Department of Mathematics
Faculty of Mechanical Engineering
Slovak University of Technology in Bratislava

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TWIST AND FOLD MODELLING
OF SUPERCOILED FILAMENTS

MAGGIONI Francesca (IT), RICCA Renzo L. (IT)

Abstract. Preliminary results on twisting and folding mechanisms of supercoiled fila-
ments are presented. We examine competing kinematic models for single and multiple coil
formation, starting from a plane circle and we evaluate the effects of curvature on writhing
and packing rates. The analysis is performed by using a simple thin filament model under
conservation of linking number. Time-dependent evolutions of epicycloid curves are used
to perform transition from twist to writhe. These results may find useful applications
in modelling natural phenomena, from magnetic field dynamos in astrophysical flows to
compaction mechanisms of DNA in cell biology.

1 Introduction

The efficiency of twist and fold of circular filaments is analyzed by this preliminary study,
examining different models of epicycloid type of evolution in terms of curvature effects on
writhing and packing rates. These results are of fundamental importance for understanding
the effects of geometric features in the morphological change of filamentary structures in small
volumes.

Examples of filamentary structures are present at a wide variety of scales in nature; these
include vortex filaments in turbulent flows, magnetic flux-tubes in magneto-hydrodynamics
and DNA molecules in cell biology. A common feature of these structures is their tendency to
re-distribute internal energy, of kinetic, magnetic or elastic origin, by changing filament shape
(Ricca, 1995). In first approximation these filaments can be modelled by thin tubes of circular
cross-section. In many istances this process consists of a pure geometric re-arrangement of the
filament axis in the ambient space without change of topology. In the case of a closed filament
in isolation, for instance, conservation of the linking number Lk implies the invariance of the
sum of two geometric quantities, the writhing number Wr and the total twist Tw, according
to the well-known formula (Călugăreanu, 1961; White, 1969)

$$Lk = Wr + Tw .$$

(1)

The writing number Wr is a measure of the amount of coiling of the filament axis, and the total twist Tw measures the winding of the constituent fibers around the filament axis. Under conservation of topology, we have $Wr + Tw = $ constant, with possible conversion of Wr and Tw during evolution, through a continuous change of curvature and torsion of the filament axis. These aspects are often mutually functional and important in nature, as in the case of the human DNA, where a molecule a few centimeters long can be stored in a micron-sized scroll of protein. This packing process depends crucially on the localized actions that induce the twisting and folding of the filament in the ambient space, often governed by energy minimization principles and guide the morphological evolution of filamentary structures to form highly complex systems (Ricca, 2005).

In this paper we want to address questions related to the geometry of writhing and coiling, in terms of single and multiple coil formation, and relative packing rate. To do this we consider a closed filament $\mathcal{F}$ given by a thin tube of length L and uniform circular cross-section of area $A = \pi a^2$, with $L \gg a$. $\mathcal{F}$ is thought to be made of a bundle of infinitesimal helical fibers, distributed inside the tube and wound around the tube axis $\mathcal{C}$ with twist. We also assume that the filament be inextensible, so that $L = $ constant. $\mathcal{C}$ is given by a smooth (at least C^3), simple (i.e. non-self-intersecting), closed curve $\mathbf{X} = \mathbf{X}(\xi)$ in $\mathbb{R}^3$, where $\xi \in [0, 2\pi]$ is a parameter on the curve. The geometry of the axis is prescribed by the curvature $c = c(\xi)$ and torsion $\tau = \tau(\xi)$ of $\mathbf{X}$ through the Frenet-Serret formulae.

The total amount of *coiling* is given by the normalized total curvature K, given by

$$K \equiv \frac{1}{2\pi} \oint_{\mathcal{C}} c(\xi) \|\mathbf{X}'(\xi)\| \, d\xi \, , \tag{2}$$

where prime denotes derivative with respect to ξ. A measure of *folding* is provided by the writhing number Wr (Fuller, 1971), given by

$$Wr \equiv \frac{1}{4\pi} \oint_{\mathcal{C}} \int_{\mathcal{C}} \frac{[d\mathbf{X} \times d\mathbf{X}^*] \cdot [\mathbf{X} - \mathbf{X}^*]}{|\mathbf{X} - \mathbf{X}^*|^3} \, , \tag{3}$$

where $\mathbf{X} = \mathbf{X}(\xi)$ and $\mathbf{X}^* = \mathbf{X}(\xi^*)$ are two points on the axis ($\{\xi, \xi^*\} \in [0, 2\pi]$).

The total winding of the infinitesimal fibers around $\mathcal{C}$ is given by *total twist* Tw; denoting by $\Omega = \Omega(\xi)$ the angular twist rate, we have

$$Tw \equiv \frac{1}{2\pi} \oint_{\mathcal{C}} \Omega(\xi) \|\mathbf{X}'(\xi)\| \, d\xi \, , \tag{4}$$

which is related to the geometry of the filament axis through the decomposition (see, for example, Moffatt & Ricca, 1992)

$$Tw = \frac{1}{2\pi} \oint_{\mathcal{C}} \tau(\xi) \|\mathbf{X}'(\xi)\| \, d\xi + \frac{1}{2\pi} [\Theta]_{\mathcal{F}} = \mathcal{T} + \mathcal{N} \, , \tag{5}$$

where the first term in the r.h.s. of (5) is the normalized total torsion $\mathcal{T}$ and the second term is the normalized intrinsic twist $\mathcal{N}$ of the fibers *around* $\mathcal{C}$.

2 Kinematic models of coil formation

By comparing different kinematic models based on the time-evolution of epicycloid type of curves, we investigate different mechanisms of coil formation through filament writhing and

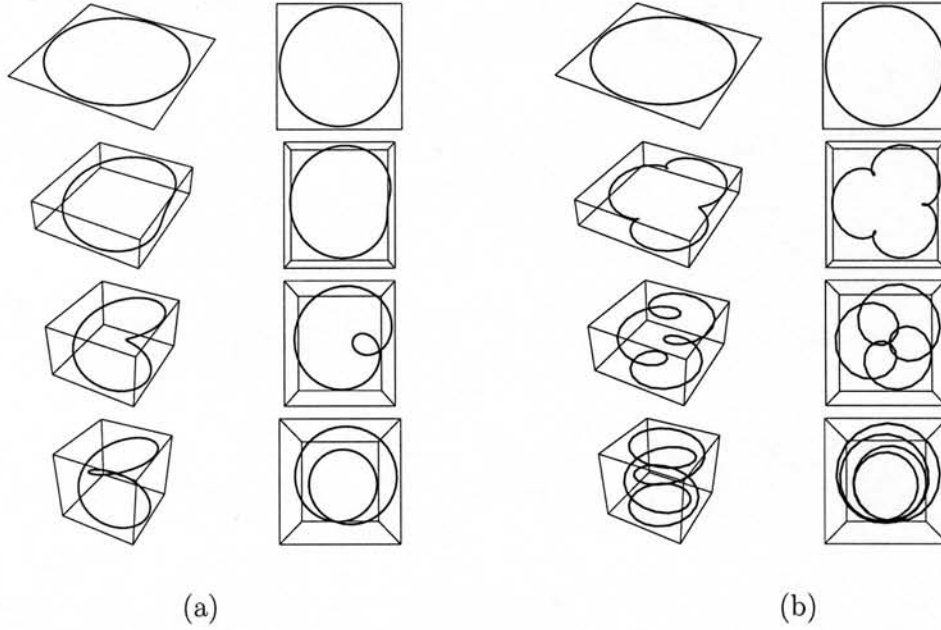| (a) | (b) |

Figure 1: Side and top view of (a) single coil formation and (b) three coil formation generated by eqs. (6) from an epicycloid type of curve (with $a = c = +1$, $b = d = -1$). In (a) $m = 1$ and $n = 2$ whereas in (b) $m = 1$ and $n = 4$. In both cases the writhing number Wr grows with time from 0 to the asymptotic value $Wr_{\max} = 1$.

folding. For this, we consider a family of time-dependent curves $\mathbf{X} = \mathbf{X}(\xi, t)$ given by an extension to three-dimensions of well-known planar curves; we propose the following general set of governing equations

$$\mathbf{X} = \mathbf{X}(\xi, t) \; : \quad \begin{cases} x = a \cos(m\xi) + bt \cos(n\xi) \\ y = c \sin(m\xi) + dt \sin(n\xi) \\ z = t \sin(\xi) \end{cases} , \tag{6}$$

where a, b, c, d take the value $+1$ or -1, $n > m > 0$, with n, m integers and t is time. For simplicity, we consider the simplest linear dependence on time, but more general non-linear relations are likely to take place in nature.

The values ± 1 for a, b, c, d exhaust in fact all possible cases (up to a scale factor). For given values of the parameters a, b, c, d (see Table 1), eqs. (6) describe the time evolution of closed

Generatrix curve	a	b	c	d	Wr-*range*
Epicycloid	$+1$	± 1	± 1	$+1$	$[-1, 0]$
Epicycloid	$+1$	∓ 1	± 1	-1	$[0, 1]$

Table 1: Types of generatrix curve for different values of parameters, for $m = 1$ and $n = 2 + 4r$, where $r \in \mathbb{N}$. Note that for these curves we have an upper bound on the writhing number given by $|Wr|_{\max} = 1$. For $n = 2 + 2r$, where $r \in \mathbb{N}$ is odd, we have the same curves, with relative range of writhing number exchanged.

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curves that originate (at $t = 0$) from a plane circle of length $L = 2\pi$ (since $a^2 = c^2 = 1$), and evolve from epicycloid generatrices to form singly or multiply coiled configurations. For simplicity we want to consider inextensible curves only, so that we must normalize $\mathbf{X} = \mathbf{X}(\xi, t)$ by the length function

$$l(t) = \frac{1}{2\pi} \int_0^{2\pi} \left[\left(\frac{\partial x}{\partial \xi}\right)^2 + \left(\frac{\partial y}{\partial \xi}\right)^2 + \left(\frac{\partial z}{\partial \xi}\right)^2 \right]^{1/2} d\xi . \tag{7}$$

Note that eq. (7) is, in general, not invertible; hence $\mathbf{X} = \mathbf{X}(\xi, t)$ cannot be parametrized by arc-length.

Single coil from planar circle: Figure 1 shows the evolution of $\mathbf{X}$ from a circular configuration to a three-dimensional curve with one single coil; this is described by eqs. (6) for $m = 1$ and $n = 2$. During evolution topology is conserved, so that Lk remains constant. For simplicity in the following we shall take $Lk = 1$. Since the original configuration is circular, eqs. (1) and (3) give $Wr = 0$ and $Tw = 1$ at $t = 0$. As t increases, the filament will form one single coil through the conversion of twist to writhe, according to the conservation of (1), and asymptotically (as $t \to \infty$) Tw will be completely converted to Wr (hence, in the limit, $Tw = 0$, $Wr = 1$).

Multiple coils formation: Figure 1(b) shows the prototype evolutions given by eqs. (6) in the case of three coils. We obtain $2k - 1$ coils for $m = 1$ and $n = 2k$ ($k \in \mathbb{N}\backslash 0$). Table 1 shows the epicicloid type of generatrix curve according to the value of the parameters and Wr-range during evolution. Due to the opposite sign of the coils, the writhing number remains bounded between 0 and 1, with $Wr \to 1$ as $t \to \infty$. Notice also that $|Wr|_{\max} = 1$ persists regardless the number of coils produced, for any $n = 2k$. For n odd we have the simultaneous production and collision of an even number of coils, generated symmetrically along the curve; so we shall exclude these values of n.

Multiple coil formation from multiple coverings of plane circle: Figure 2 show the prototype evolutions for (a) two and (b) three coil formation given by eqs. (6) for any m such that $m = n - 1$. In this case we obtain more elaborate curves generated by pseudo-epicycloid. The first $m - 1$ coils are instantly produced from m coverings of a plane circle, while the remaining coil is generated during the full evolution of the curve. In the transient the pseudo-epicycloids generate one loop, while the writhing number grows from 0 to the asymptotic value of m (see Table 2).

3   Writhing rates

We compare the kinematics considered so far in terms of relative writhing rates. Typical behaviours are shown in Figure 3. Top row diagrams refer to (a) the epicycloids of Figure 1(a)

Generatrix curve	a	b	c	d	Wr-range
Pseudo-epicycloid	$+1$	± 1	± 1	$+1$	$[-m, 0]$
Pseudo-epicycloid	$+1$	∓ 1	± 1	-1	$[0, m]$

Table 2: Case $m = n - 1$: types of generatrix curve for different values of parameters; now we have $|Wr|_{\max} = m$. The range of the writhing number shown is attained for any $n \in \mathbb{N}$.
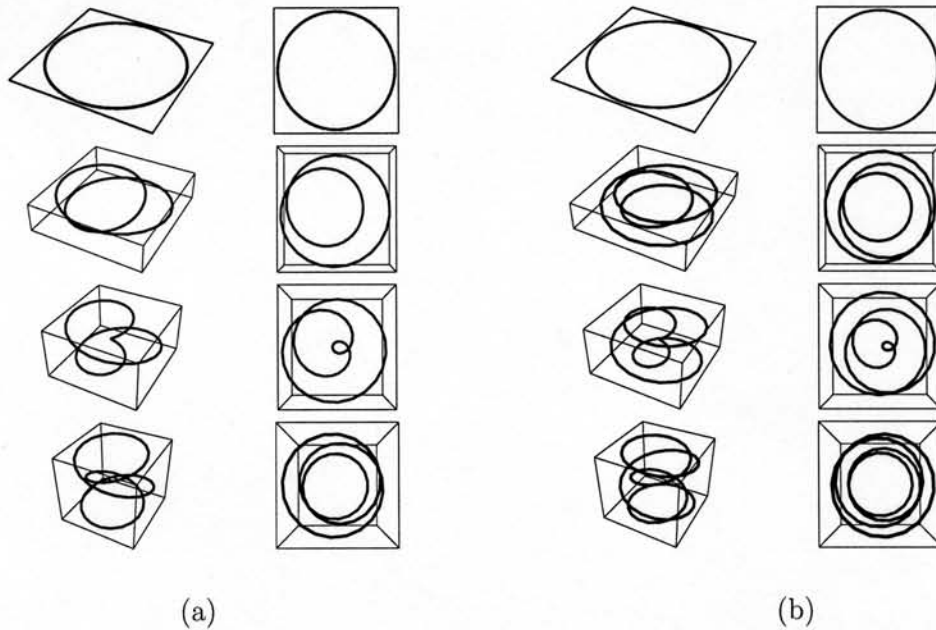
Figure 2: Side and top view of (a) two and (b) three coil formation given by eqs. (6) from pseudo-epicycloid generatrix (with $a = c = +1$, $b = d = -1$). In (a) $m = 2$ and $n = 3$, the first coil is produced instantly from a double covering of the plane circle while the second coil is generated at later time; the writhing number grows to attain the asymptotic value $Wr_{\max} = 2$. In (b) $m = 3$ and $n = 4$, the first two coils are produced instantly from a triple covering of the plane circle, while the third coil is generated at later time; the writhing number grows to attain the asymptotic value $Wr_{\max} = 3$.

and 1(b), respectively: for these cases we have $\lim_{t \to \infty} Wr = 1$. The comparison between top diagrams show that the change in writhing of the epicycloid evolution with $n = 4$ is faster than that of epicycloid with $n = 2$; this is due to the fact that in the second case three coils (instead of the one formed in the first case) are produced instantaneously. Note that the bound $Wr_{\max} = 1$ holds true for any number of coils generated, as shown in Table 1. Because of the conservation of $Lk = 1$ (cf. eq. 1), this implies also a bound on the total twist Tw.

Similarly for the bottom diagrams of Figure 3. In the case (a) we have $m = 2$, so that Wr jumps suddenly to 1 as the first coil forms, tending then asymptotically to the limit value $Wr_{\max} = 2$ with the production of the second coil. In the case (b) we have $m = 3$, so that Wr jumps suddenly to 2 as the first two coils form, tending then asymptotically to the limit value $Wr_{\max} = 3$ with the production of the third coil. In general, the first $m - 1$ coils are instantly produced from the m coverings of the plane circle and so Wr jumps instantaneously from 0 to $m - 1$ as the curve evolves. When $m = n - 1$ the writhing number has an upper bound given by $Wr_{\max} = m$.

4   Inflexional deformation

As we saw from the previous sections, coiling originates from local writhing of the filament axis to form a loop region. This mechanism consists of a passage through an inflexional state
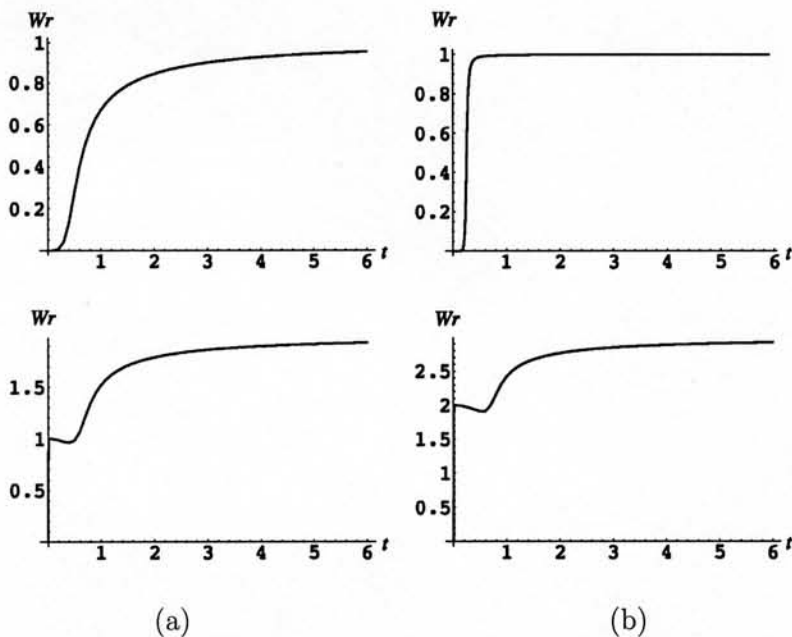
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Figure 3: Writhing number Wr plotted against time. Top row diagrams refer to the epicycloids of Figure 1(a) and (b), respectively. Bottom row diagrams refer to the pseudo-epicycloid evolutions of Figure 2(a) and (b), respectively.

(defined by vanishing curvature and local change of concavity of the curve), as it was originally recognized by Călugăreanu (1961) and analyzed in detail by Moffatt and Ricca (1992). The appearance of an inflexional state is a *generic* geometric feature, independent of the kinematics considered, and therefore it occurs during any coil formation. Moffatt and Ricca (1992) showed that at the point of inflexion the torsion is singular, but the singularity is integrable. The contribution from the integral of the total torsion through the inflexional state involves a jump $[\mathcal{T}] = 1$ in total torsion, that is compensated by an equal and opposite jump in the intrinsic twist $\mathcal{N}$, so that the twist number Tw (cfr. eq. 5) remains a smooth function of ξ and t.

In the case of the curve of Figure 1(a), since the initial conditions are given by $\mathcal{T} = 0$ and $\mathcal{N} = 1$, the initial total twist Tw is only given by pure intrinsic twist. Passage through inflexion occurs at $\xi = 0$, $t = 0.25$ and leads to the complete conversion of one full intrinsic twist to total torsion. With reference to eqs. (6), if $\mathcal{N}(0)$ is the number of full turns of twist present initially, and N is the final number of coils produced, then $\mathcal{N}(0) - N = \mathcal{N}(\infty)$ is the number of intrinsic twists present in $\mathcal{F}$ in the limit $t \to \infty$, since in this limit total torsion is zero again. Work in progress (Maggioni & Ricca, 2006) shows that this istantaneous conversion of intrinsic twist to total torsion has important consequences on the energetics of the system.

5 Compactibility and packing rate

In many physical situations filamentary structures need to be highly packed in small volumes. On macroscopic scales, for instance in astrophysical flows, the compaction of magnetic fields in small regions leads naturally to an intensification of the average field, a process that can be associated with dynamo action (for example, through a stretch-twist-fold process, as proposed

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by Moffatt & Proctor, 1985; see also Childress & Gilbert, 1995). On the other hand, on microscopic scales, the human DNA is compacted in chromosomes by a factor of about 10.000, and it may be confined into a scroll of protein with packing ratio given by $D/L = O(10^{-7})$, where D and L denote typical sizes of the proteic region and DNA length (Calladine & Drew, 1992).

We like to compare the kinematics considered here to quantify compactibility and packing rate in the light of possible applications. In the case of the generation of a single coil, at $t = 0$ we have $L = 2\pi R_0 = 2\pi$; when the coil is fully formed, the filament centreline will tend, on average, to a double covering of a circle of radius R. Since L is kept constant, the average radius of the new curve will, in the limit $t \to \infty$, be half of the original, that in our case corresponds to $R = 1/2$. In general, if N is the total number of coils produced, then we have:

$$L = 2\pi = (N+1)2\pi R \qquad \to \qquad R = \frac{1}{N+1} . \tag{8}$$

In general, then, if $N = N(t)$ is the number of coils produced per unit time, the *packing rate* $\rho = \rho(t)$ will be given by $\rho(t) = [N(t) + 1]$.

6 Conclusions

In this preliminary report we have analyzed competing kinematic models of coiling formation, based on epicycloid evolutions and we have shown how efficiency of coiling and compaction mechanisms depend on geometric quantities such as writhing, folding and inflexional configurations associated with exchange of twist to writhe. We have seen that some of the kinematics considered have $Wr_{\max} = 1$, regardless the number of coils formed, and we have underlined that this fact implies a bound on the total twist Tw converted. In effect, this will imply a bound on the torsional energy converted into bending energy. We have also estimated the efficiency of filament packing into small volumes. Work is in progress to apply these results to investigate further localized coiling for DNA modelling (Ricca & Maggioni, 2006) and magnetic dynamo actions.

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Current address

Francesca Maggioni,
Department of Mathematics & Applications, University of Milano-Bicocca, Via Cozzi 53, 20125 Milano, ITALY, e-mail: francesca.maggioni@unimib.it

Renzo L. Ricca,
Department of Mathematics & Applications, University of Milano-Bicocca, Via Cozzi 53, 20125 Milano, ITALY, e-mail: renzo.ricca@unimib.it