Hydrodynamics of magnetic chains, and flexible fibres with a twist

Brennan Sprinkle

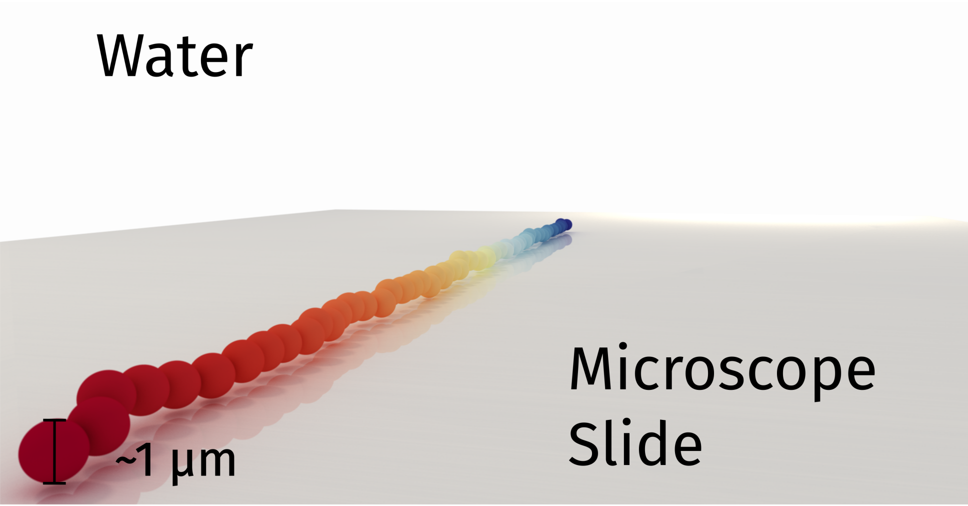
April 30, 2020

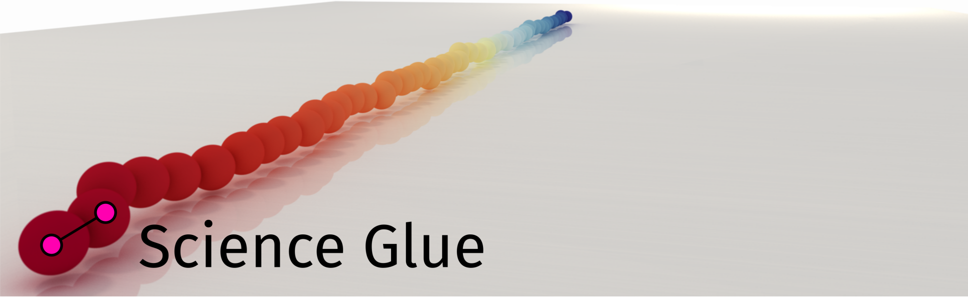
Outline

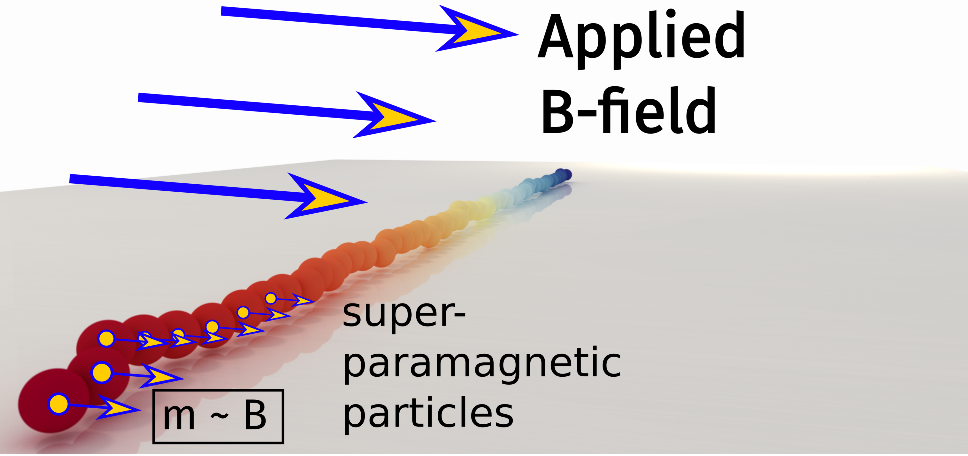
Orders of business

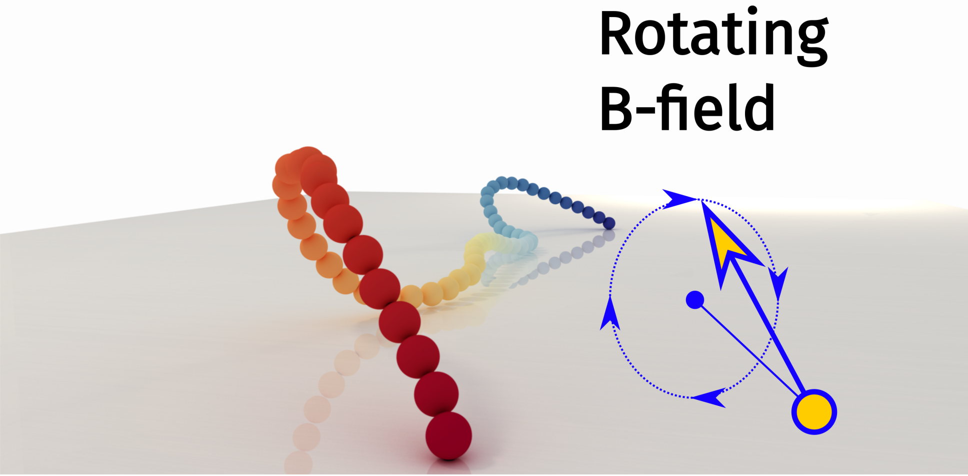
1. Problem set up
2. The model/method we used
3. Towards a new method

Colloidal Chains


Water
Microscope
Slide
~1 µm


Science Glue


Applied
B-field
super-
paramagnetic
particles
m ~ B


Rotating
B-field

Experiments

Simulation

Magnetic Model

Magnetic Force

Superparamagnetic particles (almost) instantaneously develop a magnetic moment $\bar{\boldsymbol{m}}$ aligned with the applied magnetic field $\boldsymbol{B}(t)$ so that

$$\bar{\boldsymbol{m}} \propto \boldsymbol{B}(t) = B_{\mathrm{DC}}\hat{\boldsymbol{x}} + B_{\mathrm{AC}} \sin\left(2\pi(50\mathrm{Hz})t\right)\hat{\boldsymbol{y}} + B_{\mathrm{AC}} \sin\left(2\pi(50\mathrm{Hz})t\right)\hat{\boldsymbol{z}}.$$

In a chain of N beads, the magnetic force on bead i due to the interaction with bead j is

$$\boldsymbol{f}_{i,j}^{\mathrm{mag}} = \frac{F_0}{(r_{i,j}/a)^4}\left(2\left(\bar{\boldsymbol{m}}\cdot\hat{\boldsymbol{r}}_{i,j}\right)\bar{\boldsymbol{m}} - \left(5\left(\bar{\boldsymbol{m}}\cdot\hat{\boldsymbol{r}}_{i,j}\right)^2 - 1\right)\hat{\boldsymbol{r}}_{i,j}\right), \quad (1)$$

where $F_0 = 2.6\times10^{-12}\mathrm{N}$ is the strength of the magnetic interactions.

Magic Angle

We can define the 'angle' β of the magnetic field

$$\boldsymbol{B}(t) = B_{\text{DC}}\hat{\boldsymbol{x}} + B_{\text{AC}} \sin\left(2\pi(50\text{Hz})t\right) \hat{\boldsymbol{y}} + B_{\text{AC}} \sin\left(2\pi(50\text{Hz})t\right) \hat{\boldsymbol{z}}.$$

as

$$\beta = \arctan\left(\frac{B_{\text{AC}}}{B_{\text{DC}}}\right).$$

And it was observed in experiments that the chains formed a helix shape for

$$\beta \approx 55^\circ,$$

where stretching from B_{DC}, and twirling from B_{AC} are in balance.

Chain Model

Requirements

- We maintain inextensibility between the centers of neighboring beads $\boldsymbol{x}_i$ and $\boldsymbol{x}_{i+1}$
- The particles in the chain are bonded together so they shouldn't 'twist' much relative to each other.
- The chain should be able to bend with modulus κ_b

Heterogeneity in Bending

The chains in experiments clearly have a preferred chirality from a heterogeneity built into them during synthesis. We model this as a linearly decaying bending stiffness

$$\kappa_b\left(s\right) = \kappa_b^{\text{const.}} \frac{3 + 2(i/N)}{5}$$

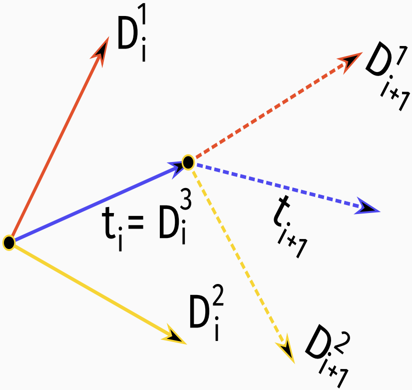
Kirchhoff Rods

Particle orientation

At each bead, we affix an othonormal triad

$$Q_i = [D_i^1, D_i^2, D_i^3],$$

and constrain $D_i^3 = (x_{i+1} - x_i) \approx x'(s) = t(s)$.



Assume the frames at two neighboring beads only differ by a small rotation

Let s be arclength along the chain.

$$\partial_s \boldsymbol{Q} = \boldsymbol{\Omega} \times \boldsymbol{Q}$$

Using

$$\boldsymbol{D}^1 = \boldsymbol{D}^2 \times \boldsymbol{D}^3, \ \cdots$$

we get

$$\begin{aligned} \boldsymbol{\Omega} &= \Omega_1 \boldsymbol{D}^1 + \Omega_2 \boldsymbol{D}^2 + \Omega_3 \boldsymbol{D}^3 && (2) \\ &= \left(\boldsymbol{D}_s^2 \cdot \boldsymbol{D}^3\right) \boldsymbol{D}^1 + \left(\boldsymbol{D}_s^3 \cdot \boldsymbol{D}^2\right) \boldsymbol{D}^2 + \left(\boldsymbol{D}_s^1 \cdot \boldsymbol{D}^2\right) \boldsymbol{D}^3 && (3) \end{aligned}$$

and discretize $\boldsymbol{D}_s^k \approx \boldsymbol{D}_{i+1/2}^k - \boldsymbol{D}_{i-1/2}^k$

Penalty Method

Lim and Peskin give forces and torques on the particles as

$$-\boldsymbol{f}^{ch} = \overbrace{\partial_s \boldsymbol{\Lambda}}^{(1)} \tag{4}$$

$$-\boldsymbol{\tau}^{ch} = \partial_s \underbrace{\boldsymbol{M}(s)}_{(2)} + \underbrace{(\partial_s \boldsymbol{x}) \times \boldsymbol{\Lambda}}_{(3)} \tag{5}$$

where $\boldsymbol{\Lambda}$ enforces that the triad be orthogonal and that $\boldsymbol{D}_i^3 = (\boldsymbol{x}_{i+1} - \boldsymbol{x}_i) \approx \partial_s \boldsymbol{x} = \boldsymbol{t}(s)$.

$$\boldsymbol{\Lambda} = \Lambda_1 \boldsymbol{D}^1 + \Lambda_2 \boldsymbol{D}^2 + \Lambda_3 \boldsymbol{D}^3 \tag{6}$$

$$= \underbrace{\kappa_S \left(\boldsymbol{D}^1 \cdot \boldsymbol{t}\right) \boldsymbol{D}^1 + \kappa_S \left(\boldsymbol{D}^2 \cdot \boldsymbol{t}\right) \boldsymbol{D}^2}_{(a)} + \underbrace{\kappa_S \left(\boldsymbol{D}^3 \cdot \boldsymbol{t} - 1\right) \boldsymbol{D}^3}_{(b)} \tag{7}$$

And

$$\boldsymbol{M}(s) = \left(\kappa_b \left[\Omega_1 \boldsymbol{D}^1 + \Omega_2 \boldsymbol{D}^2\right] + \kappa_T \Omega_3 \boldsymbol{D}^3\right)$$

Force and Torque on the Chain

The force and torque on bead i in the chain is

$$\boldsymbol{f}_i = \boldsymbol{f}_i^{ch} + \sum_{j>i} \boldsymbol{f}_{i,j}^{\text{mag}} \tag{8}$$

$$\boldsymbol{\tau}_i = \boldsymbol{\tau}_i^{ch} + \sum_{j>i} \boldsymbol{\tau}_{i,j}^{\text{mag}} \tag{9}$$

hydrodynamics

Equation of motion

Chains are small enough that steady Stokes equations govern hydrodynamics. Linearity of Stokes means that we can write

$$\begin{bmatrix} U_1 \\ \vdots \\ U_N \end{bmatrix} = \mathcal{N}(x_1, \cdots, x_n) \cdot \begin{bmatrix} F_1 \\ \vdots \\ F_N \end{bmatrix}, \quad U_i = \begin{bmatrix} \boldsymbol{u}_i \\ \boldsymbol{\omega}_i \end{bmatrix}, \; F_i = \begin{bmatrix} \boldsymbol{f}_i \\ \boldsymbol{\tau}_i \end{bmatrix} \tag{10}$$

Mobility

- $\mathcal{N}(x_1, \cdots, x_n)$ is a 'Friction' or 'Mobility' operator that depends of the configuration of every particle in the chain and the geometry of the domain (e.g. bottom wall)

Update position

we integrate $\boldsymbol{x}_i, \boldsymbol{Q}_i$ according to

$$\partial_t \boldsymbol{x}_i = \boldsymbol{u}_i, \tag{11}$$

$$\partial_t \boldsymbol{Q}_i = \boldsymbol{\omega}_i \times \boldsymbol{Q}_i, \tag{12}$$

Details in Hydrodynamics

- Chains are small enough that hydrodynamics also must include terms which capture thermal fluctuations from the fluid. These are included but we won't really discuss them.
- Since the beads are so close together, we include lubrication corrections in the mobility

$$\bar{\mathcal{N}} = \left(\mathcal{N}^{-1} - \mathcal{N}^{-1}_{\text{close particles}} + \left(\mathcal{N}^{\text{asymptotics}}_{\text{close particles}}\right)^{-1}\right)^{-1}$$

and steric repulsion to keep the beads from overlapping

Comparison With experiments

Another Way

Problems With Kirchhoff

1. Unnecessary degrees of freedom (position and orientation of every particle in the chain)
2. Penalty formulation imposes a potentially large time step restriction

New Coordinates

We should be able to model chains using only their unit tangent vectors $\boldsymbol{t}_i$ and a scalar 'twist' θ_i off of a reference axis (more on θ_i in coming slides). Given a set of unit tangent vectors

$$\{\boldsymbol{t}_1, \boldsymbol{t}_2, \cdots, \boldsymbol{t}_N\}$$

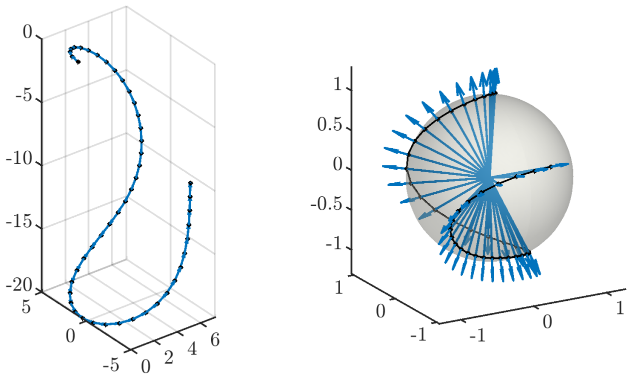
we can find

$$\boldsymbol{x}_i = \boldsymbol{x}_0 + \sum_{j=1}^{i-1} \boldsymbol{t}_i \approx \boldsymbol{x}_0 + \int_0^s \boldsymbol{t}(s')ds'$$

as a map from

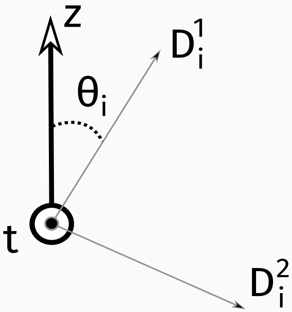
$$\boldsymbol{t} \in S^2 \to \boldsymbol{x} \in \mathbb{R}^3$$

New Coordinates



New Coordinates

For a straight chain pointing *into* the page, we can define ***z*** as a reference axis and measure the local twist θ_i off of this axis.



But what about a curved chain?

Bishop Frame

Recall

$$\partial_s \boldsymbol{t} = \boldsymbol{\Omega} \times \boldsymbol{t}$$

We can write

$$\boldsymbol{\Omega} = m(s)\boldsymbol{t} + \boldsymbol{t} \times \boldsymbol{t}_s$$

where $m(s) = \left(\boldsymbol{D}^1_s\right) \cdot \boldsymbol{D}^2$ is the 'rate of twist'.

The material frame

$$\boldsymbol{Q}(s) = [\boldsymbol{D}^1(s), \boldsymbol{D}^2(s), \boldsymbol{D}^3(s)],$$

is to be determined by the physics of the problem.

But we can define a new ‘intrinsic frame’ (Bishop frame) so that the rate of twist vanishes.

$$\boldsymbol{B}(s) = [\boldsymbol{t}(s), \boldsymbol{u}(s), \boldsymbol{v}(s)] \qquad \text{such that} \tag{13}$$

$$m_B(s) = \boldsymbol{u}_s \cdot \boldsymbol{v} = 0 \tag{14}$$

and

$$\boldsymbol{\Omega}_B = \cancel{m_B(s)\boldsymbol{t}} + \boldsymbol{t} \times \boldsymbol{t}_s$$

Bishop Frame

In the Bishop frame

$$\partial_s \boldsymbol{u} = (\boldsymbol{t} \times \boldsymbol{t}_s) \times \boldsymbol{u} \text{ (no twist)}$$

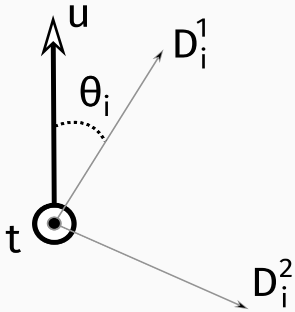
which is integrable as

$$\boldsymbol{u}(s) = \underbrace{\exp\left(s\ \ [\boldsymbol{t} \times \boldsymbol{t}_s]_\times\right)}_{P} \boldsymbol{u}(0), \qquad \boldsymbol{v}(s) = \boldsymbol{t}(s) \times \boldsymbol{u}(s)$$

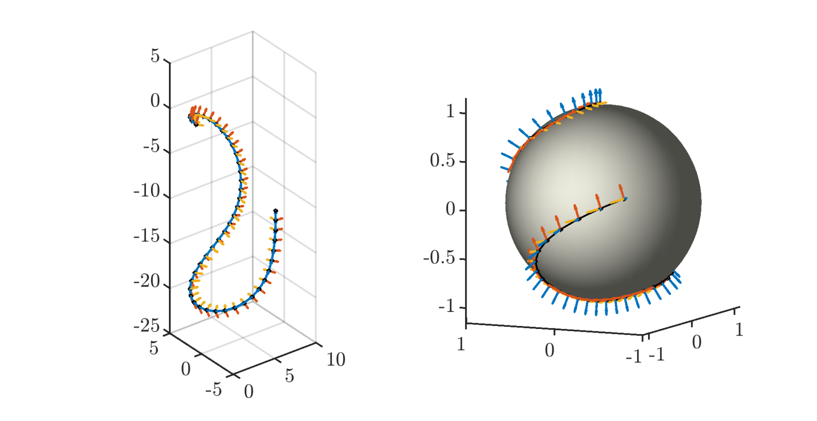
where $\boldsymbol{P}$ is a rotation matrix such that $\boldsymbol{t}(s + ds) = \boldsymbol{P} \cdot \boldsymbol{t}(s)$, or a *parallel transport map*.

Bishop Frame

Given $\boldsymbol{t}(s)$ and $\boldsymbol{u}(0), \boldsymbol{v}(0)$ (which are arbitrary), the Bishop frame is completely determined. We use the bishop frame as a reference frame for measuring θ.



New Coordinates



Bishop Frame

From the Bishop frame and $\theta(s)$, we compute the material frame as

$$D^1 = \cos(\theta)u + \sin(\theta)v \tag{15}$$

$$D^2 = -\sin(\theta)u + \cos(\theta)v \tag{16}$$

Hence

$$m(s) = \left(D^1_s\right) \cdot D^2 = \theta_s$$

and

$$\boldsymbol{\Omega} = \underbrace{\theta_s}_{\Omega_3} t + \underbrace{t \times t_s}_{\Omega_1 D^1 + \Omega_2 D^2} \tag{17}$$

Energy

$$\boldsymbol{\Omega} = \underbrace{\theta_s}_{\Omega_3} \boldsymbol{t} + \underbrace{\boldsymbol{t} \times \boldsymbol{t}_s}_{\Omega_1 \boldsymbol{D}^1 + \Omega_2 \boldsymbol{D}^2}$$

The energy functional for a constrained ($\boldsymbol{x}_s = \boldsymbol{t}$) Kirchhoff rod is

$$E = \frac{1}{2} \int_0^L \kappa_b \left(\Omega_1^2 + \Omega_2^2\right) + \kappa_T \Omega_3^2 + \overbrace{\Lambda(s)}^{\text{Lagrange mult.}} \quad ds \tag{18}$$

$$= \frac{1}{2} \int_0^L \kappa_b \left(||\boldsymbol{t} \times \boldsymbol{t}_s||^2\right) + \kappa_T \left(\theta_s\right)^2 + \Lambda(s) \tag{19}$$

$$= \frac{1}{2} \int_0^L \kappa_b \underbrace{\left(||\boldsymbol{t}_s||^2\right)}_{\text{Euler Beam}} + \kappa_T \left(\theta_s\right)^2 + \Lambda(s) \tag{20}$$

Variation of the energy

We get the torque on out particles from $\boldsymbol{E}$ easily by varying theta

$$\boldsymbol{\tau} = -\frac{\delta}{\delta\theta}\boldsymbol{E} = -\kappa_T\theta_{ss}$$

The force is a bit more nuanced.
We vary the center-line $\boldsymbol{x}(s) \leftarrow \boldsymbol{x}(s) + \delta\boldsymbol{x}(s)$ and compute

$$\boldsymbol{f} = -\frac{\delta \boldsymbol{E}}{\delta \boldsymbol{x}} - \frac{\delta \boldsymbol{E}}{\delta\theta_s}\frac{\delta\theta_s}{\delta \boldsymbol{x}}$$

Variation of the energy

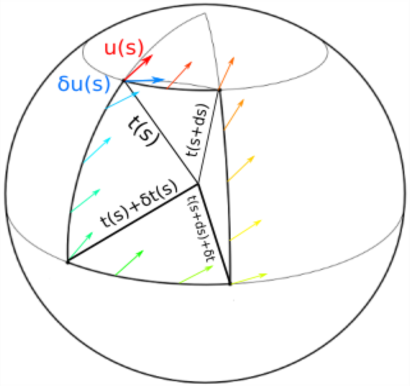
The quantity

$$\frac{\delta\theta_s}{\delta x}$$

is tantamount to the variation of the Bishop frame along centerline

$$\frac{\delta\theta_s}{\delta x} = u_s \triangleleft \frac{\delta u_s}{\delta x}$$

Holonomy



$$\frac{\delta\theta_s}{\delta x} = u \angle \delta u \approx ||t_s \times \delta x_s|| = (t \times t_s) \cdot \delta x_s ds$$

Variation of the energy

$$\boldsymbol{\tau} = -\frac{\delta}{\delta\theta}E = -\kappa_T\theta_{ss} \tag{21}$$

$$\boldsymbol{f} = -\frac{\delta E}{\delta \mathbf{x}} - \frac{\delta E}{\delta \theta_s}\frac{\delta \theta_s}{\delta \mathbf{x}} \tag{22}$$

$$= \kappa_b \mathbf{x}_{ssss} - \kappa_T\Big(\underbrace{\theta_s}_{\text{from } \frac{\delta E}{\delta \theta_s}} \overbrace{(\boldsymbol{t}\times\boldsymbol{t}_s)}^{\text{from } \frac{\delta \theta_s}{\delta \mathbf{x}}}\Big)_s + (\Lambda \boldsymbol{t})_s \tag{23}$$

Next Steps

Open question:
How to do hydrodynamics with constrained chains and twist.