Stable knots with no self-contact

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Knots are everywhere

Long enough polymers are (almost) certainly knotted

750 knotted proteins in the ProteinDataBank (1%)
catalyse enzymatic reactions (Lim+Jackson 2015)
stabilize protein structure (Wagner et al 2005)

knots in DNA
ejection from capsides (Marenduzzo 2013)
replication / transcription - cell death (Deibler 2007)

Olavarrieta JMB 2002
Tensile strength of a wire


fishing line

10 kg
Tensile strength of a wire

fishing line with knot

6 kg

Pieranski EPJE (2001)

Elastic knots

self-contact

Circular cross-section
Bending and twist

Clauvelin J MPS 2009
Applying torsion

numerical simulations: M. Bergou (SIGGRAPH) 2008
role of friction: Jawed (PRL) 2015
unstable !
do stable open trefoil knotted configurations exist?

Closed configurations (Elastic Rings)

Global Bifurcation Diagram
Dichmann (1996)

Kirchhoff equations for elastic rods

**kinematics**

\[
\begin{align*}
x' &= d_{3x} \\
y' &= d_{3y} \\
z' &= d_{3z} \\
d'_{3x} &= u_2 d_{1x} - u_1 d_{2x} \\
d'_{3y} &= u_2 d_{1y} - u_1 d_{2y} \\
d'_{3z} &= u_2 d_{1z} - u_1 d_{2z} \\
d'_{1x} &= u_3 d_{2x} - u_2 d_{3x} \\
d'_{1y} &= u_3 d_{2y} - u_2 d_{3y} \\
d'_{1z} &= u_3 d_{2z} - u_2 d_{3z} \\
d'_{2x} &= u_1 d_{3x} - u_3 d_{1x} \\
d'_{2y} &= u_1 d_{3y} - u_3 d_{1y} \\
d'_{2z} &= u_1 d_{3z} - u_3 d_{1z} 
\end{align*}
\]

**dynamics**

\[
\begin{align*}
n'_1 &= n_2 u_3 - n_3 u_2 - f_1 + \rho A (\ddot{x} d_{1x} + \ddot{y} d_{1y} + \ddot{z} d_{1z}) \\
n'_2 &= n_3 u_1 - n_1 u_3 - f_2 + \rho A (\ddot{x} d_{2x} + \ddot{y} d_{2y} + \ddot{z} d_{2z}) \\
n'_3 &= n_1 u_2 - n_2 u_1 - f_3 + \rho A (\ddot{x} d_{3x} + \ddot{y} d_{3y} + \ddot{z} d_{3z}) \\
m'_1 &= m_2 u_3 - m_3 u_2 + n_2 \\
m'_2 &= m_3 u_1 - m_1 u_3 - n_1 \\
m'_3 &= m_1 u_2 - m_2 u_1 
\end{align*}
\]

**constitutive relations**

\[
m_1 = K_1 u_1 , \quad m_2 = K_2 u_2 , \quad m_3 = K_3 u_3
\]

21 non linear PDE (arclength & time)
equilibrium & stability
BVP (collocation)
umerical path following
Obtaining a good knot

\[
\begin{aligned}
\text{fixed} & \left\{ \begin{array}{c}
z^* = 0.115 \\
\delta = 0.05
\end{array} \right.
\end{aligned}
\]
Obtaining a good knot

\[
\text{fixed } \begin{cases} 
  z^* &= 0.115 \\
  \delta &= 0.05 
\end{cases}
\]
Obtaining a good knot

\[
\text{fixed} \left\{ \begin{array}{c}
\dot{z}^* = 0.115 \\
\delta = 0.05
\end{array} \right. 
\]
Obtaining a good knot

\[
\begin{align*}
\text{fixed} \left\{ \begin{array}{c}
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Obtaining a good knot

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\begin{aligned}
\text{fixed } & \left\{ \begin{array}{c}
\dot{z}^* = 0.115 \\
\delta = 0.05
\end{array} \right.
\end{aligned}
\]
'All' the good knots

fixed $\delta = 0.05$
All the good knots

elastic strip model

- good (w=0)
- unknotted
- unwalled
Equations for elastic strips

**kinematics**

\[
x' = d_{3x}
\]
\[
y' = d_{3y}
\]
\[
z' = d_{3z}
\]
\[
d'_{3x} = u_2 d_{1x} - u_1 d_{2x}
\]
\[
d'_{3y} = u_2 d_{1y} - u_1 d_{2y}
\]
\[
d'_{3z} = u_2 d_{1z} - u_1 d_{2z}
\]
\[
d'_{1x} = u_3 d_{2x} - u_2 d_{3x}
\]
\[
d'_{1y} = u_3 d_{2y} - u_2 d_{3y}
\]
\[
d'_{1z} = u_3 d_{2z} - u_2 d_{3z}
\]
\[
d'_{2x} = u_1 d_{3x} - u_3 d_{1x}
\]
\[
d'_{2y} = u_1 d_{3y} - u_3 d_{1y}
\]
\[
d'_{2z} = u_1 d_{3z} - u_3 d_{1z}.
\]

**dynamics**

\[
n'_1 = n_2 u_3 - n_3 u_2 - f_1 + \rho A (\ddot{x} d_{1x} + \dot{y} d_{1y} + \ddot{z} d_{1z})
\]
\[
n'_2 = n_3 u_1 - n_1 u_3 - f_2 + \rho A (\ddot{x} d_{2x} + \dot{y} d_{2y} + \ddot{z} d_{2z})
\]
\[
n'_3 = n_1 u_2 - n_2 u_1 - f_3 + \rho A (\ddot{x} d_{3x} + \dot{y} d_{3y} + \ddot{z} d_{3z})
\]
\[
m'_1 = m_2 u_3 - m_3 u_2 + n_2
\]
\[
m'_2 = m_3 u_1 - m_1 u_3 - n_1
\]
\[
m'_3 = m_1 u_2 - m_2 u_1
\]

**nonlinear constitutive relations**

\[
m_1 = K \left( 1 - \frac{u_3^4}{u_1^4} \right) u_1
\]
\[
u_2 = 0
\]
\[
m_3 = 2K \left( 1 + \frac{u_3^2}{u_1^2} \right) u_3
\]

Dias & Audoly (JMPS) 2014
Experiments with $\delta = 0.10$

PVC 3GPa
$h = 200$ microns
$L = 26.3$ cm
$w = 1.5$ cm ($w/h=75$)

$z^* = 0.17$

$\varphi = 0.78$

gravity:
$\Gamma = \frac{Mg}{EI/L^2} \approx 25$
Conclusions

Importance of the w/h ratio experiments: h = 200 microns and w from 0.6 cm to 1.5 cm

- Elastic rod behavior (jump to contact)
- Match with Dias model
- No jump

Stable closed knots with no self-contact?
- Natural curvature?
- Varying stiffness?