Stable knots with no self-contact

Derek Moulton (Math Oxford UK)
Paul Grandgeorge (Flexlab EPFL Switzerland)
Sebastien Neukirch (d'alembert UPMC Paris France)

Knots are everywhere

Long enough polymers are (almost) certainly knotted

Sumners+Whittington, J. Phys. A : Math. Gen. 1988

750 knotted proteins in the ProteinDataBank (1%)

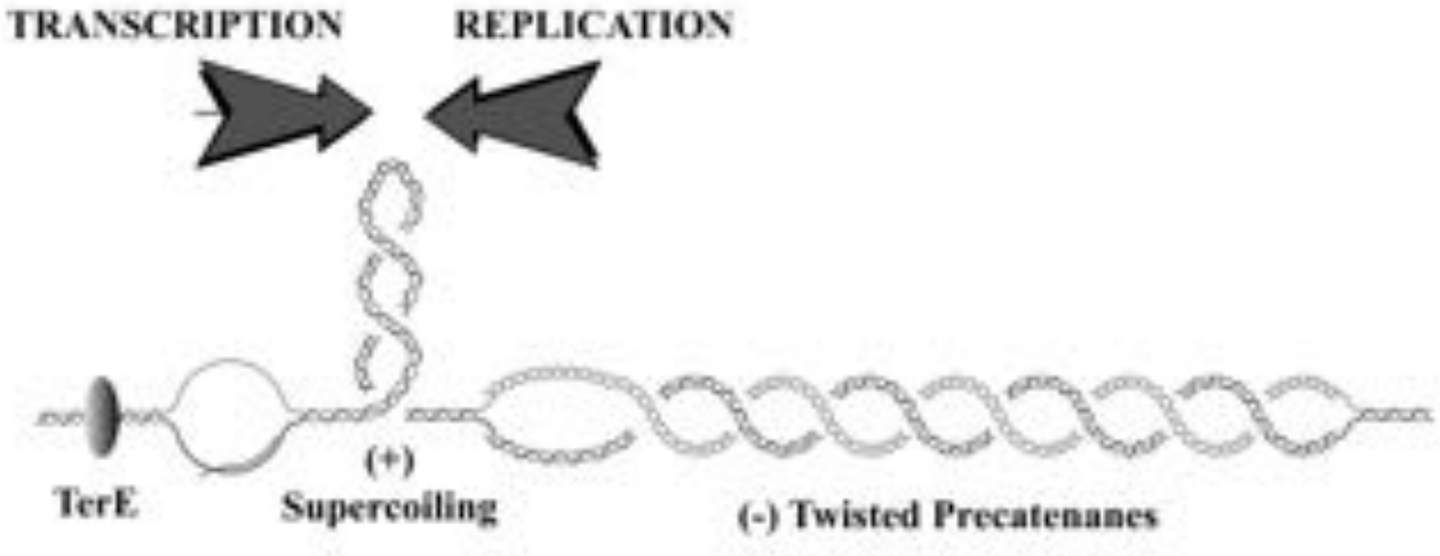
catalyse enzymatic reactions (Lim+Jackson 2015)

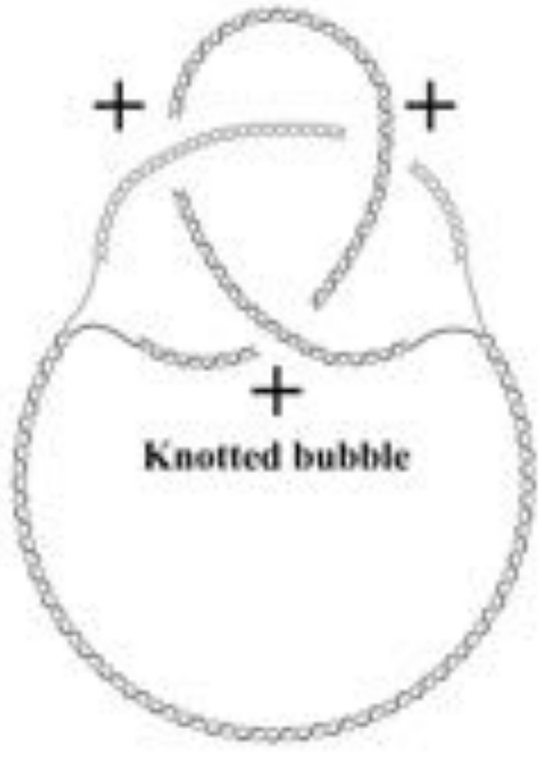
stabilize protein structure (Wagner et al 2005)

knots in DNA

ejection from capsides (Marenduzzo 2013)

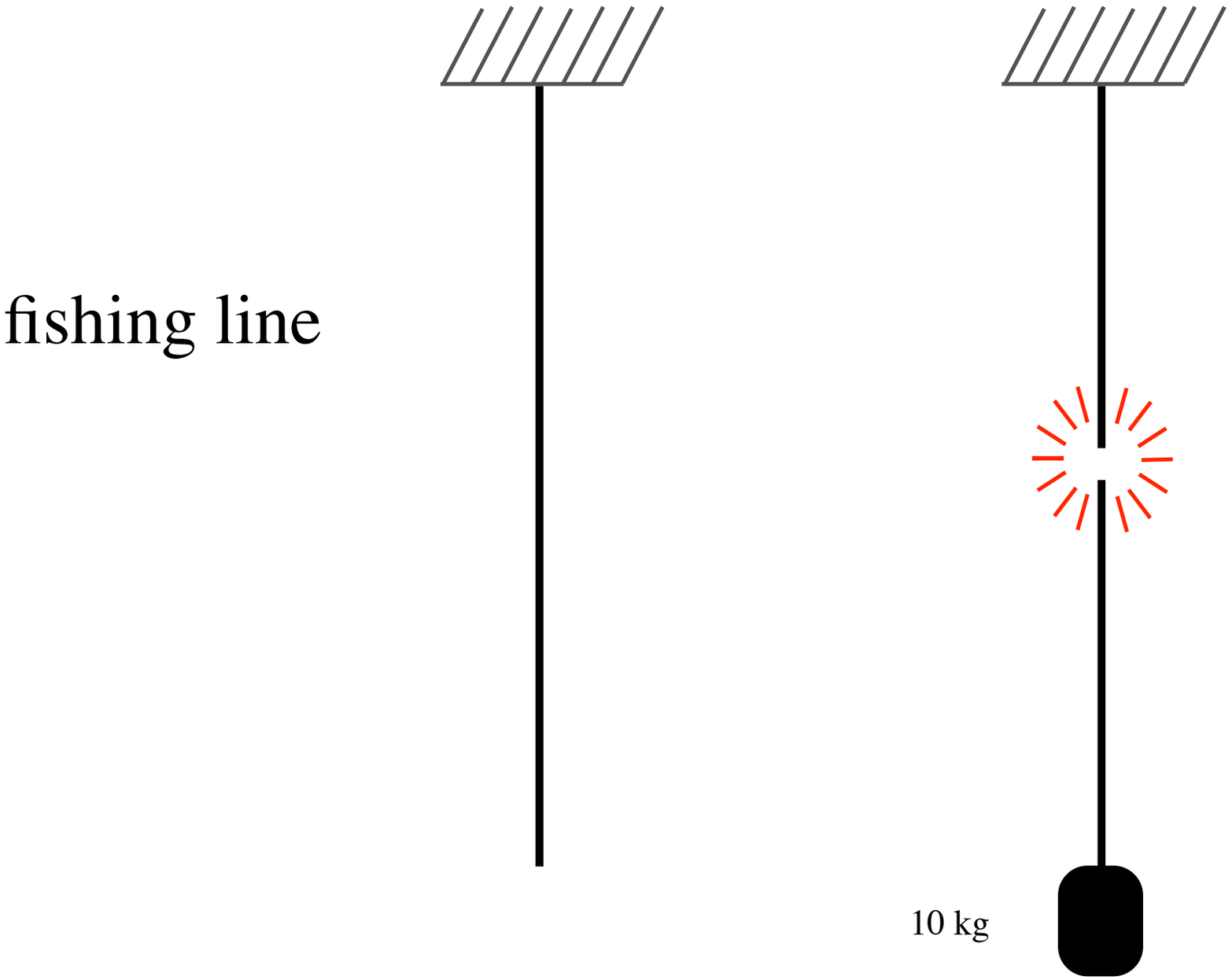
replication / transcription - cell death (Deibler 2007)





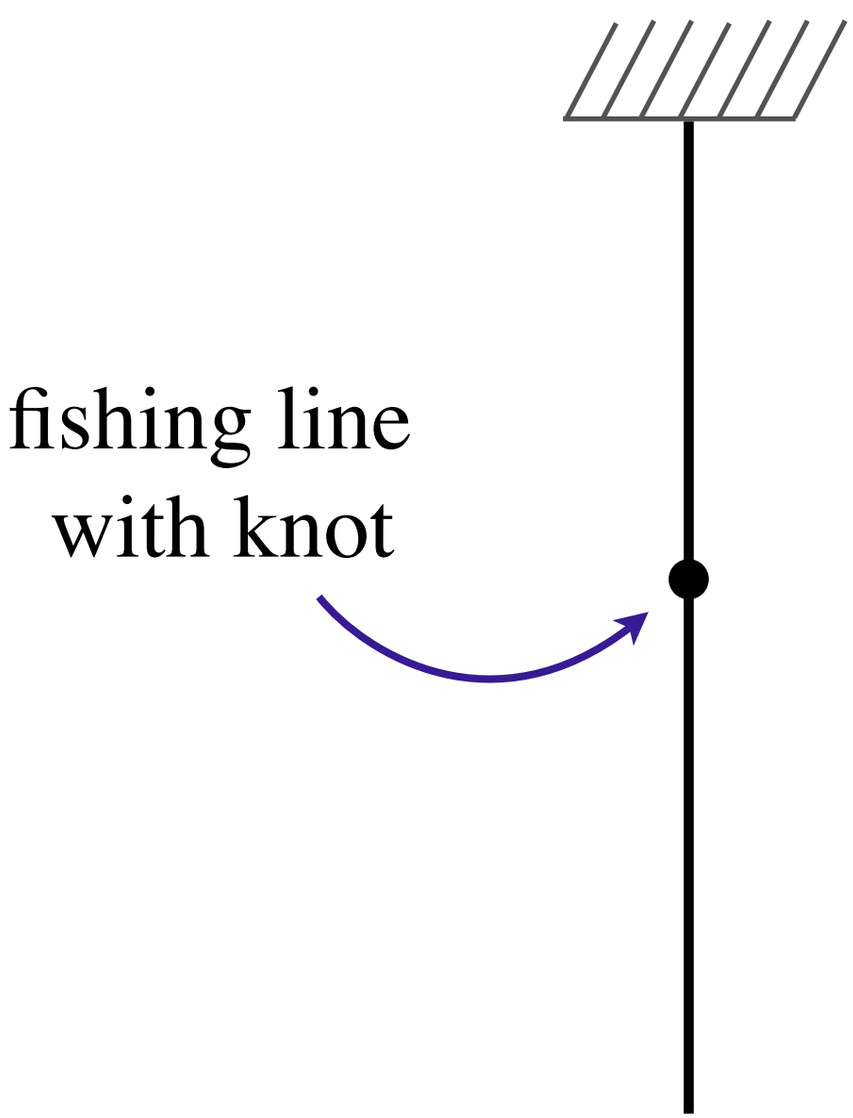
Olavarrieta JMB 2002

Tensile strength of a wire

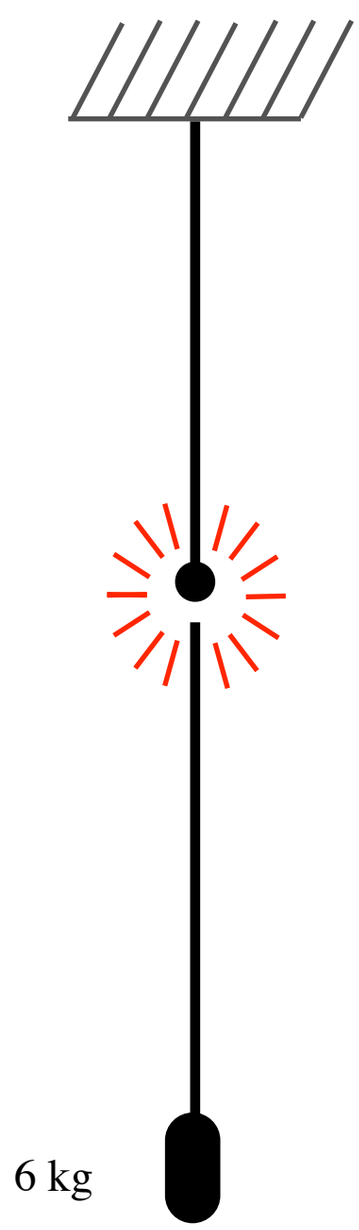


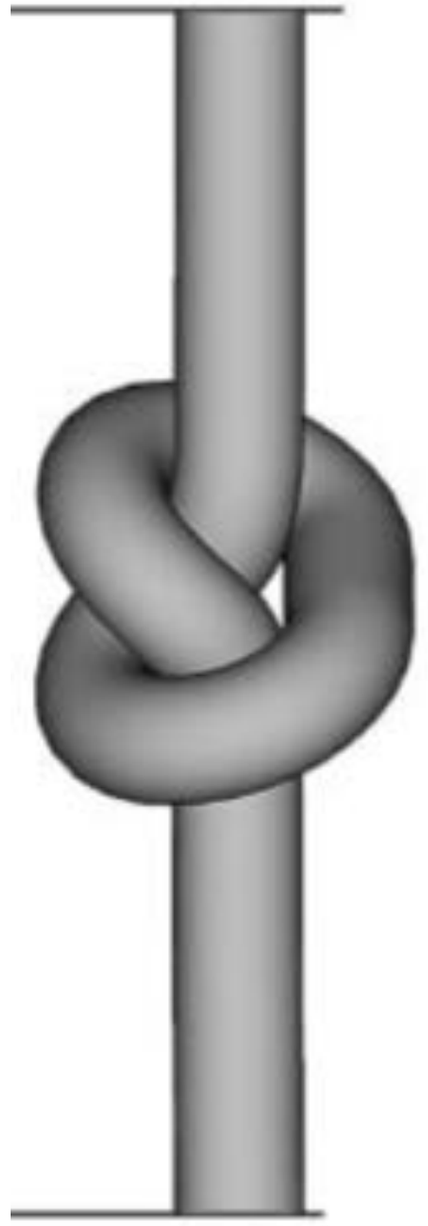
Stasiak et al, *Science* (1999)

Tensile strength of a wire



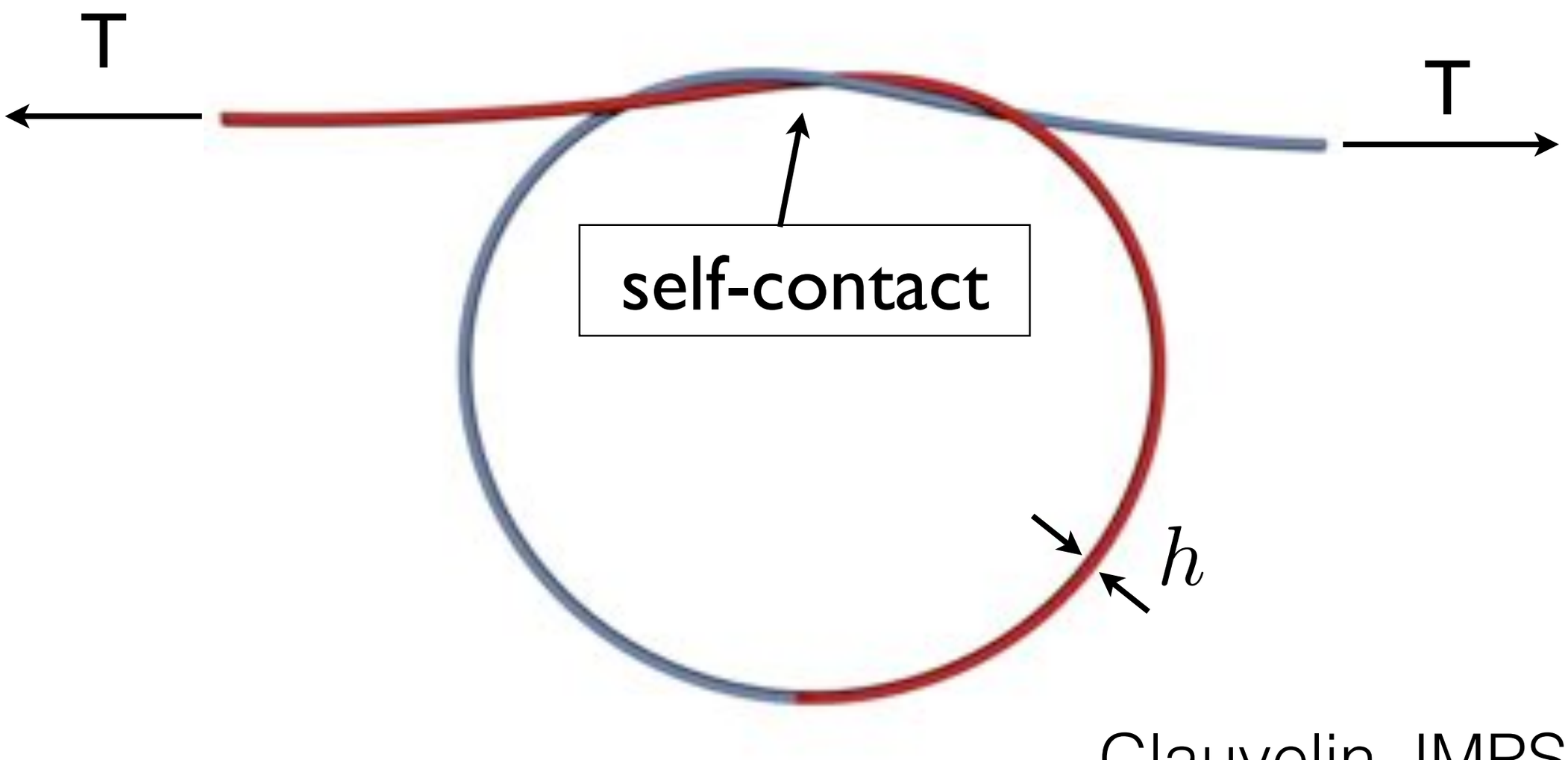
Stasiak et al, *Science* (1999)





Pieranski EPJE (2001)

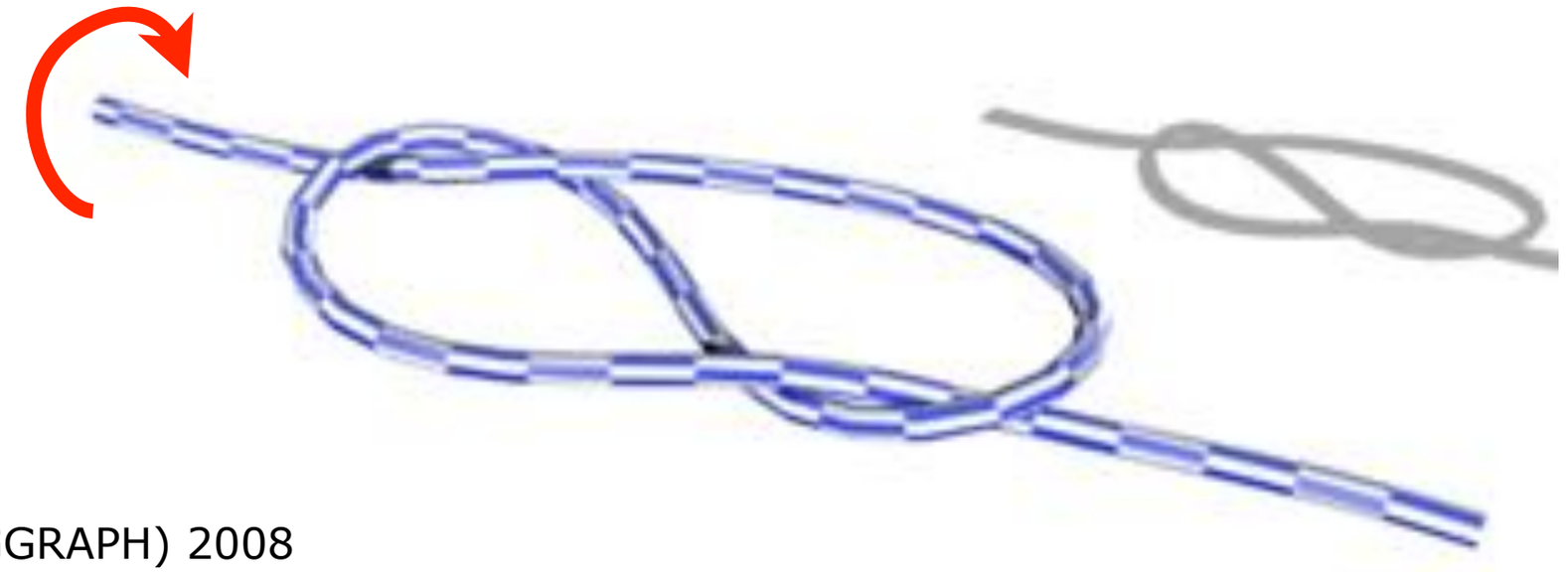
Elastic knots



Clauvelin JMPS 2009

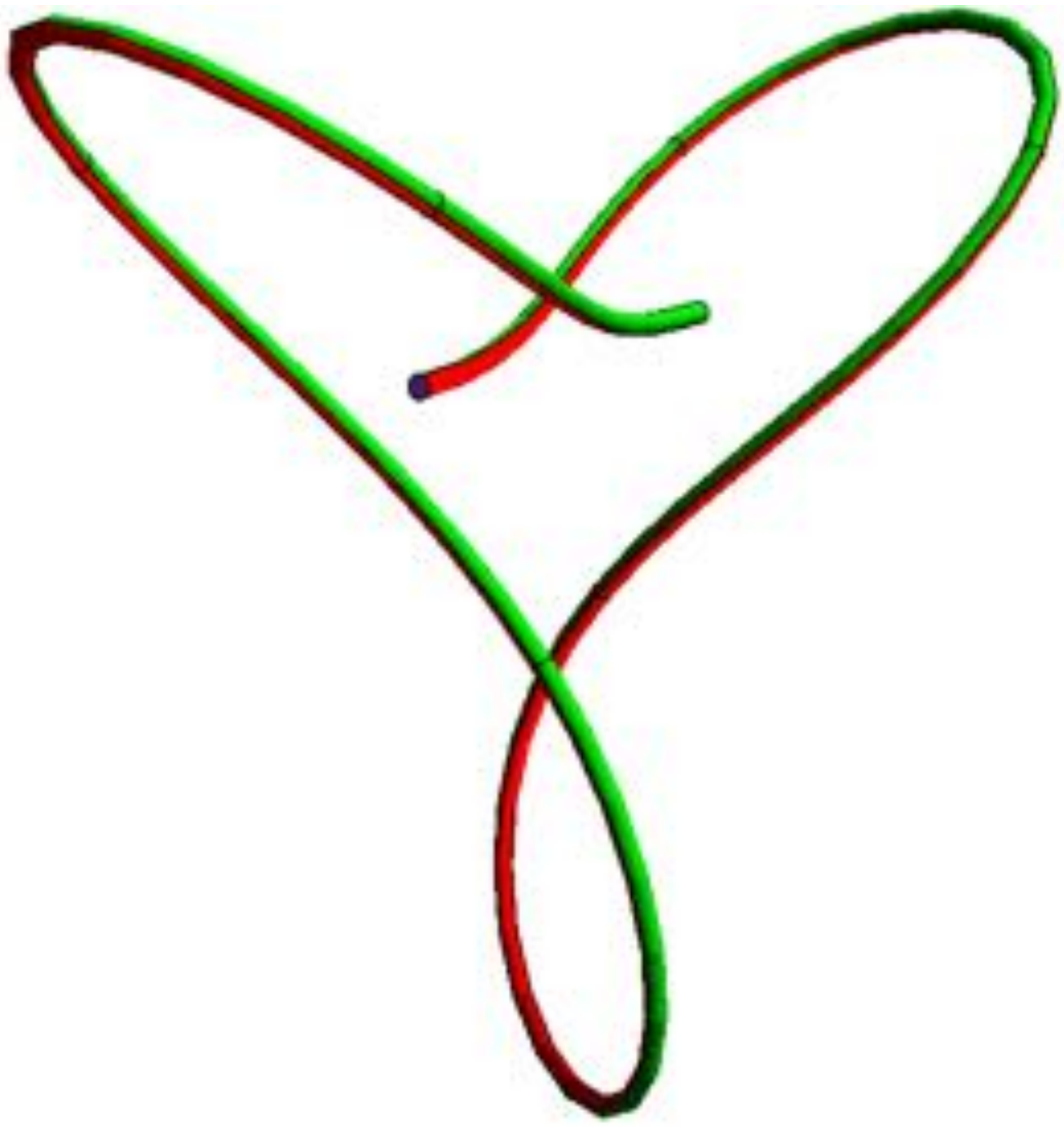
circular cross-section
bending and twist

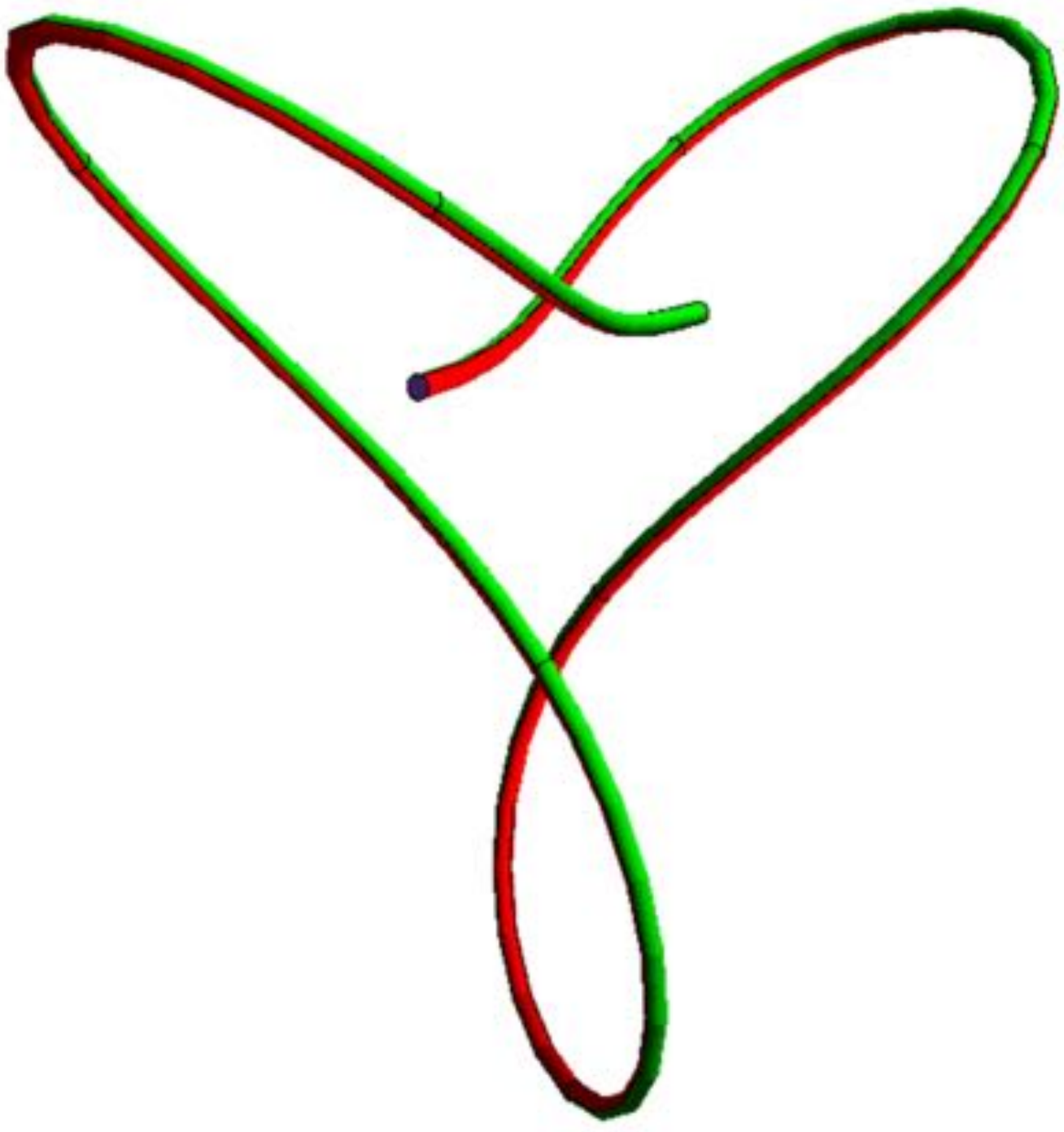
Applying torsion



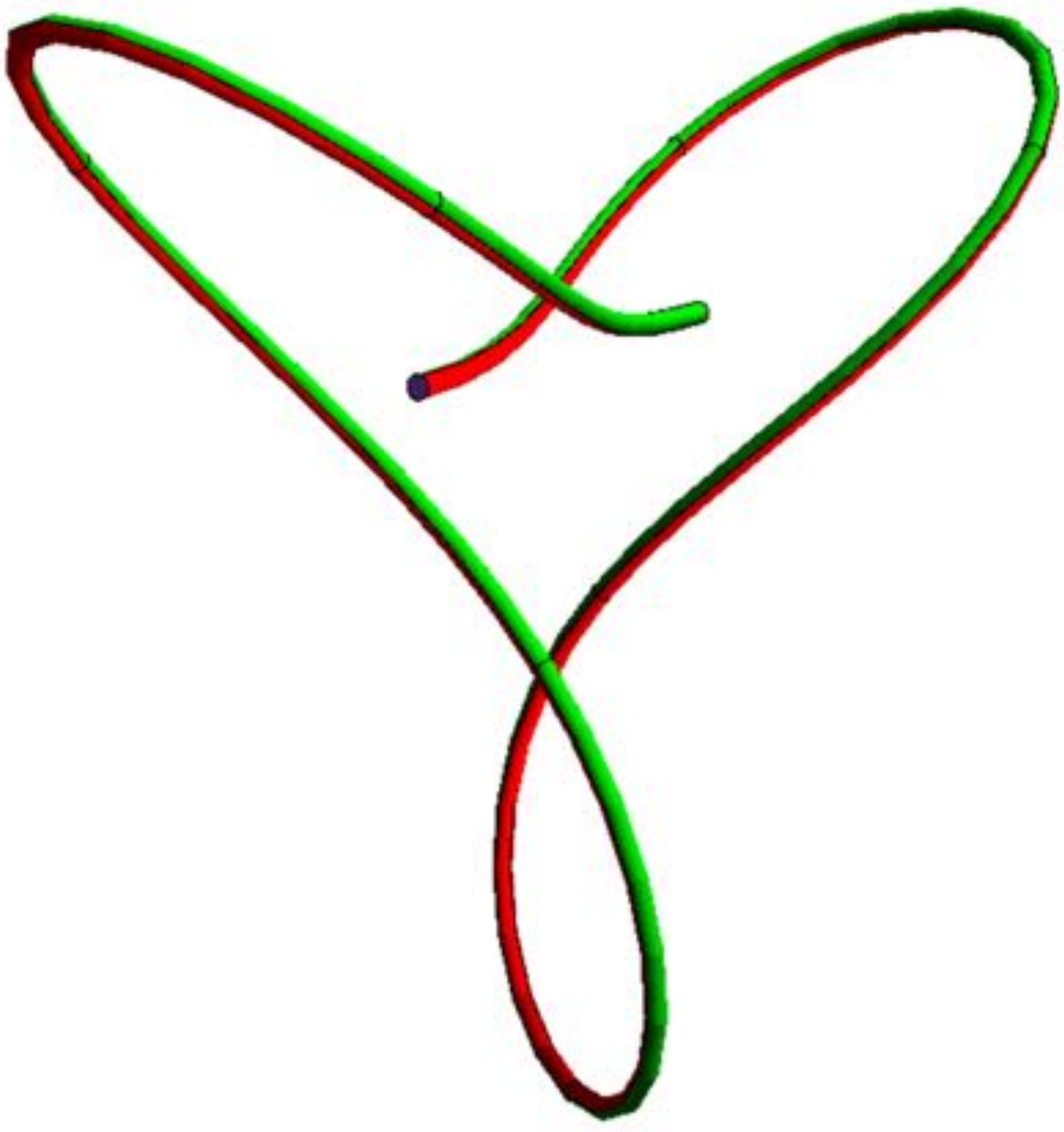
numerical simulations: M. Bergou (SIGGRAPH) 2008

role of friction: Jawed (PRL) 2015



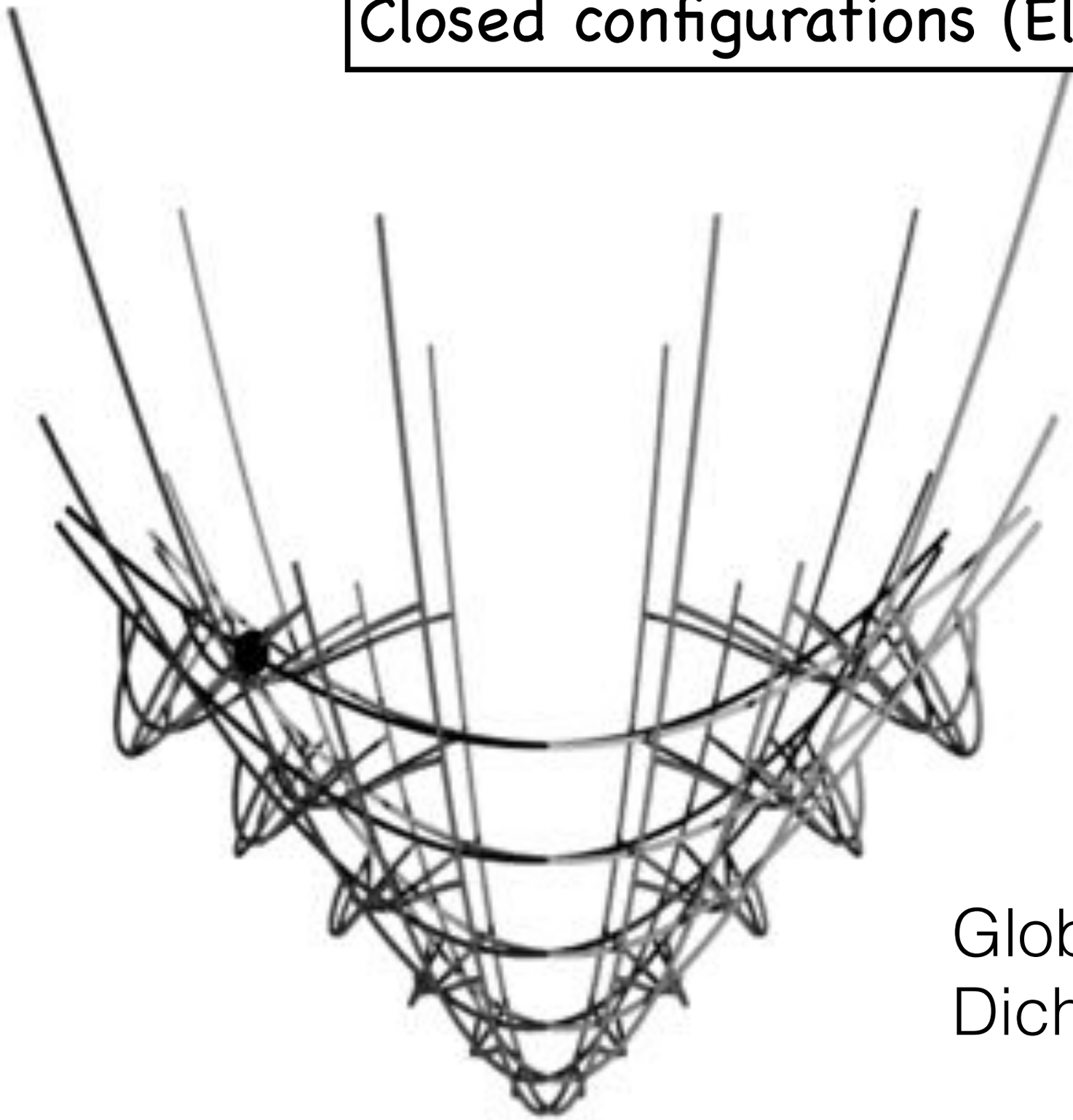


unstable !



do stable open trefoil knotted configurations exist ?

Closed configurations (Elastic Rings)



Global Bifurcation Diagram
Dichmann (1996)

Langer & Singer (1984) conjecture: no stable solution

Kirchhoff equations for elastic rods

kinematics

$$
\begin{aligned}
x' &= d_{3x} \\
y' &= d_{3y} \\
z' &= d_{3z} \\
d'_{3x} &= u_2\, d_{1x} - u_1\, d_{2x} \\
d'_{3y} &= u_2\, d_{1y} - u_1\, d_{2y} \\
d'_{3z} &= u_2\, d_{1z} - u_1\, d_{2z} \\
d'_{1x} &= u_3\, d_{2x} - u_2\, d_{3x} \\
d'_{1y} &= u_3\, d_{2y} - u_2\, d_{3y} \\
d'_{1z} &= u_3\, d_{2z} - u_2\, d_{3z} \\
d'_{2x} &= u_1\, d_{3x} - u_3\, d_{1x} \\
d'_{2y} &= u_1\, d_{3y} - u_3\, d_{1y} \\
d'_{2z} &= u_1\, d_{3z} - u_3\, d_{1z}.
\end{aligned}
$$

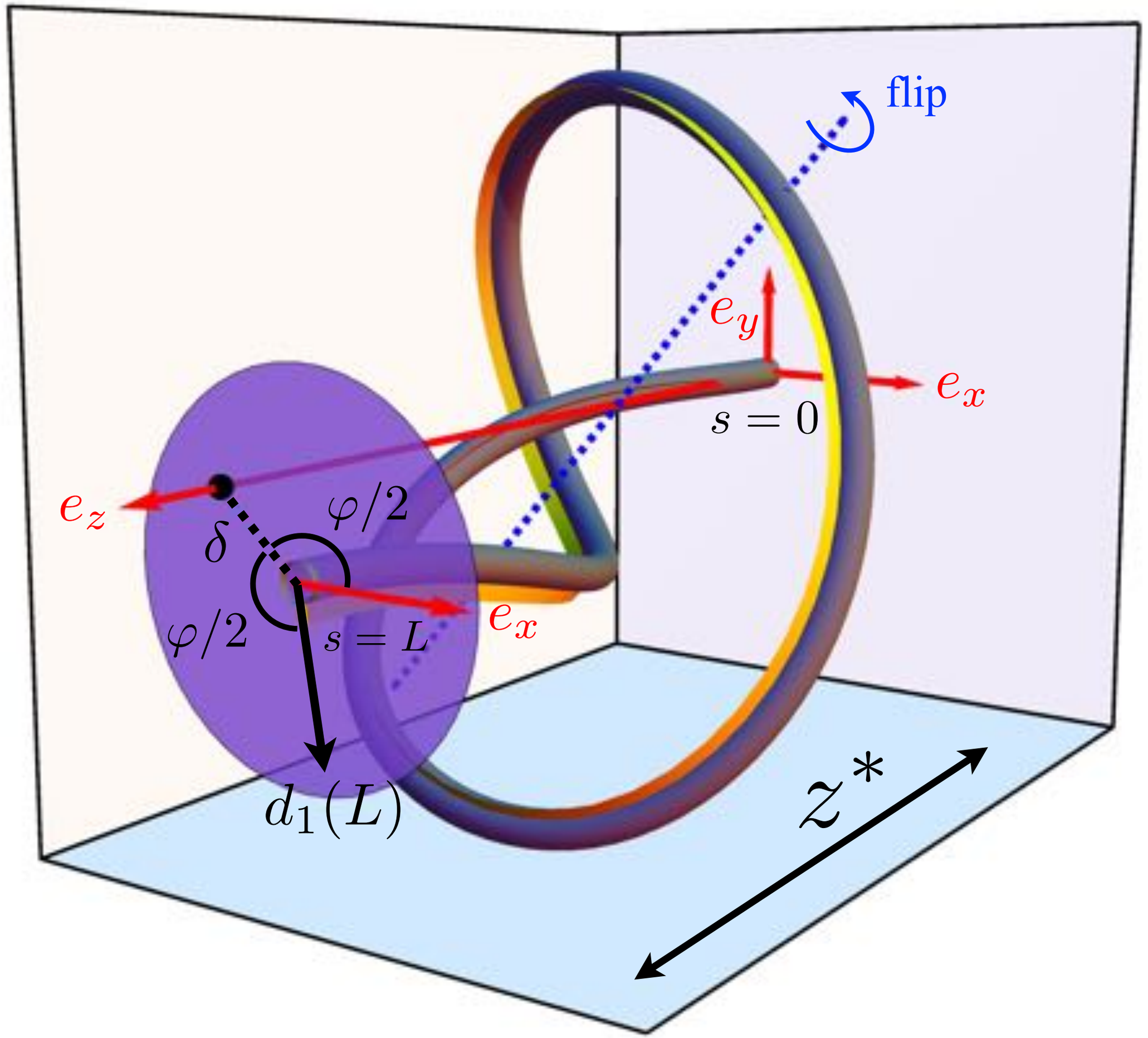
dynamics

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

constitutive relations

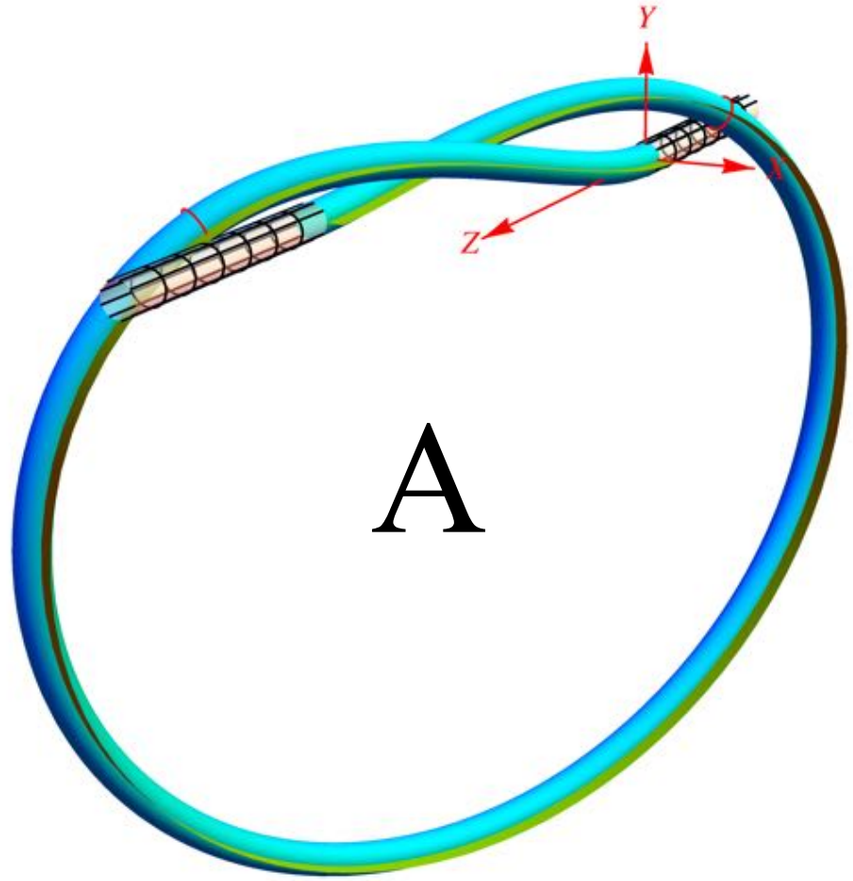
$$
m_1 = K_1\, u_1\,, \quad m_2 = K_2\, u_2\,, \quad m_3 = K_3\, u_3
$$

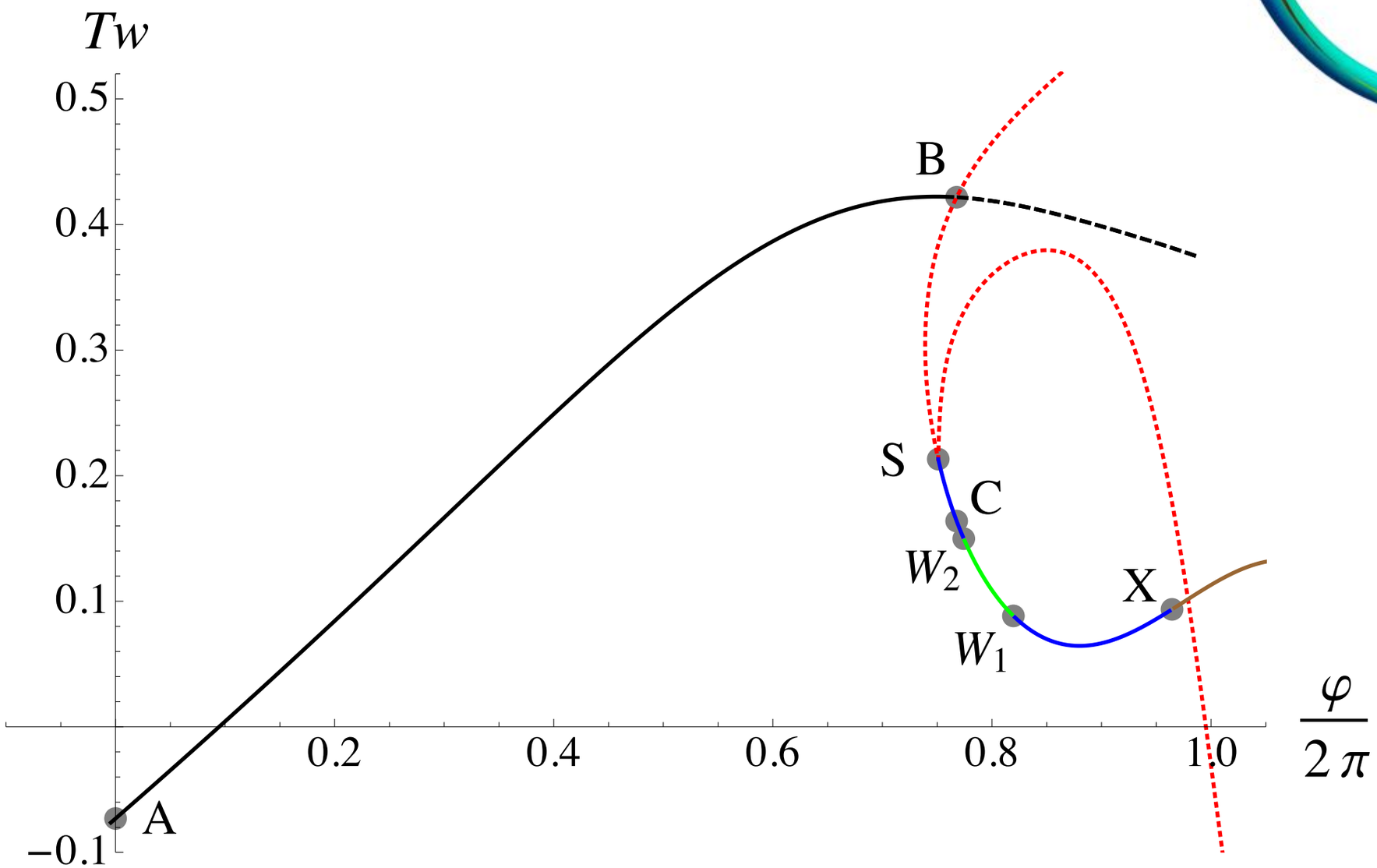
21 non linear PDE (arclength & time)
equilibrium & stability
BVP (collocation)
numerical path following


flip
e_y
e_x
$s = 0$
e_z
δ
$\varphi/2$
$\varphi/2$
$s = L$
e_x
$d_1(L)$
z^*

Obtaining a good knot

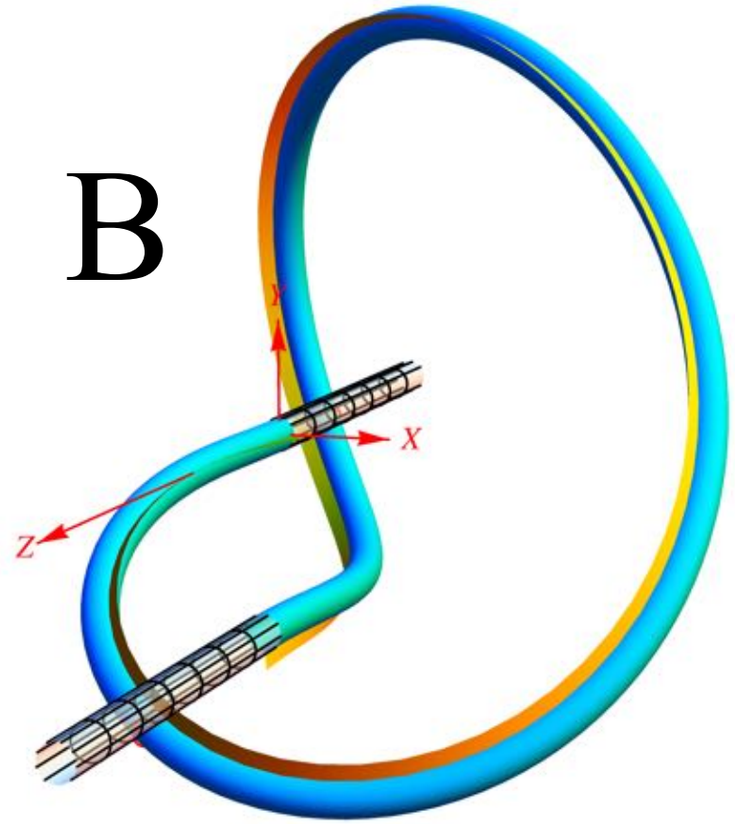
$$\text{fixed}\begin{cases} z^* &= 0.115 \\ \delta &= 0.05 \end{cases}$$

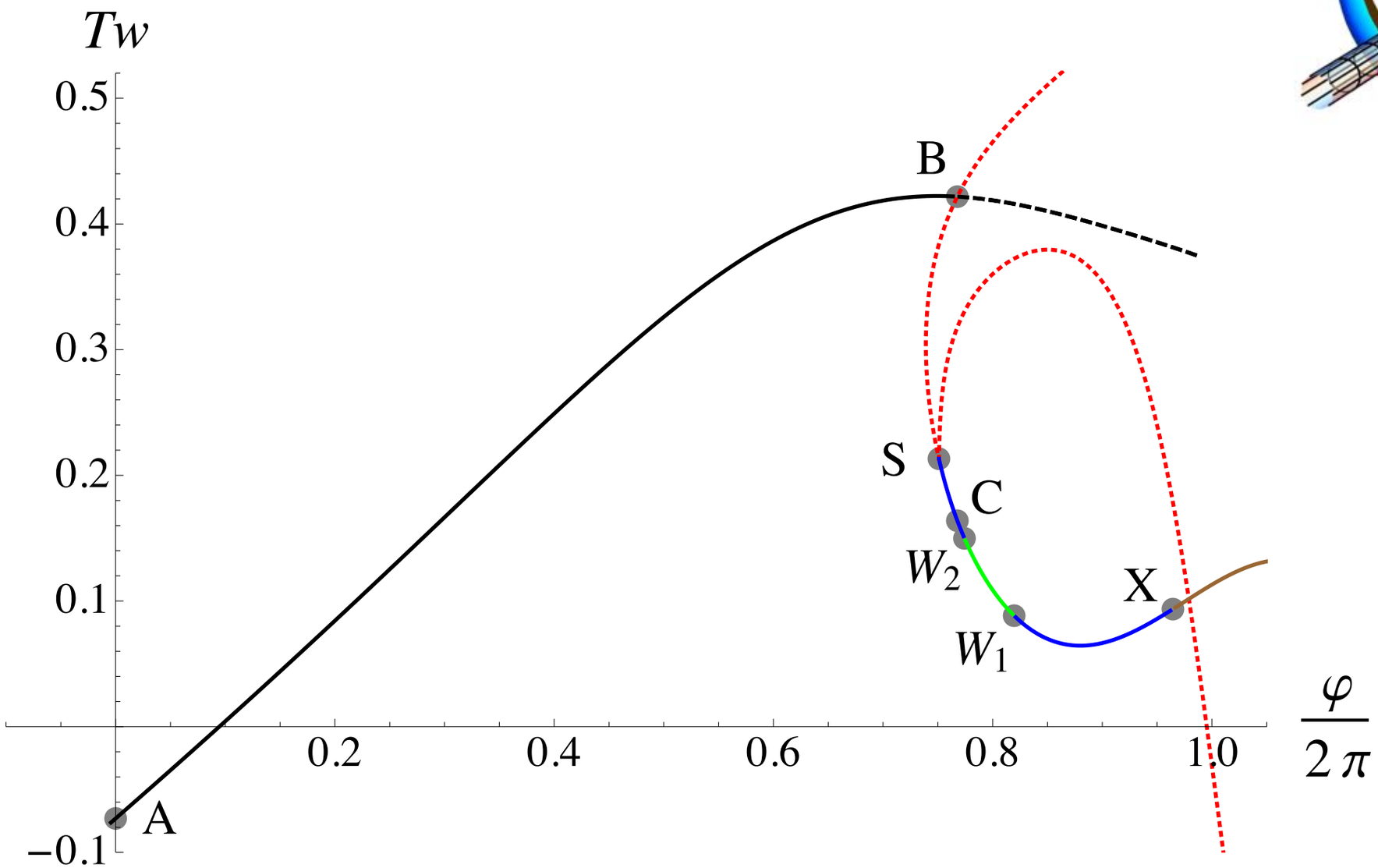




Obtaining a good knot

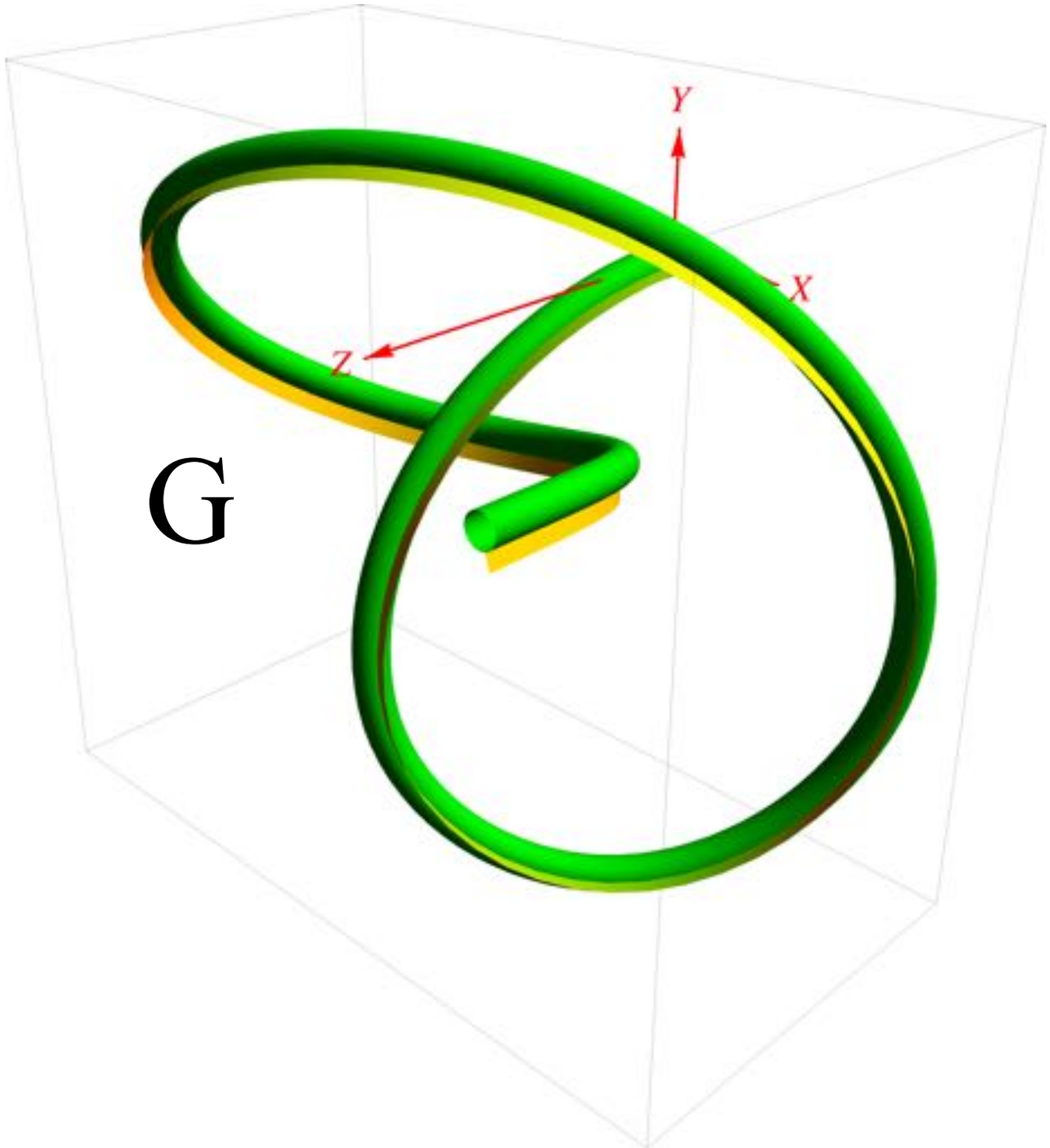
$$\text{fixed}\begin{cases} z^* &= 0.115 \\ \delta &= 0.05 \end{cases}$$

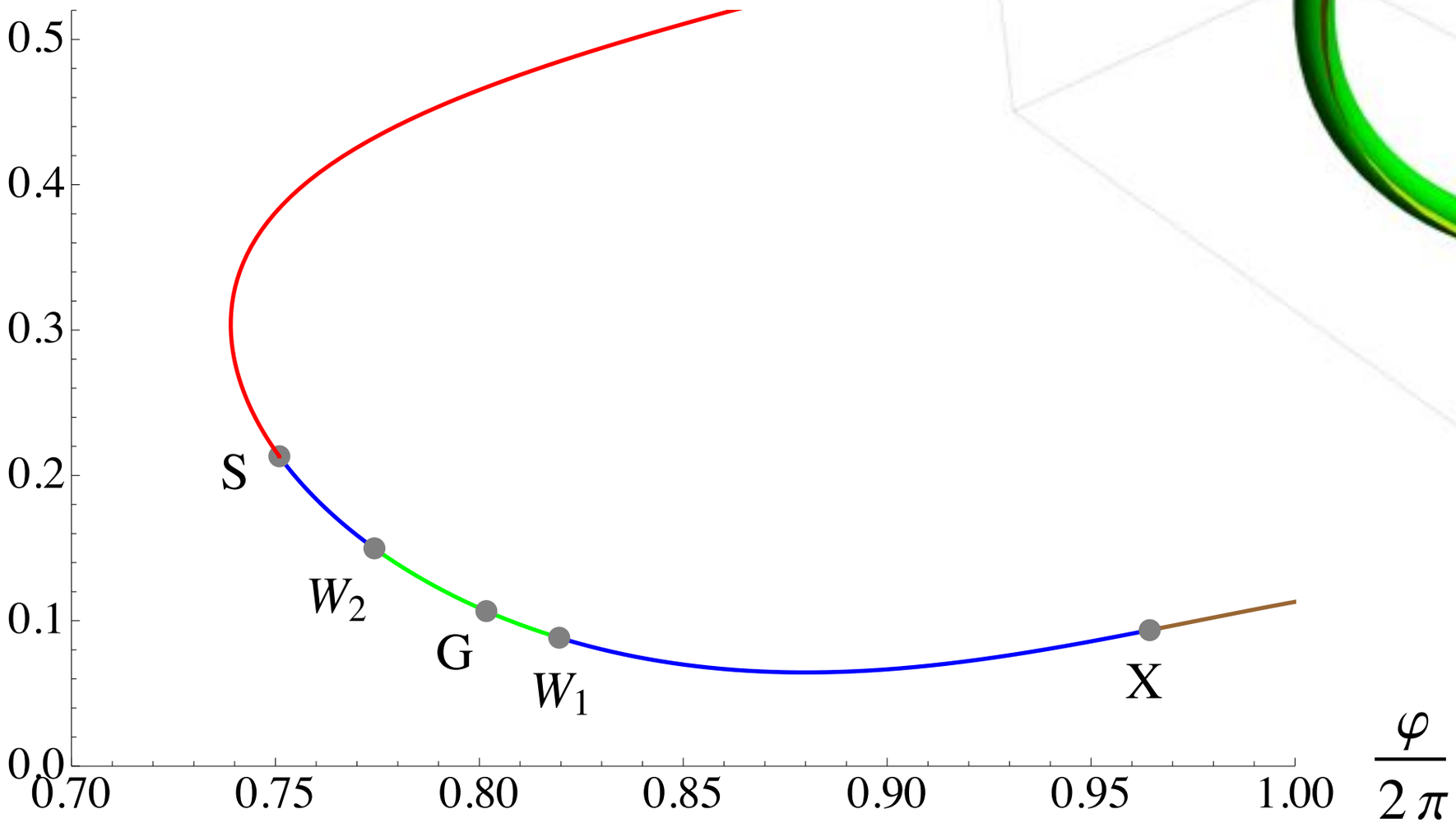




Obtaining a good knot

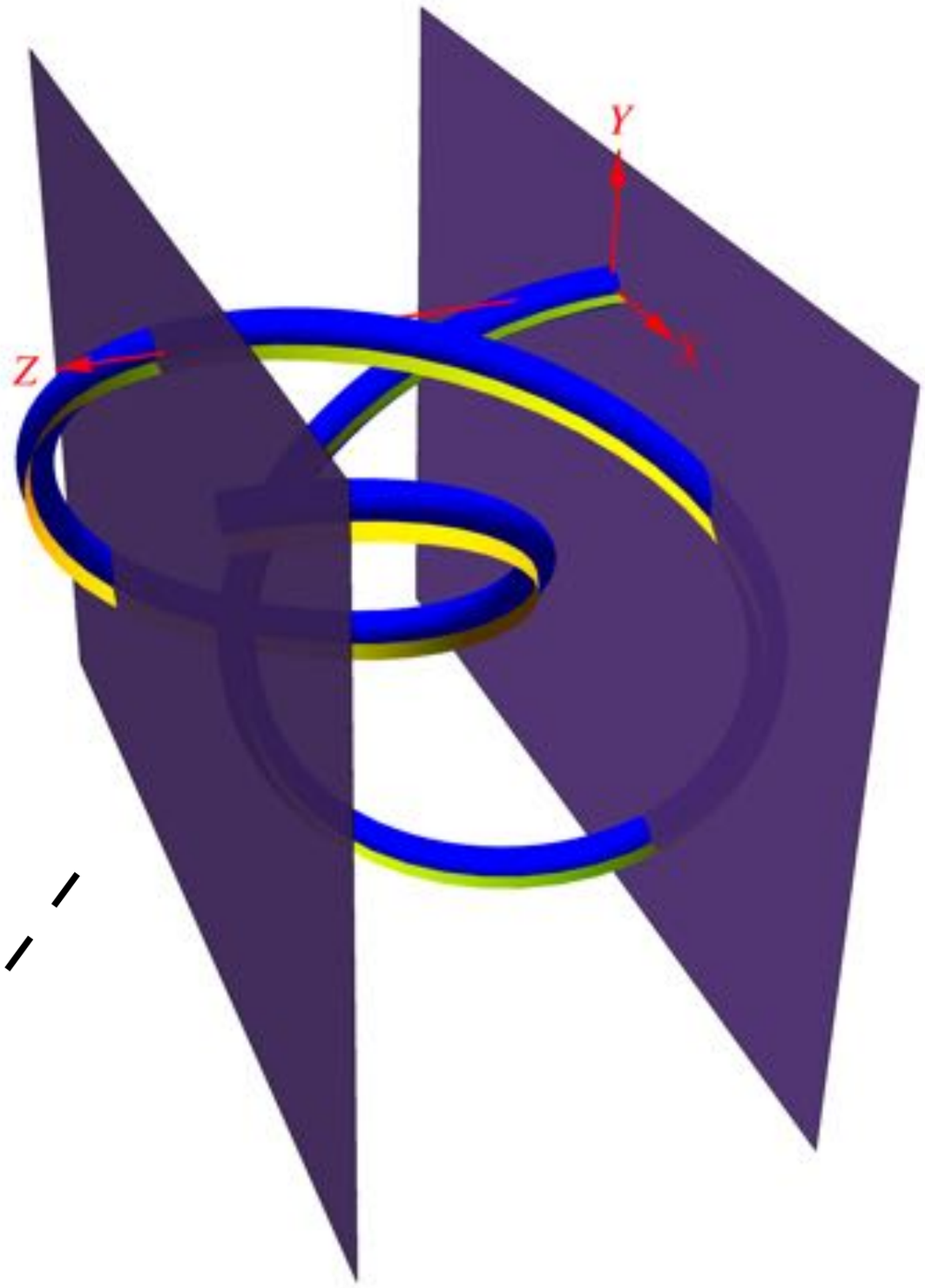
$$\text{fixed}\begin{cases} z^* &= 0.115 \\ \delta &= 0.05 \end{cases}$$

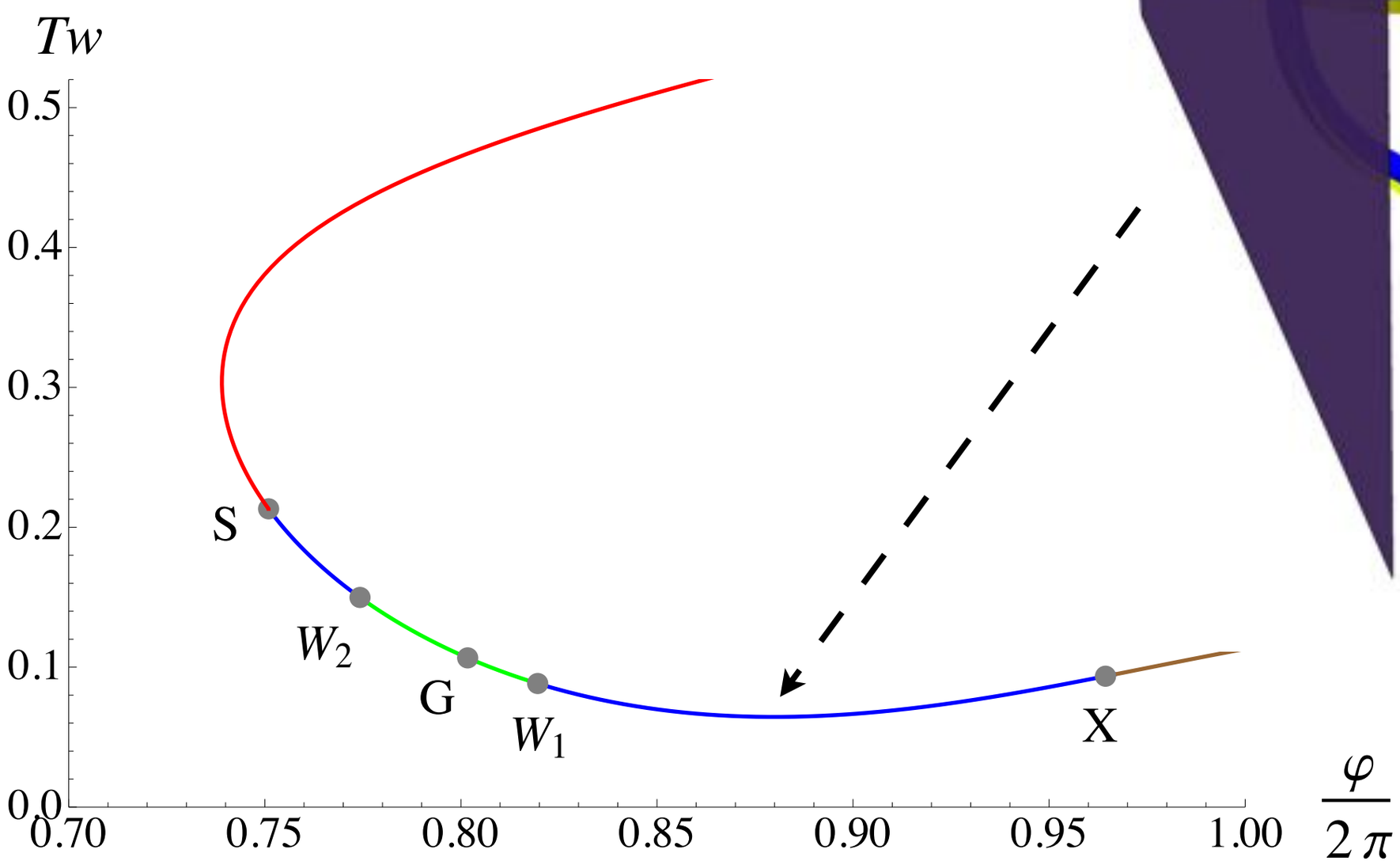




Obtaining a good knot

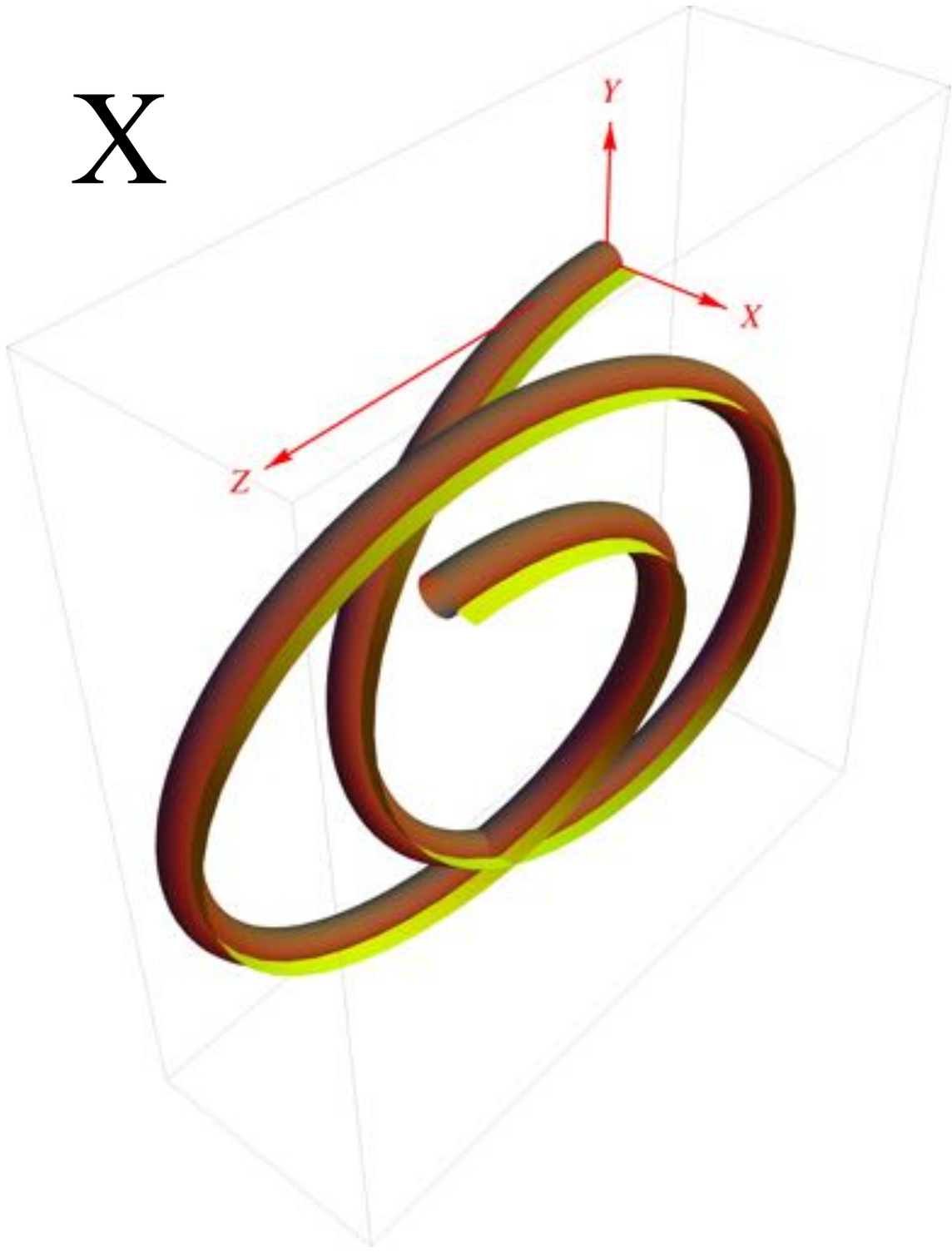
$$\text{fixed}\begin{cases} z^* &= 0.115 \\ \delta &= 0.05 \end{cases}$$

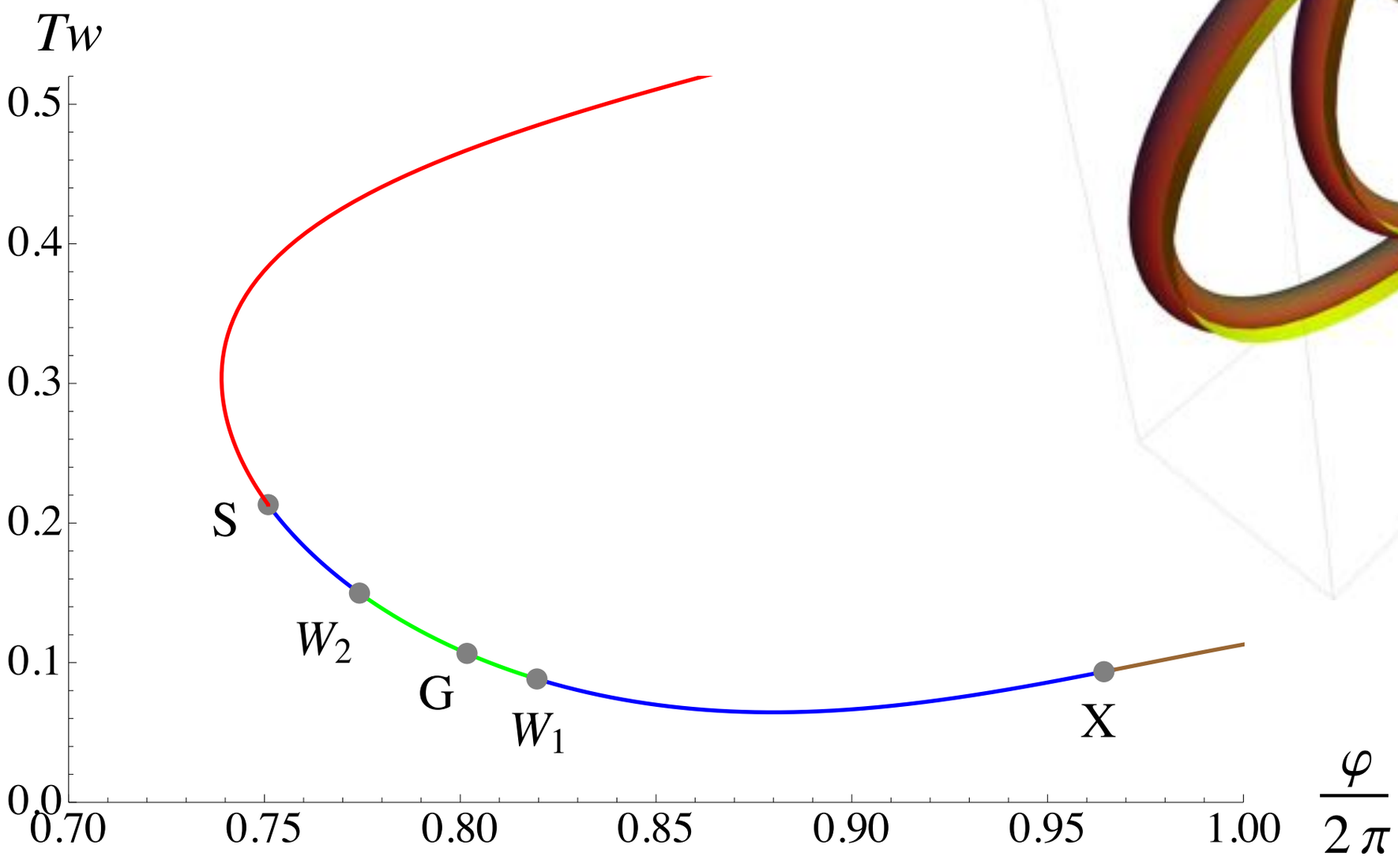




Obtaining a good knot

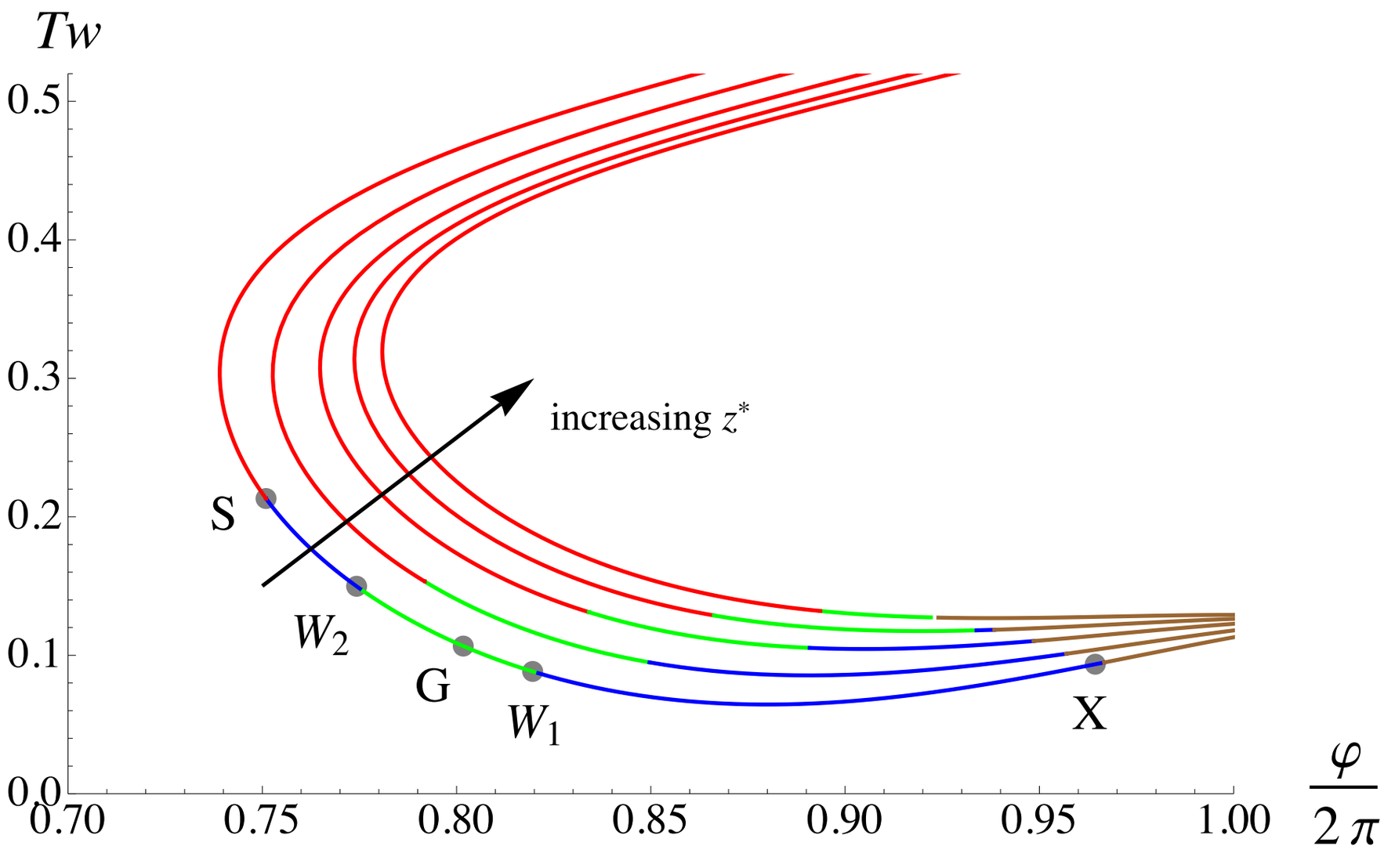
$$\text{fixed}\begin{cases} z^* &= 0.115 \\ \delta &= 0.05 \end{cases}$$





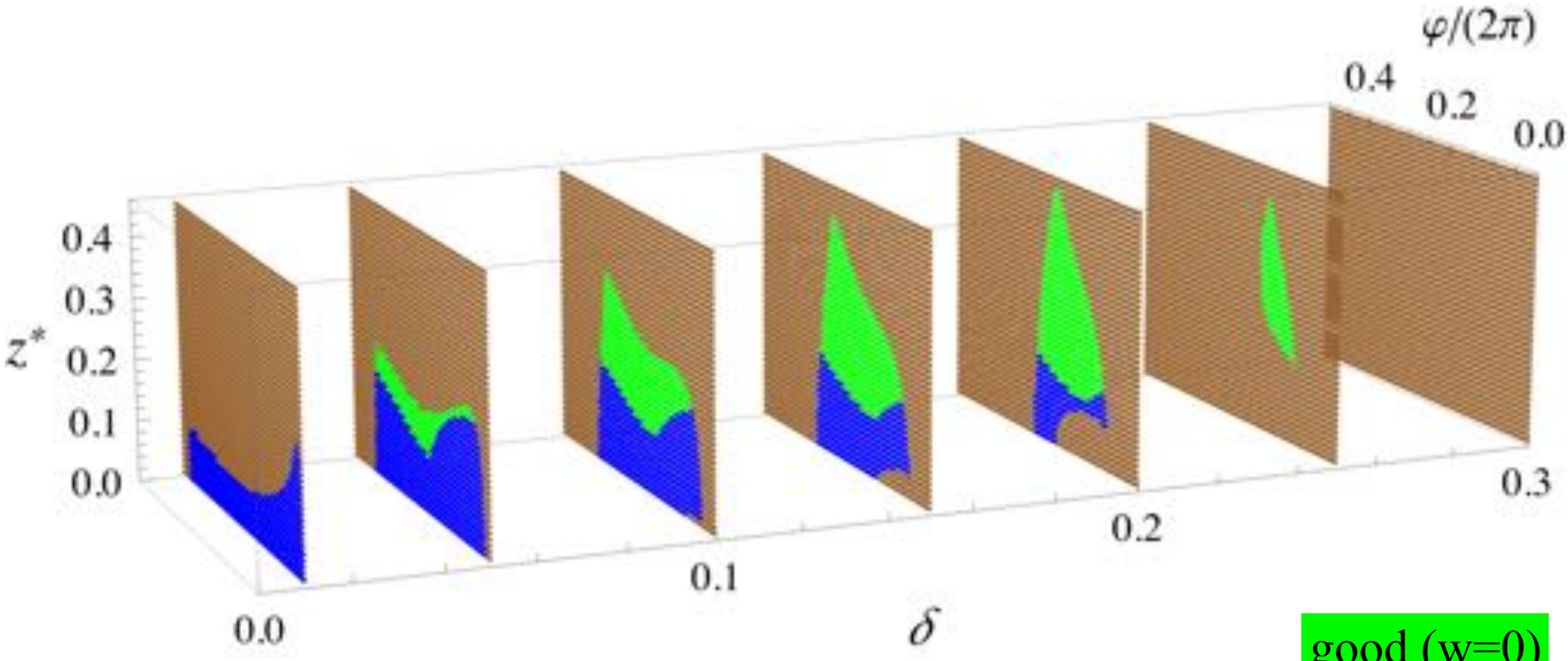
'All' the good knots

fixed $\delta = 0.05$



All the good knots

elastic strip model



good (w=0)

unknotted

unwalled

Equations for elastic strips

kinematics

$$
\begin{aligned}
x' &= d_{3x} \\
y' &= d_{3y} \\
z' &= d_{3z} \\
d'_{3x} &= u_2\, d_{1x} - u_1\, d_{2x} \\
d'_{3y} &= u_2\, d_{1y} - u_1\, d_{2y} \\
d'_{3z} &= u_2\, d_{1z} - u_1\, d_{2z} \\
d'_{1x} &= u_3\, d_{2x} - u_2\, d_{3x} \\
d'_{1y} &= u_3\, d_{2y} - u_2\, d_{3y} \\
d'_{1z} &= u_3\, d_{2z} - u_2\, d_{3z} \\
d'_{2x} &= u_1\, d_{3x} - u_3\, d_{1x} \\
d'_{2y} &= u_1\, d_{3y} - u_3\, d_{1y} \\
d'_{2z} &= u_1\, d_{3z} - u_3\, d_{1z}.
\end{aligned}
$$

dynamics

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

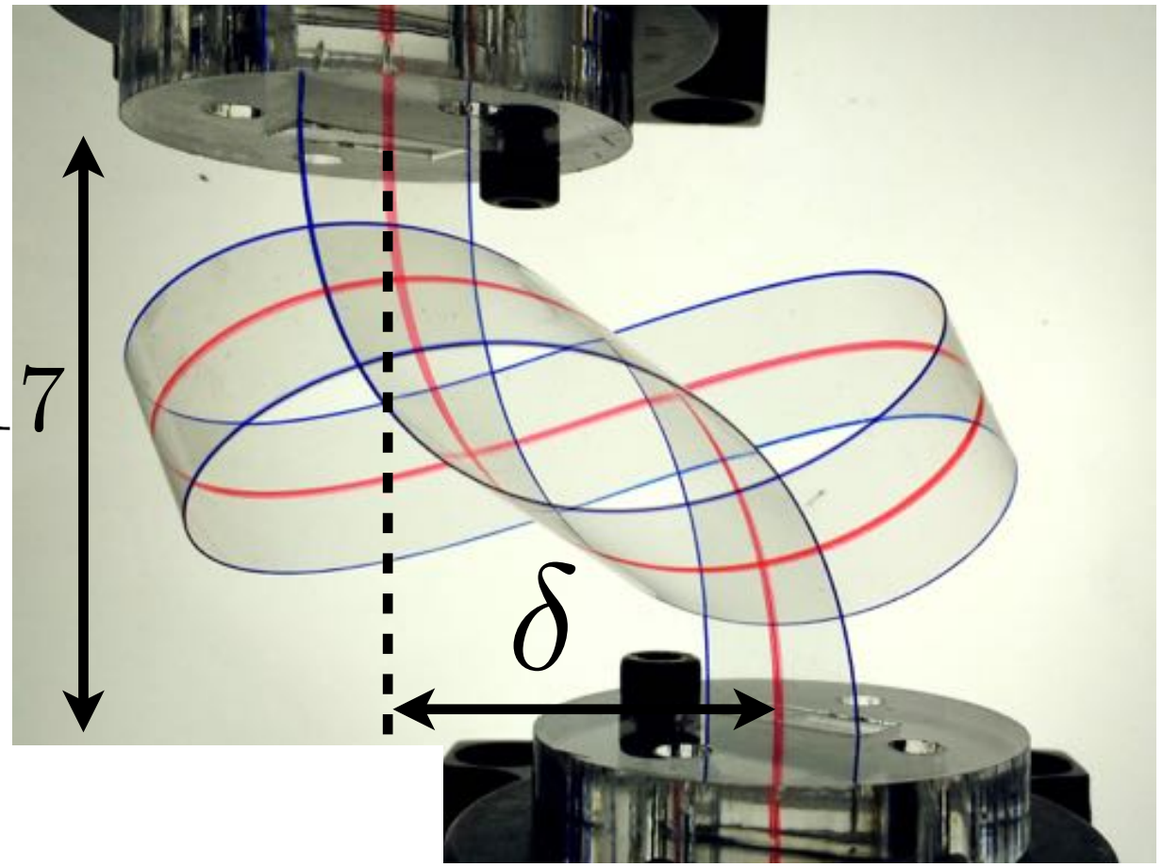
nonlinear constitutive relations

$$
\begin{aligned}
m_1 &= K\left(1 - \frac{u_3^4}{u_1^4}\right) u_1 \\
u_2 &= 0 \\
m_3 &= 2K\left(1 + \frac{u_3^2}{u_1^2}\right) u_3
\end{aligned}
$$

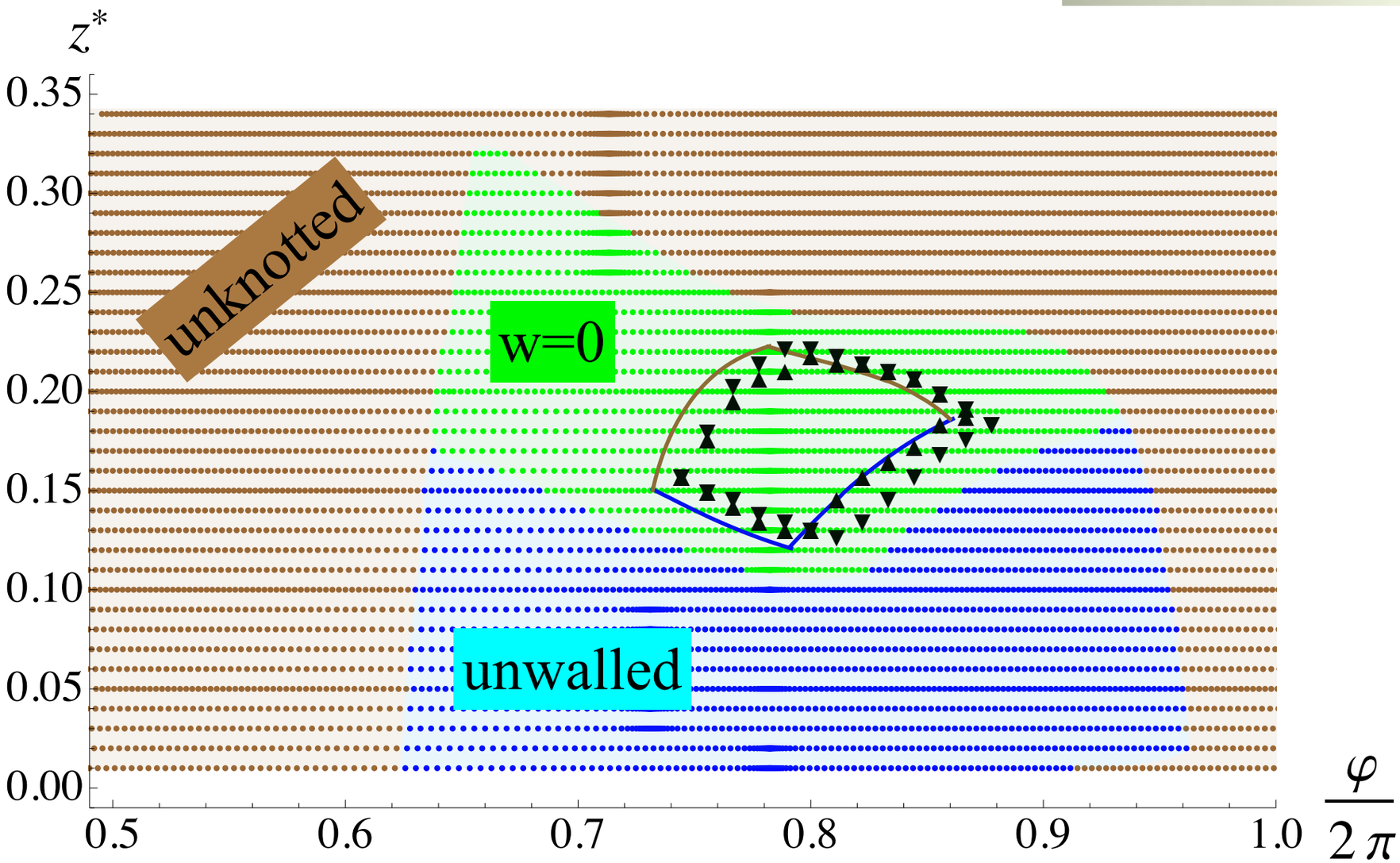
Dias & Audoly (JMPS) 2014

Experiments with $\delta = 0.10$

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



$$\frac{\varphi}{2\pi} = 0.78$$



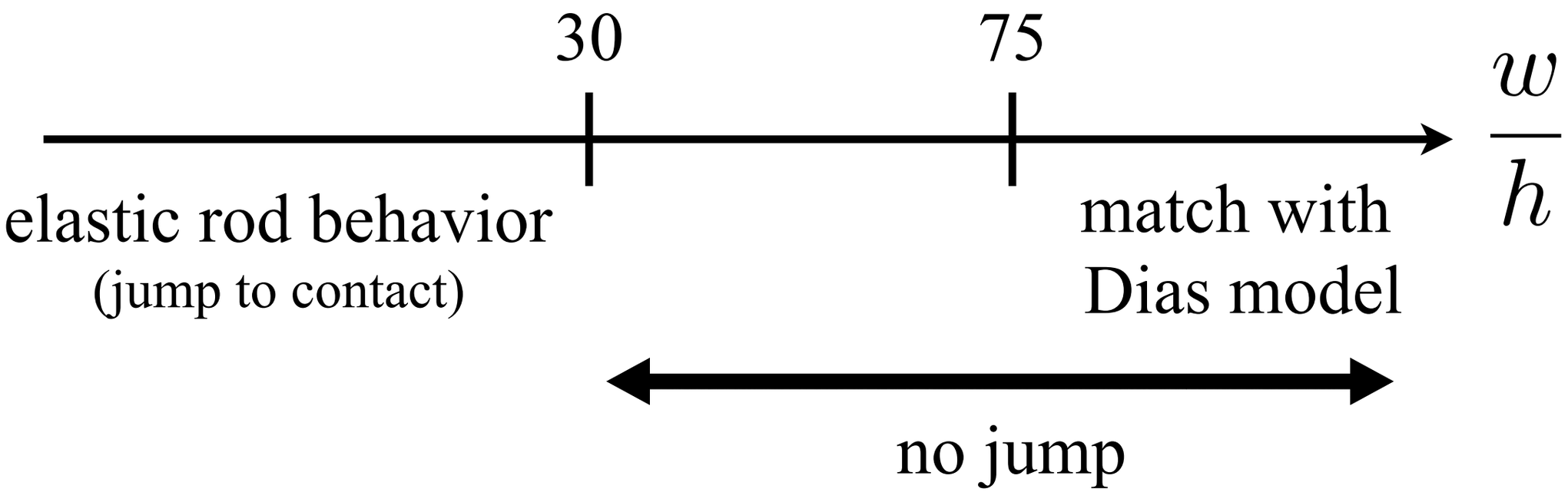
gravity:

$$\Gamma = \frac{Mg}{EI/L^2} \simeq 25$$

Conclusions

Importance of the w/h ratio

experiments: h = 200 microns and w from 0.6 cm to 1.5 cm



Stable *closed* knots with no self-contact ?

natural curvature ?

varying stiffness ?