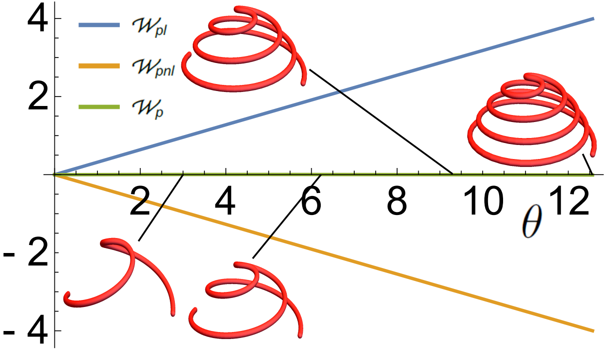
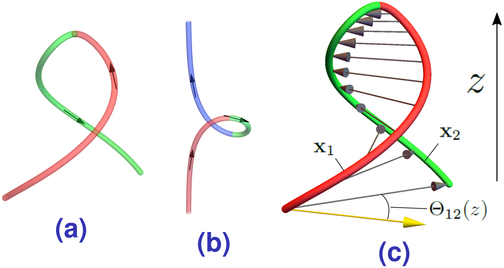


Figure: Polar writhe decomposition as a function of the winding angle θ for a parabola for which $W_p = 0$.

Calculating it

Split the curve



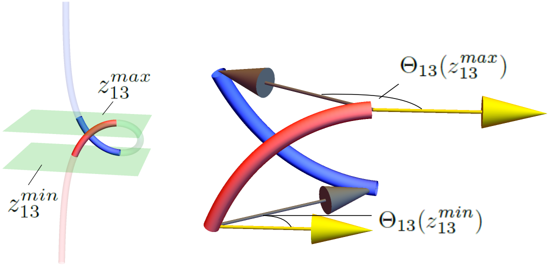
Local writhe for each section:

$$W_{pl}(\mathbf{x}) = \frac{1}{2\pi}\sum_{i=1}^{n}\int_{z_i^{min}}^{z_i^{max}} \frac{\hat{z}\cdot\mathbf{T}_i \times \frac{\mathrm{d}\mathbf{T}_i}{\mathrm{d}z}}{1+\|\hat{z}\cdot\mathbf{T}\|}\,\mathrm{d}z \qquad (8)$$

Non local:

$$W_{pnl} = 2\sigma_1\sigma_2\frac{\Delta\Theta_{12}}{2\pi} = -\frac{\theta}{\pi}. \qquad (9)$$

Non local writhe



(a) **(b)**

$$W_{pnl}(\mathbf{x}_1, \mathbf{x}_3) = 2\sigma_1\sigma_3 \frac{\Delta\Theta_{13}}{2\pi} = \frac{\Theta_{13}(z_{13}^{max}) - \Theta_{13}(z_{13}^{min})}{\pi}, \qquad (10)$$

In general

$$W_{pnl} = \sum_{i=1}^{n} \sum_{\substack{j=1 \\ i \neq j}}^{n} \frac{\sigma_i \sigma_j}{2\pi} \int_{z_{ijmin}}^{z_{ij}{}^{max}} \frac{\mathrm{d}\Theta_{ij}(z)}{\mathrm{d}z} \mathrm{d}z, \qquad (11)$$

Loop formation

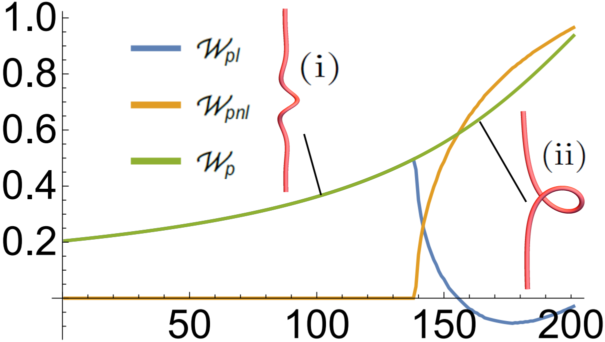
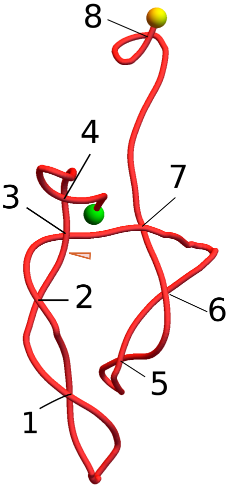


Figure: W_p values of a loop forming curve deformation.

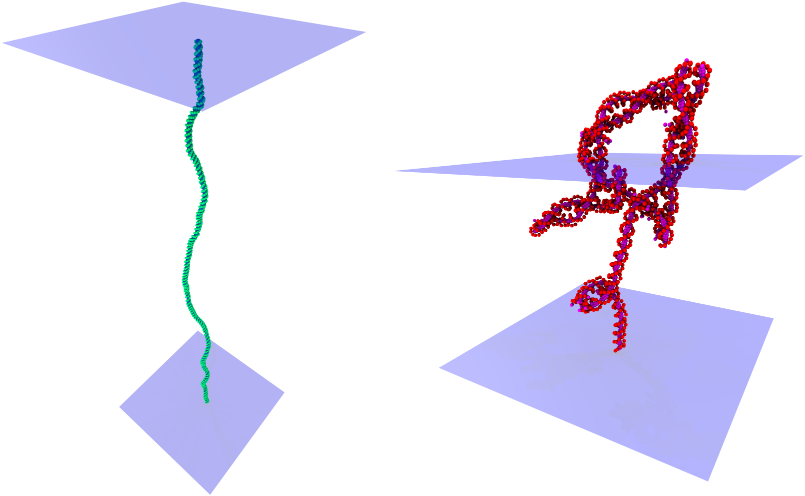
Again the local non-local decomposition tells us a lot more that W_p. In DNA models this is a prototype for plectoneme formation.

Plectoneme



$W_p = 8.88$, $W_{pnl} = 8.55$, $W_{pl} = 0.33$ (all to 3.s.f).

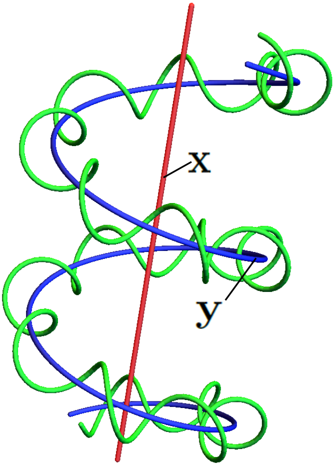
DNA models (Courtesy of Zack



(a) (b)

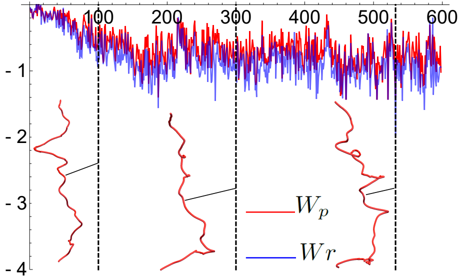
Over and under twisting

The ribbbon axis is actually the supercoiling axis.

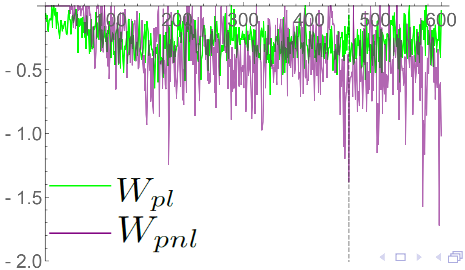


(12)

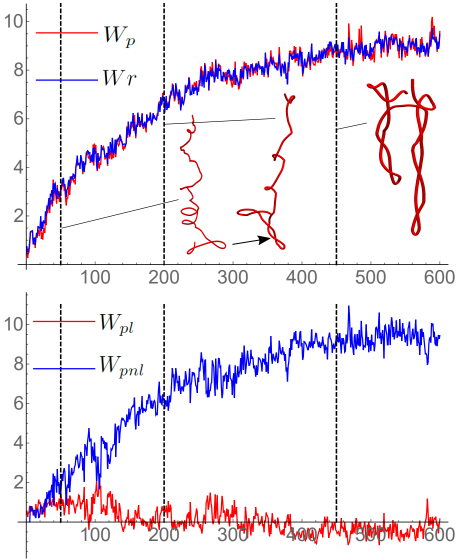
Under-twisted results



(a)

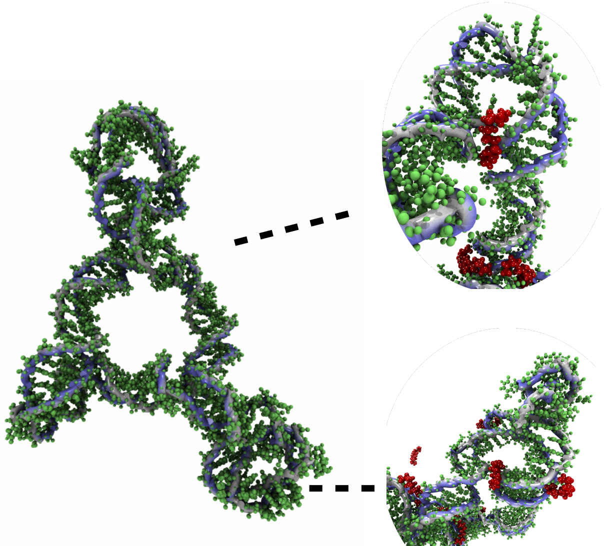


Over-twisted results



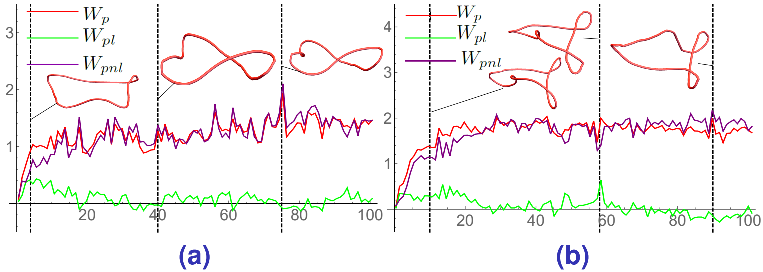
Spermine bridging

Spermine (red) acts to stabalise helical structures but also increases inflexibility. Can be used to form interesting minicircle topologies.



Detecting spermine action

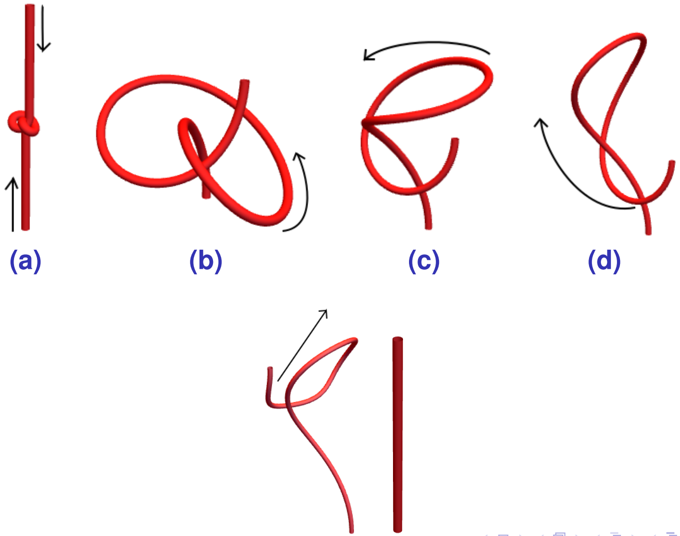
Two experiments with differing Spermine solutions.



Writhe increasing over 1 $\Rightarrow$ loop formation. The shape spikes in local/non local writhe in the second case indicate failed loop formation. Subsequent investigations indicated it was due t sporadic spermine binding.

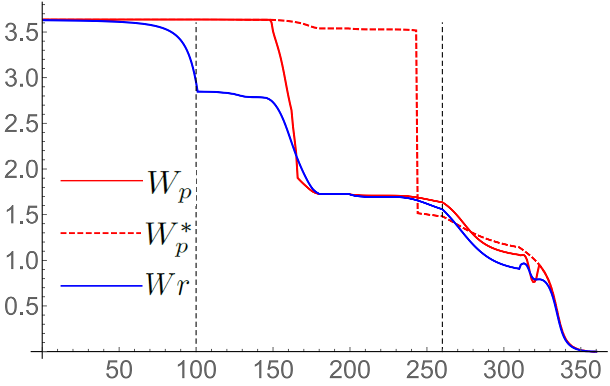
Knot undoing (Prior and Neukirch 2016)

Can modify the polar writhe to detect pulled tight knotting changes.



Pulled tight change

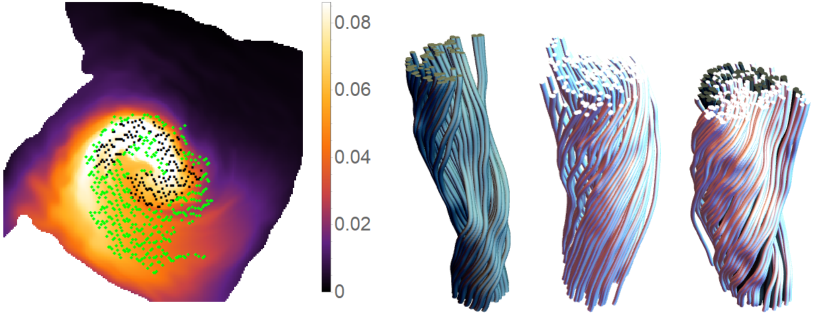
Detect a change in the pulled tight configuration as an integer jump.



The star polar writhe is introduced in Prior and Neukirch 2016 where an unknotting deformation is found.

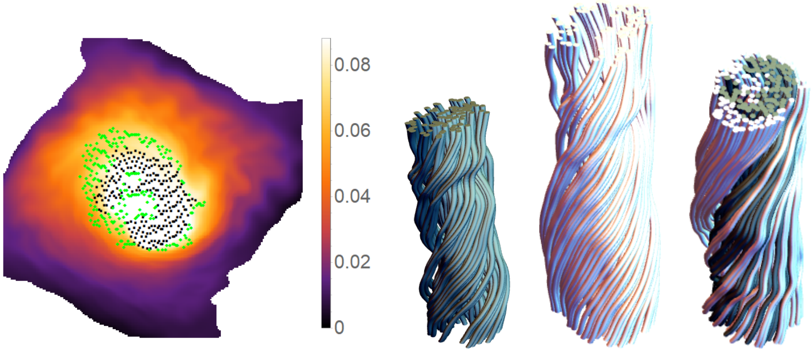
Other uses: Plasma topology i

Prior, C., Yeates, A. R. (2018). Quantifying reconnective activity in braided vector fields. Physical Review E, 98(1), 013204.



(a) (b) (c) (d)

Other uses: Plasma topology II



(a) (b) (c) (d)

Referenes

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