La molécule d'ADN vue comme une poutre élastique : application aux expériences de pinces magnétiques

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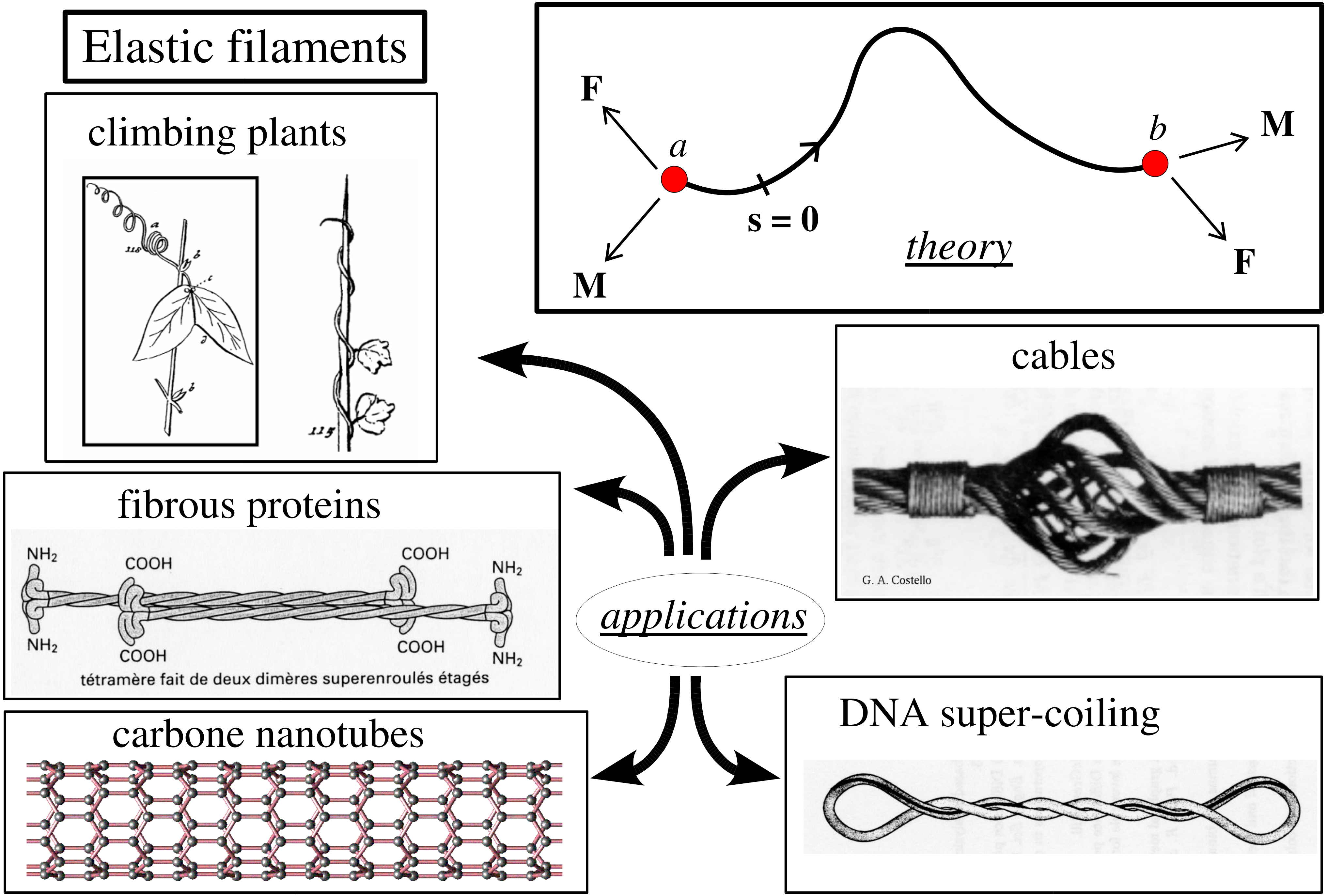
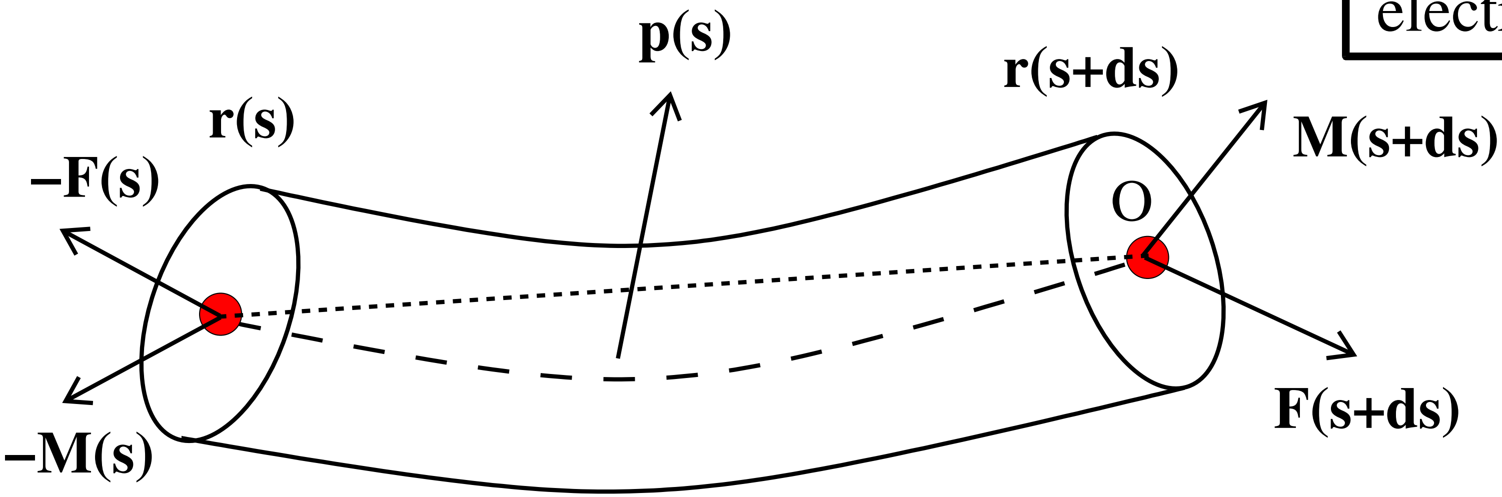

Elastic filaments
climbing plants
theory
F
M
a
b
s = 0
cables
G. A. Costello
fibrous proteins
NH2
COOH
tétramère fait de deux dimères superenroulés étagés
applications
carbone nanotubes
DNA super-coiling

Elastic rod in equilibrium

p(s) = external force
gravity, contact,
electrostatic, ...



force balance

$$p(s)\,\delta s + F(s+\delta s) - F(s) = 0$$

$$\boxed{p(s) + F'(s) = 0}$$

momentum balance

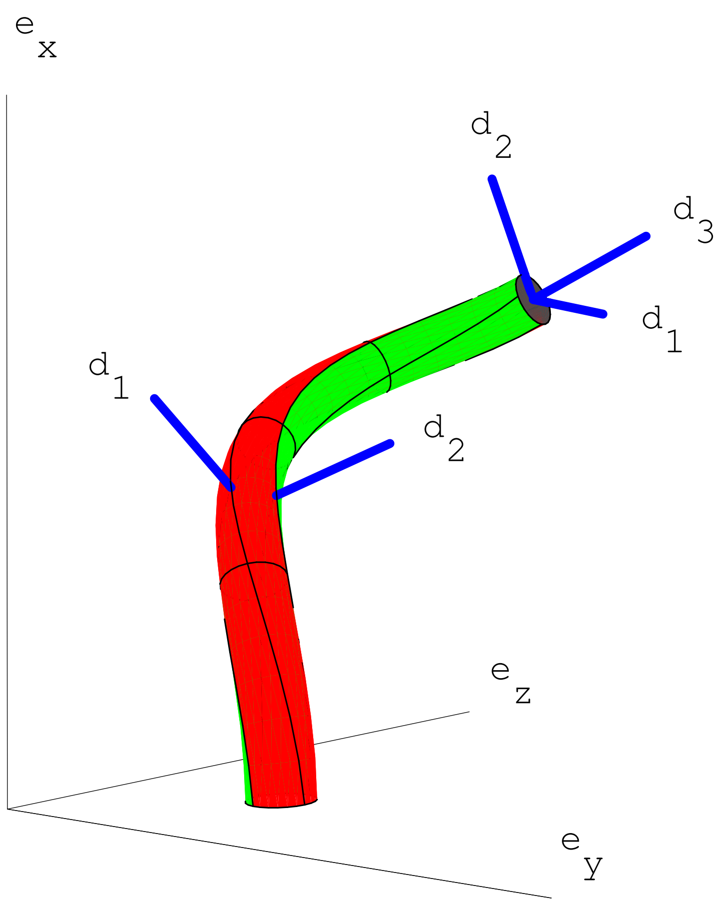
$$M(s+\delta s) - M(s) + \Pi_O[F(s+\delta s)] + \Pi_O[-F(s)] = 0$$

$$M(s+\delta s) - M(s) + 0 + (r(s) - r(s+\delta s)) \wedge (-F(s)) = 0$$

$$\boxed{M'(s) + r'(s) \wedge F(s) = 0}$$

Cosserat model for 1D elasticity

3 directors $\vec{d}_1, \vec{d}_2, \vec{d}_3$ on the top of $\vec{r}(s)$



no shear
no extension

$$\vec{r}\,'(s) = \vec{d}_3(s)$$

$$\begin{cases} \vec{d}_1\,'(s) = \vec{u}(s) \wedge \vec{d}_1 \\ \vec{d}_2\,'(s) = \vec{u}(s) \wedge \vec{d}_2 \\ \vec{d}_3\,'(s) = \vec{u}(s) \wedge \vec{d}_3 \end{cases}$$

evolution in SO(3)

$$\vec{u}(s) = \{u_1,\, u_2,\, u_3\}_{\vec{d}_1, \vec{d}_2, \vec{d}_3}$$

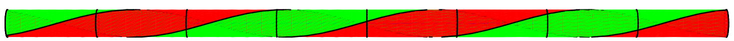
$$\vec{u}(s) = \{\kappa_1,\, \kappa_2,\, \tau\}_{\vec{d}_1, \vec{d}_2, \vec{d}_3}$$

u_1, u_2 : curvature and u_3 : twist

Linear Constitutive Relations

Bending stiffness : K_0

$$\vec{M}\cdot\vec{d}_1 = K_0\, u_1$$
$$\vec{M}\cdot\vec{d}_2 = K_0\, u_2$$



Twist stiffness : K_3

$$\vec{M}\cdot\vec{d}_3 = K_3\, u_3$$

$K_0 = E\, I$

I : moment of inertia

E : Young's modulus

filament	E
Microtubule	1 GPa
DNA	1 GPa
Actine	2 GPa
Collagen	2 GPa
Rubber	2 GPa
Steel	200 GPa

Kirchhoff equations

21 ODEs with variable : s

ordinary differential equations

$$\frac{d}{ds}\vec{F}=\vec{p}$$

$$\frac{d}{ds}\vec{M}=\vec{F}\wedge\vec{d}_3$$

$$\frac{d}{ds}\vec{r}=\vec{d}_3$$

$$\frac{d}{ds}\vec{d}_i=\vec{u}\wedge\vec{d}_i$$

$$m_i=K_i u_i$$

linear elasticity

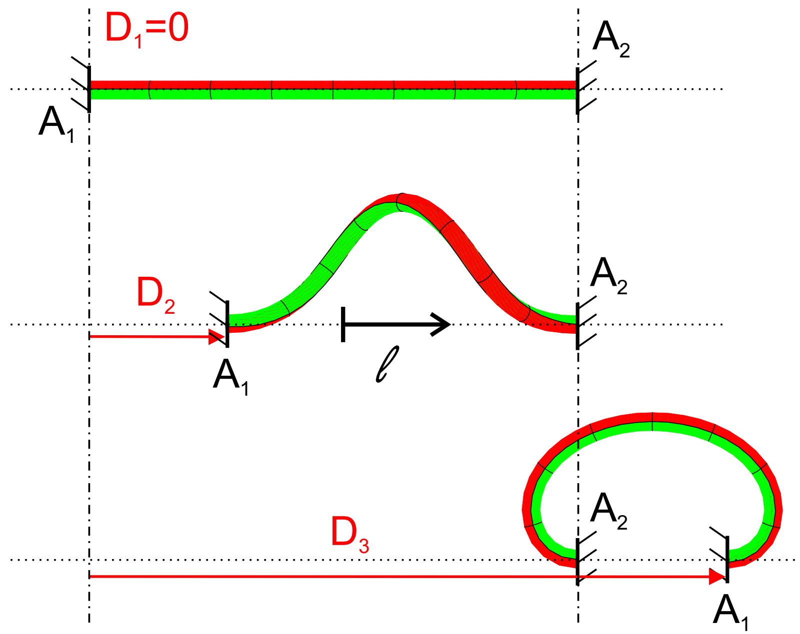
21 unknowns

$$\vec{F}(s)$$
$$\vec{M}(s)$$
$$\vec{r}(s)$$
$$\vec{d}_3(s)$$
$$\vec{d}_2(s)$$
$$\vec{d}_3(s)$$
$$\vec{u}(s)$$

$$i=1,2,3$$

boundary conditions

- how the rod is held
- few solutions are admissibles



$$\vec{d}_3(A_1)=\vec{d}_3(A_2)$$

$$\vec{r}(A_2)-\vec{r}(A_1)=k\,\vec{d}_3(A_2)$$

$$(D=L-k)$$

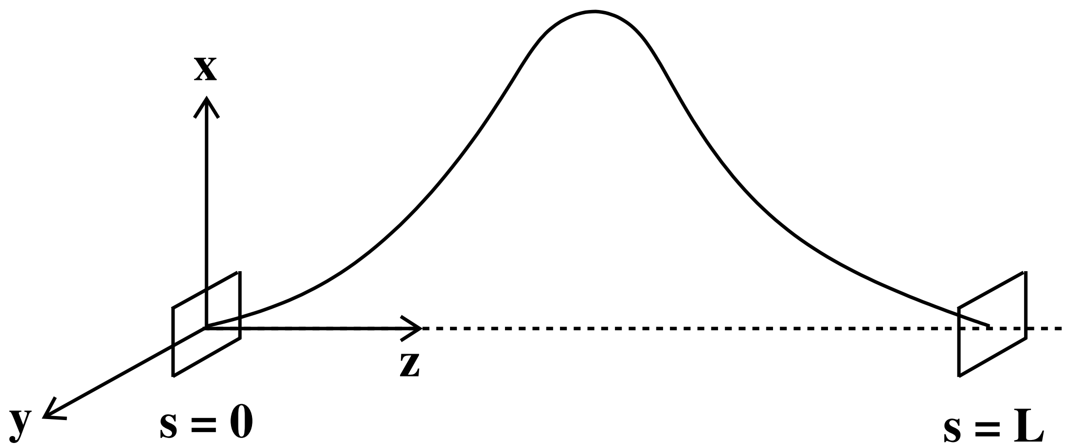
Find admissible equilibrium solutions : shooting method

initial conditions

$$r(0)=(0,0,0)$$
$$d_1(0)=(1,0,0)$$
$$d_2(0)=(0,1,0)$$
$$d_3(0)=(0,0,1)$$

parameters

$$\vec{F}(0), \vec{M}(0)$$



end conditions

$$\left.\begin{array}{l} x(L)=0 \\ y(L)=0 \\ d_3x(L)=0 \\ d_3y(L)=0 \end{array}\right\}\phi$$

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solution of ODEs

$$\phi(\overbrace{\vec{F}(0), \vec{M}(0)}^{u})=0$$
$$\Leftrightarrow \phi(u)=0$$

$$\phi \in \mathbb{R}^L$$
$$u \in \mathbb{R}^P$$

this defines a *P-L* solution manifold

1D solution manifold : path following predictor-corrector scheme

1D solution manifold
$$\begin{cases}\phi_1(u_1,u_2,u_3)=0\\ \phi_2(u_1,u_2,u_3)=0\end{cases}$$

At each point :

1-(predictor)

we take a guess : Z_i

2-(corrector)

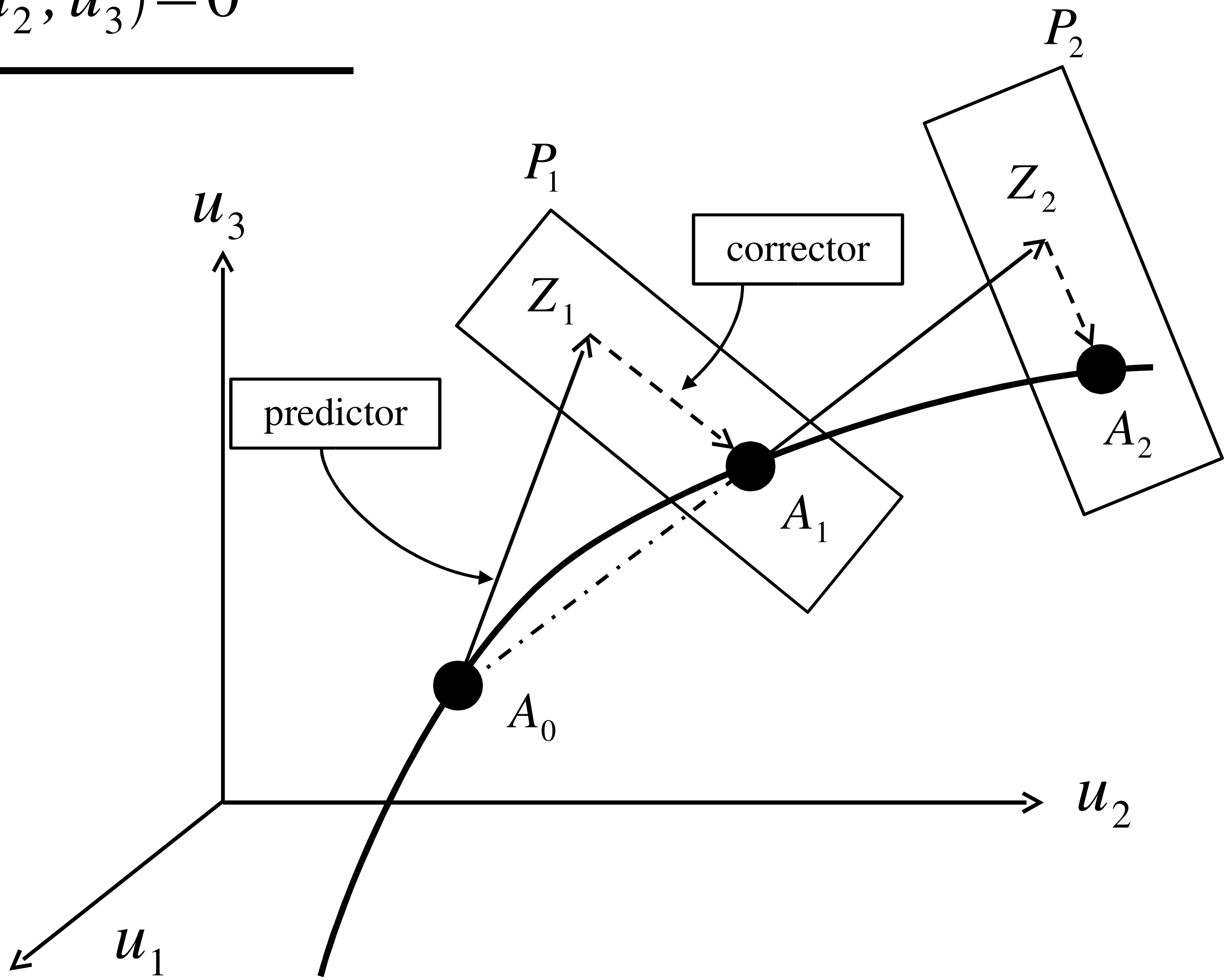
we define a projection :

$P_i(u_1,u_2,u_3)=0$

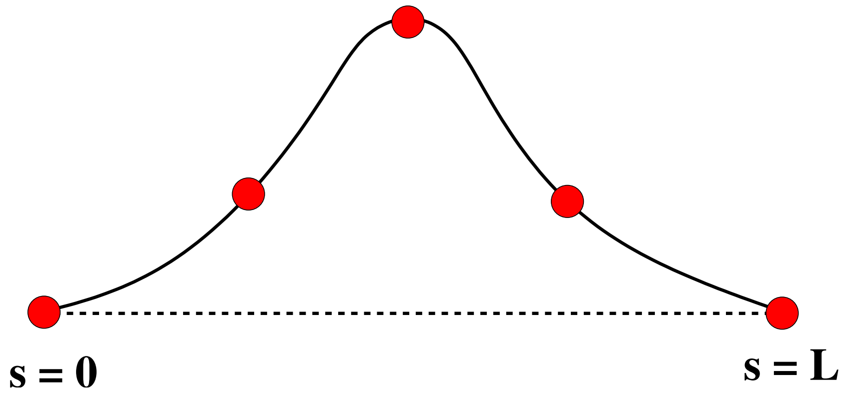
and we solve :

$$\begin{cases}\phi_1(u_1,u_2,u_3)=0\\ \phi_2(u_1,u_2,u_3)=0\\ P_i(u_1,u_2,u_3)=0\end{cases}$$

to obtain A_i



Find admissible equilibrium solutions : discretization methods



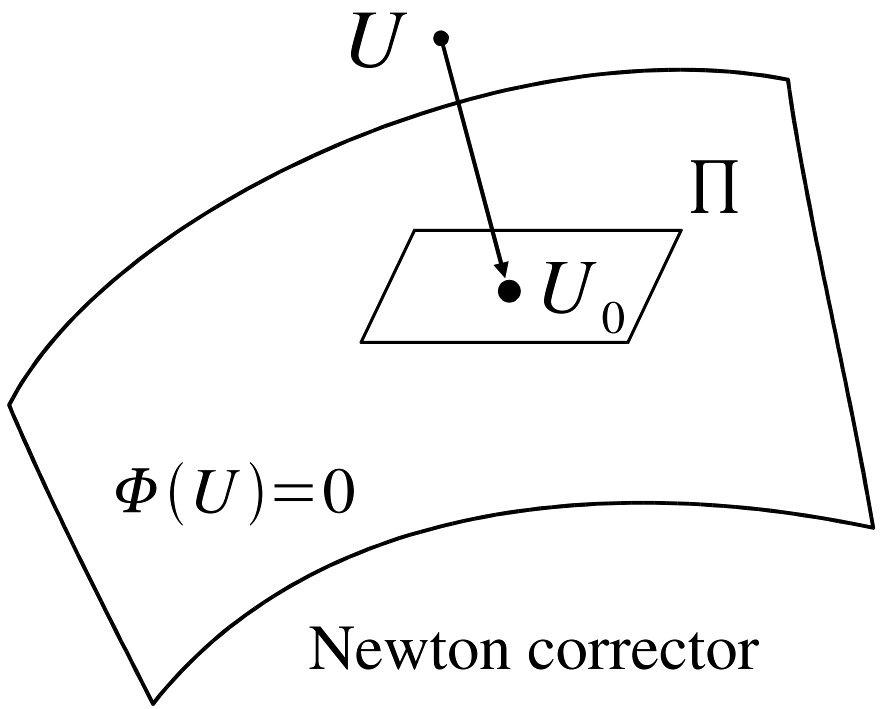
discretization over N intervals

$$\Phi(U)=0$$

→ boundary conditions

→ matching conditions

system of nonlinear algebraic equations



$$\underbrace{\Phi(U_0)}_{=0}=\Phi(U)+\frac{D\Phi}{DU}(U_0-U)+\dots$$

1-we take a point U

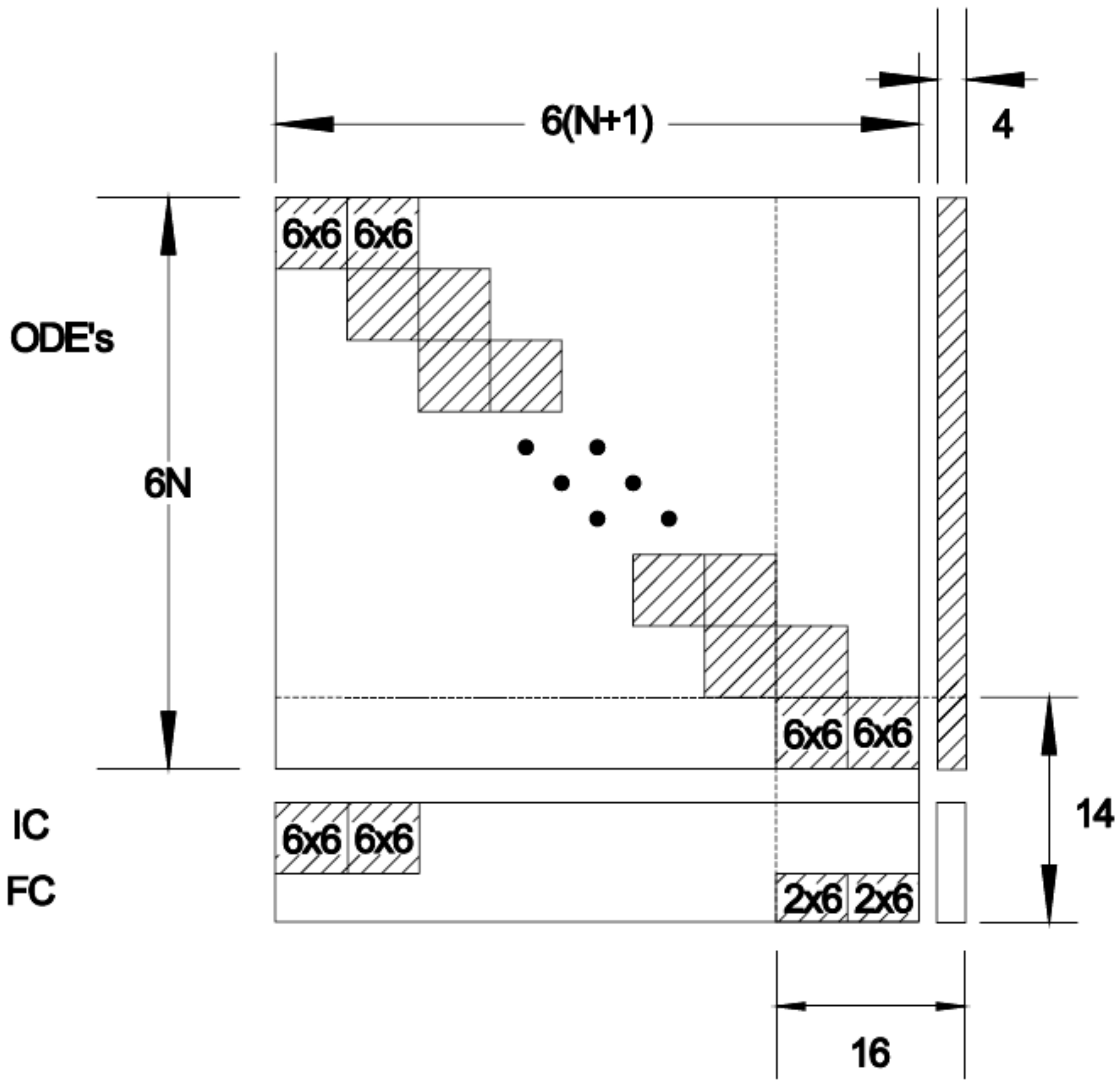
2-compute Jacobian

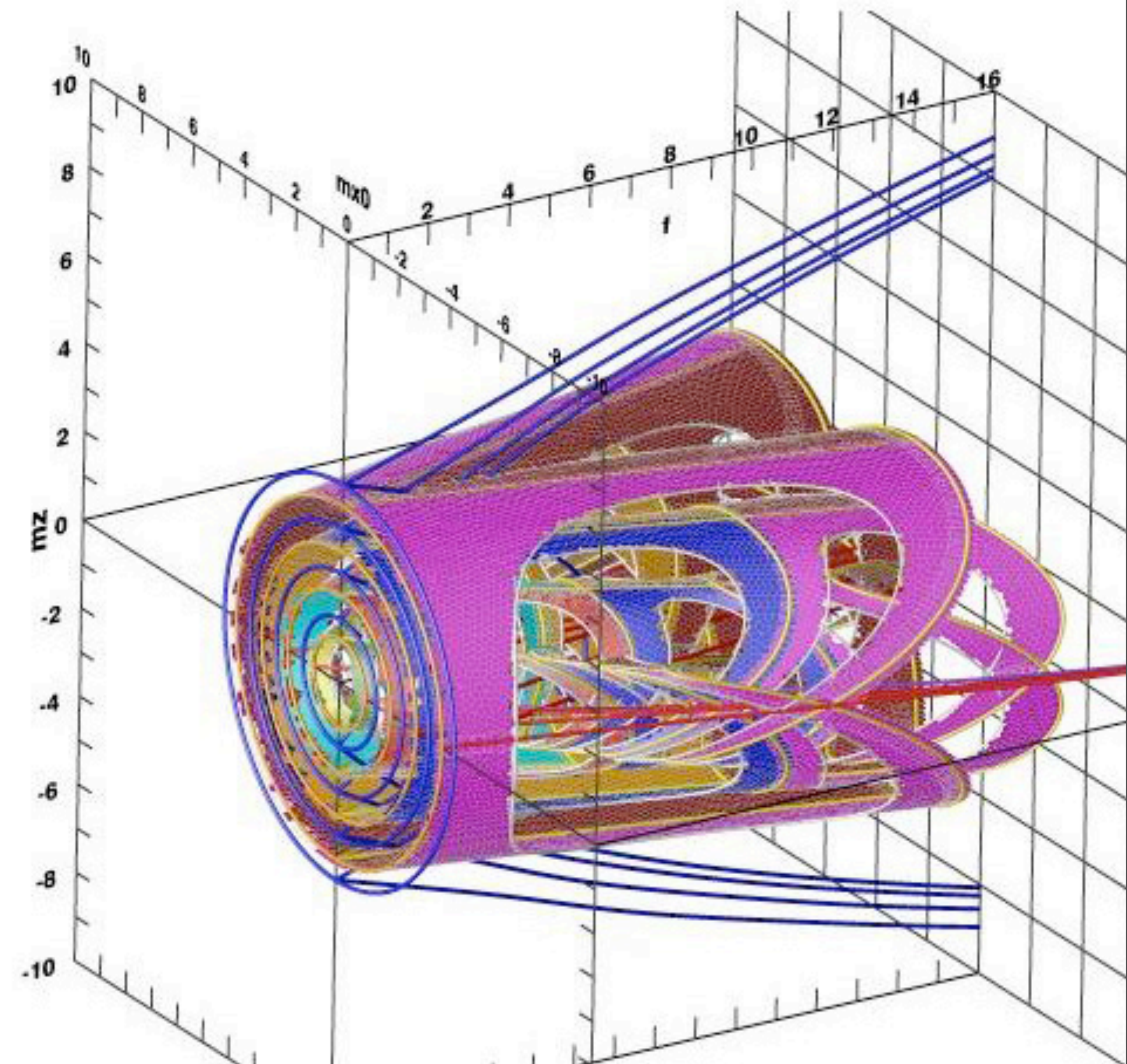
3-kernel is tangent plane Π

4-we project orthogonaly : $U \rightarrow U_0$

2D solution manifold

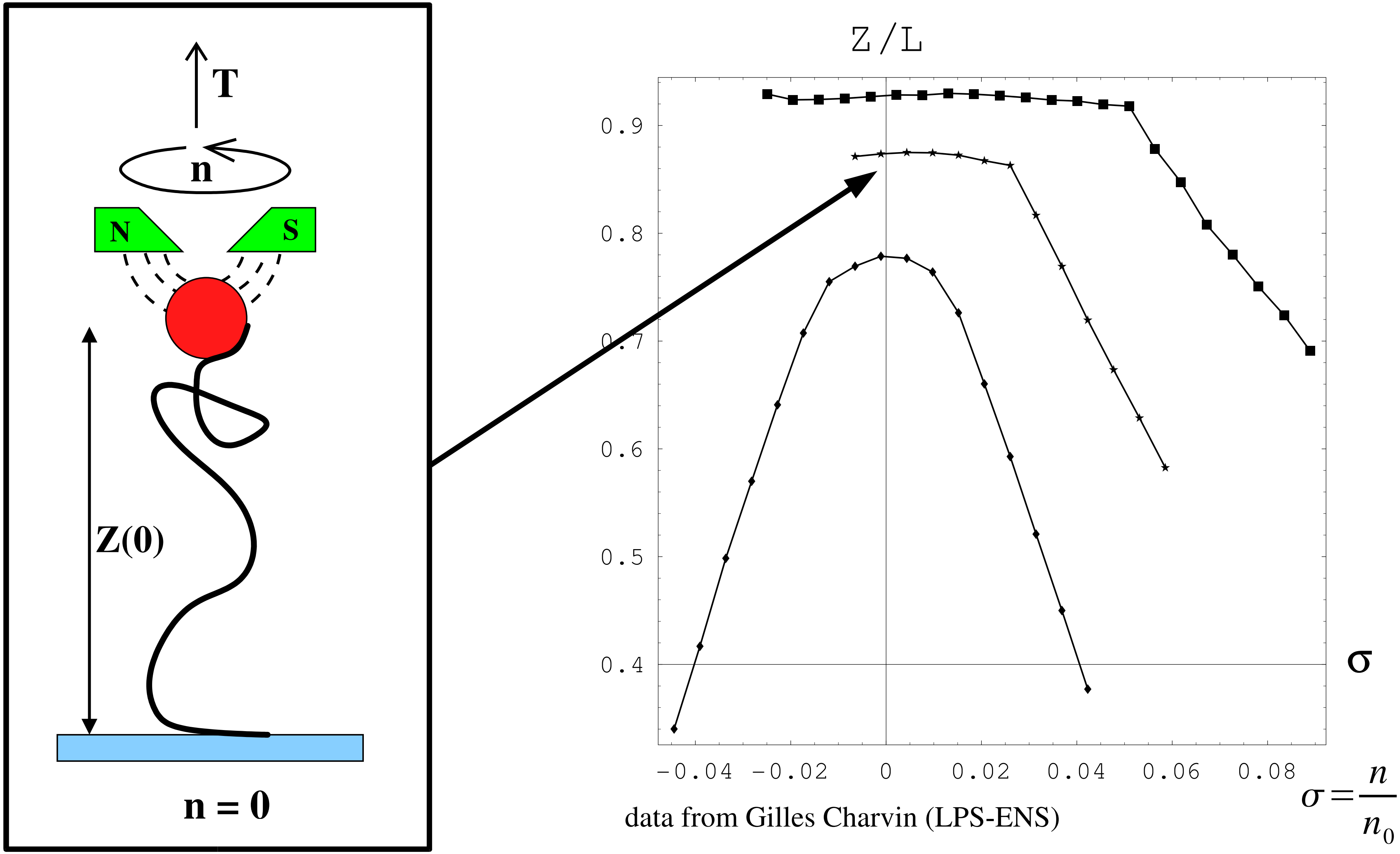
$$\dot{x} = d_{3y}$$
$$\dot{y} = d_{3y}$$
$$\dot{z} = d_{3z}$$
$$\dot{d}_{3x} = fxd_{3z} - m_z d_{3y}$$
$$\dot{d}_{3y} = fyd_{3z} - m_{x0}d_{3z} + m_z d_{3x}$$
$$\dot{d}_{3z} = -fxd_{3x} - fyd_{3y} + m_{x0}d_{3y}$$





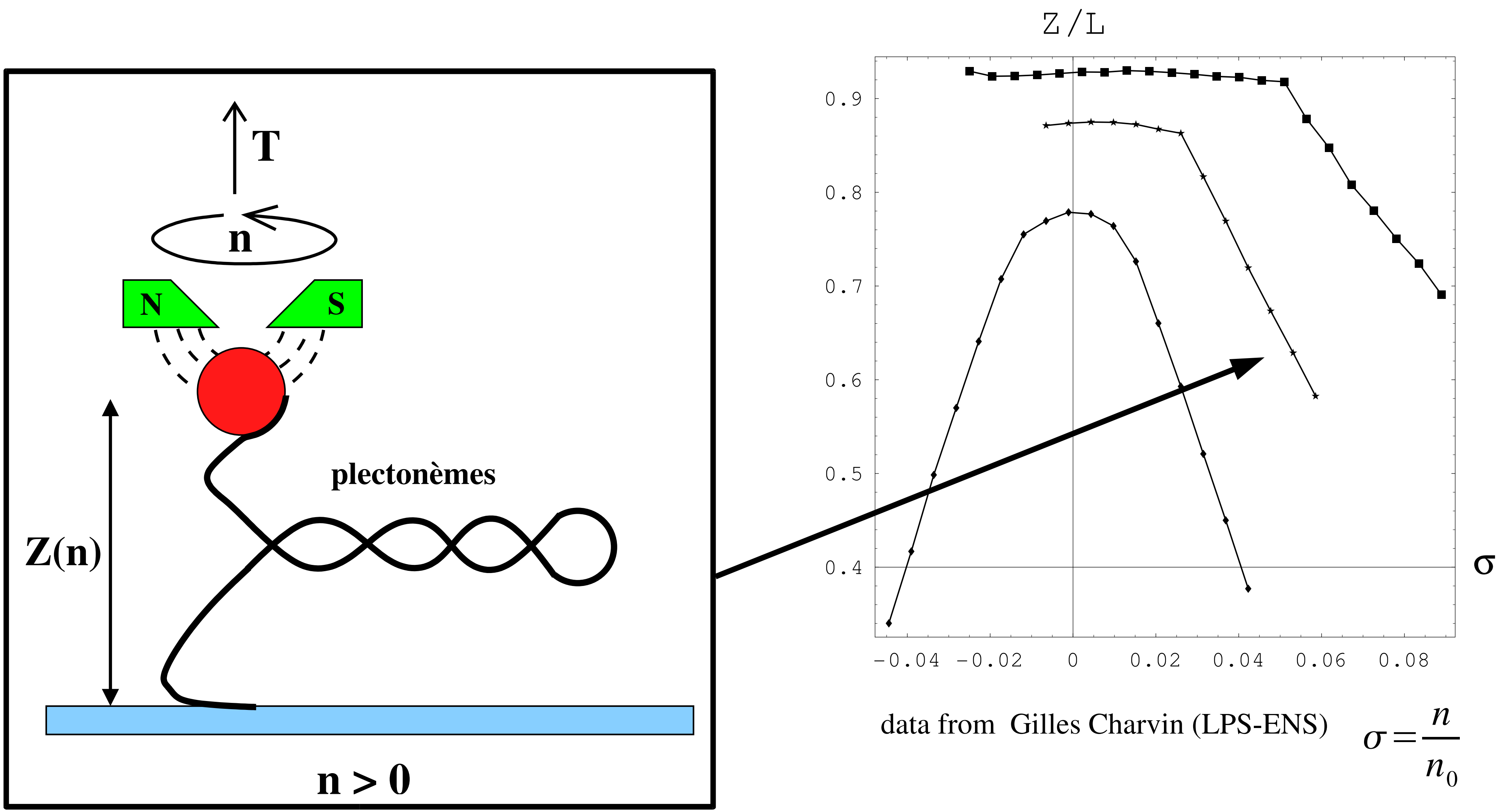
Michael Henderson (IBM)

Pulling and twisting DNA



data from Gilles Charvin (LPS-ENS)

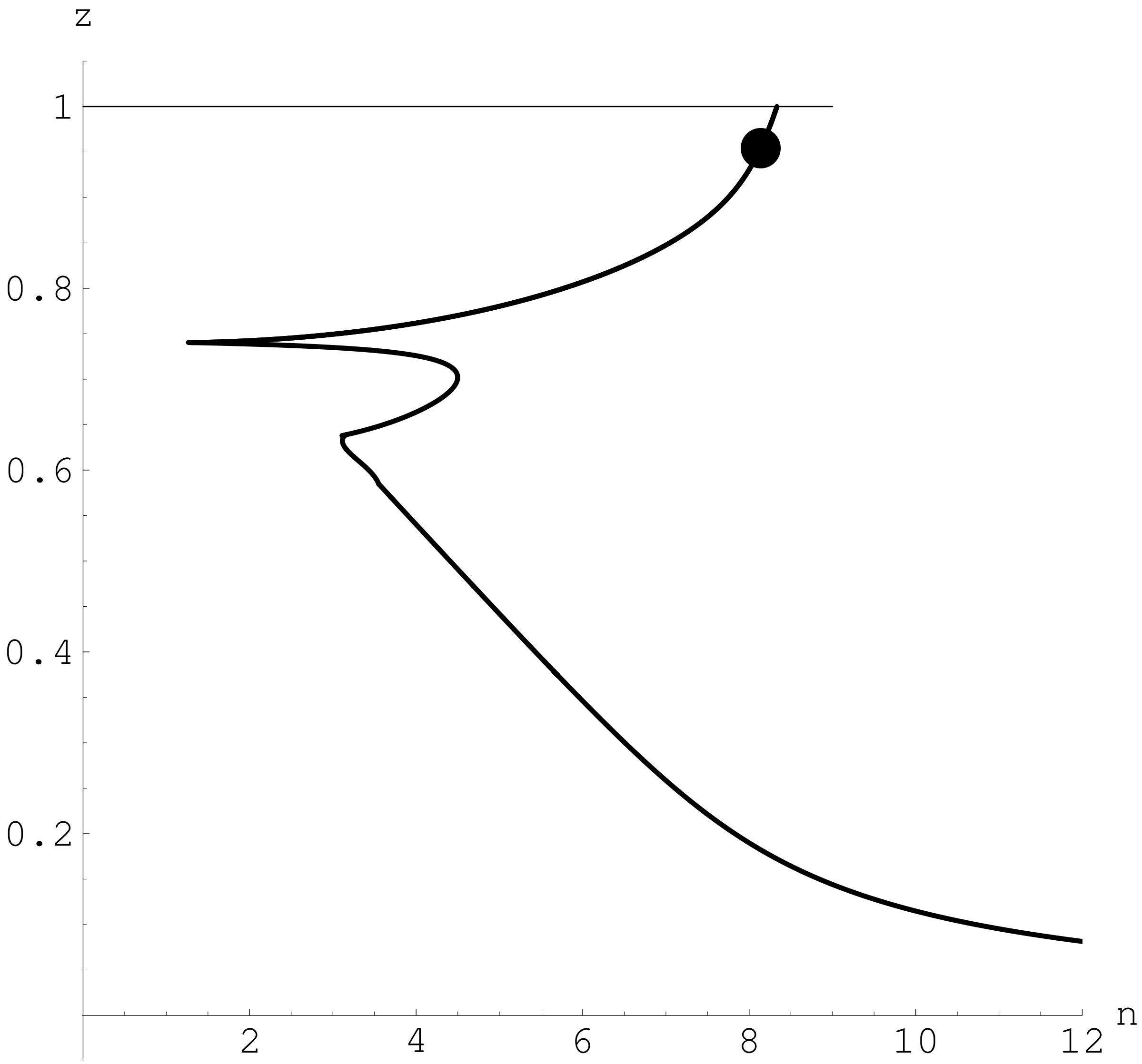
Pulling and twisting DNA

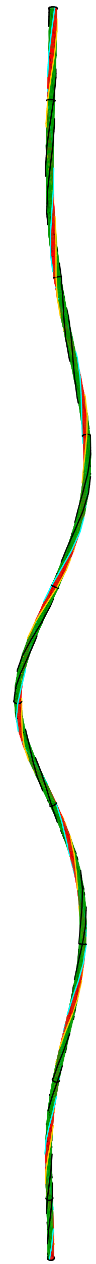


data from Gilles Charvin (LPS-ENS)

$$\sigma = \frac{n}{n_0}$$

Results : how a twisted rod coils





$$\frac{L}{2R} = 170$$

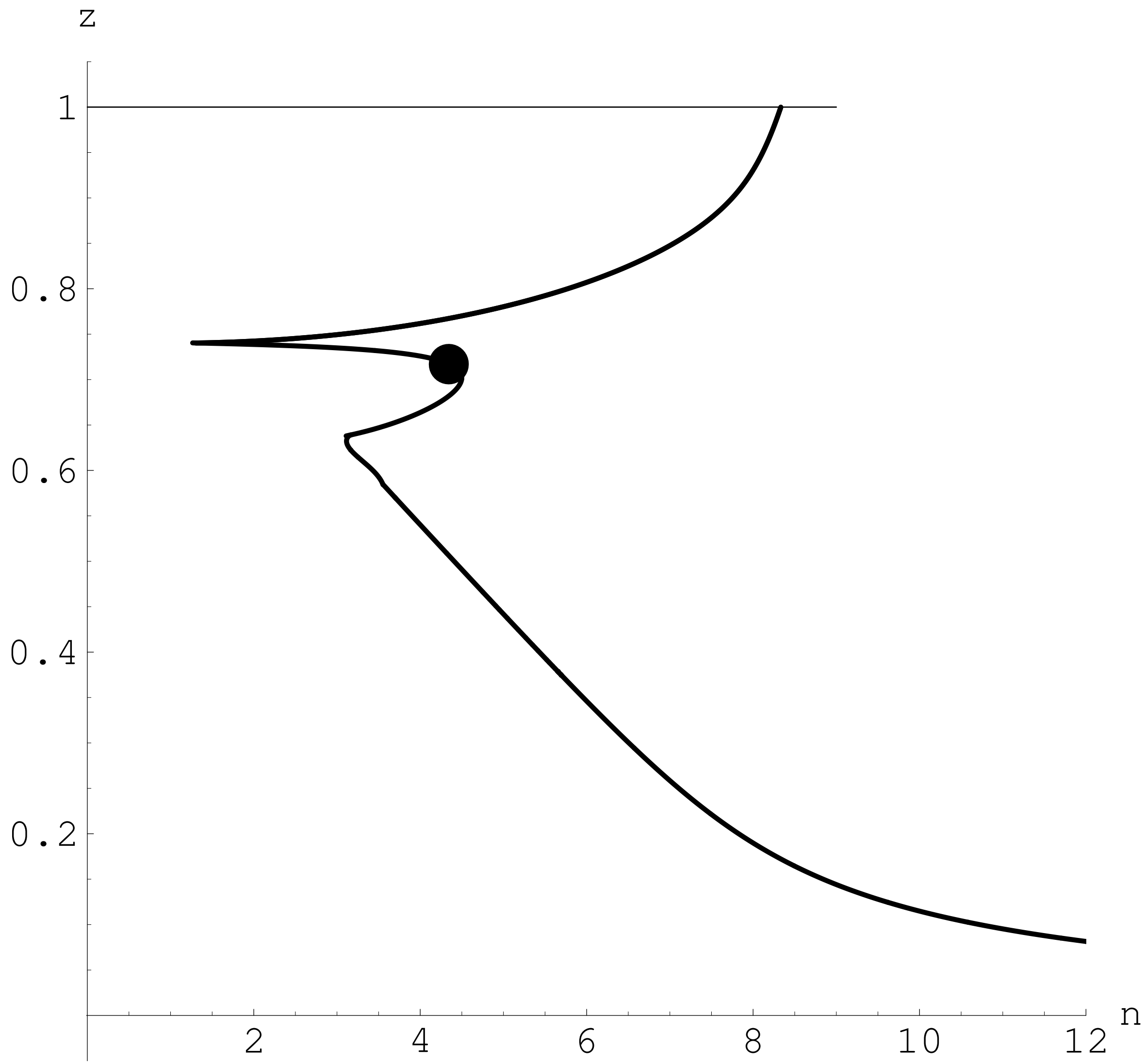
$$t = \frac{TL^2}{4\pi^2 K_0} = 6$$

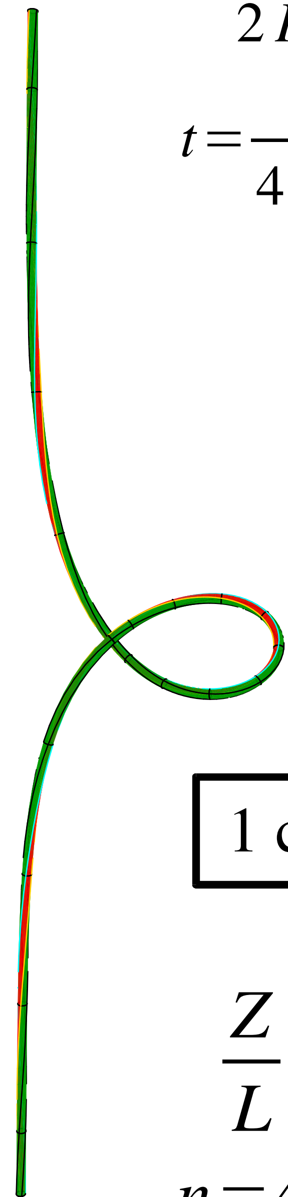
0 contact(s)

$$\frac{Z}{L} = 0.95$$

$$n = 8.1\ turns$$

Results : how a twisted rod coils





$$\frac{L}{2R} = 170$$

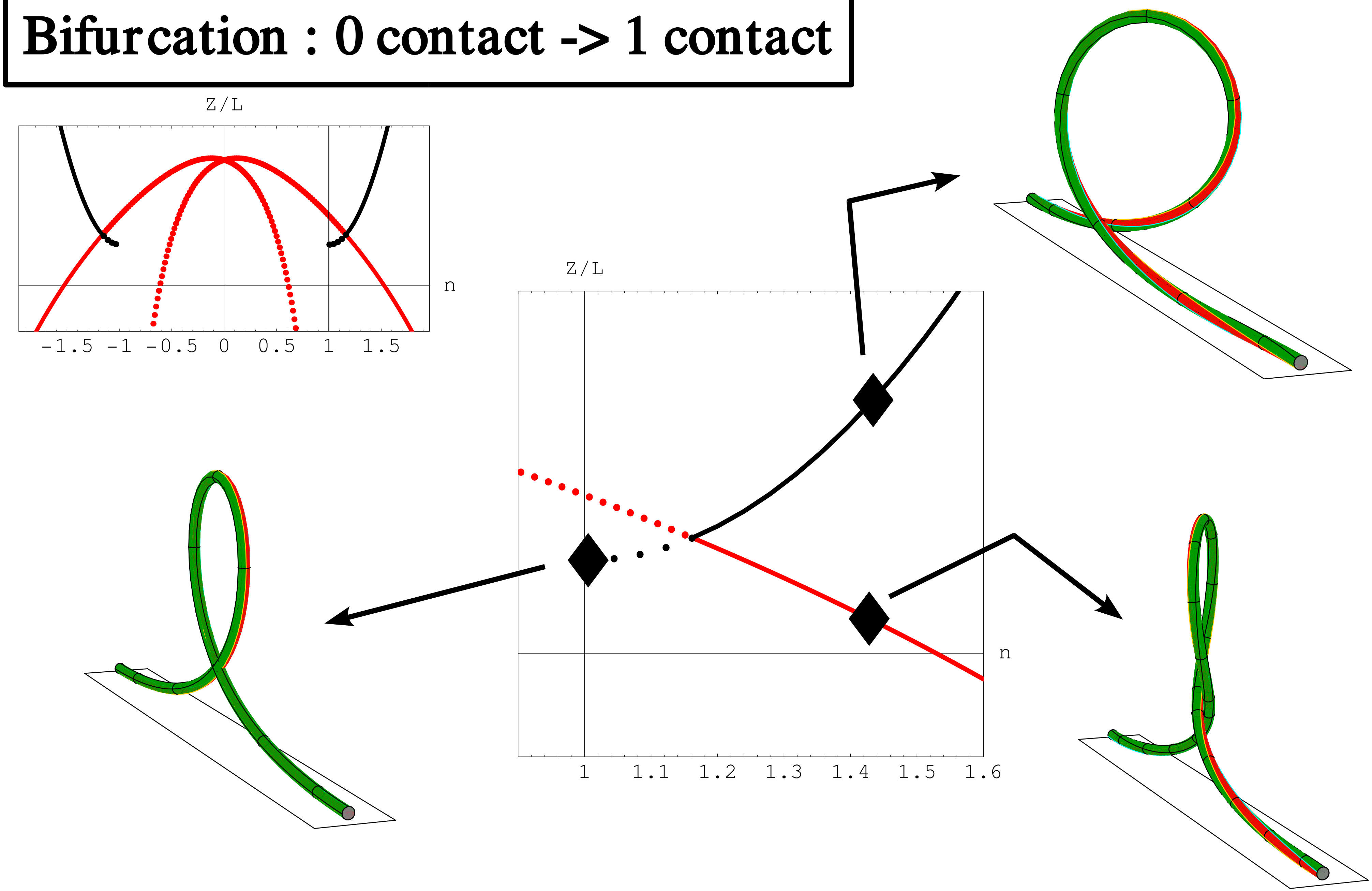
$$t = \frac{TL^2}{4\pi^2 K_0} = 6$$

1 contact(s)

$$\frac{Z}{L} = 0.72$$

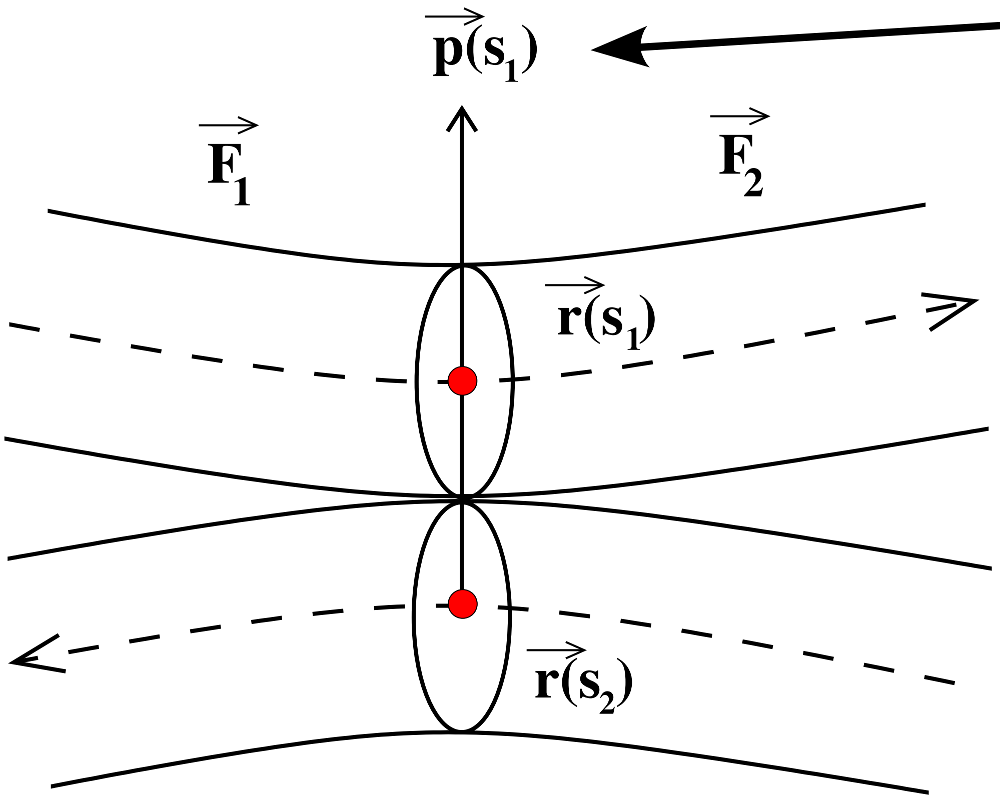
$n = 4.3$ turns

Bifurcation : 0 contact -> 1 contact



Hard-wall contact, no friction

force from strand at s_2 acting on strand at s_1



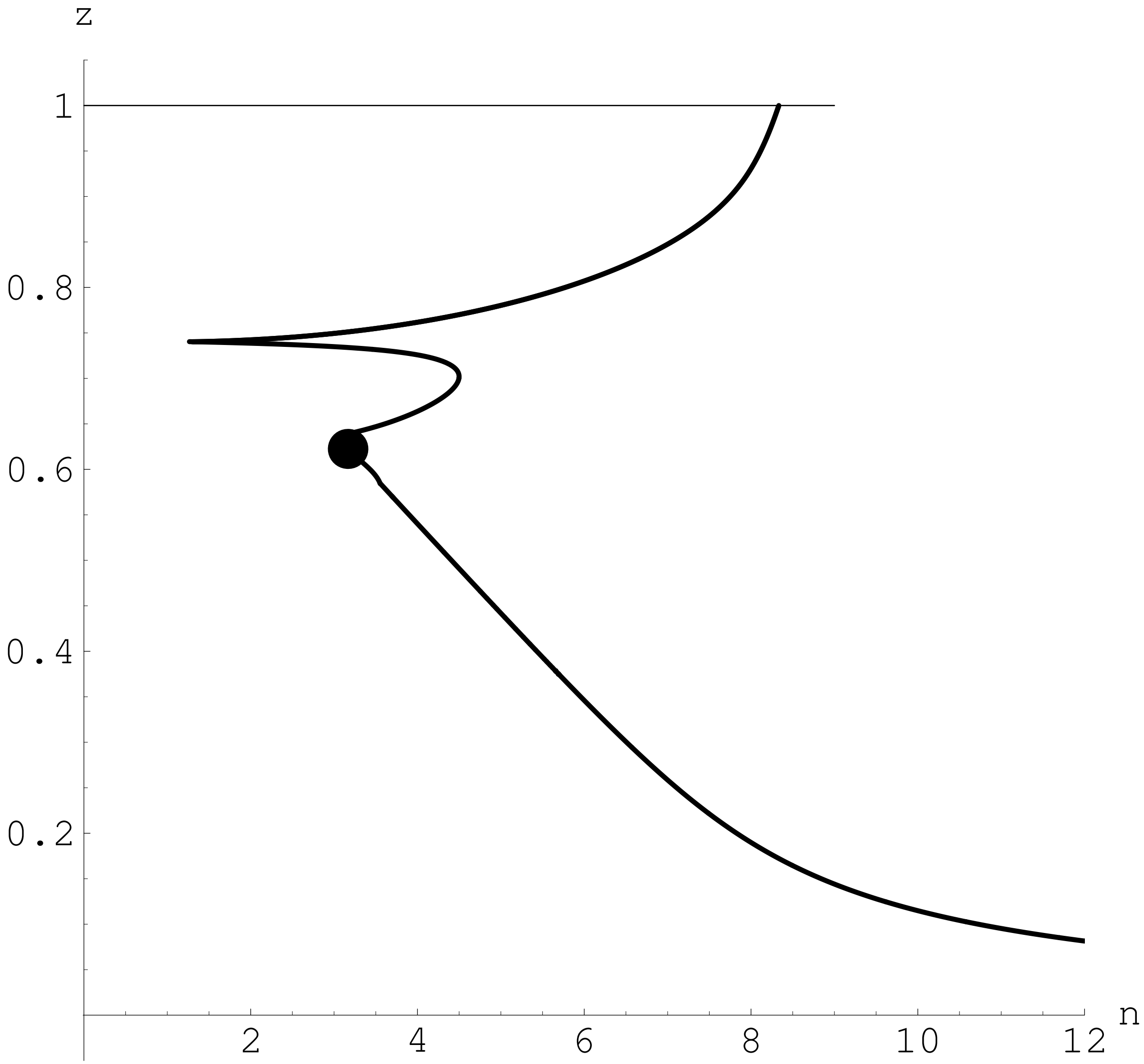
$$\vec{F}_1 = \vec{p} + \vec{F}_2$$

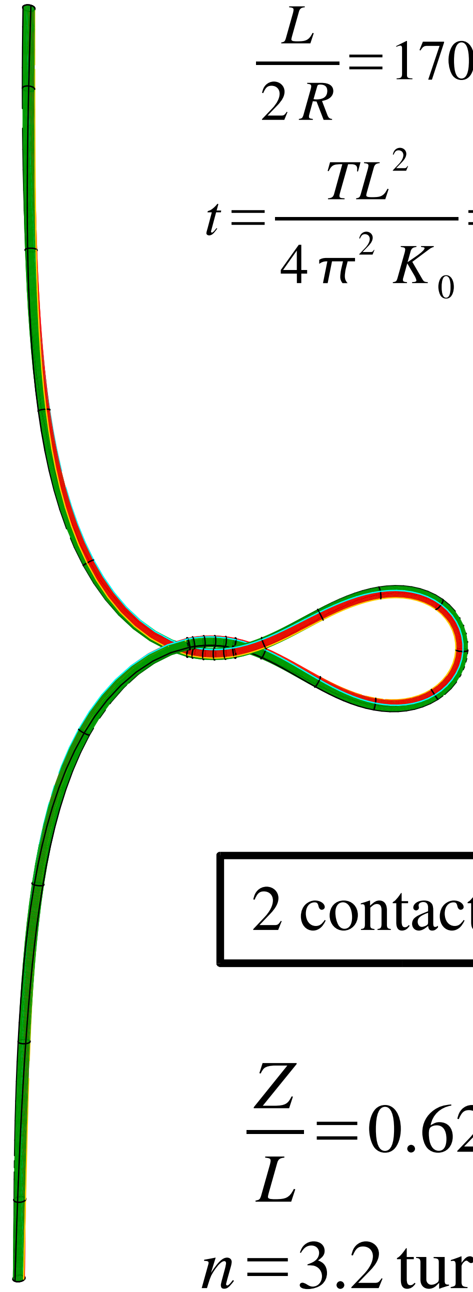
$$\vec{p} = p \frac{\vec{r}(s_1) - \vec{r}(s_2)}{|\vec{r}(s_1) - \vec{r}(s_2)|}$$

touching conditions :

$$\begin{cases} |\vec{r}(s_1) - \vec{r}(s_2)| = \text{thickness} \\ (\vec{r}(s_1) - \vec{r}(s_2)) \perp \vec{d}_3(s_1) \\ (\vec{r}(s_1) - \vec{r}(s_2)) \perp \vec{d}_3(s_2) \end{cases}$$

Results : how a twisted rod coils





$$\frac{L}{2R} = 170$$

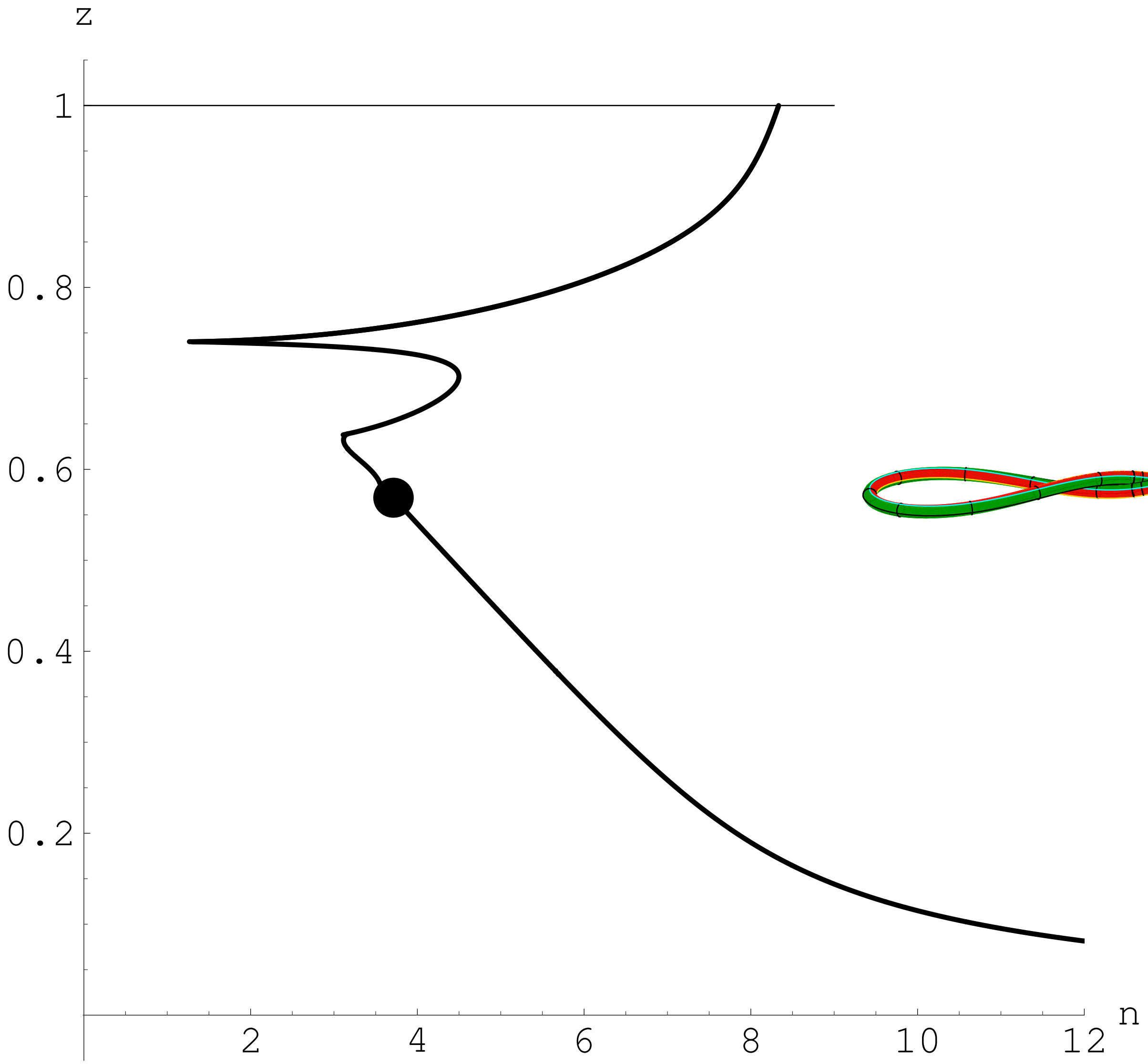
$$t = \frac{TL^2}{4\pi^2 K_0} = 6$$

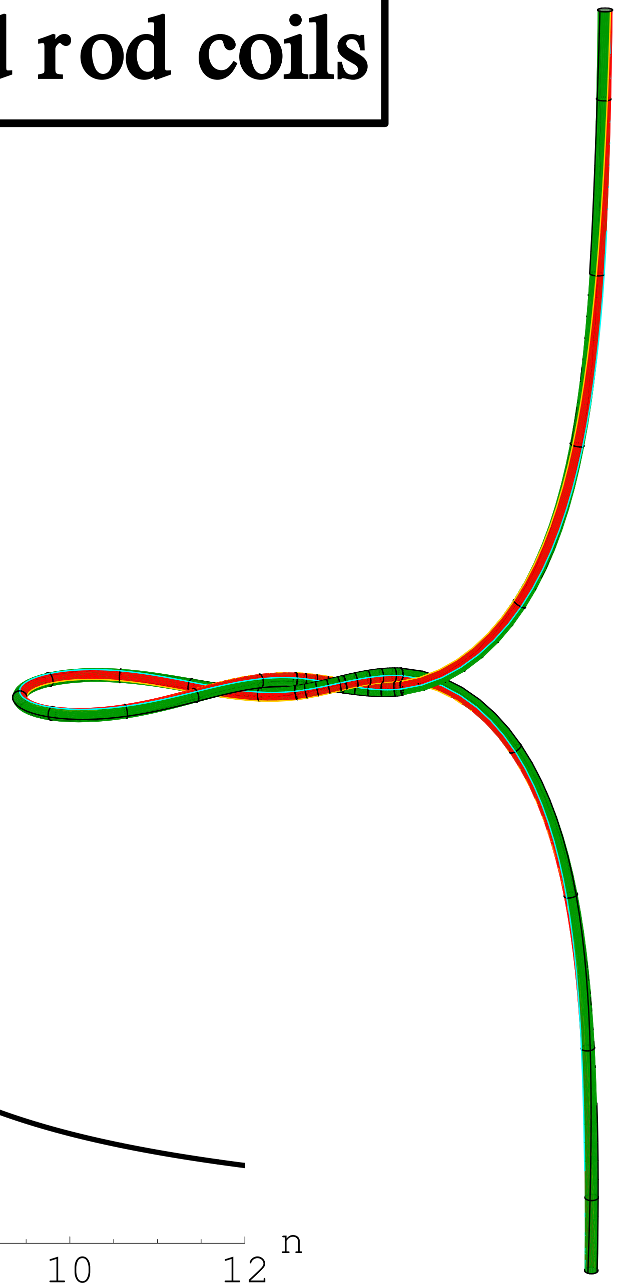
2 contact(s)

$$\frac{Z}{L} = 0.62$$

$n = 3.2$ turns

Results : how a twisted rod coils





$$\frac{L}{2R} = 170$$

$$t = \frac{TL^2}{4\pi^2 K_0} = 6$$

3 contact(s)

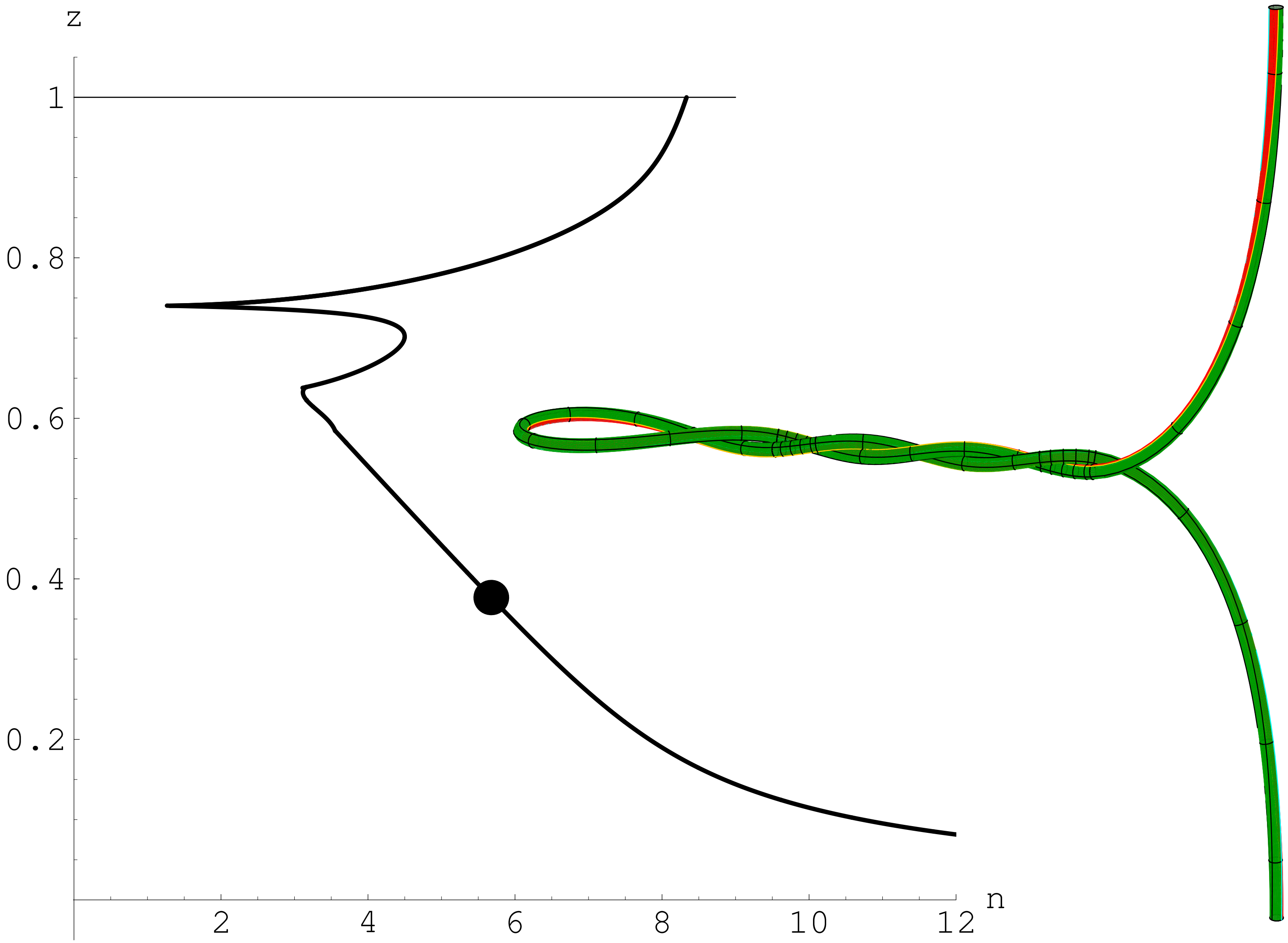
$$\frac{Z}{L} = 0.57$$

$n = 3.7$ turns

Results : how a twisted rod coils

$$\frac{L}{2R} = 170$$

$$t = \frac{TL^2}{4\pi^2 K_0} = 6$$

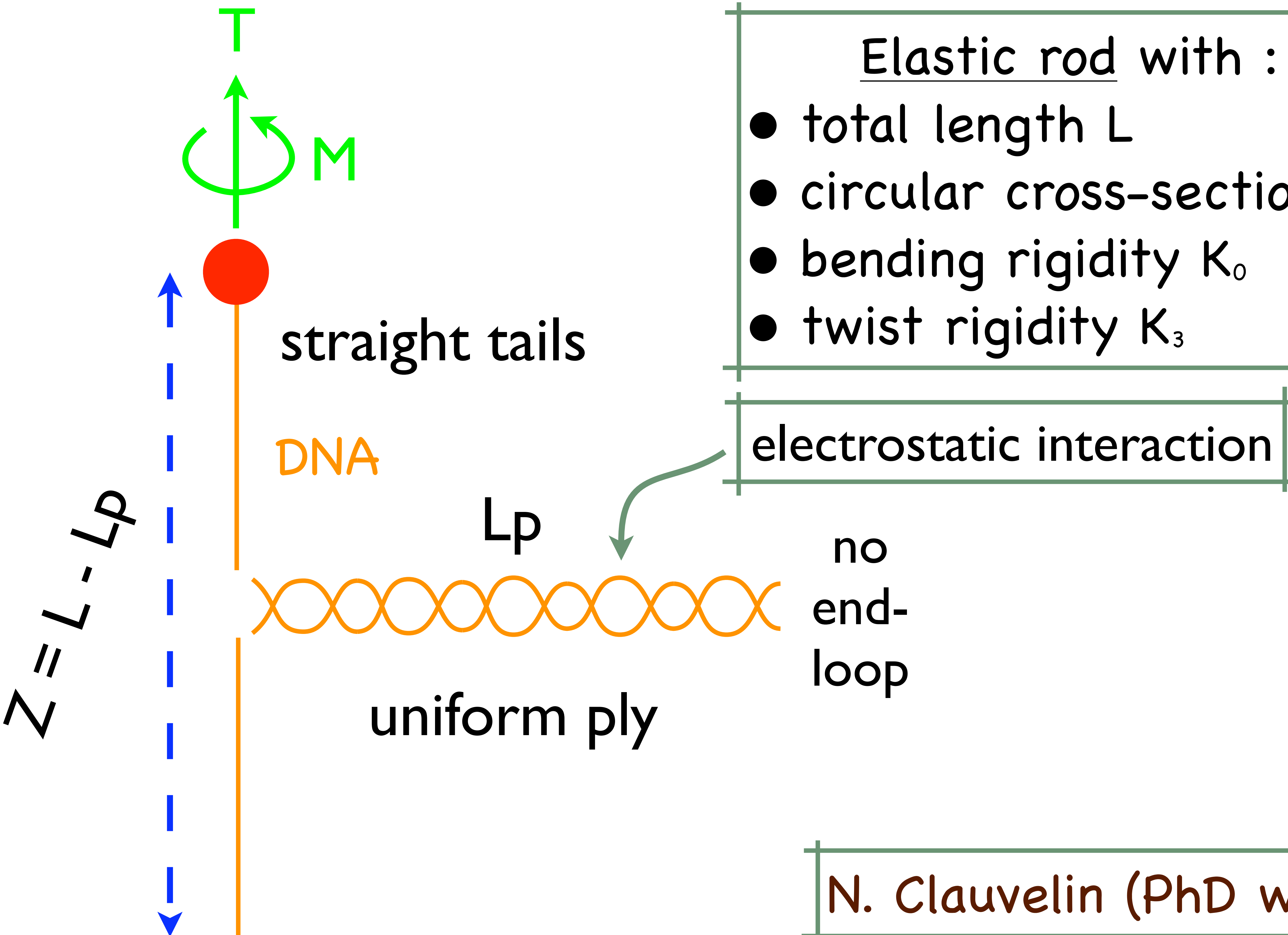


1L1 contact(s)

$$\frac{Z}{L} = 0.38$$

$n = 5.7$ turns

Analytical model for plectonemic DNA



Elastic rod with :

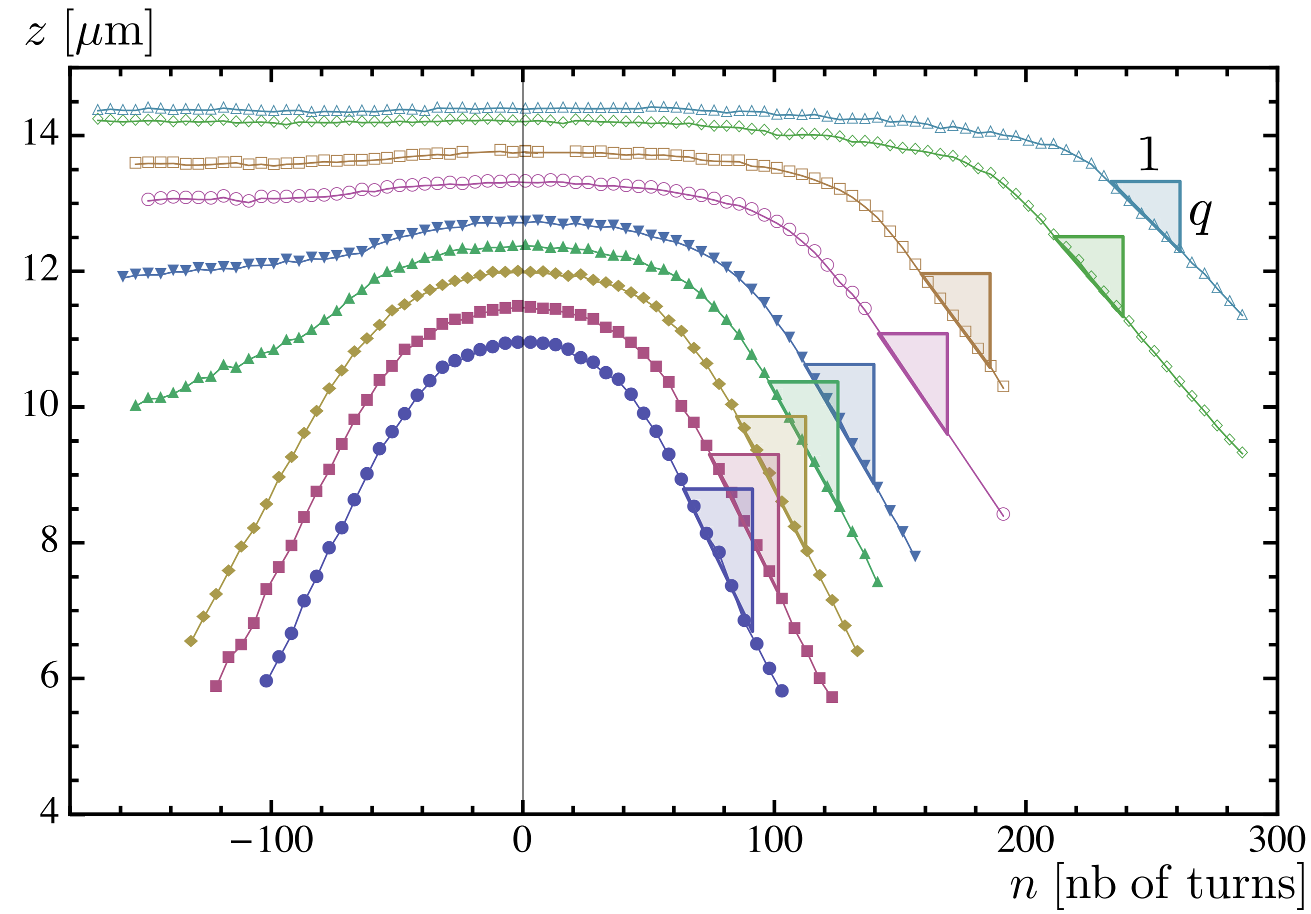
- total length L
- circular cross-section R_0
- bending rigidity K_0
- twist rigidity K_3

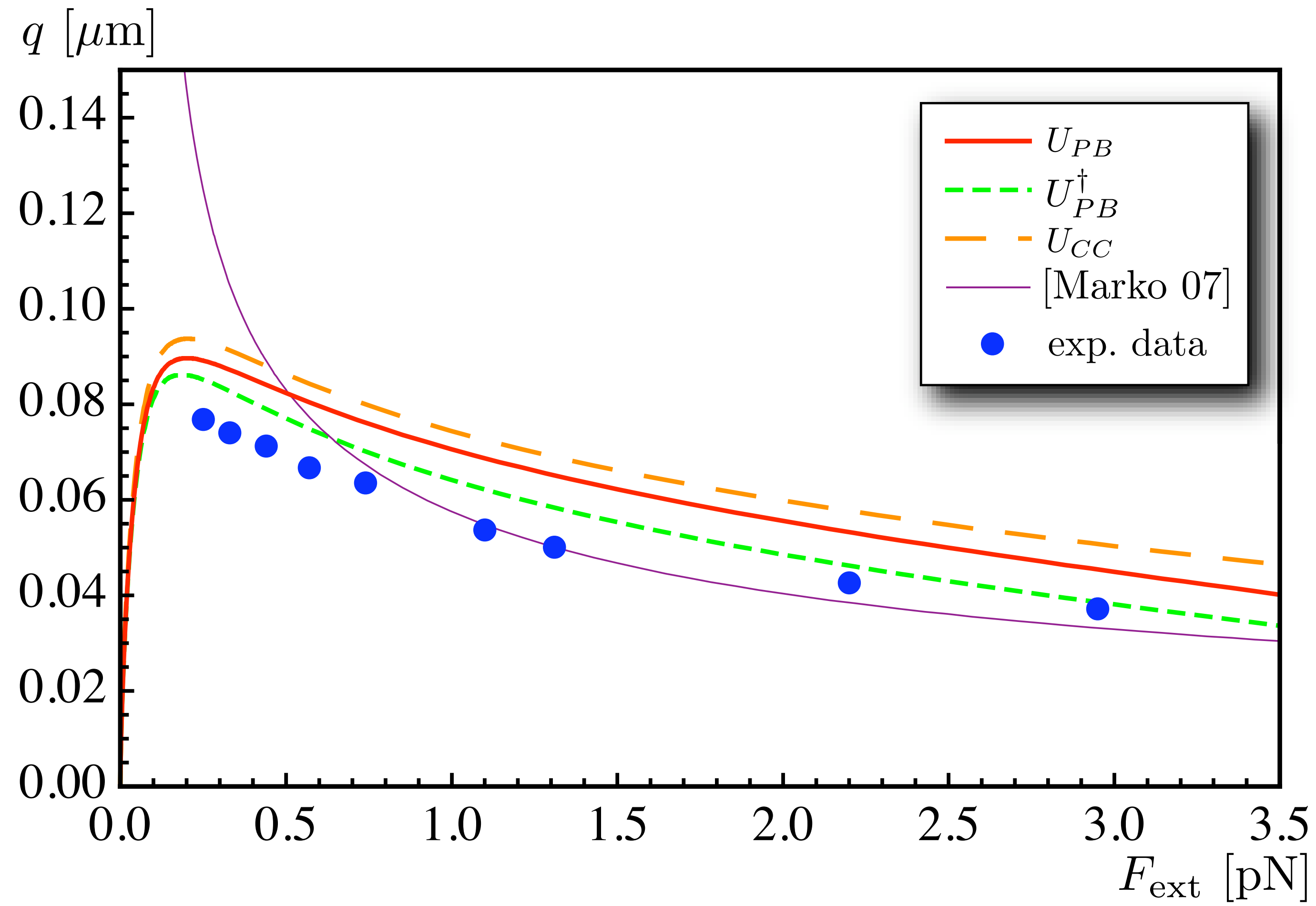
N. Clauvelin (PhD work)

Results

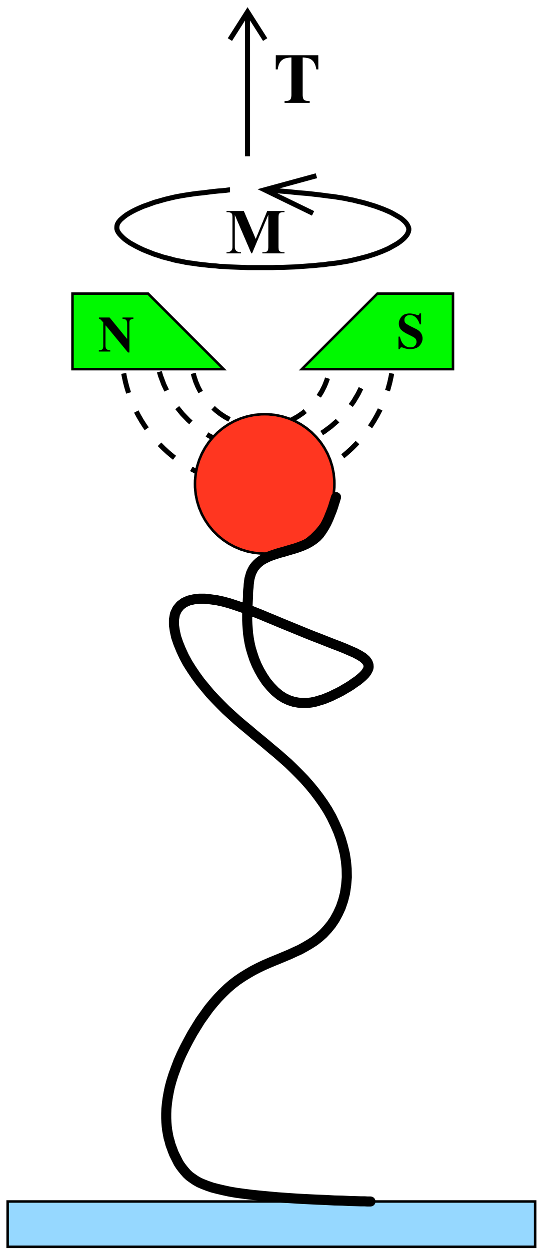
data from V. Croquette (LPS-ENS)

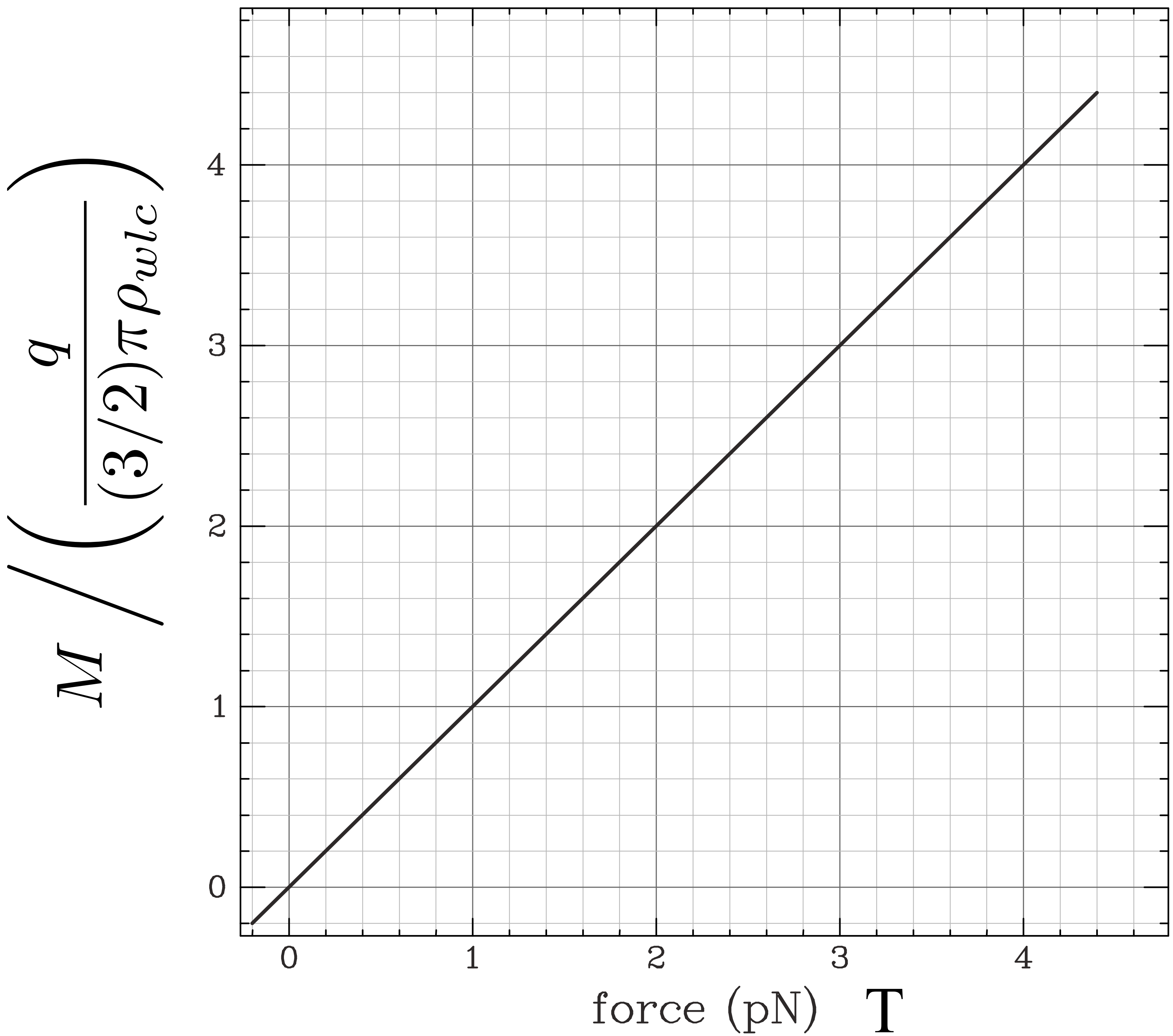
DNA lambda phage 48kbp
phosphate buffer 10 mM





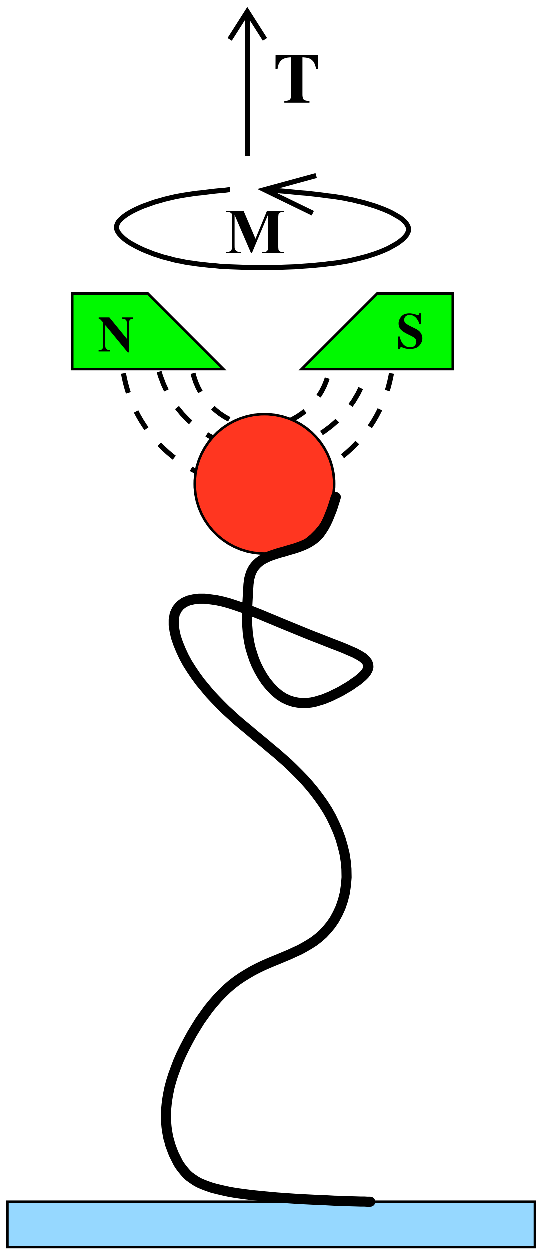
Torque prediction

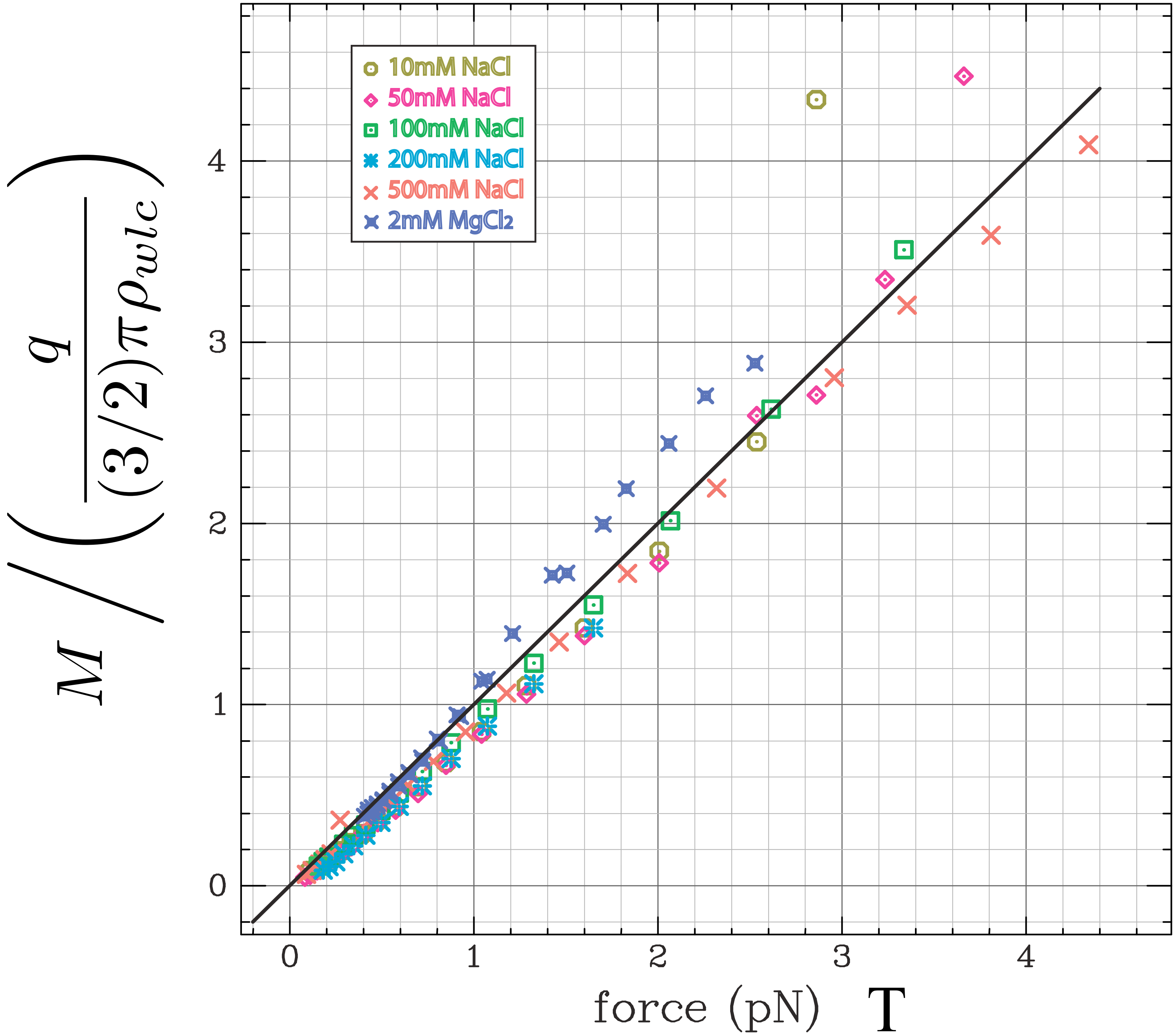




$$M = \frac{q}{(3/2)\pi\rho_{wlc}} T$$

Torque prediction





$$M = \frac{q}{(3/2)\pi\rho_{wlc}} T$$

data from F. Mosconi (LPS-ENS)

Conclusion

molécule d'ADN $\approx$ tige élastique

Perspective

simulations numériques avec potentiel électrostatique

=> système intégro-différentiel