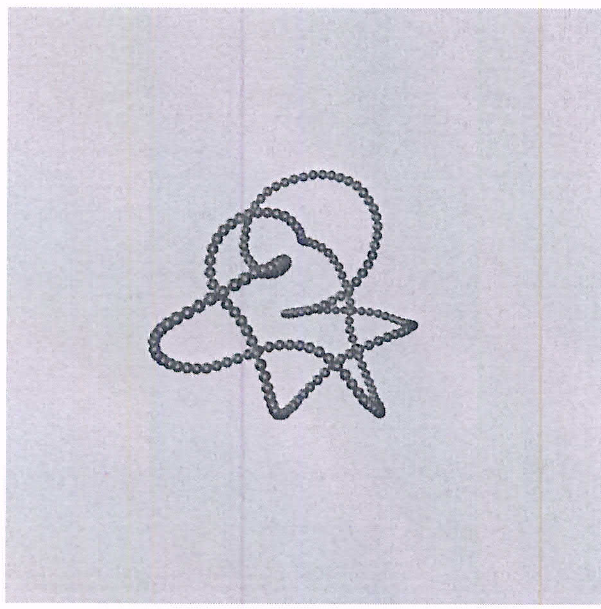
Sedimentation dynamics of rigid, knotted filaments

O. Gonzalez (Univ of Texas, Austin)



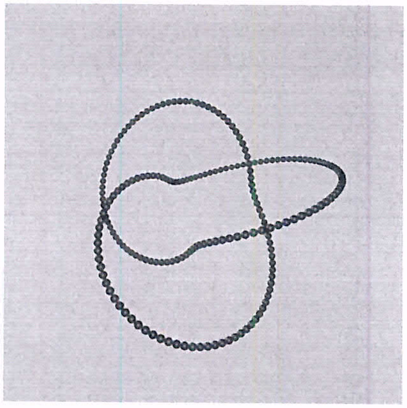
How do they move?

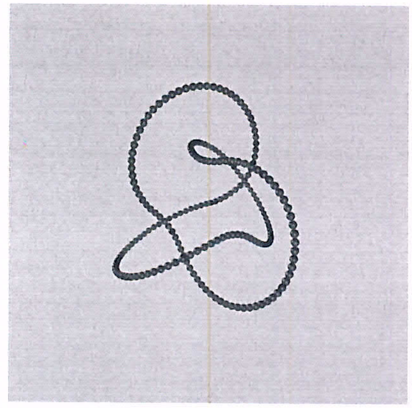
Do knots separate?

Are ideal shapes special?

Example filaments

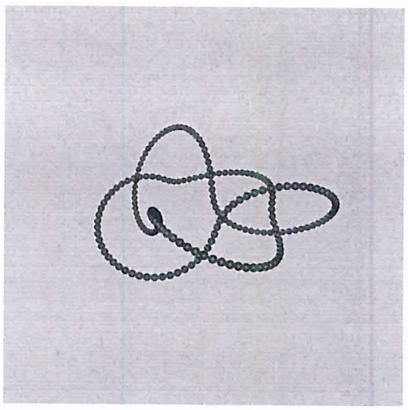
3_1

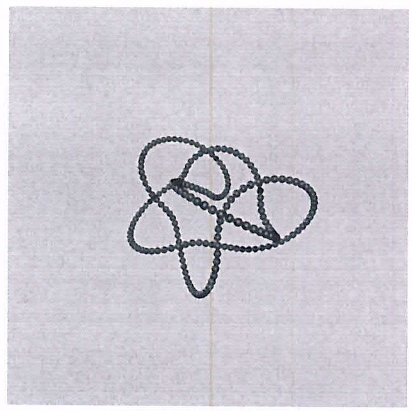




4_1

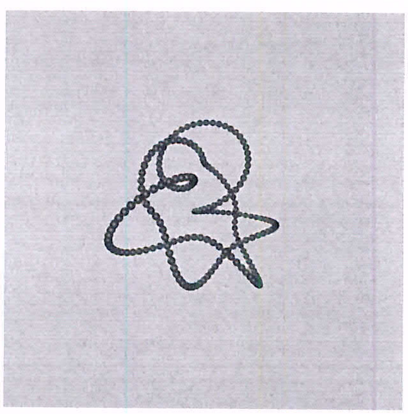
5_1

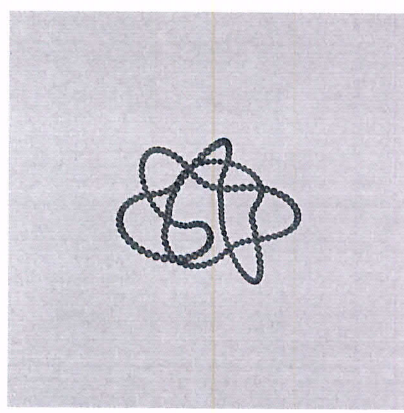




6_1

7_1





7_7

all have same length L and diameter d with $d/L \ll 1$

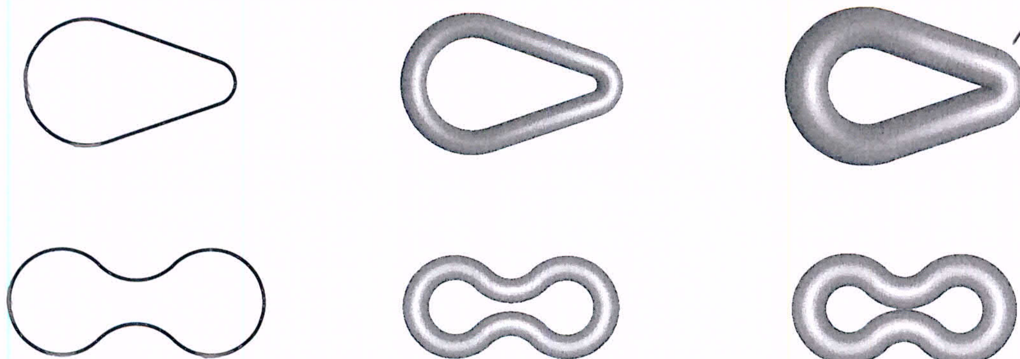
Ideal shapes

Curves $\gamma \in Q$

$$Q = \{\gamma \in C^1(S, \boldsymbol{R}^3) \mid \quad |\gamma'(s)| = 1, \quad s \in S\}$$

circle w/unit perim

Thickness functional $\Delta : Q \to R$



Ideal shapes γ_*

$$\Delta[\gamma_*] = \sup \Delta[\gamma], \quad \gamma \in Q, \quad \gamma \simeq \boldsymbol{k}$$

$\boldsymbol{k}$:

γ_* :

J. Mol. Biol. (1998) **278**, 1–3

JMB

COMMUNICATION

Sedimentation and Electrophoretic Migration of DNA Knots and Catenanes

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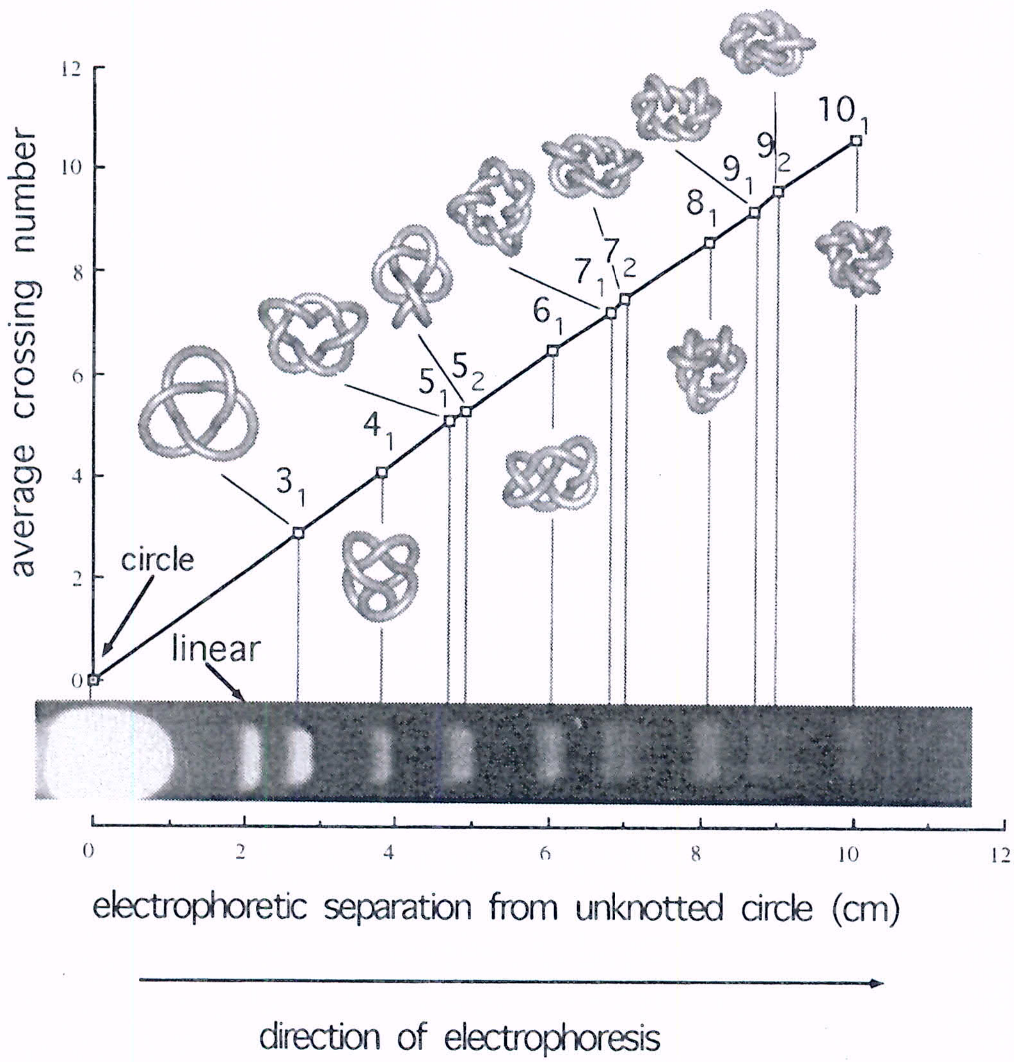
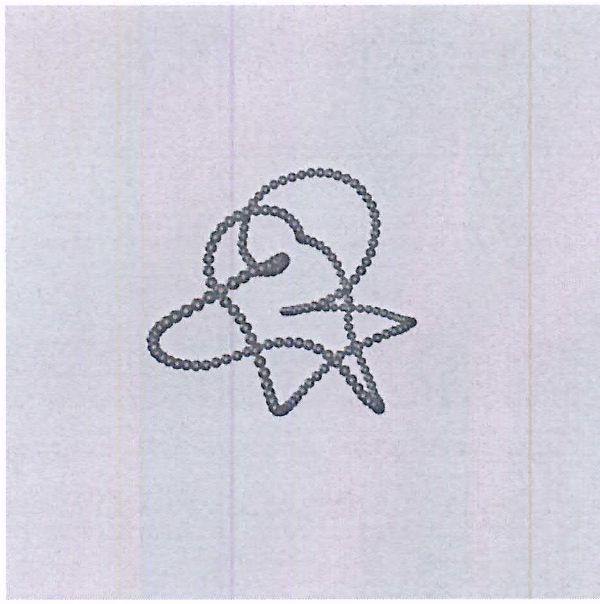
Piotr Pieranski[4], Vsevolod Katritch[5], Jacques Dubochet[6]
and Andrzej Stasiak[6]*



Outline

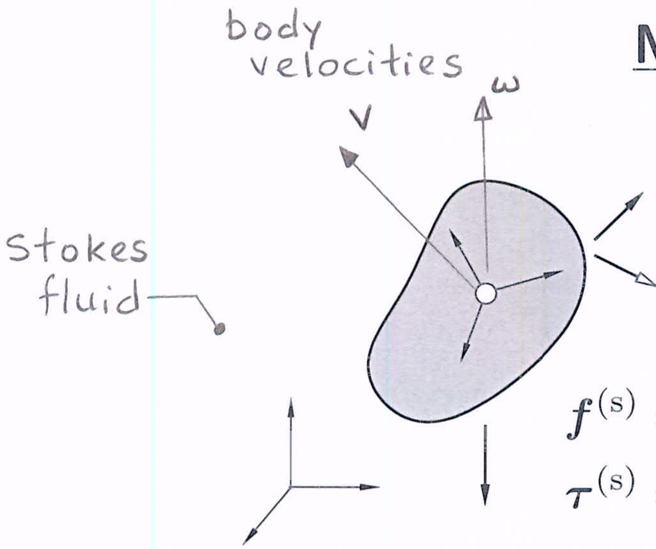


- Setup/Questions
  - How do they move?
  - Do knots separate?
  - Are ideal shapes special?

- Model
  - Body balance laws.
  - Stokes resistance tensors.

- Results
  - Steady states.
  - Stability.
  - Sedimentation speed.

Model



$$\left.\begin{aligned} \boldsymbol{f}^{(\mathrm{d})} &= -\boldsymbol{L}_1\boldsymbol{v} - \boldsymbol{L}_3\boldsymbol{\omega} \\ \boldsymbol{\tau}^{(\mathrm{d})} &= -\boldsymbol{L}_2\boldsymbol{v} - \boldsymbol{L}_4\boldsymbol{\omega} \end{aligned}\right\}$$ hydrodynamic loads (drag)

$$\left.\begin{aligned} \boldsymbol{f}^{(\mathrm{s})} &= \boldsymbol{\eta} \\ \boldsymbol{\tau}^{(\mathrm{s})} &= \boldsymbol{0} \end{aligned}\right\}$$ hydrostatic loads (gravity, buoyancy)

Balance equations

$\boldsymbol{p} = m\boldsymbol{v}, \quad \boldsymbol{\pi} = \boldsymbol{C}\boldsymbol{\omega}$

$$\begin{cases} \dot{\boldsymbol{\eta}} = \boldsymbol{0} & \text{constant gravity} \\ \dot{\boldsymbol{p}} = -\boldsymbol{L}_1\boldsymbol{v} - \boldsymbol{L}_3\boldsymbol{\omega} + \boldsymbol{\eta} & \text{linear momentum} \\ \dot{\boldsymbol{\pi}} = -\boldsymbol{L}_2\boldsymbol{v} - \boldsymbol{L}_4\boldsymbol{\omega} & \text{angular momentum} \end{cases}$$

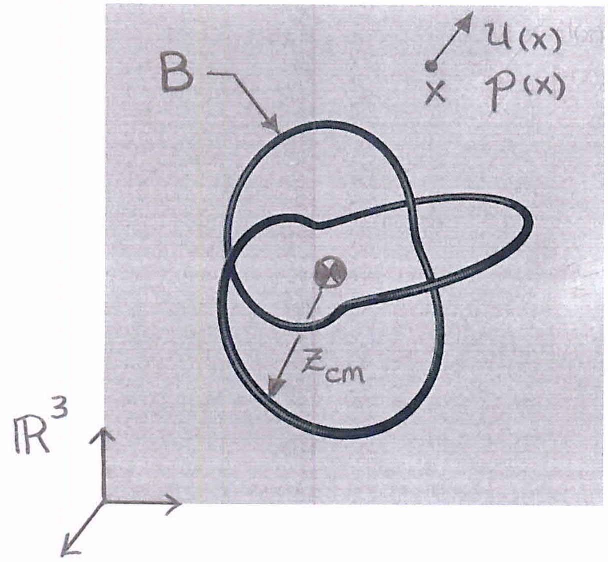
Main parameters

$\alpha = \lvert\boldsymbol{\eta}\rvert > 0$	hydrostatic load
$\mu > 0$	viscosity
$m > 0$	mass
$l > 0$	body size
$C \in \boldsymbol{R}^{3\times 3}$	inertia matrix
$L = \begin{pmatrix} L_1 & L_3 \\ L_2 & L_4 \end{pmatrix} \in \boldsymbol{R}^{6\times 6}$	Stokes resistance matrix — use bead approx.

$$\begin{pmatrix} M_1 & M_3 \\ M_2 & M_4 \end{pmatrix} = \begin{pmatrix} L_1 & L_3 \\ L_2 & L_4 \end{pmatrix}^{-1}$$

↑ important

Stokes resistance tensors



Stokes flow

$$
\begin{array}{rcll}
\mu\Delta \boldsymbol{u} & = & \nabla p & \text{in } \boldsymbol{R}^3 - B \\
\nabla \cdot \boldsymbol{u} & = & 0 & \text{in } \boldsymbol{R}^3 - B \\
\boldsymbol{u} & = & \boldsymbol{V}[v, \omega] & \text{on } \partial B \\
\boldsymbol{u} & \to & \boldsymbol{0} & \text{as } |\boldsymbol{x}| \to \infty
\end{array}
$$

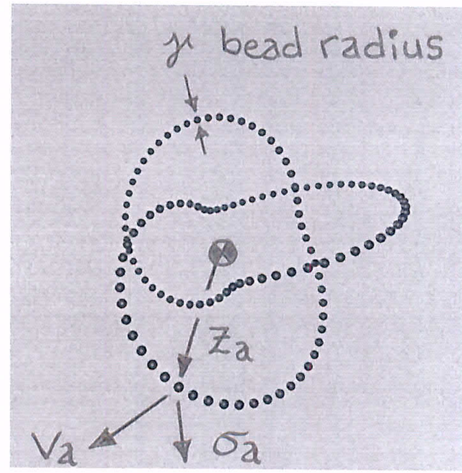
Resultant loads

stress tensor

$$
\begin{array}{rcccl}
\boldsymbol{f}^{(\mathrm{d})} & = & \int_{\partial B} \boldsymbol{\sigma}[\boldsymbol{u}] \cdot \boldsymbol{n}\, dA & = & -\boldsymbol{L}_1 \boldsymbol{v} - \boldsymbol{L}_3 \boldsymbol{\omega} \\
\boldsymbol{\tau}^{(\mathrm{d})} & = & \int_{\partial B} \boldsymbol{z}_{\mathrm{cm}} \times \boldsymbol{\sigma}[\boldsymbol{u}] \cdot \boldsymbol{n}\, dA & = & -\boldsymbol{L}_2 \boldsymbol{v} - \boldsymbol{L}_4 \boldsymbol{\omega}
\end{array}
$$

Bead model for resistance tensors

J. Rotne and S. Prager, J Chem Phys 50 (1969) 4831–4837



force — velocity

- $\sigma_a = -\sum_{b=1}^{n} A_{ab} V_b, \ (a = 1, \ldots, n)$
- $A = (A_{ab}) = D^{-1} \in \boldsymbol{R}^{3n \times 3n}$
- $D = (D_{ab})$ with diagonal blocks $(a = b)$

$$D_{aa} = \frac{1}{6\pi\mu\gamma}\mathrm{Id}$$

and off-diagonal blocks $(a \neq b)$

$$D_{ab} = \frac{1}{8\pi\mu|z_{ab}|^3}\Big[\left(\mathrm{Id}|z_{ab}|^2 + z_{ab} \otimes z_{ab}\right) + \frac{2\gamma^2}{|z_{ab}|^2}\left(\frac{1}{3}\mathrm{Id}|z_{ab}|^2 - z_{ab} \otimes z_{ab}\right)\Big]$$

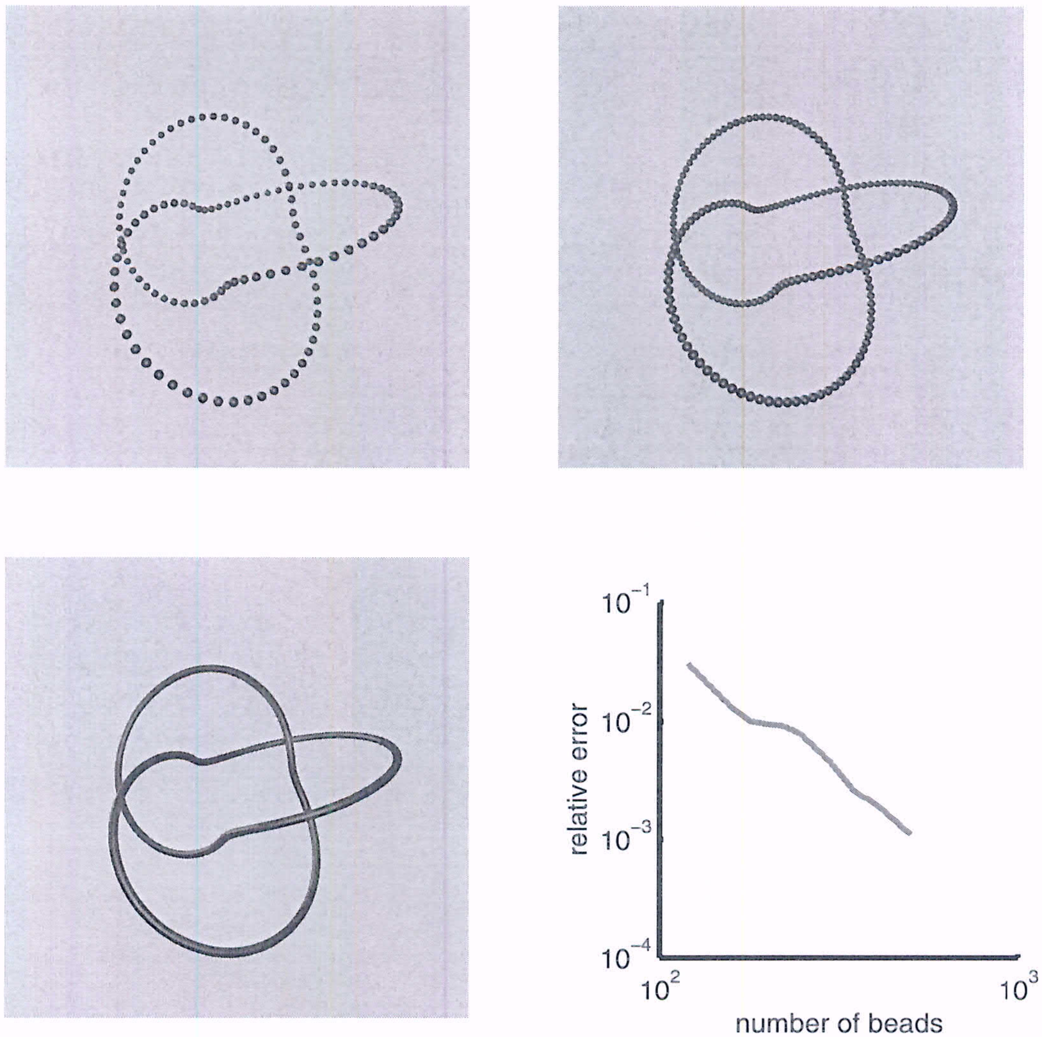
- $f^{(\mathrm{d})} = \sum_{a=1}^{n} \sigma_a$ and $\tau^{(\mathrm{d})} = \sum_{a=1}^{n} z_a \times \sigma_a$ imply

$$L_1 = \sum_{a,b=1}^{n} A_{ab} \qquad L_3 = \sum_{a,b=1}^{n} A_{ab}[z_b \times]^T$$

$$L_2 = \sum_{a,b=1}^{n} [z_a \times] A_{ab} \qquad L_4 = \sum_{a,b=1}^{n} [z_a \times] A_{ab} [z_b \times]^T$$

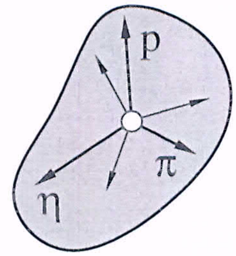
Effect of number of beads

(arclength and bead radius fixed)



$$\text{relative error} = \frac{||L(n) - L(n_*)||}{||L(n_*)||}, \quad n_* = 750$$

Perturbation analysis



Nondimensional IVP (in body frame)

Find $\eta(t)$, $p(t)$, $\pi(t) \in \boldsymbol{R}^3$ such that

$$\left.\begin{aligned} \dot{\eta} + \omega \times \eta &= 0 \\ \varepsilon[\dot{p} + \omega \times p] &= -L_1 v - L_3 \omega + \eta \\ \varepsilon[\dot{\pi} + \omega \times \pi] &= -L_2 v - L_4 \omega \end{aligned}\right\}, \qquad t > 0$$

$$\eta(0) = \eta_0, \quad p(0) = p_0, \quad \pi(0) = \pi_0, \quad \varepsilon = \frac{m\alpha}{\mu^2 l^3} \ll 1$$

Leading-order solution (singular perturbation)

$$\begin{Bmatrix} p(t) \\ \pi(t) \end{Bmatrix} = \underbrace{\exp(-At/\varepsilon) \begin{Bmatrix} p_0 - mM_1\eta_0 \\ \pi_0 - CM_2\eta_0 \end{Bmatrix}}_{\text{exponential decay}} + \underbrace{\begin{Bmatrix} mM_1\eta(t) \\ CM_2\eta(t) \end{Bmatrix}}_{\text{coupling}}$$

where $A \in \boldsymbol{R}^{6\times 6}$ and $\eta(t)$ satisfies

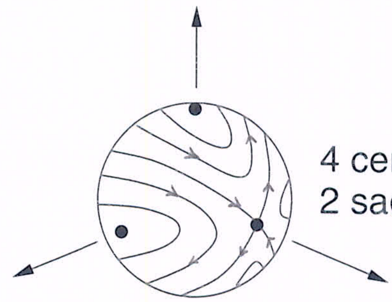
$$\underline{\underline{\dot{\eta} = \eta \times M_2 \eta, \qquad \eta(0) = \eta_0}}$$

∴ "Generalized Euler equation" determines leading-order soln

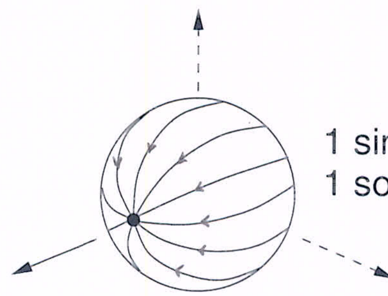
Generalized Euler equation

$$\dot{\eta} = \eta \times M_2 \eta, \quad M_2 \in \boldsymbol{R}^{3\times 3}, \quad |\eta(0)| = 1.$$

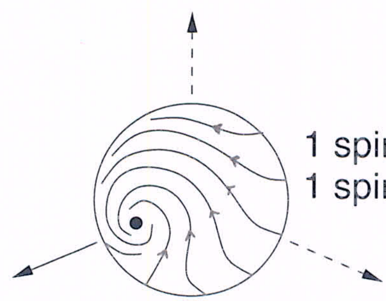
- $M_2^T = M_2$ (w/distinct eigvals).



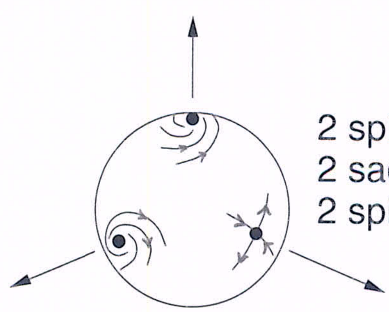
- $M_2^T = -M_2$.



- M_2 w/ 1 real, 2 cmplx eigvals.



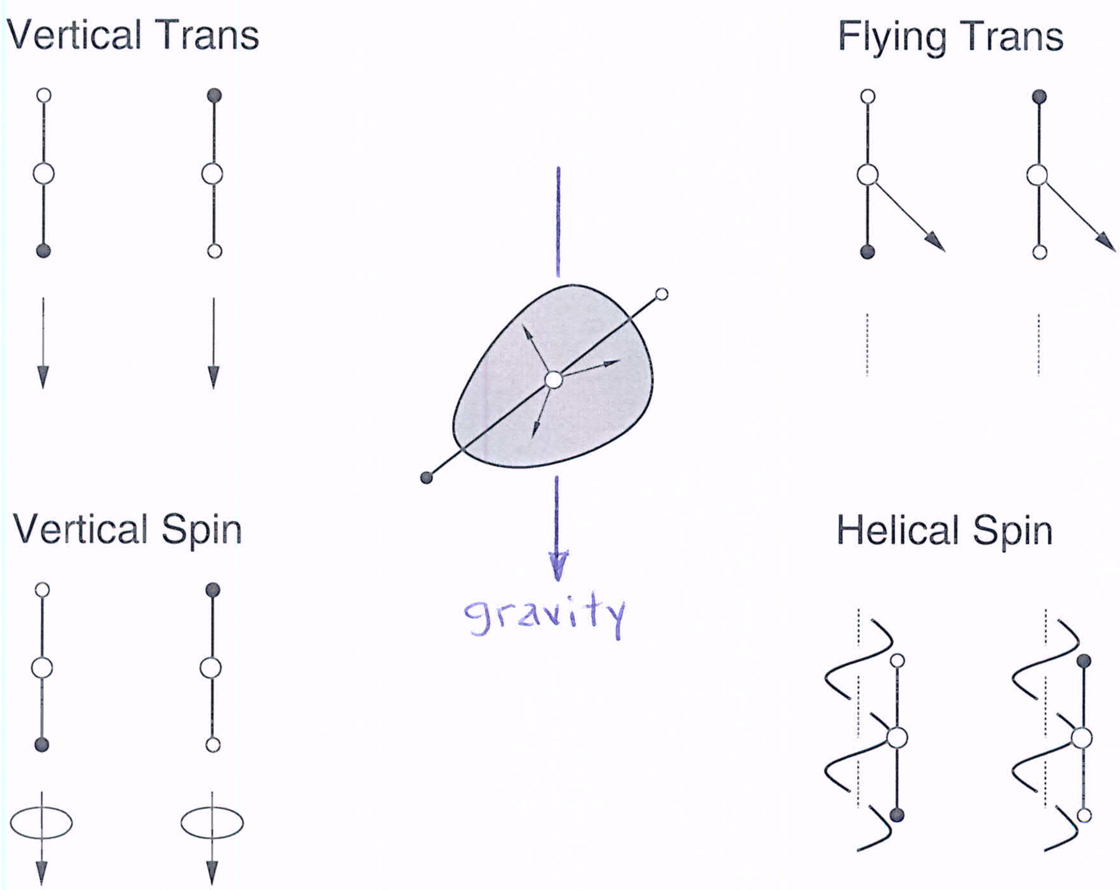
- M_2 w/ 3 real, distinct eigvals and "oblique" eigvecs.



Characterization of steady states

$$\dot{\eta} = \eta \times M_2 \eta, \quad M_2 \in \mathbf{R}^{3\times 3}$$

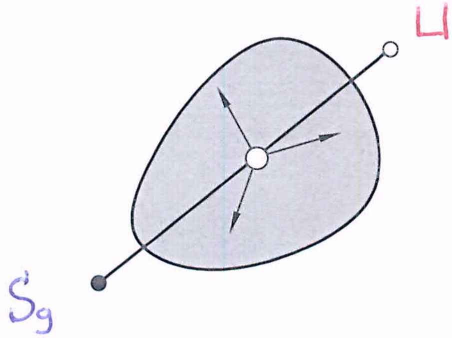
- real eigvec of M_2 $\Rightarrow$ hydrodynamic axis
- hydrodynamic axis $\Rightarrow$ steady state pair
- steady state pair $\in$ {VT, FT, VS, HS}



Stability of steady states

$$\dot{\eta} = \eta \times M_2 \eta, \quad M_2 \in \mathbf{R}^{3\times 3}$$

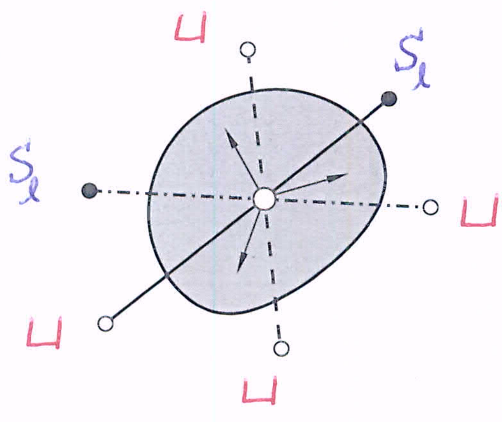
- M_2 w/ 1 real, 2 complex eigvals



U = unstable

S_g = globally, asymp stable

- M_2 w/ 3 real distinct eigvals; oblique eigvecs



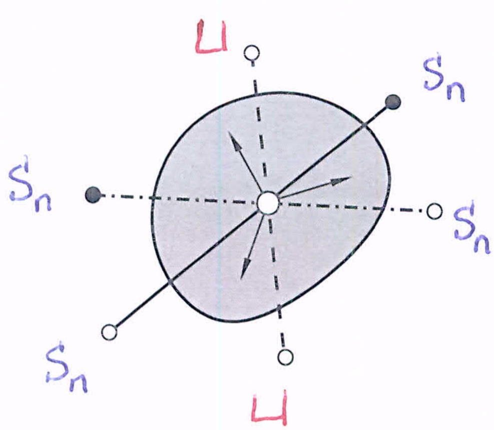
S_ℓ = locally, asymp stable

—•—• min axis

- - - - - mid axis

——— max axis

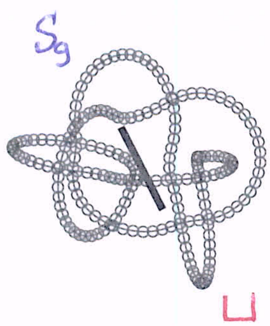
- M_2 w/ 3 real distinct eigvals; orthog eigvecs



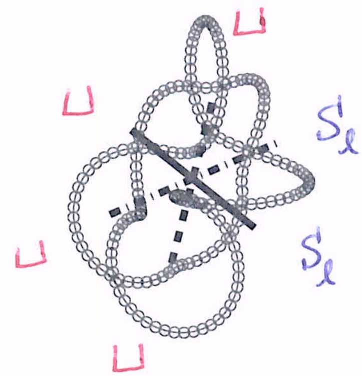
S_n = neutrally stable

Sedimentation simulations

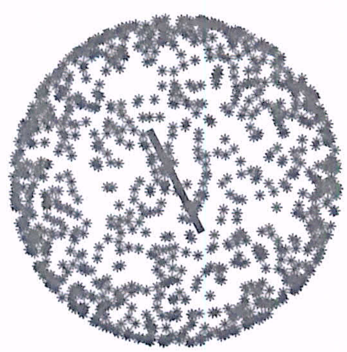
ideal 7_7 and 7_1 knots



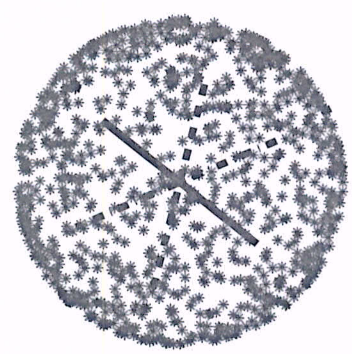
7_7



7_1

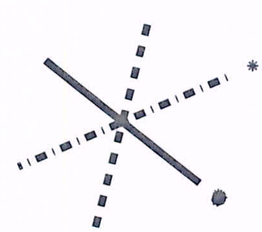


(t=0)



(t=0)

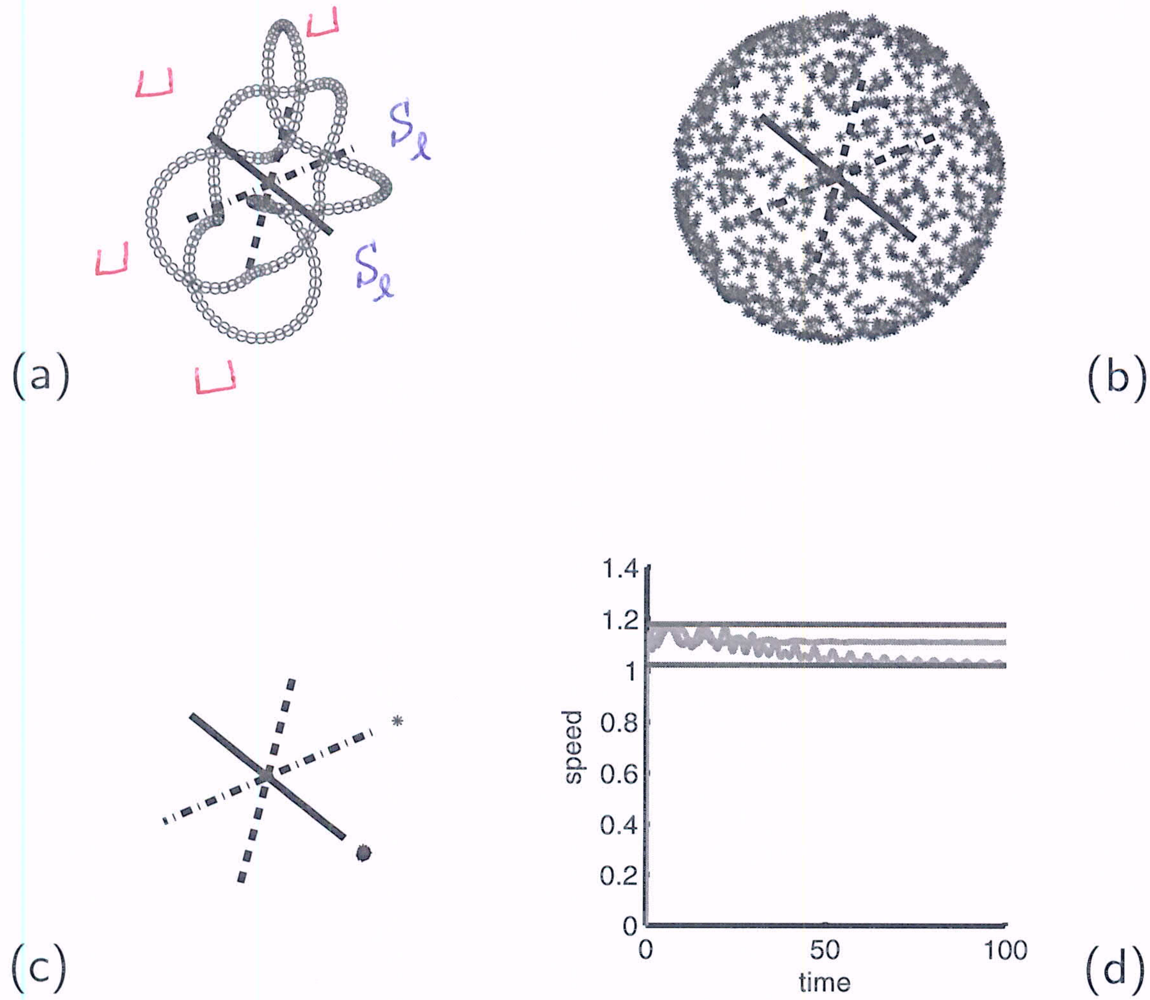
(t=200)



(t=200)

Sedimentation simulation

ideal 7_1 knot



(a) hydrodynamic axes of knot

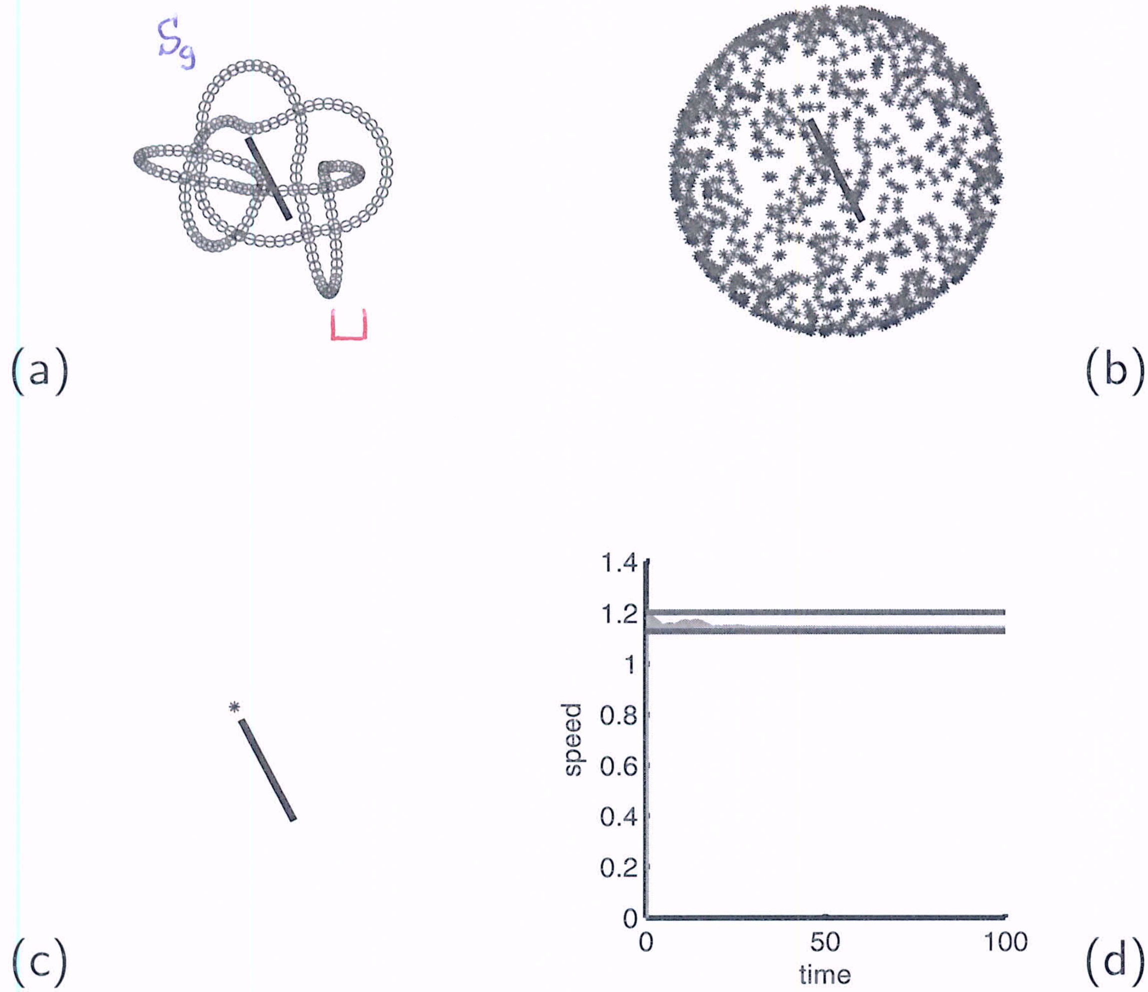
(b) initial distribution of gravity directions (in body frame)

(c) final distribution of gravity directions ($t = 200,\ \varepsilon = 0.01$)

(d) sedimentation speed vs time (a few members from sample)

Sedimentation simulation

ideal 7_7 knot



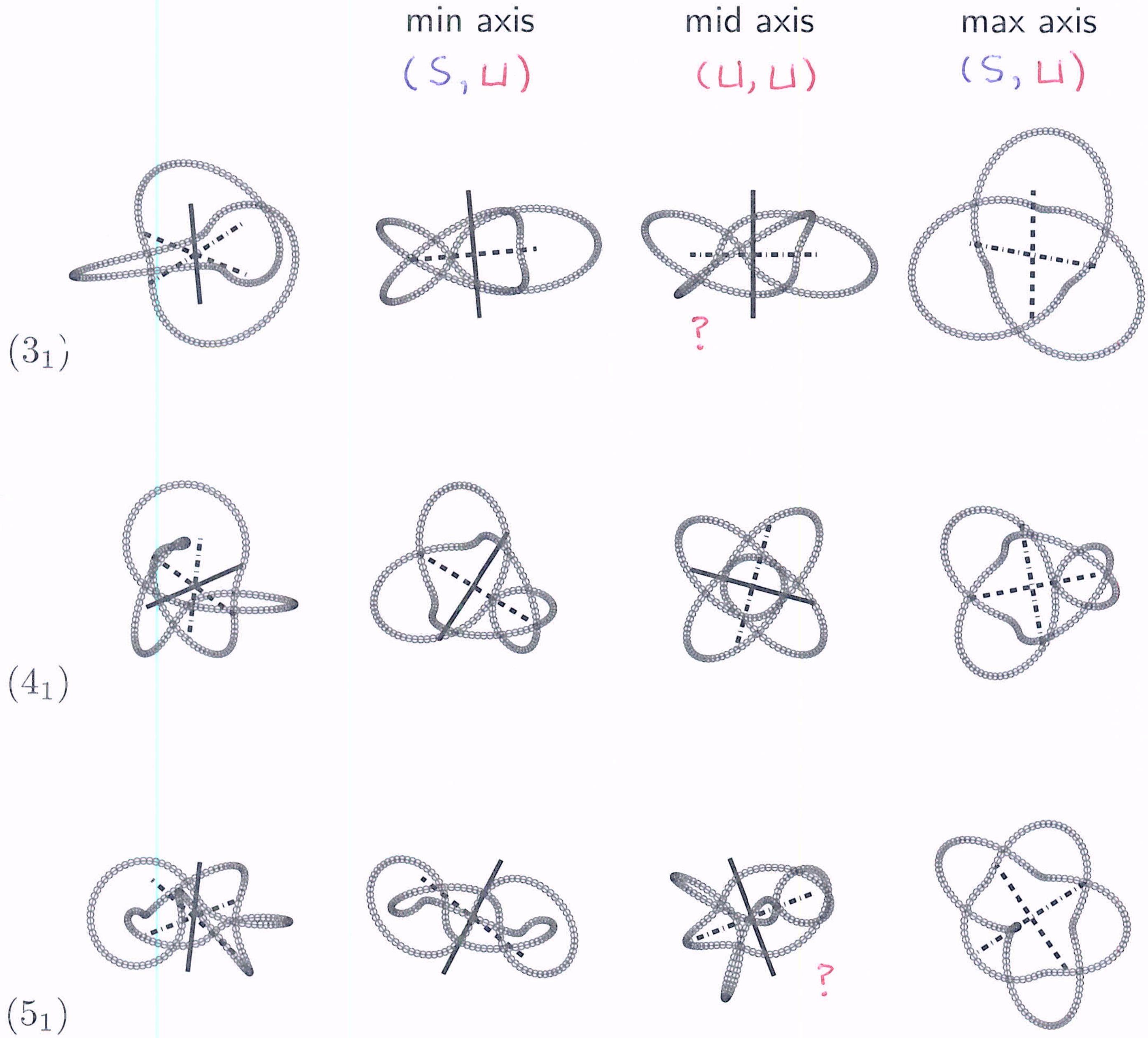
(a) hydrodynamic axes of knot

(b) initial distribution of gravity directions (in body frame)

(c) final distribution of gravity directions ($t = 200,\ \varepsilon = 0.01$)

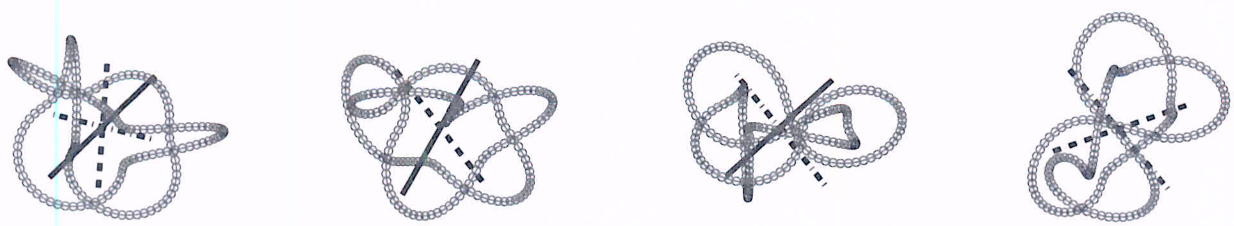
(d) sedimentation speed vs time (a few members from sample)

Hydrodynamic axes of ideal shapes



Hydrodynamic axes of ideal shapes

	min axis	mid axis	max axis
	(S, U)	(U, U)	(S, U)



(6_1)

(7_1)

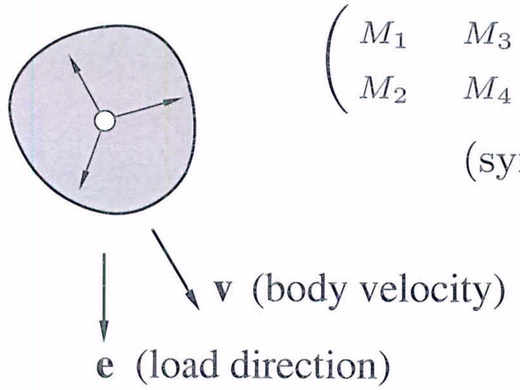
(7_7)

Steady states of ideal shapes

	spin rate	helix rad	helix pitch	stability
	-0.506 ?	1.09×10^{-3}	11.6	
3_1	-0.495 ?	6.67×10^{-4}	11.9	
	$+0.634$	5.86×10^{-4}	7.97	
	-0.796	2.32×10^{-3}	7.61	S,U
4_1	$+0.007$?	2.03×10^{-1}	931	U,U
	$+0.781$	2.29×10^{-3}	7.71	S,U
	-0.769	1.53×10^{-3}	8.22	S,U
5_1	-0.407	1.37×10^{-1}	16.4	U,U
	$+0.801$	3.86×10^{-2}	7.28	S,U
	-0.896	3.32×10^{-2}	7.45	S,U
6_1	$+0.253$	1.40×10^{-1}	27.0	U,U
	$+0.722$	5.36×10^{-2}	9.13	S,U
	-0.825	2.27×10^{-2}	8.47	S,U
7_1	-0.470	6.77×10^{-2}	15.7	U,U
	$+0.786$	2.41×10^{-2}	8.18	S,U
	-0.414	2.18×10^{-2}	17.3	S,U
7_7	$0.25 + i0.6$	–	–	–
	$0.25 - i0.6$	–	–	–

- arclength $= 1$, 6_1 bounding radius $\approx 6 \times 10^{-2}$

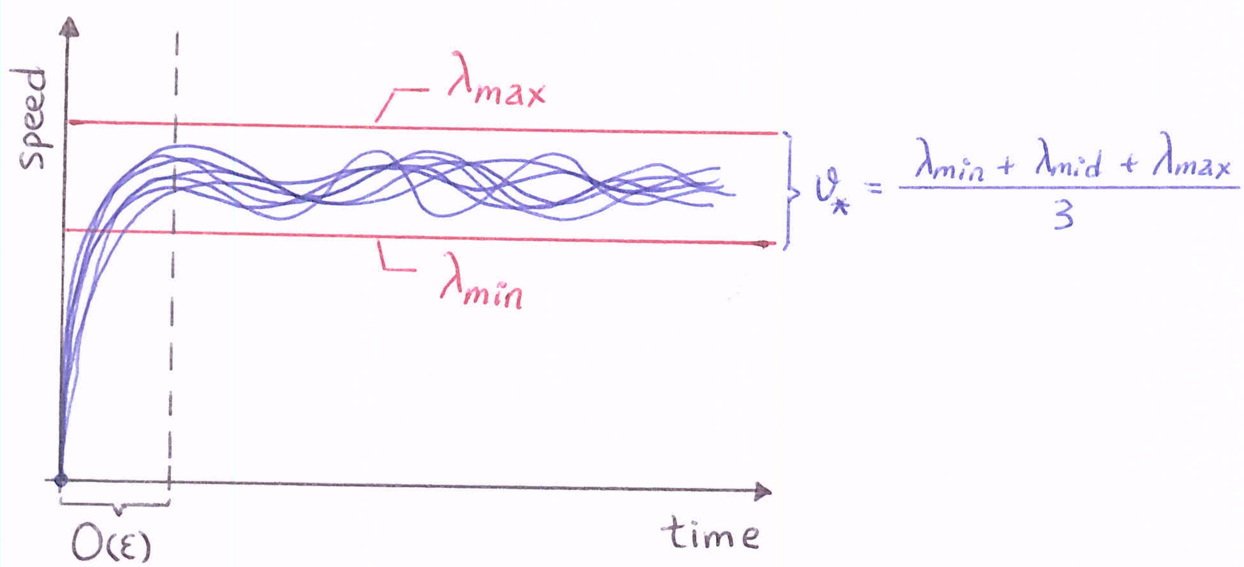
Sedimentation speed



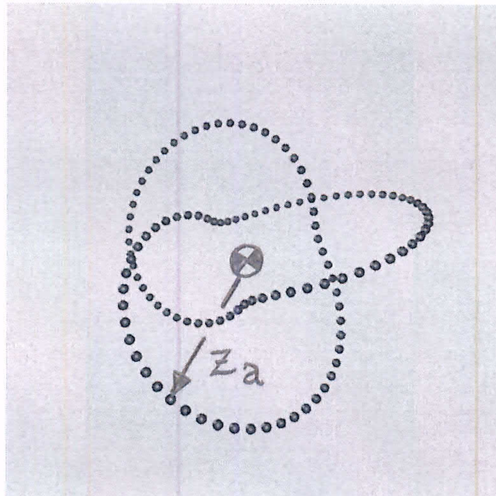
$$\begin{pmatrix} M_1 & M_3 \\ M_2 & M_4 \end{pmatrix} = \begin{pmatrix} L_1 & L_3 \\ L_2 & L_4 \end{pmatrix}^{-1}$$

(sym, pos-def)

- Definition: $\vartheta(t) := \boldsymbol{v}(t) \cdot \boldsymbol{e}$
- Bounds: $\lambda_{\min}(M_1) \leq \vartheta(t) \leq \lambda_{\max}(M_1), \quad t \geq O(1)$
- Characteristic value: $\vartheta_* := \frac{1}{3}\,\mathrm{tr}(M_1)$



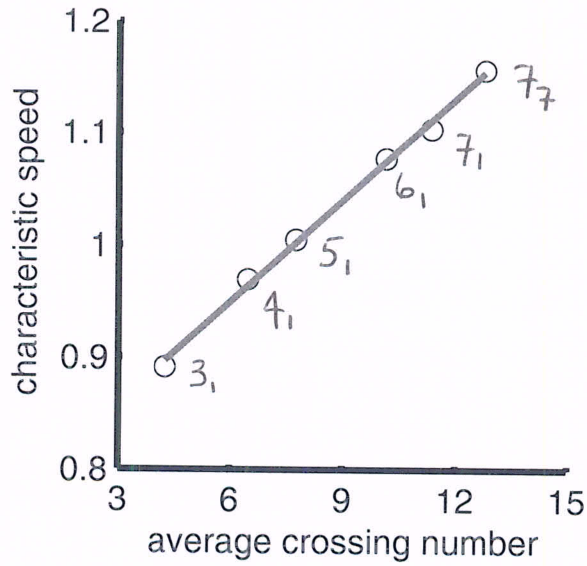
Characteristic speed function



$$\text{nodes } z_a \in \boldsymbol{R}^3 \ (a = 1, \ldots, n)$$
$$\downarrow$$
$$D \in \boldsymbol{R}^{3n \times 3n}$$
$$\downarrow$$
$$A = D^{-1}$$
$$\downarrow$$
$$L \in \boldsymbol{R}^{6 \times 6}$$
$$\downarrow$$
$$M = L^{-1}$$
$$\downarrow$$
$$M_1 \in \boldsymbol{R}^{3 \times 3}$$
$$\downarrow$$
$$\text{speed } \vartheta_* = \tfrac{1}{3} \operatorname{tr}(M_1)$$

Characteristic speed vs avg crossing number

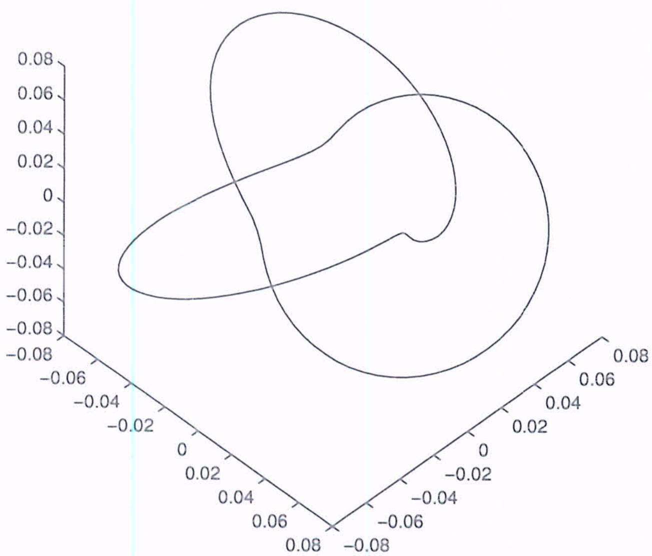
ideal 3_1, 4_1, 5_1, 6_1, 7_1 and 7_7 knots



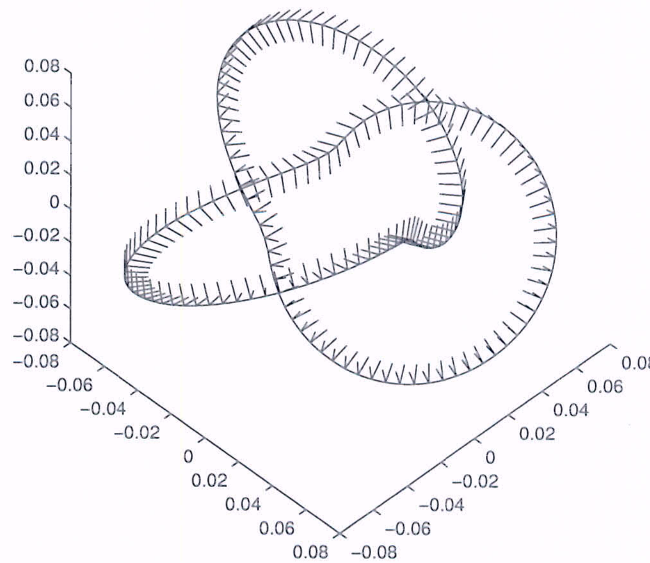
- results are for single shapes for each knot type
- suggests different knots would separate
- same ordering as for electrophoresis data
- what about nearby shapes within knot type?

Construction of nearby, random shapes

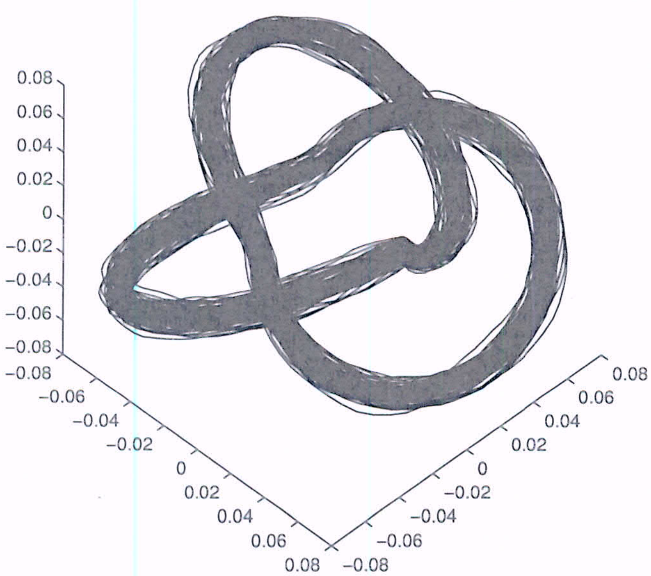
Knot centerline



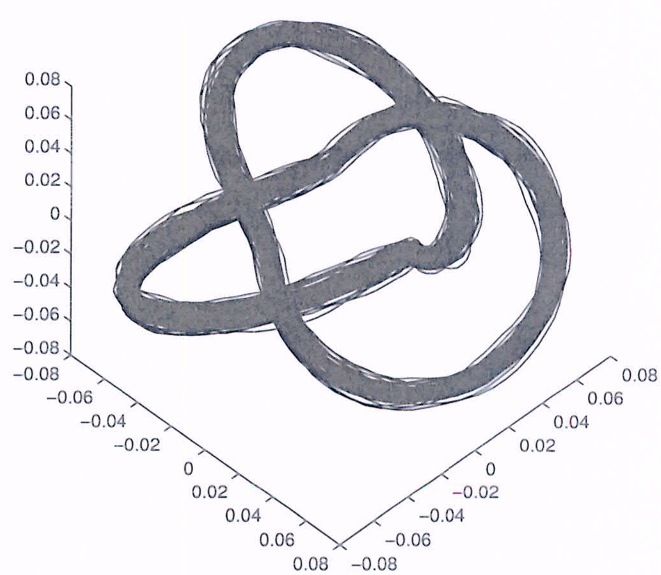
Coordinates in normal tube



Gaussian distribution in normal tube

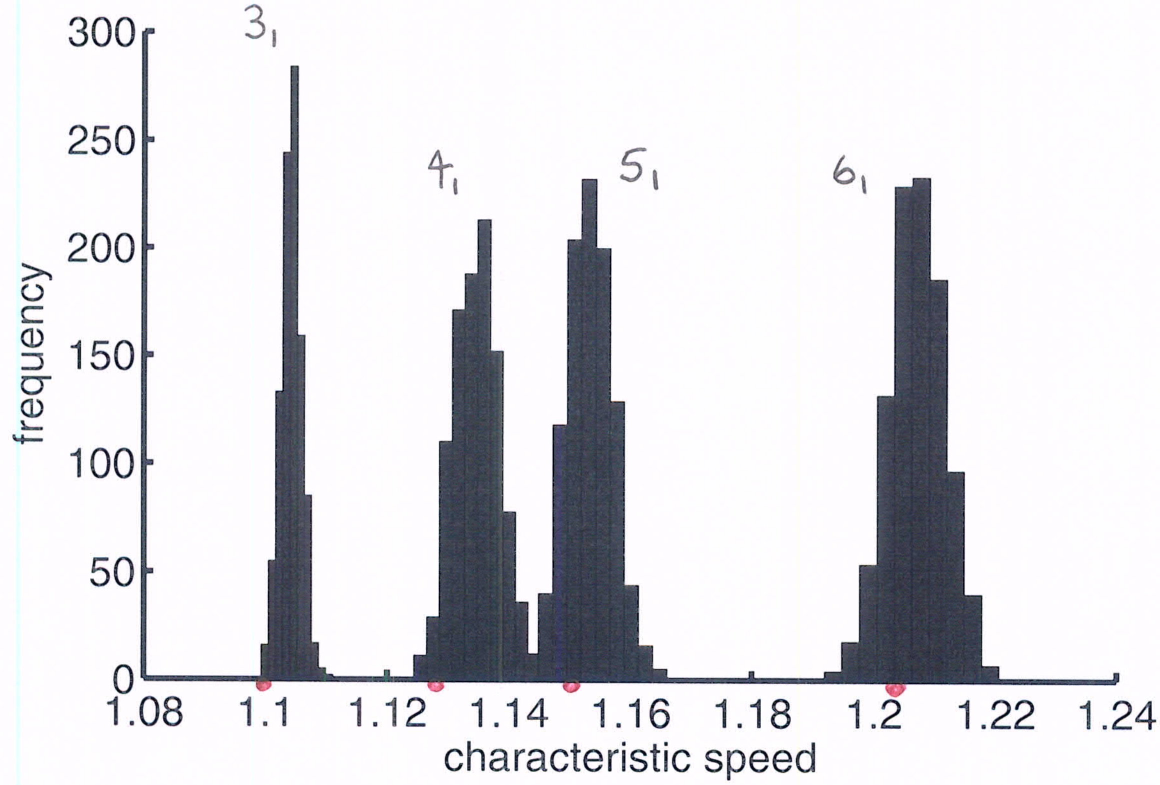


Transformed distribution (unit arclength)



Characteristic speed distribution

neighborhood of ideal 3_1, 4_1, 5_1, 6_1 knots



- results show well-separated peaks
- suggests slightly distorted knots would separate
- are ideal shapes special?

Summary

- Generalized Euler eq drives sedimentation dynamics

- Multiple, stable steady-states are possible

- A characteristic speed functional is

$$\gamma \mapsto \vartheta_*(\gamma) := \frac{1}{3}\,\mathrm{tr}[M_1(\gamma)]$$

- $\vartheta_*(\gamma)$ orders example filaments by knot type

- Several open questions about $\vartheta_*(\gamma)$

  - possible scaling laws
  - properties of optimizers
  - approximation techniques (e.g. Rotne-Prager)