Élasticité des biofilaments

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collaborations :

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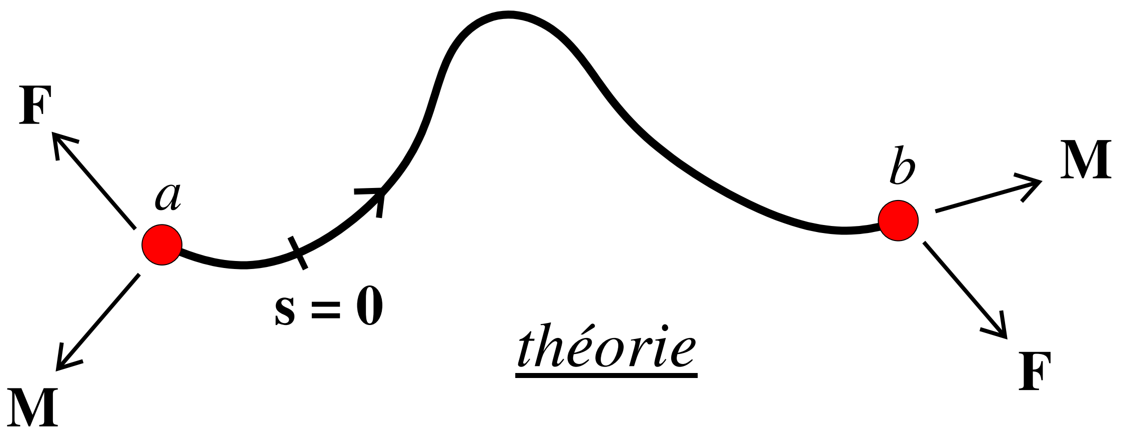
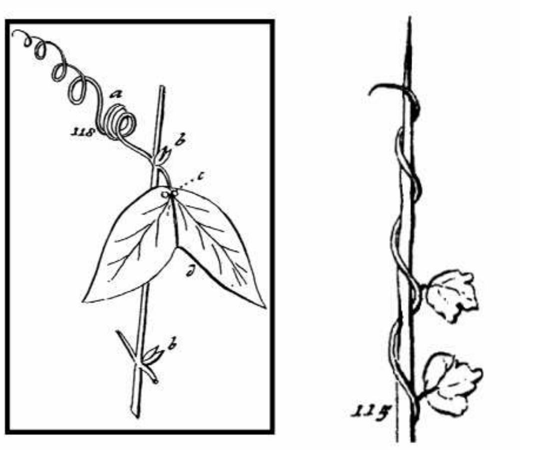
- Alain Goriely (Math. Univ. Arizona)

Quelques exemples

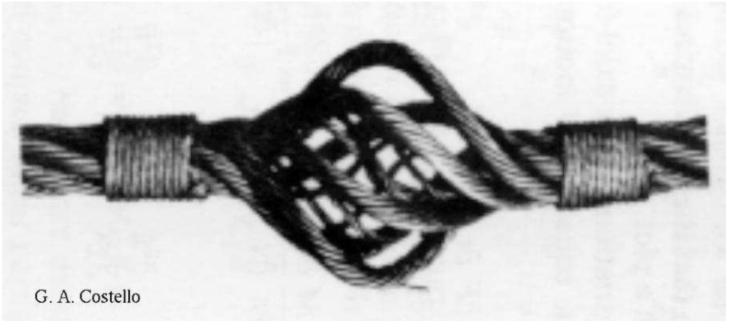


théorie

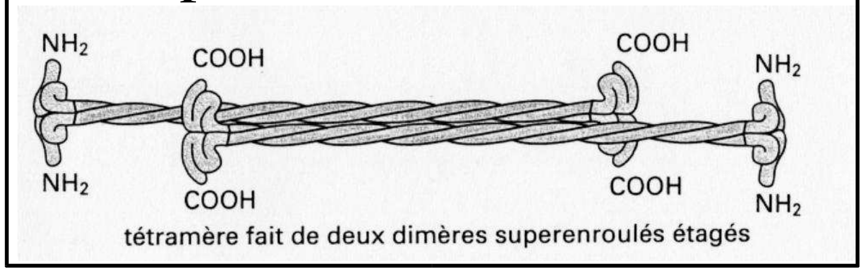
plantes grimpantes



câbles


G. A. Costello

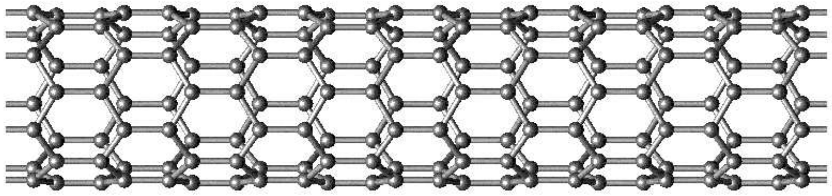
protéines fibreuses



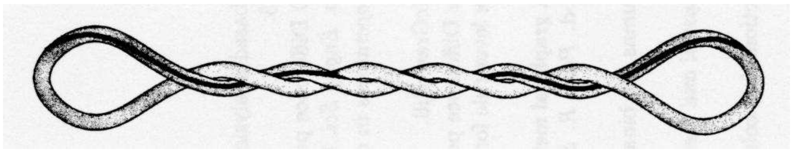
tétramère fait de deux dimères superenroulés étagés

applications

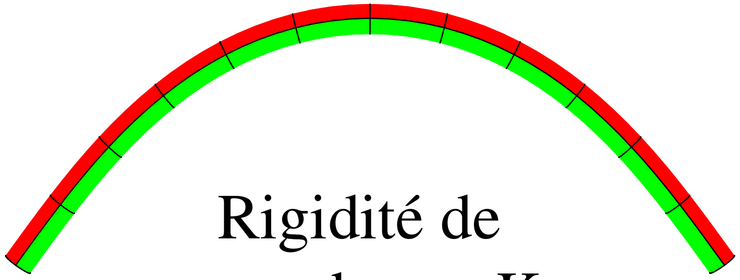
nanotubes de carbone



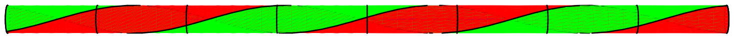
sur-enroulement de l'ADN



Loi de comportement élastique



Rigidité de courbure : K_0



Rigidité de torsion : K_3

Energie déformation élastique

$$V = \frac{1}{2} \int_0^L \left[K_0 \, \kappa^2(s) + K_3 \, \tau^2(s) \right] ds$$

$K_0 = E\, I$

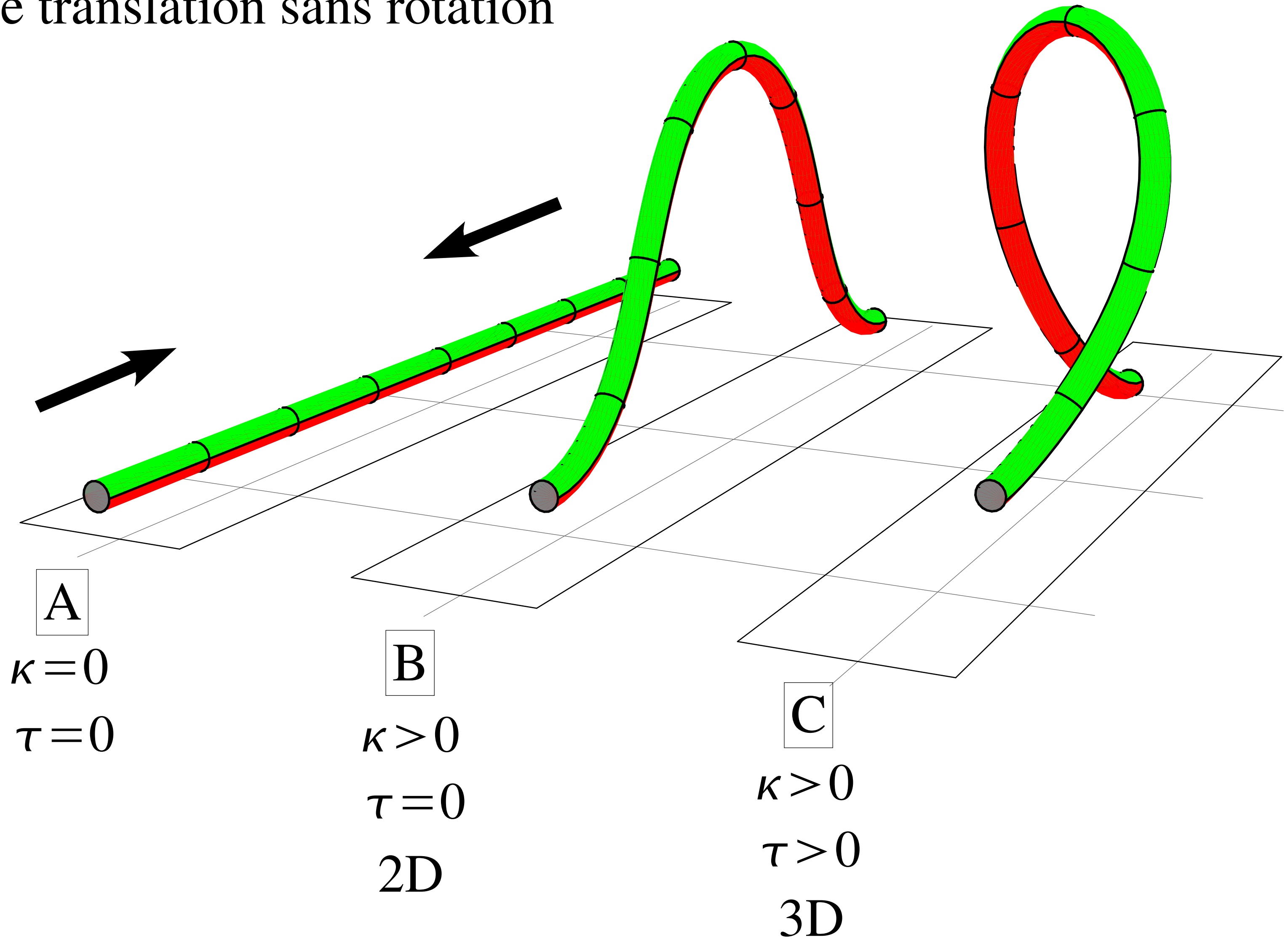
I : moment d'inertie section

E : module de Young

filament	E
Microtubule	1 GPa
ADN	1 GPa
Actine	2 GPa
Collagène	2 GPa
Caoutchouc	2 GPa
Acier	200 GPa

Courbure et torsion sont liées

Expérience de translation sans rotation



A

$\kappa = 0$

$\tau = 0$

B

$\kappa > 0$

$\tau = 0$

2D

C

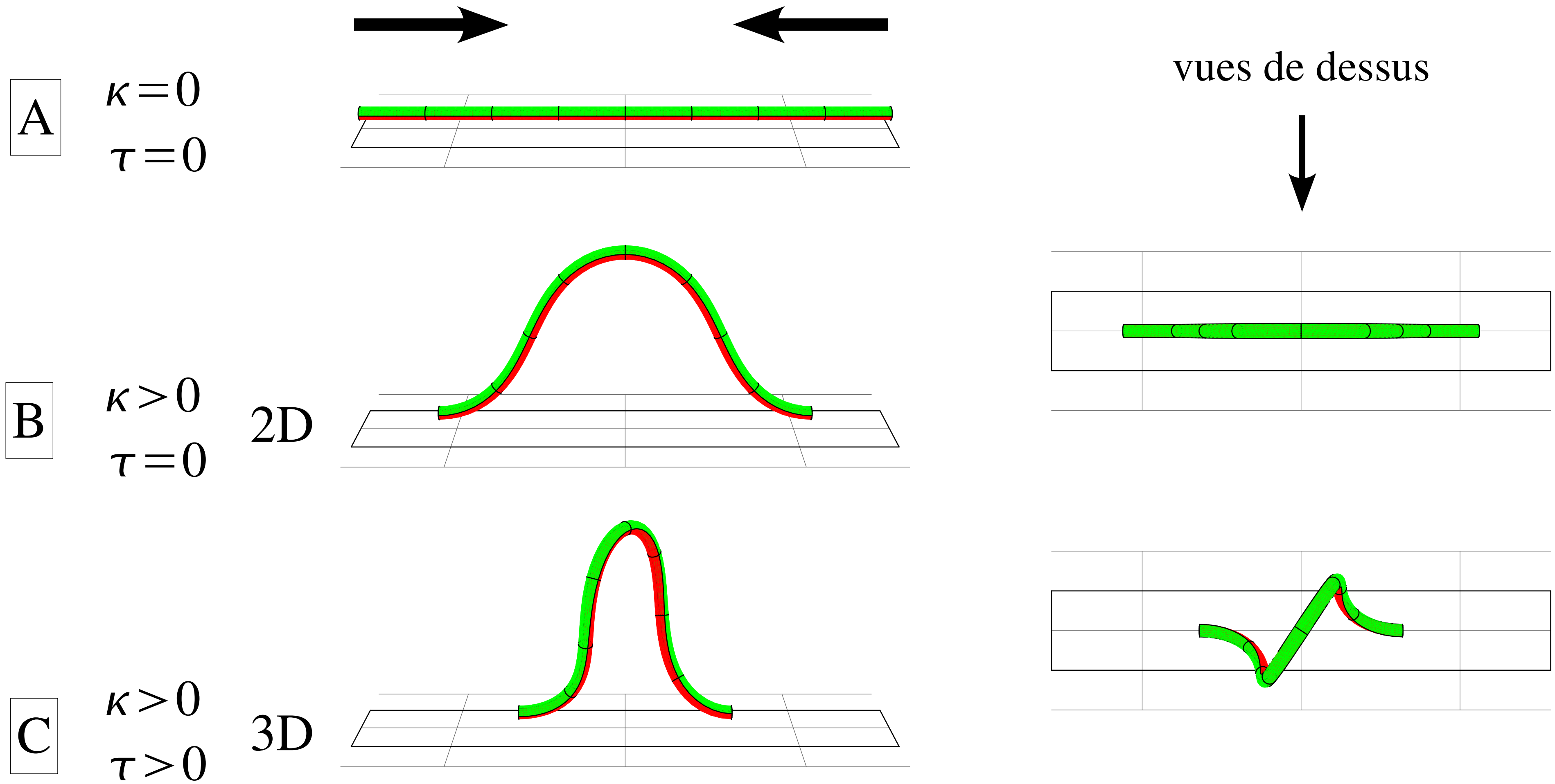
$\kappa > 0$

$\tau > 0$

3D

Courbure et torsion sont liées

Expérience de translation sans rotation



vues de dessus

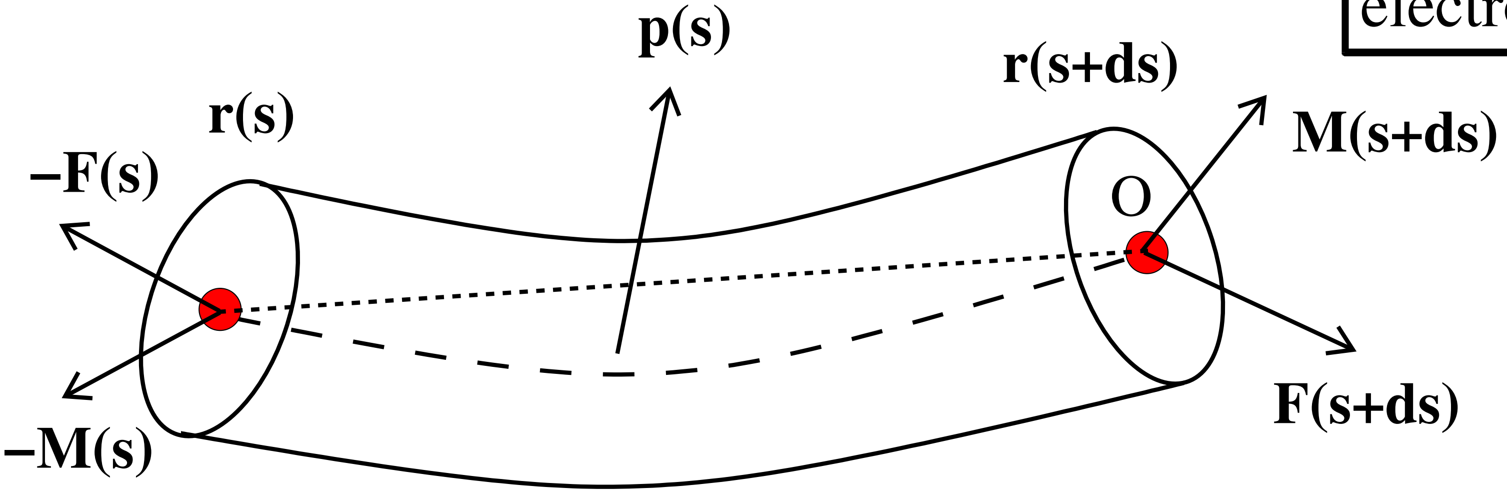
A $\kappa=0$ $\tau=0$

B $\kappa>0$ $\tau=0$ 2D

C $\kappa>0$ $\tau>0$ 3D

Équilibre mécanique d'une tige

p(s) = force externe :
pesanteur, contact,
electrostatique, ...



eq. forces $p(s)\delta s+F(s+\delta s)-F(s)=0$

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

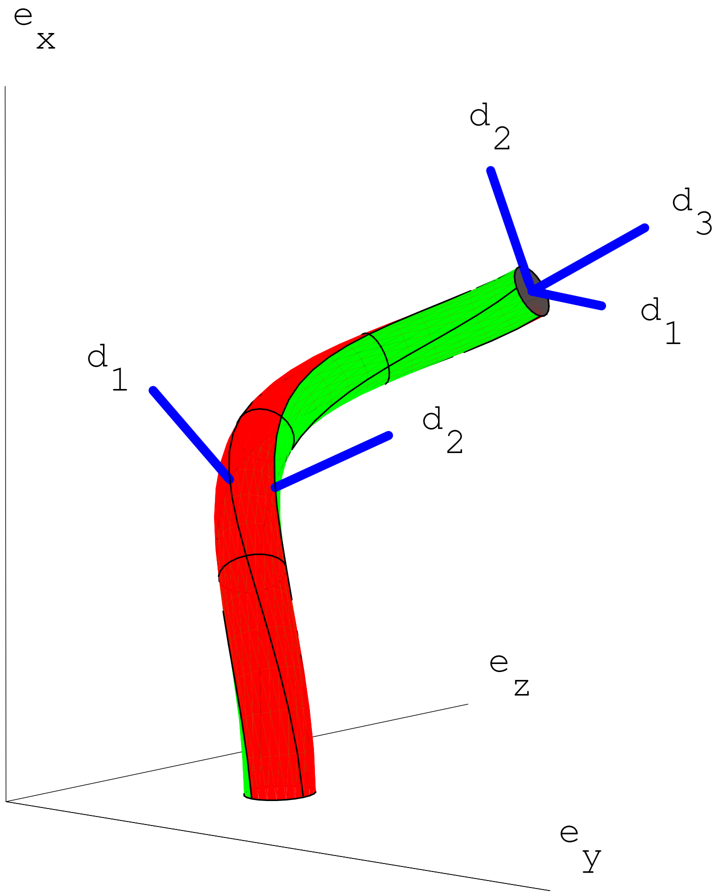
eq. moments $M(s+\delta s)-M(s)+\Pi_O[F(s+\delta s)]+\Pi_O[-F(s)]=0$

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

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

Structure mince : modèle de Cosserat

directeurs orthonormés $\vec{d}_1, \vec{d}_2, \vec{d}_3$ en plus de $\vec{r}(s)$



pas cisaillement
pas d'extension

$$\left.\begin{array}{l}\text{pas cisaillement}\\ \text{pas d'extension}\end{array}\right\} \vec{r}\,'(s)=\vec{d}_3(s)$$

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

évolution 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 : courbures et u_3 : twist

Équations de Kirchhoff

21 équations diff.
variable indép. : s

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

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

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

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

$$m_i=K_i u_i$$

élasticité linéaire

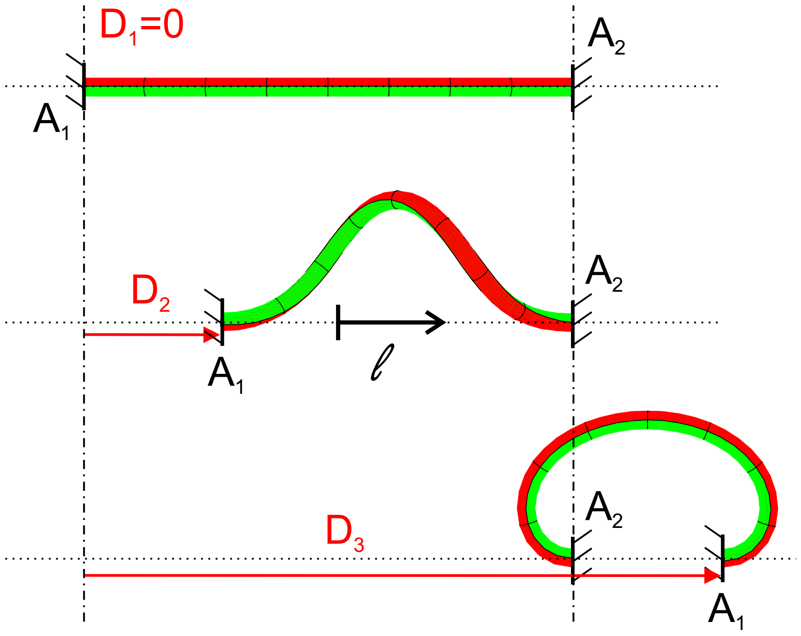
21 inconnues

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

$i=1,2,3$

Conditions de bords

- Façon dont on tient la tige
- Seulement certaines solutions sont acceptables

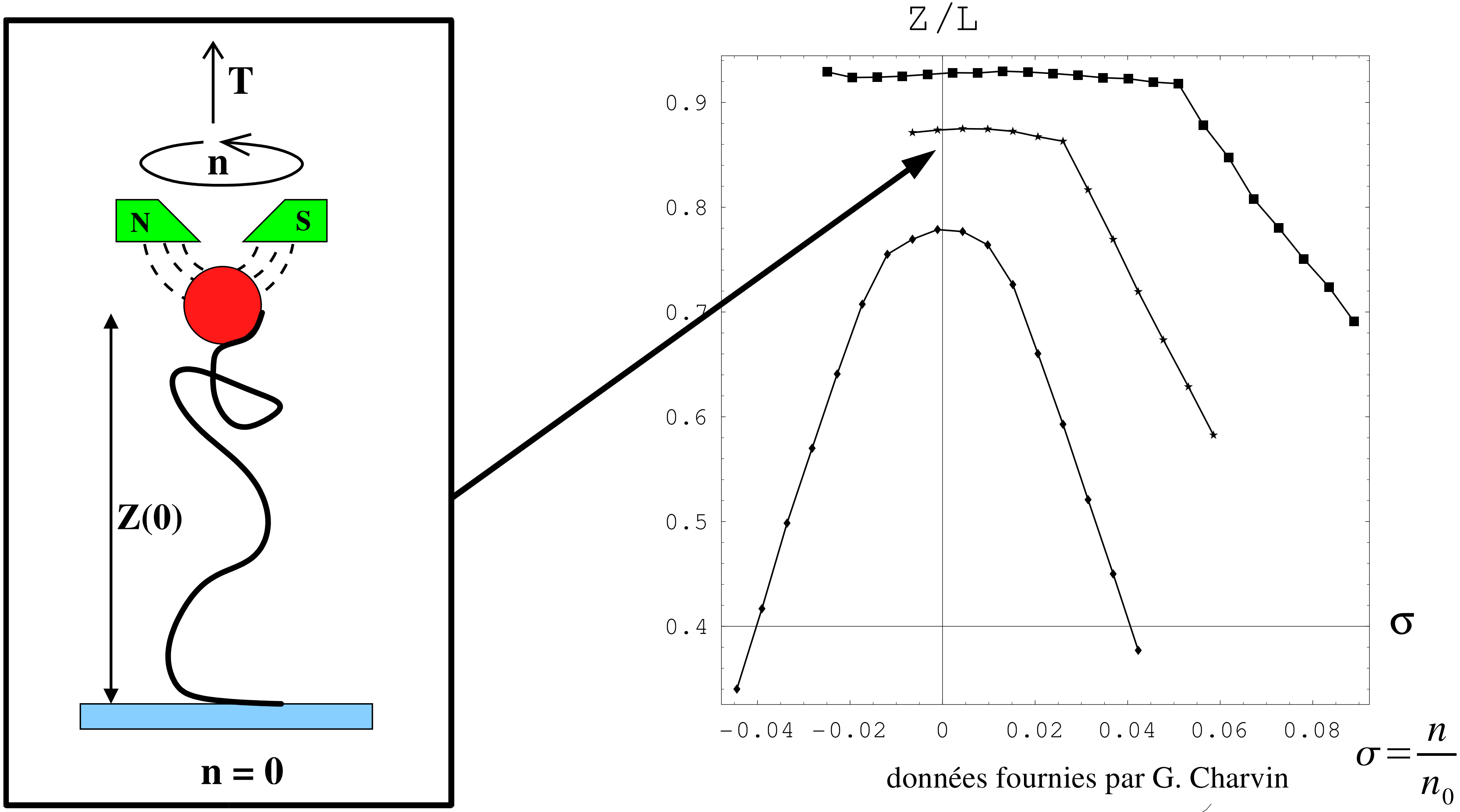


$$\vec{d}_3(A_1)=\vec{d}_3(A_2)$$

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

$$(D=L-k)$$

Étirement d'ADN sous contrainte de torsion



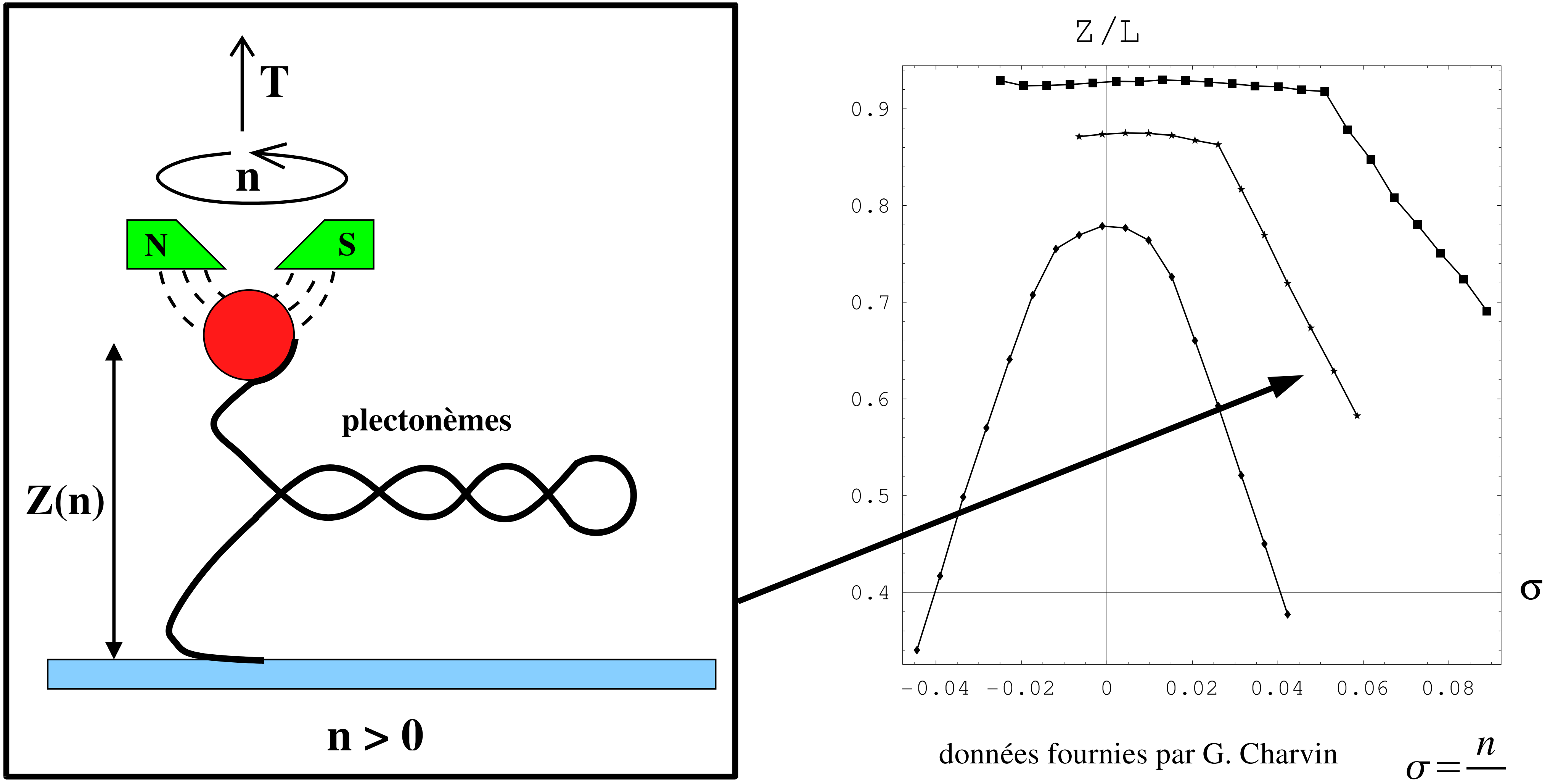
$\sigma = \dfrac{n}{n_0}$

données fournies par G. Charvin

autres équipes : C. Bustamante, L. Finzi, J.-L. Viovy (Bancaud)

équipe : V. Croquette - D.Bensimon

Étirement d'ADN sous contrainte de torsion



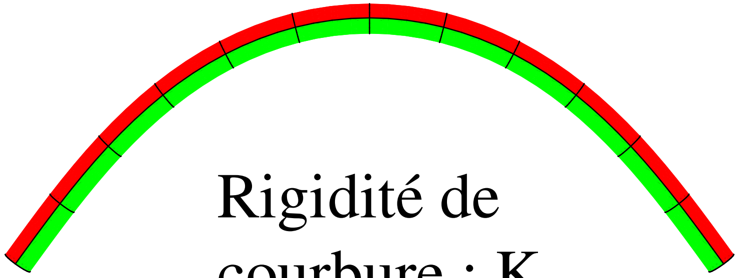
données fournies par G. Charvin

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

Modélisation : tige élastique avec contact

- Elasticité des structures minces
- Equations de Kirchhoff
- Problème avec conditions de bords
- Méthode du tir
- Méthode de relaxation

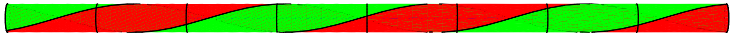
  (différences finies ou éléments finis)
- Méthode de cheminement numérique
- Contact : type sphères dures (condition de contact unilatéral de Signorini)
- Problème raide (points de selle)



Rigidité de courbure : K_0

K_0 : moyenne petit/grand sillon

[Maddocks+Kehrbaum 2000]



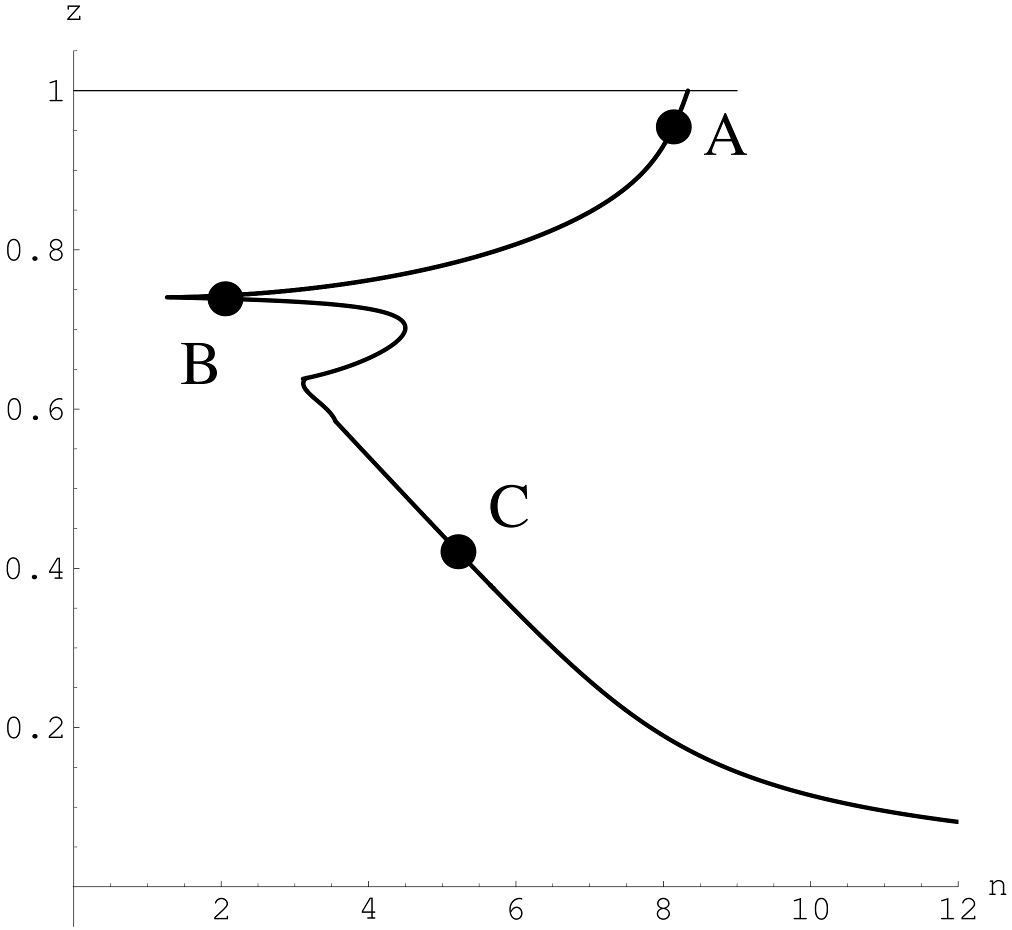
Rigidité de torsion : K_3

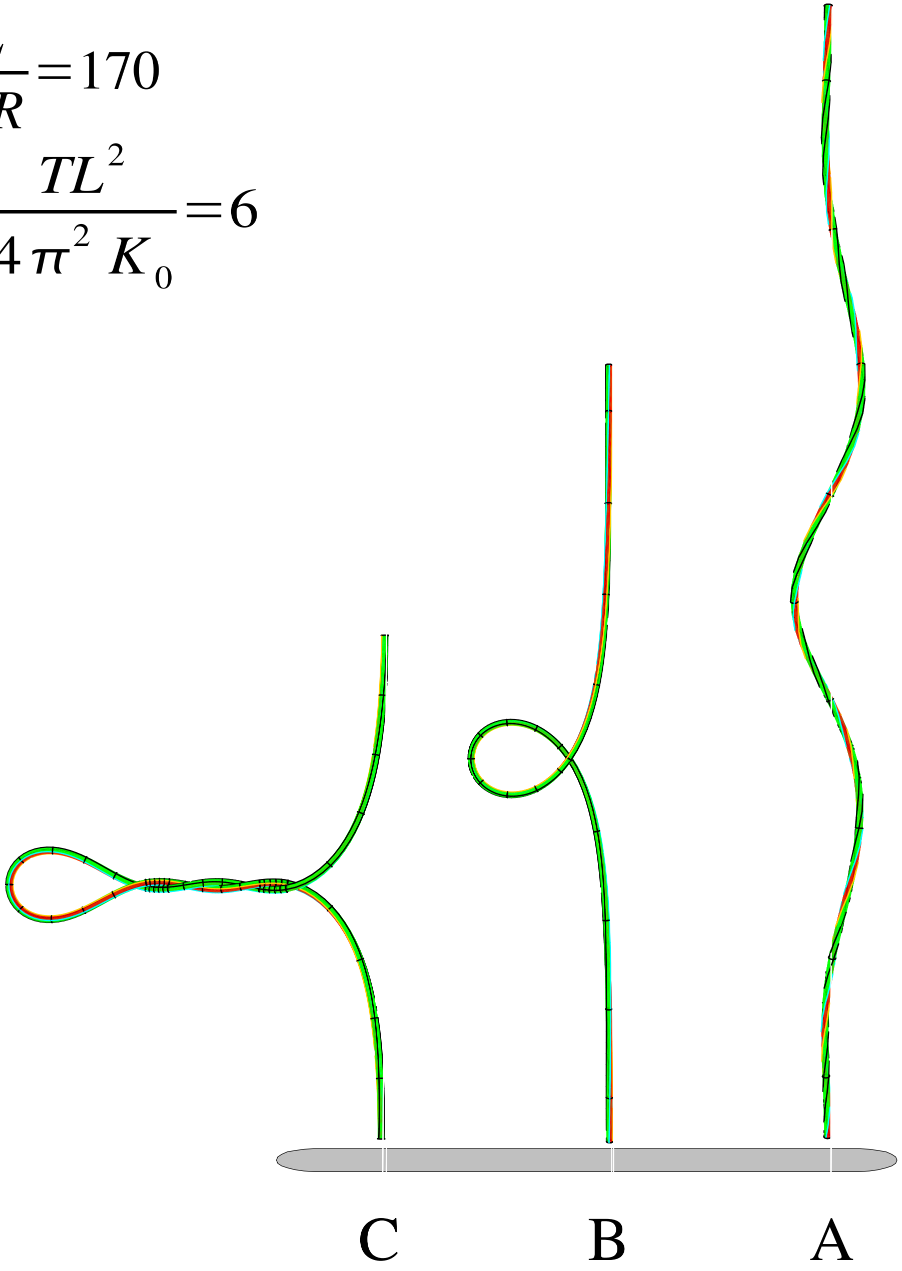
$$V=\frac{1}{2}\int_0^L \left[K_0\,\kappa^2(s)+K_3\,\tau^2(s)\right]ds$$

Numerical simulations

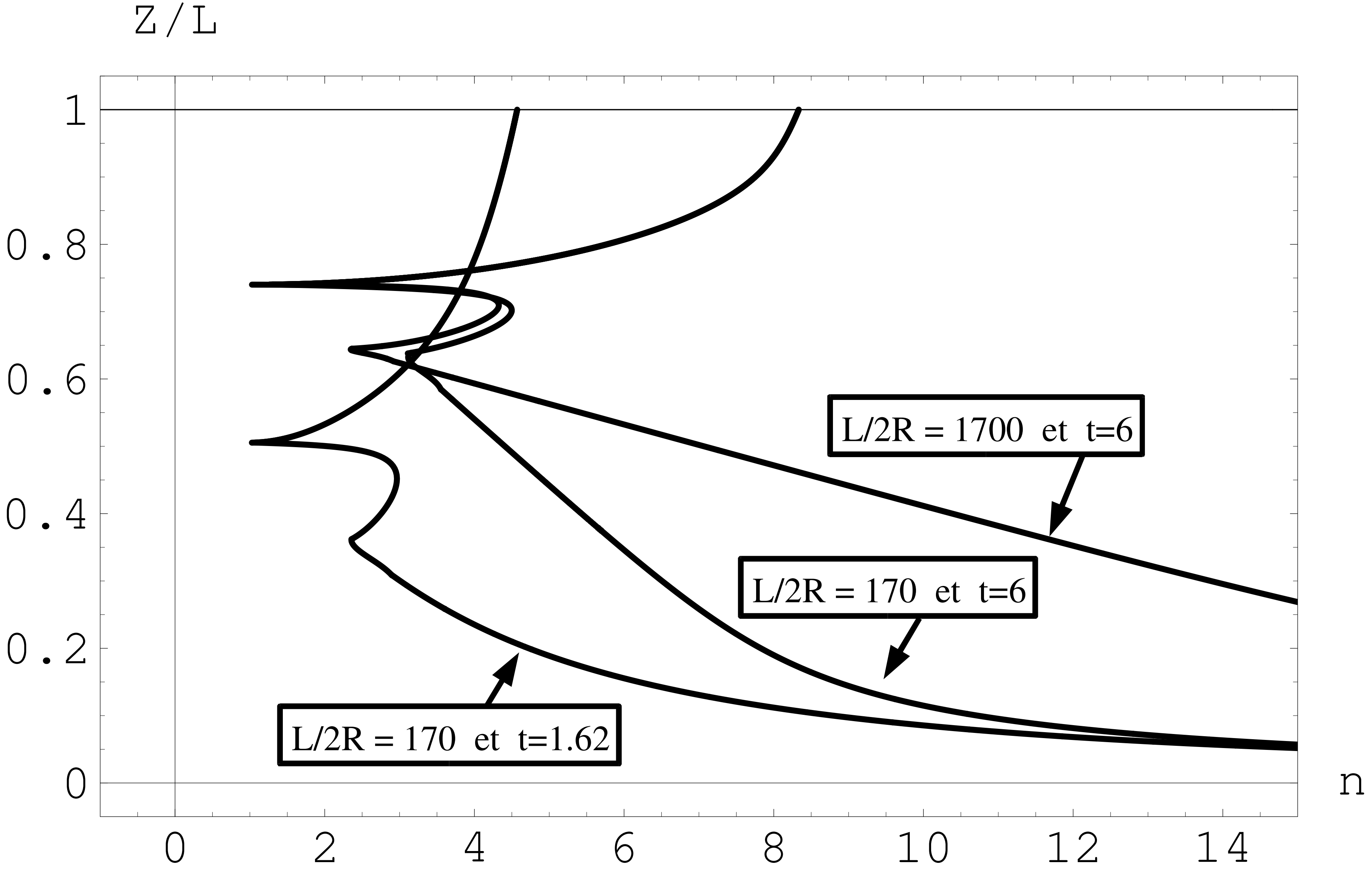
slenderness ratio: $\frac{L}{2R} = 170$

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





Variation de la pente en fonction de *t* et de *L*/*R*



Équilibre mécanique : formules approchées

$$\theta \simeq 0.88\left(\frac{R^2 T}{K_0}\right)^{1/4}$$

angle de la super hélice

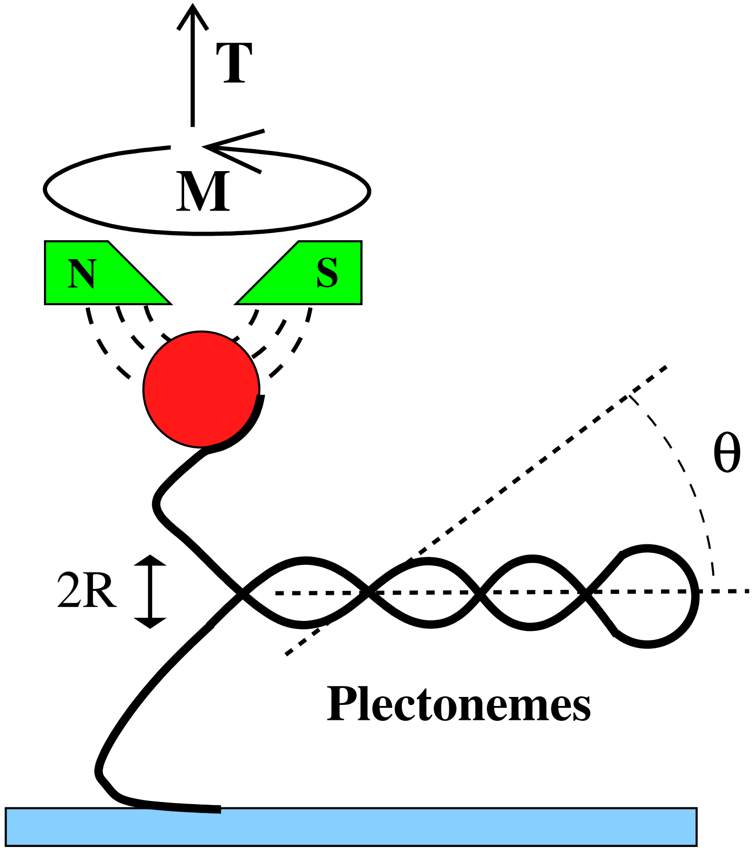
$$p=\frac{K_0}{R^3}\,\frac{\sin^4\theta}{\cos 2\theta}$$

pression de contact

$$M=\frac{K_0}{2R}\left(\tan 2\theta-\sin 2\theta\right)$$

couple de torsion

$$Tw=\frac{L}{2\pi}\,\frac{M}{K_3}$$



Géométrie :
vrillage des
plectonèmes :

$$Wr\simeq\frac{L_{Plecto}}{4\pi R}\sin 2\theta$$

Calugareano, White, Fuller ($Lk = Tw + Wr$)

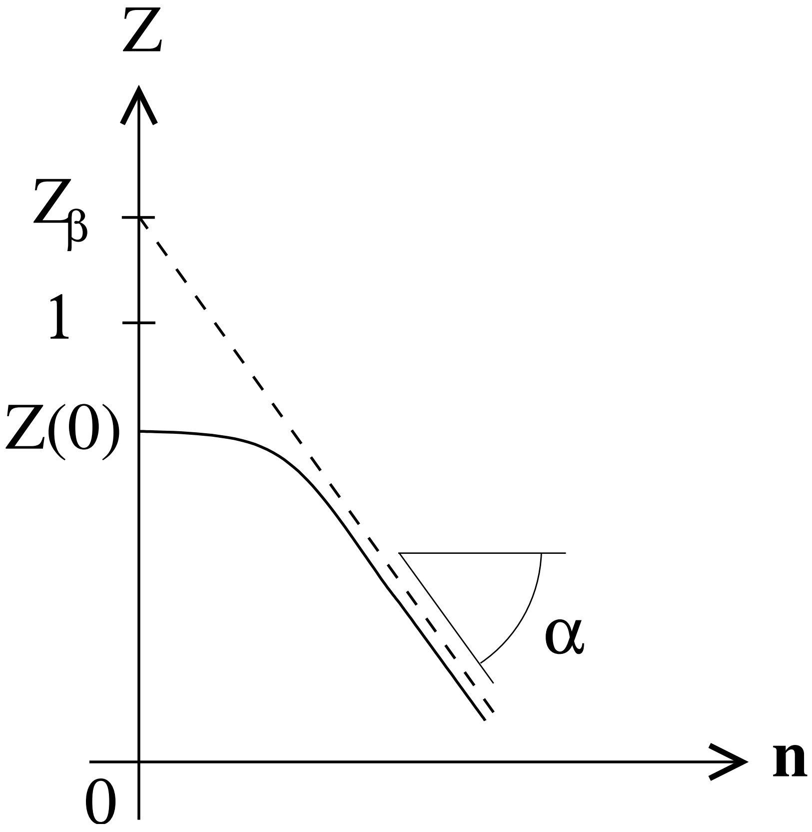
$$Lk=\frac{L}{4\pi R}\left\{\frac{K_0}{K_3}\left(\tan 2\theta-\sin 2\theta\right)+\sin 2\theta\left(1-\frac{Z}{Z(0)}\right)\right\}$$

Équation approchée pour la partie linéaire

$$Z = \underbrace{Z(0)\left\{1+\frac{K_0}{K_3}\left(\frac{1}{\cos 2\theta}-1\right)\right\}}_{Z_\beta} - \underbrace{\frac{4\,\pi}{\sin 2\theta}\,\frac{R}{L}\,Z(0)}_{\alpha}\,n \qquad (n \equiv Lk)$$

$$\begin{cases} \theta \simeq 0.88\left(\dfrac{R^2 T}{K_0}\right)^{1/4} \\ \alpha = \dfrac{4\,\pi}{\sin 2\theta}\,\dfrac{R}{L}\,Z(0) \\ Z_\beta = Z(0)\left\{1+\dfrac{K_0}{K_3}\left(\dfrac{1}{\cos 2\theta}-1\right)\right\} \end{cases}$$

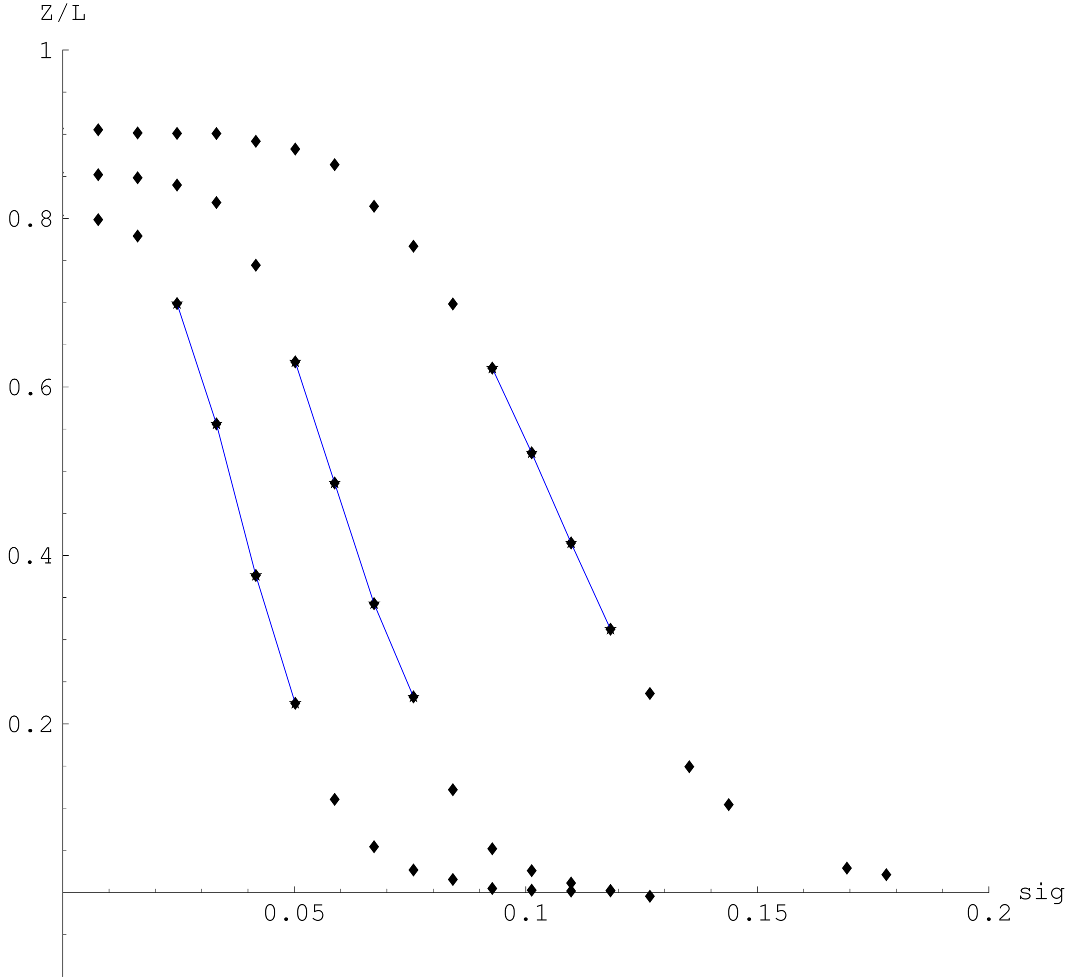
3 inconnues : (R , θ , K_0 / K_3)



Results

buffer solution = monovalent salt (PB) 10mM

molecule ~ 6kb



$$B = \frac{K_0}{k_B T} = 46 \ nm$$ (worm-like chain)

T (pn)	θ (rad)	R (nm)	C/B	P pN/µm
0,45	0,43	5,03	1,13	64
0,90	0,46	4,14	0,98	155
3,00	0,54	3,37	1,21	646

$$C = \frac{K_3}{k_B T} = 50 \pm 5 \ nm$$

data from Gilles Charvin (LPS-ENS)

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

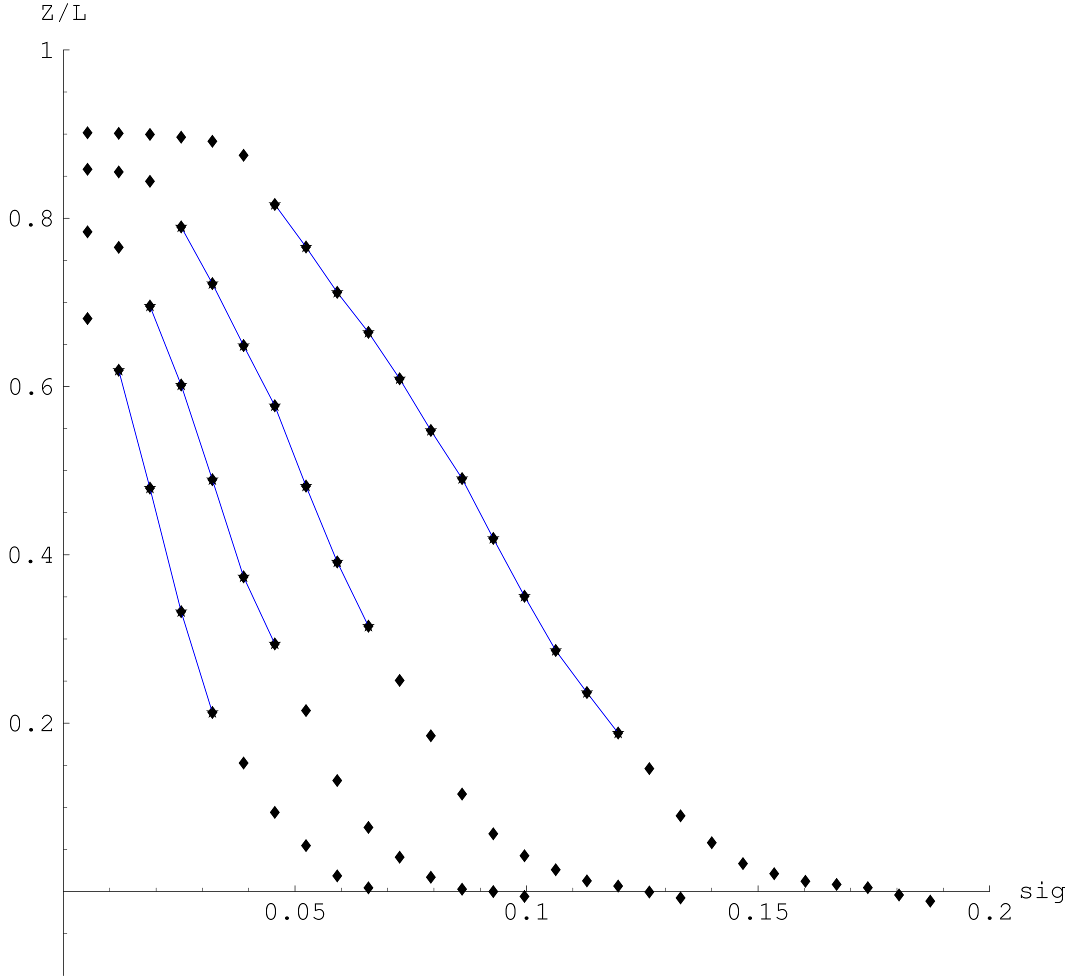
Results

buffer solution = monovalent salt (PB) 100mM

molecule ~ 6kb

$$B = \frac{K_0}{k_B T} = 49\ nm$$

(worm-like chain)



T (pn)	θ (rad)	R (nm)	C/B	P pN/µm
0,20	0,37	5,56	1,35	26
0,45	0,37	3,72	1,31	87
0,90	0,37	2,67	1,19	242
3,00	0,44	2,12	1,54	1 007

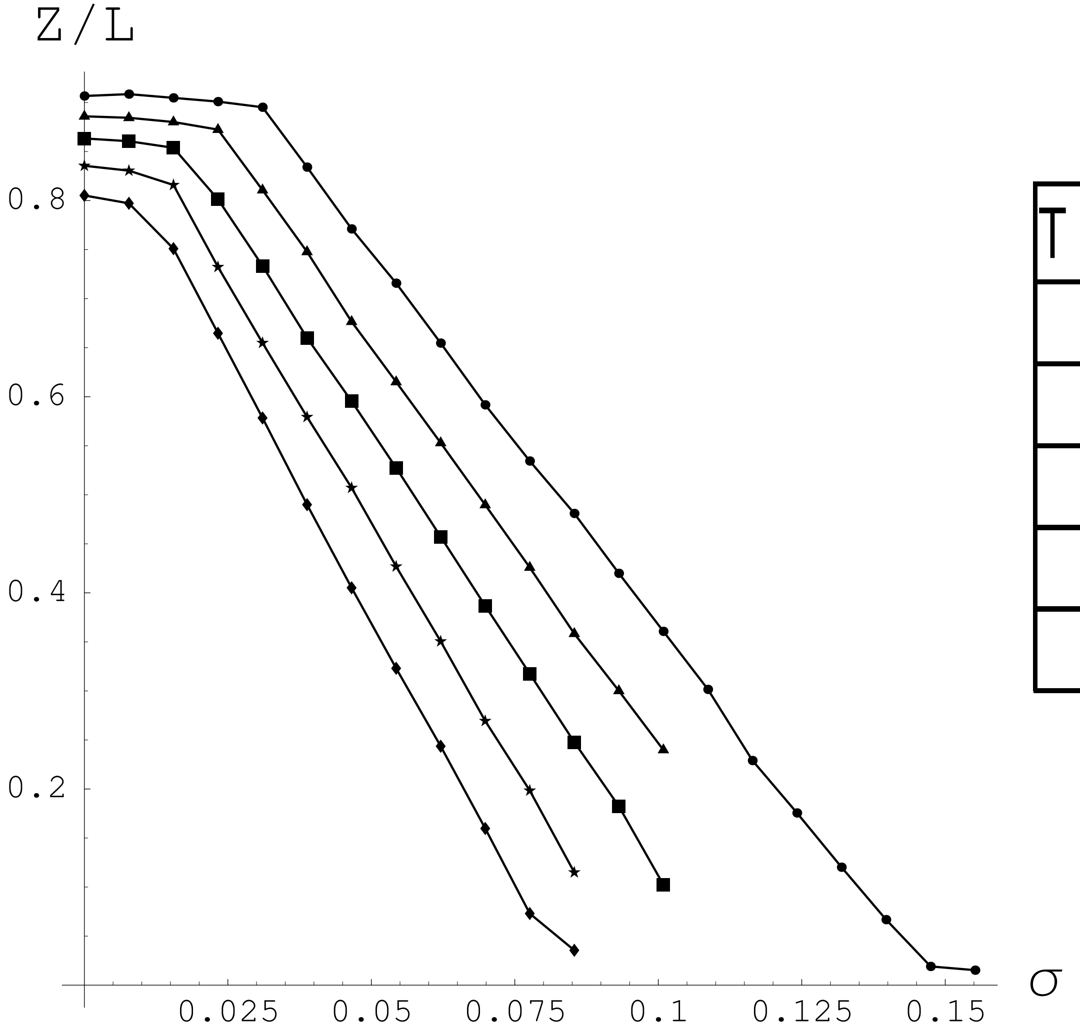
$$C = \frac{K_3}{k_B T} = 66 \pm 8\ nm$$

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

data from Gilles Charvin (LPS-ENS)

Results

buffer solution = monovalent salt (NaCl) 500mM



data from par R. Fulconis (Institut Curie)

molecule ~ 9kb

$$B = \frac{K_0}{k_B T} = 40\ nm$$

(worm-like chain)

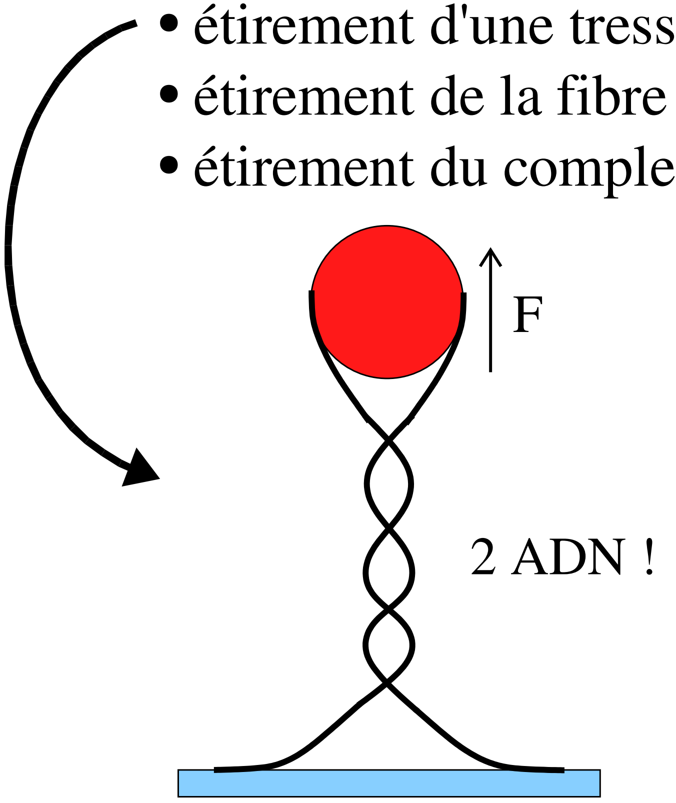
T (pn)	θ (rad)	R (nm)	C/B	P pN/µm
0,62	0,34	2,38	2,02	187
0,95	0,36	2,23	2,12	310
1,30	0,37	1,95	2,02	485
1,80	0,38	1,81	1,90	729
2,70	0,41	1,76	1,92	1 150

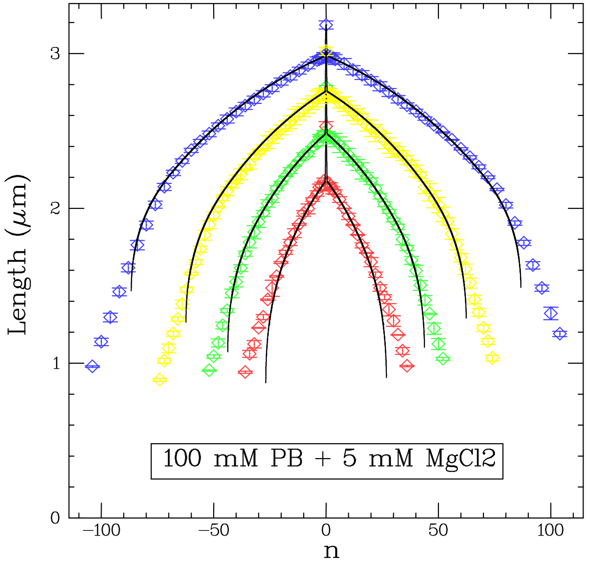
$$C = \frac{K_3}{k_B T} = 80 \pm 4\ nm$$

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

Perspectives : Mécanique de la molécule d'ADN

- → Inclure :
  - chiralité et couplage extension-rotation
  - répulsion électrostatique (thèse Nicolas Clauvelin)
- → Etude théorique des expériences :
  - étirement d'une tresse de 2 molécules d'ADN (Gilles Charvin)
  - étirement de la fibre de chromatine de 10 nm (A. Bancaud & J.-L. Viovy)
  - étirement du complexe ADN+RecA (R. Fulconis & J.-L. Viovy)





Lien entre *n* et σ

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

$L = 0.34\ nbp\ nm$

σ : ratio de sur-enroulement

n : nombre de tours de la bille

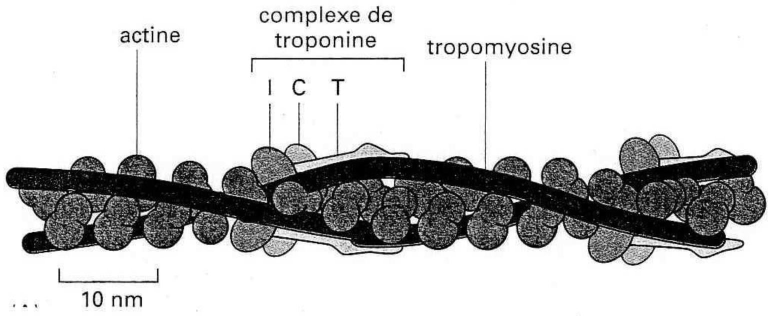
$n_0 = L / H$: twist intrinsèque de la double hélice

H = 3.57 nm : pas de la double hélice d'ADN

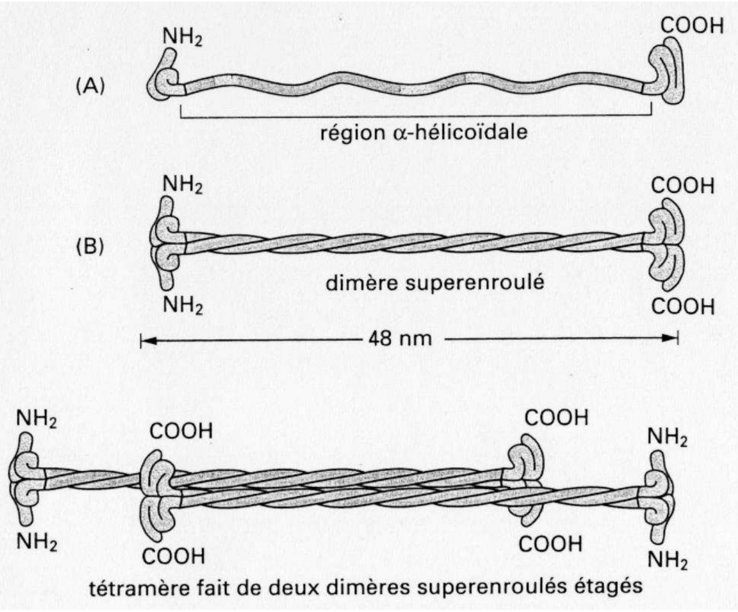
L : longueur totale de la molécule

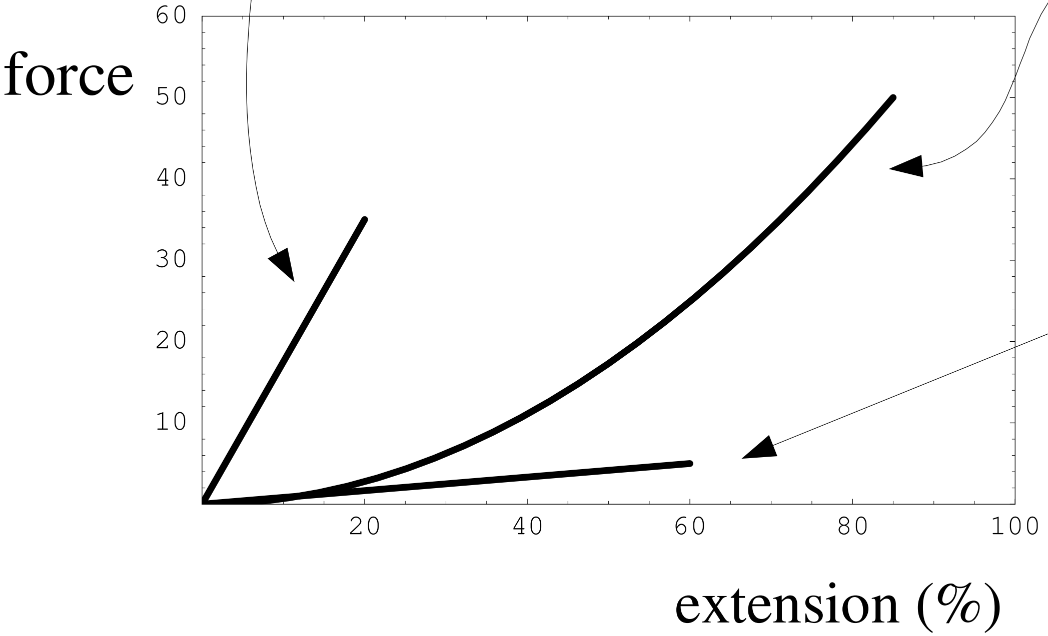
Protéines fibreuses

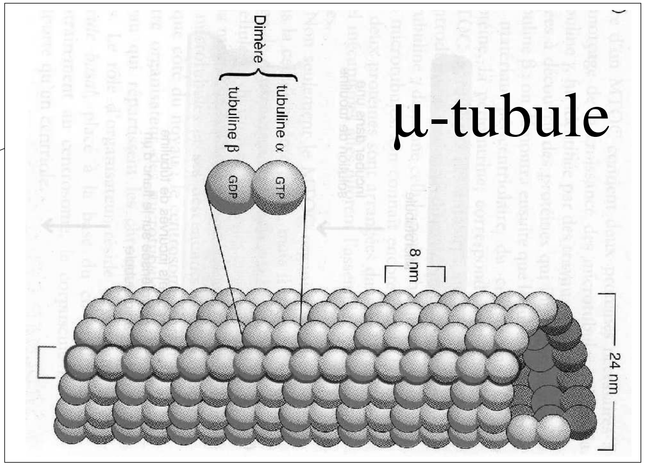
complexe actine-myosine



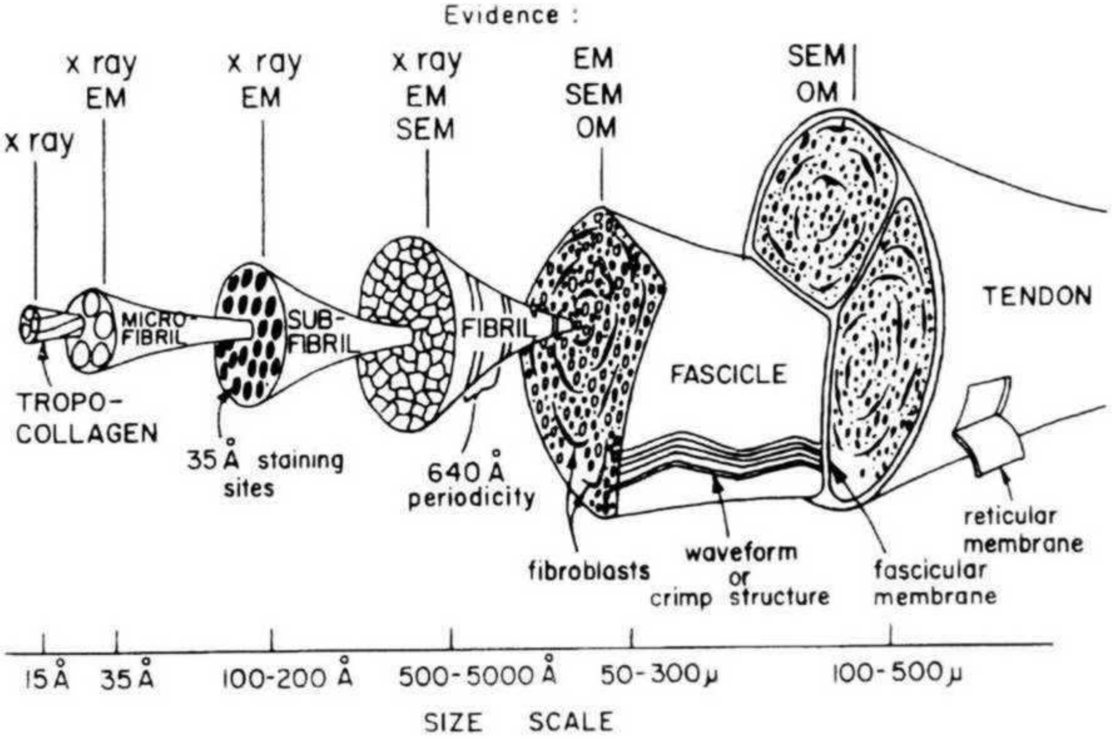
α-kératine



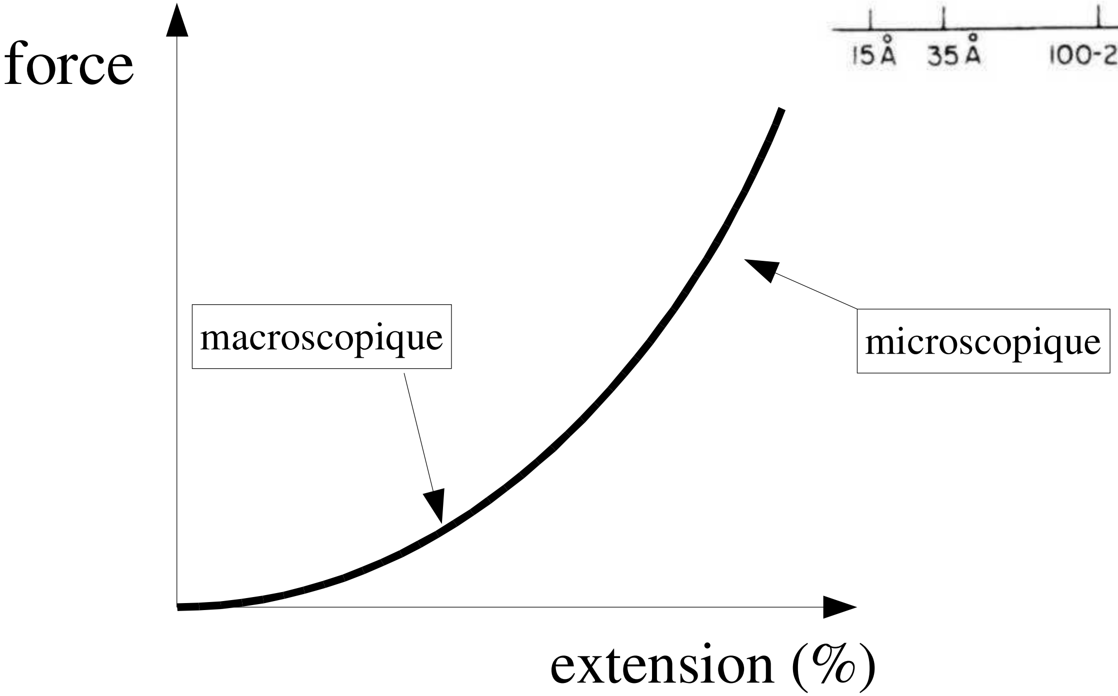



μ-tubule

Structure hiérarchique : e.g. collagène



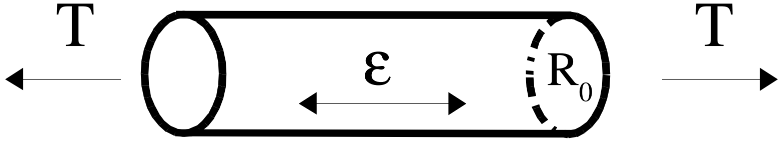
P. Fratzl



Les câbles : flexibilité et résistance à la traction

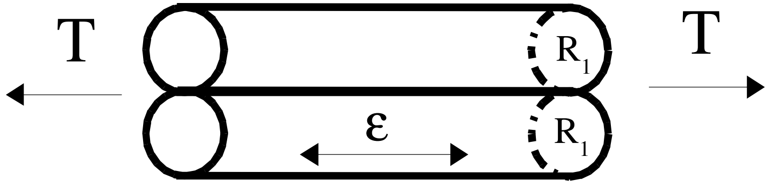
- Rôle d'un câble : résister à une traction
- Pourquoi un câble (avec n brins) et pas un gros fil (n fois plus gros)?

Extension



$$\left(A_0 = \pi R_0^2\right)$$

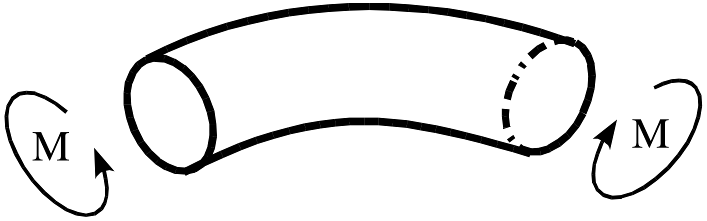
$$T = \underbrace{EA_0}_{k_0}\ \varepsilon$$



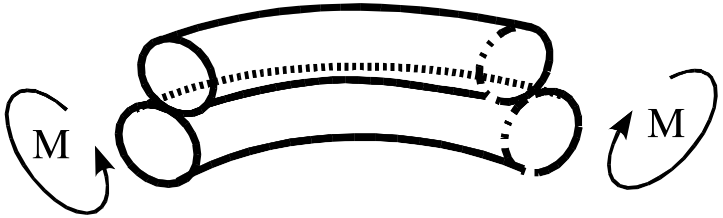
si on veut
la même
extensibilité

$$k_1 = k_0 \Rightarrow R_1 = \frac{R_0}{\sqrt{2}}$$

Flexion



rigidité de courbure : $K_0 = EI_0$

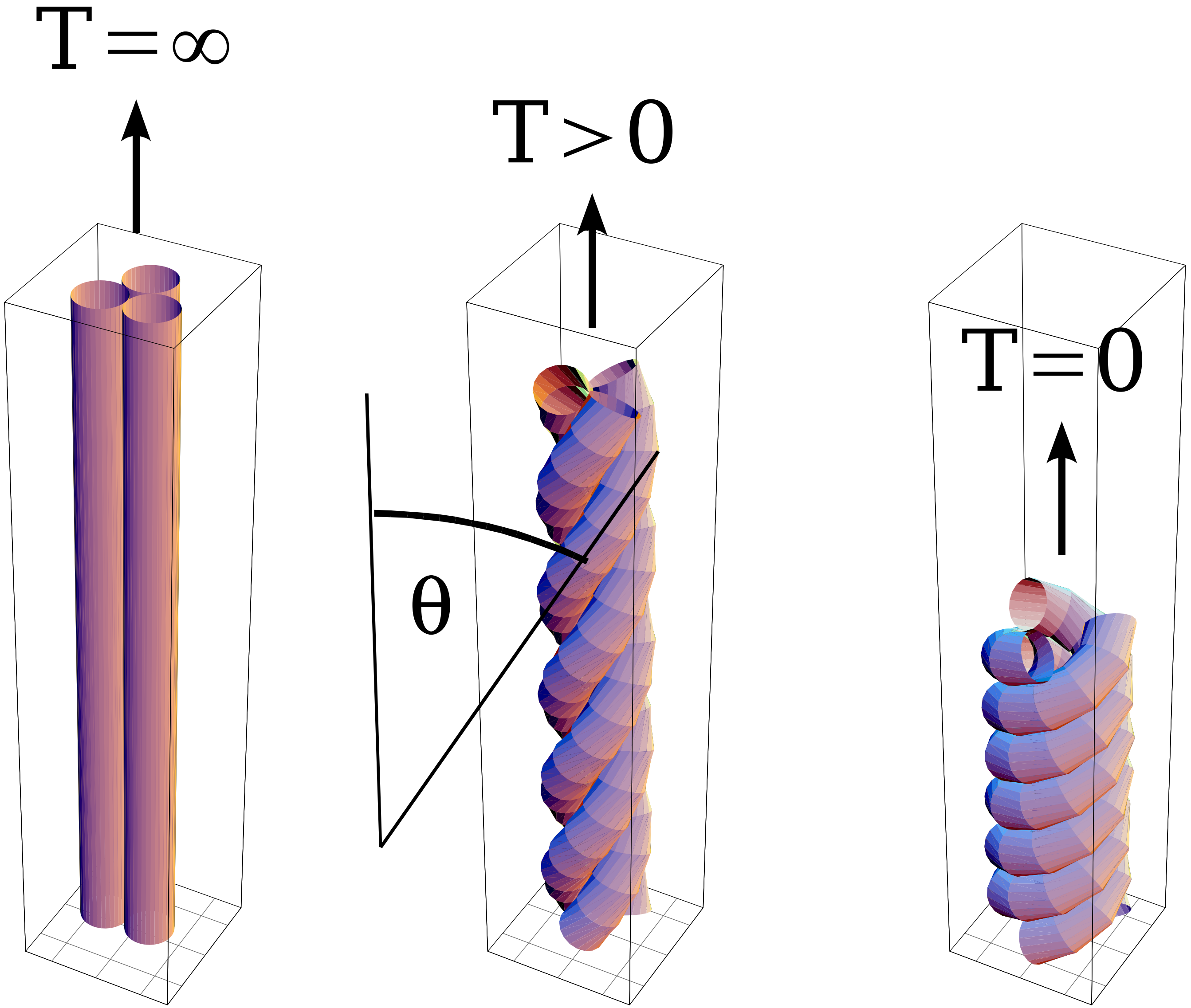


$$R_1 = \frac{R_0}{\sqrt{2}} \Rightarrow K_1 = \frac{K_0}{2}$$

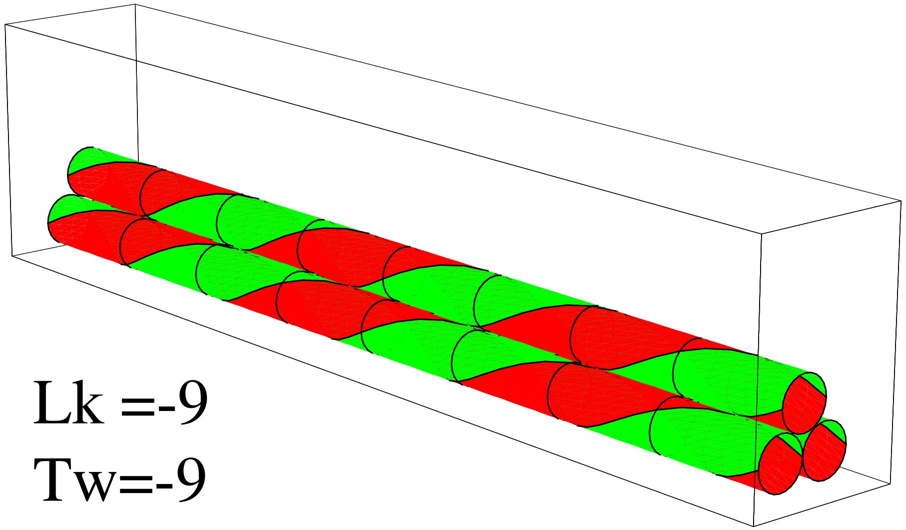
le câble est
deux fois
plus flexible

Les câbles : extensibles par construction

(M=0)



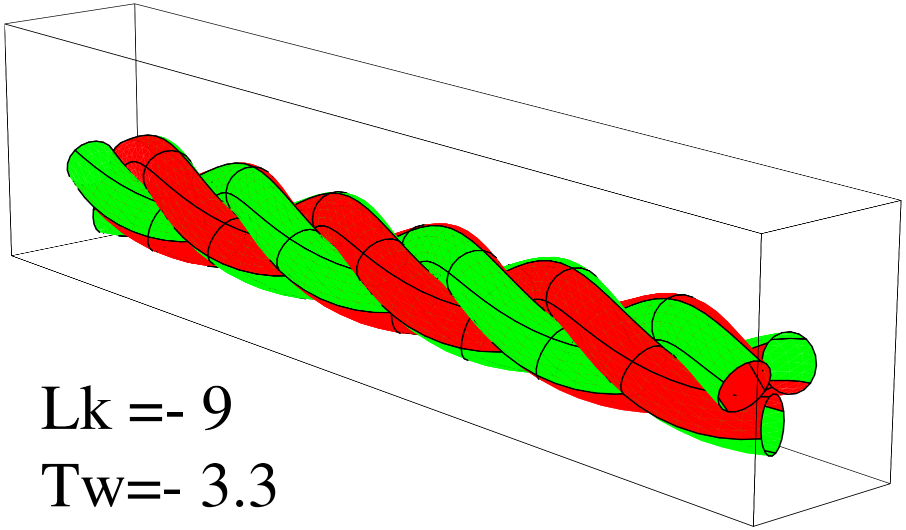
Câbles / torsades : modèle mécanique



Lk =-9

Tw=-9

Wr= 0



Lk =- 9

Tw=- 3.3

Wr= -5.7

équilibre : $2\ n \sin^3\theta\ \cos\theta+\frac{n}{4}\frac{K_3}{K_0}\sin(4\ \theta)+2\ \pi n\ Lk\ \frac{R}{L}\ \frac{K_3}{K_0}\cos(2\ \theta)+\frac{R^2\ T}{K_0}\sin\theta-\frac{R\,M}{K_0}\cos\theta=0$

pression de contact : $\frac{P\,R^3}{K_0}=\frac{\sin^2\theta}{\cos(2\ \theta)}\left[\sin^2\theta+\frac{R^2\ T}{n\,K_0}\cos\theta-\frac{R\,M}{n\,K_0}\sin\theta\right]$

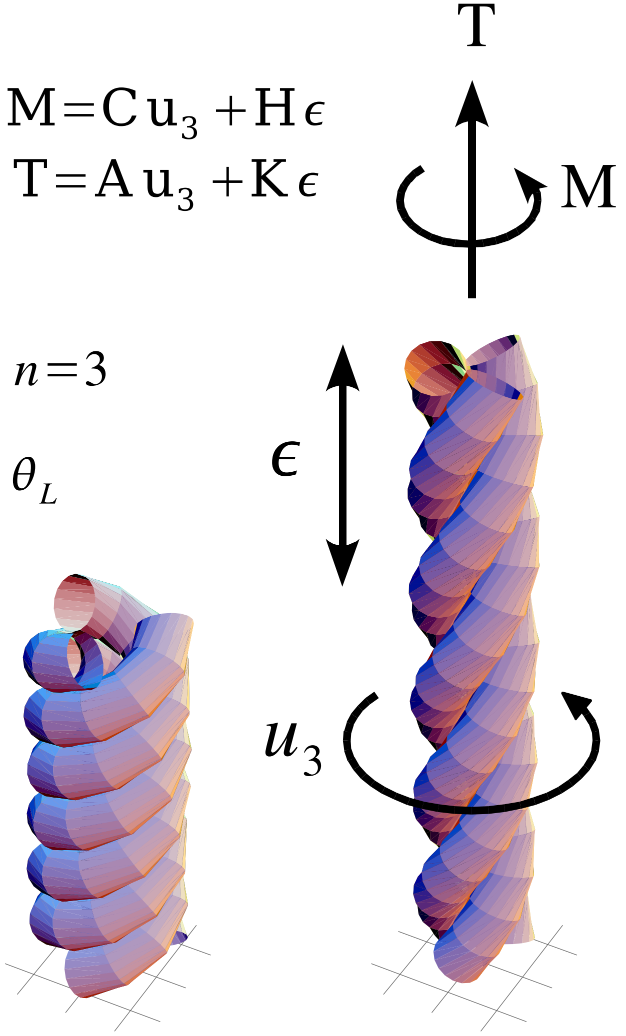
Câbles / torsades : étage par étage

$M = C u_3 + H \epsilon$

$T = A u_3 + K \epsilon$

$n = 3$

θ_L



libre

contraint

étage i+1

étage i

rigidités

twist $\bar{C} = n\left(C + (A+H) R \theta_L\right) + O(\theta_L^2)$

extension $\bar{K} = n\left(K - \frac{A}{R}\theta_L\right) + O(\theta_L^2)$

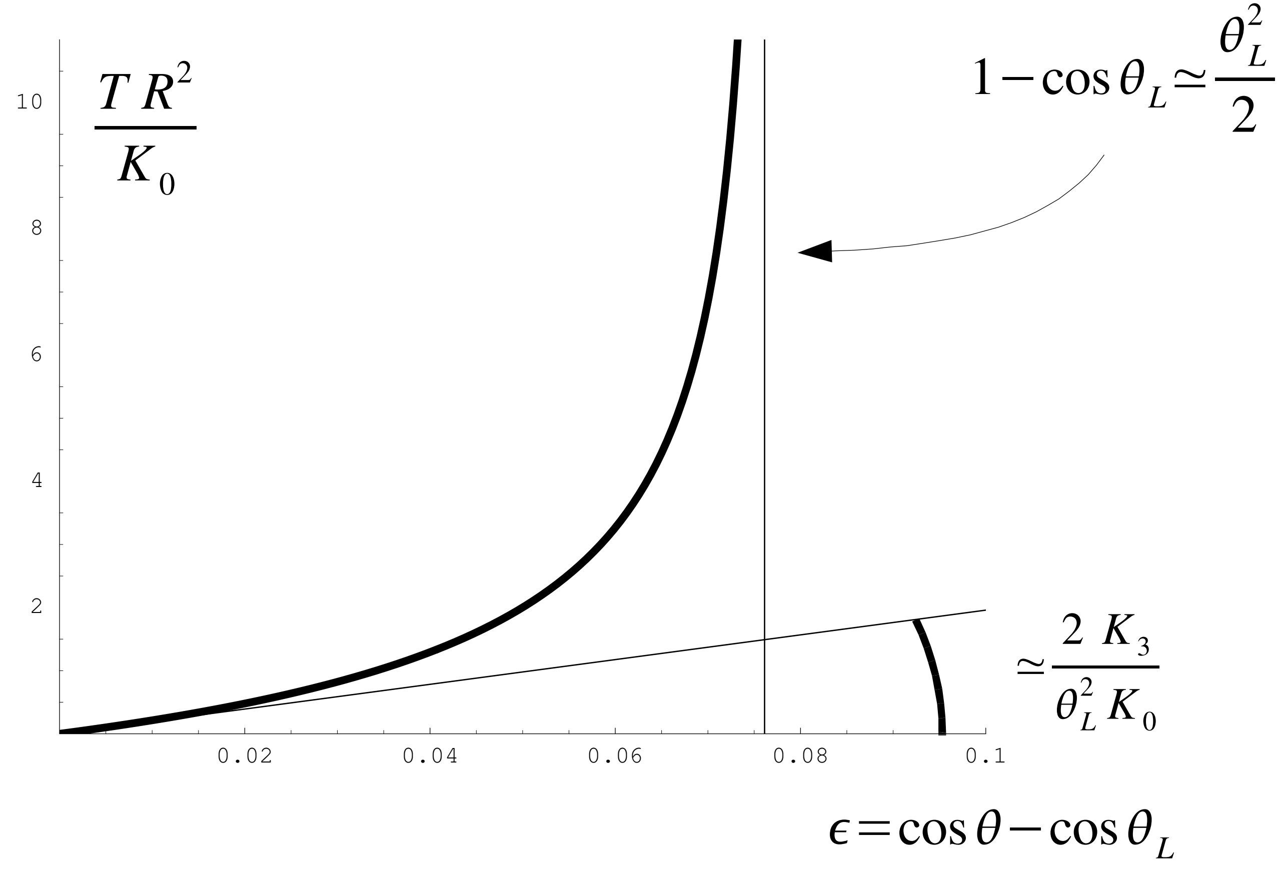
couplage $\bar{A} = n\left(A + KR\theta_L\right) + O(\theta_L^2)$

couplage $\bar{H} = n\left(H + \left(KR - \frac{C}{R}\right)\theta_L\right) + O(\theta_L^2)$

Câbles / torsades : diagramme force-extension

équilibre torsade avec n=2 et M=0 : $\frac{R^2 T}{K_0} = -4 \sin^2\theta \cos\theta - \frac{K_3}{K_0}\frac{\sin(4\,\theta)}{2\sin\theta} + 4\,\pi\,\mathrm{Lk}\,\frac{R}{L}\,\frac{K_3}{K_0}\,\frac{\cos(2\,\theta)}{\sin\theta}$

torsade libre : $T = 0 \Leftrightarrow \theta = \theta_L$



$\frac{T\,R^2}{K_0}$

$1 - \cos\theta_L \simeq \frac{\theta_L^2}{2}$

$\simeq \frac{2\,K_3}{\theta_L^2\,K_0}$

$\epsilon = \cos\theta - \cos\theta_L$

diffraction X sur α-kératine
J. Doucet
F. Briki
LPSolides (Orsay)

Remarques

Ne sont pas pris en compte :

- contribution entropique : physique statistique en mécanique
- interaction longue portée : difficile numériquement
- interaction croissance – élasticité

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