Numerical methods for inextensible slender fibers in Stokes flow

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Outline

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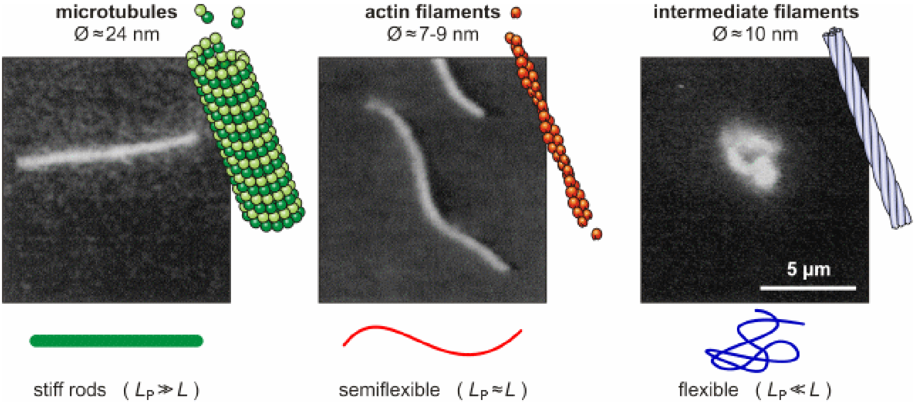
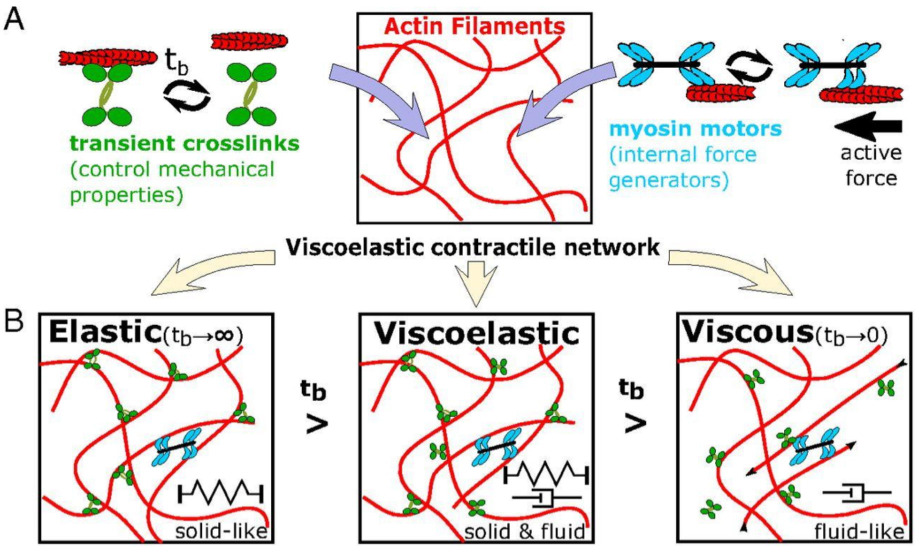
Fibers involved in cell mechanics



Pawlizak and Käs, University of Leipzig

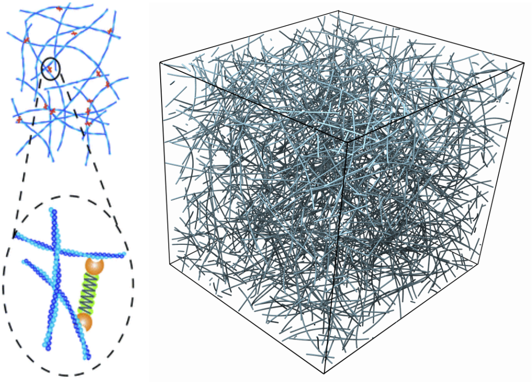
L_p =persistence length, L =fiber length, $a = \epsilon L$ =fiber radius, ϵ =slenderness ratio

Cytoskeleton rheology



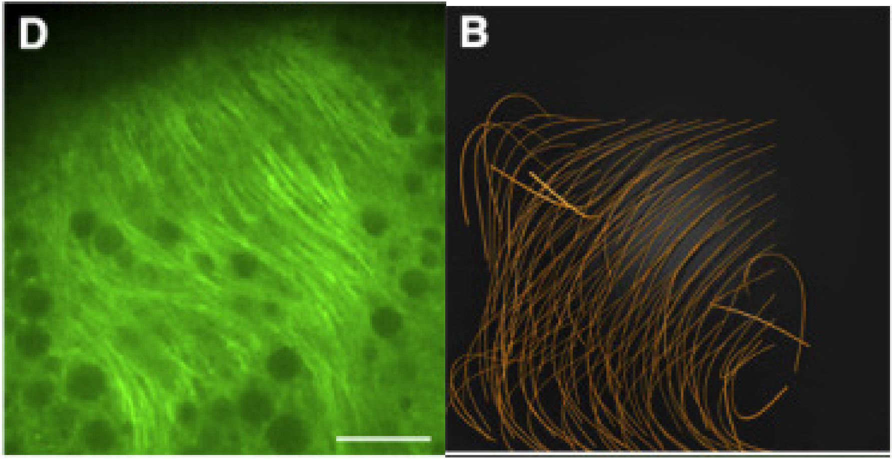
Ahmed and Betz. *PNAS*. (2015)

Cross-linked actin gels



- Very **slender semi-flexible fibers** (aspect ratio $10^2 - 10^4$) suspended in a **viscous solvent**.
- For now **cross linkers** modeled as simple elastic springs.
- **Periodic cyclically sheared** unit cell: **viscoelastic moduli**.

Does nonlocal hydrodynamics matter?



Monteith et al. Biophysics Journal. (2016)

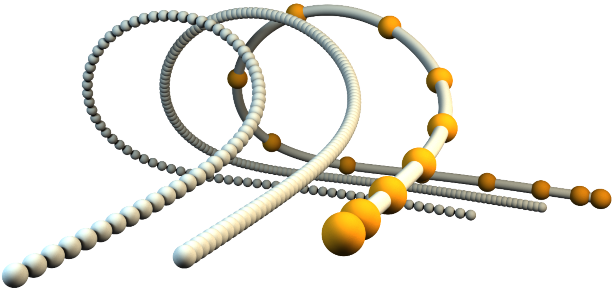
Does nonlocal hydrodynamics matter?

- Sometimes flows created by individual fibers add up constructively to produce **large-scale flows**, which advect network.
- For example, cytoplasmic streaming on previous slide or contraction of a myosin-actin gel (must expel liquid out).
- Flow is generated at scales of fiber thickness: **multiscale problem**.
- Role of **long-ranged (nonlocal) hydrodynamics** unclear for rheology of cross-linked actin gels.
- For background consult:
  Dynamics of Flexible Fibers in Viscous Flows and Fluids, Annual Review of Fluid Mechanics 51:539, Olivia du Roure, Anke Lindner, Ehssan N. Nazockdast, and Michael J. Shelley

Outline

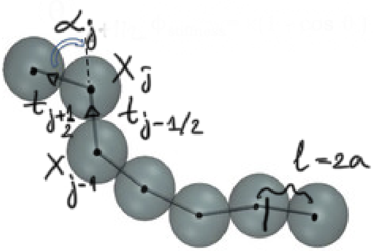
Fiber Representation

Simple approach is to represent a fiber as a **discrete chain** of beads/blobs: **multiblob model**



More efficient approach is to represent a fibers as **continuum curve**
O. Maxian, A. Mogilner and A. Donev, **ArXiv:2007.11728**
An integral-based spectral method for inextensible slender fibers in Stokes flow [1]

Inextensible multiblob chains



Worm-like polymer chain

- Inextensibility: $\|\mathbf{X}_{j+1} - \mathbf{X}_j\| = l \sim a$ (e.g., a or $2a$).
- Tangent vectors: $\boldsymbol{\tau}_{j+1/2} = (\mathbf{X}_{j+1} - \mathbf{X}_j)/l$
- Bending angles: $\cos\alpha_j = \boldsymbol{\tau}_{j+1/2} \cdot \boldsymbol{\tau}_{j-1/2}$
- Elastic energy (bending modulus κ_b)

$$E_b = \frac{2\kappa_b}{l} \sum_{j=1}^{N-1} \sin^2\left(\frac{\alpha_j}{2}\right)$$

Inextensible continuum fibers

- Persistence length due to thermal fluctuations $\xi = 2\kappa_b / (k_B T) \gg l$ gives us a **continuum limit**, $\alpha_j \ll 1$.
- Fiber centerline $\mathbf{X}(s)$ where the **arc length** $0 \leq s \leq L$.
- The tangent vector is $\boldsymbol{\tau} = \partial \mathbf{X} / \partial s = \mathbf{X}_s$, and the **fibers are inextensible**,

$$\boldsymbol{\tau}(s,t) \cdot \boldsymbol{\tau}(s,t) = 1 \quad \forall (s,t).$$

- Bending energy functional is integral of inverse curvature squared:

$$E_b(\mathbf{X}) = \frac{2\kappa_b}{l} \sum_{j=1}^{N-1} \left(\frac{\alpha_j}{2}\right)^2 \quad \Rightarrow \quad E_b[\mathbf{X}(\cdot)] = \frac{\kappa_b}{2} \int ds \, \|\mathbf{X}_{ss}(s)\|^2$$

Bending elasticity

- Bending force $\mathbf{F}_j^{(b)}$ on each blob j in the interior gives us **elastic force density** $\mathbf{f}_b(s,t)$

$$\mathbf{F}_j^{(b)} = -\frac{\partial E_b}{\partial \mathbf{X}_j} = \frac{\kappa_b}{l^3}\left(-\mathbf{X}_{j-2} + 4\mathbf{X}_{j-1} - 6\mathbf{X}_j + 4\mathbf{X}_{j+1} - \mathbf{X}_{j+2}\right)$$

$$\mathbf{F}_b \approx -l\kappa_b\,\mathbf{D}^4\mathbf{X} \quad \Rightarrow \quad \mathbf{f}_b = -\frac{\delta E_{\text{bend}}}{\delta X} = -\kappa_b \mathbf{X}_{ssss}$$

- Endpoints naturally handled discretely, giving in continuum natural BCs for **free fibers**:

$$\mathbf{X}_{ss}\left(0/L\right) = 0, \quad \mathbf{X}_{sss}\left(0/L\right) = 0.$$

- **Tensions** $T_{j+1/2} \to T(s)$ are **unknown** and resist stretching,

$$\boldsymbol{\Lambda}_i = T_{i+1/2}\boldsymbol{\tau}_{i+1/2} - T_{i-1/2}\boldsymbol{\tau}_{i-1/2} \quad \Rightarrow \quad \boldsymbol{\lambda} = \left(T\boldsymbol{\tau}\right)_s.$$

Fluid dynamics

- For multiblob chains in **Stokes flow**, fluid velocity $\mathbf{v}(\mathbf{r}, t)$ satisfies $\boldsymbol{\nabla} \cdot \mathbf{v} = \mathbf{0}$ and

$$\boldsymbol{\nabla}\pi = \eta \boldsymbol{\nabla}^2 \mathbf{v} + \sum_j \mathbf{F}_j \, \delta_a (\mathbf{X}_j - \mathbf{r}),$$

where δ_a is a **regularized delta/blob function** whose width is proportional to a, and

$$\mathbf{F} = -l\kappa_b \, \mathbf{D}^4 \mathbf{X} + \boldsymbol{\Lambda}$$

- Blobs/fiber are advected by fluid

$$\mathbf{U}_j = d\mathbf{X}_j/dt = \int d\mathbf{r} \; \mathbf{v}(\mathbf{r}, t) \, \delta_a (\mathbf{X}_j - \mathbf{r}) \, .$$

- Continuum limit is obvious

$$\boldsymbol{\nabla}\pi (\mathbf{r}, t) = \eta \boldsymbol{\nabla}^2 \mathbf{v}(\mathbf{r}, t) + \int_0^L ds \; \mathbf{f}(s, t) \delta_a (\mathbf{X}(s, t) - \mathbf{r})$$

$$\mathbf{U}(s, t) = \partial_t \mathbf{X}(s, t) = \int d\mathbf{r} \; \mathbf{v}(\mathbf{r}, t) \, \delta_a (\mathbf{X}(s, t) - \mathbf{r})$$

$$\mathbf{f} = -\kappa_b \mathbf{X}_{ssss} + \boldsymbol{\lambda}$$

Multiblob chains in Stokes flow

- We can (temporarily) eliminate the fluid velocity to write an equation for **fiber only**.
- Define the positive semi-definite **hydrodynamic kernel**
$$\mathcal{R}\left(\mathbf{r}_1,\mathbf{r}_2\right)=\int \delta_a\left(\mathbf{r}_1-\mathbf{r}'\right)\mathbb{G}\left(\mathbf{r}',\mathbf{r}''\right)\delta_a\left(\mathbf{r}_2-\mathbf{r}''\right)d\mathbf{r}'d\mathbf{r}'',$$
where $\mathbb{G}$ is the Green's function for (periodic) Stokes flow.
- Define $\mathbf{M}\left(\mathbf{X}\right)\succeq\mathbf{0}$ to be the symmetric positive semidefinite (SPD) **mobility matrix** with blocks
$$\mathbf{M}_{ij}\left(\mathbf{X}_i,\mathbf{X}_j\right)=\mathcal{R}\left(\mathbf{X}_i,\mathbf{X}_j\right)=\mathcal{R}\left(\mathbf{X}_i-\mathbf{X}_j\right).$$
- Discrete dynamics = **inextensibility** +
$$\mathbf{U}=d\mathbf{X}/dt=\mathbf{M}\left(\mathbf{X}\right)\mathbf{F}\left(\mathbf{X}\right)=\mathbf{M}\left(-l\kappa_b\,\mathbf{D}^4\mathbf{X}+\mathbf{\Lambda}\right)$$

Inextensible fibers in Stokes flow

- Define a positive semidefinite **mobility operator**

$$(\mathcal{M}[\mathbf{X}(\cdot)]\,\mathbf{f}(\cdot))(s) = \int_0^L ds'\,\mathcal{R}\left(\mathbf{X}(s), \mathbf{X}(s')\right)\mathbf{f}(s')$$

- Continuum dynamics is a **non-local PDE**

$$\mathbf{U} = \mathbf{X}_t = \mathcal{M}[\mathbf{X}]\left(-\kappa_b \mathbf{X}_{ssss} + \boldsymbol{\lambda}\right)$$
$$\boldsymbol{\tau}(s,t)\cdot\boldsymbol{\tau}(s,t) = 1 \quad \forall(s,t).$$

- Is this PDE well-posed (weak, strong)? Since $\boldsymbol{\lambda}$ only appears inside spatial integrals, this is a sort of first-kind integral equation.
- Recent work by Ohm and Mori defines a "**slender-body PDE**" that is *probably* well-posed (not proven yet for inextensible fibers or for cylindrical fibers with free ends) but too difficult for computation.

Rotne-Prager-Yamakawa kernel

$$\mathcal{R}\left(\mathbf{r}_1,\mathbf{r}_2\right)=\int \delta_a\left(\mathbf{r}_1-\mathbf{r}'\right)\mathbb{G}\left(\mathbf{r}',\mathbf{r}''\right)\delta_a\left(\mathbf{r}_2-\mathbf{r}''\right)d\mathbf{r}'d\mathbf{r}''$$

- Taking the regularization kernel and unbounded Stokes flow

$$\delta_a\left(\mathbf{r}\right)=\left(4\pi a^2\right)^{-1}\delta\left(r-a\right)$$

gives the **Rotne-Prager-Yamakawa (RPY) kernel**

$$\mathcal{R}\left(\mathbf{r}\right)=\begin{cases}\left(8\pi\eta\right)^{-1}\left(\mathcal{S}\left(\mathbf{r}\right)+\dfrac{2a^2}{3}\mathcal{D}\left(\mathbf{r}\right)\right), & r>2a\\ \left(6\pi a\eta\right)^{-1}\left[\left(1-\dfrac{9r}{32a}\right)\mathbf{I}+\left(\dfrac{3r}{32a}\right)\dfrac{\mathbf{r}\otimes\mathbf{r}}{r^2}\right], & r\leq 2a\end{cases}$$

$$\mathcal{S}\left(\mathbf{r}\right)=\frac{1}{8\pi\eta r}\left(\mathbf{I}+\hat{\mathbf{r}}\hat{\mathbf{r}}^T\right)\equiv\mathbb{G},\quad \text{and}\quad \mathcal{D}\left(\mathbf{r}\right)=\frac{1}{8\pi\eta r^3}\left(\mathbf{I}-\hat{\mathbf{r}}\hat{\mathbf{r}}^T\right)$$

Matched asymptotics

$$\left(\mathcal{M}\left[\mathbf{X}\left(\cdot\right)\right]\,\mathbf{f}\left(\cdot\right)\right)(s)=\int_{0}^{L}ds'\,\mathcal{R}\left(\mathbf{X}(s)-\mathbf{X}(s')\right)\mathbf{f}(s')$$

- **Matched asymptotics** gives (away from endpoints)

  $(\mathcal{M}\,\mathbf{f})(s)\approx(\mathcal{M}_{\text{SBT}}\,\mathbf{f})(s)=(\mathcal{M}_{\text{loc}}\,\mathbf{f})(s)+(\mathcal{M}_{\text{FP}}\,\mathbf{f})(s)=$

  $$=\frac{1}{8\pi\mu}\left(\log\left(\frac{(L-s)s}{4a^2}\right)\left(\mathbf{I}+\boldsymbol{\tau}(s)\boldsymbol{\tau}(s)^T\right)+4\mathbf{I}\right)\mathbf{f}(s)$$

  $$+\frac{1}{8\pi\mu}\int_0^L ds'\left(\mathcal{S}\left(\mathbf{X}(s)-\mathbf{X}(s')\right)\mathbf{f}\left(s'\right)-\left(\frac{\mathbf{I}+\boldsymbol{\tau}(s)\boldsymbol{\tau}(s)^T}{|s-s'|}\right)\mathbf{f}(s)\right)$$

- For a special choice of blob radius $a=\left(e^{3/2}/4\right)\epsilon L=1.12\epsilon L$, this formula matches the widely-used **Slender Body Theory** (SBT).
- Our approach automatically works for **multiple fibers**, and also gives us a natural **regularization of the endpoints** (not shown).

Slender body theory

$$\mathcal{M} = \mathcal{M}_{\textbf{loc}} + \mathcal{M}_{\textbf{FP}} = \mathcal{O}\left(\log\left(\frac{(L-s)s}{a^2}\right)\right) + \mathcal{O}(1)$$

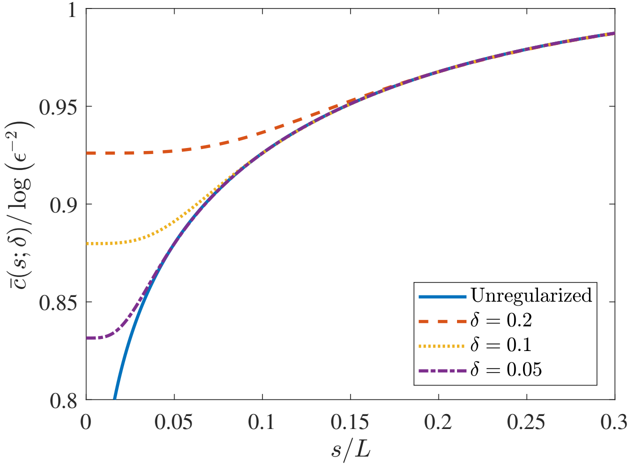
- SBT is great for numerics since it involves **quadratures** that can be computed accurately for smooth $\mathbf{f}$ to **spectral accuracy**.
- Problem 1: The local drag term is logarithmically **singular at endpoints** for cylindrical fibers.
  Many use (unphysical) **ellipsoidal fibers**: $\mathcal{M}_{\text{loc}} = \mathcal{O}(\log(L/a))$.
- Problem 2: The finite-part mobility $\mathcal{M}_{\text{FP}}$ has **spurious negative eigenvalues** for high spatial frequencies, so $\mathcal{M}_{\text{SBT}}$ is **not SPD**, and equations are definitely **not well posed**.
  Previous works starting with Tornberg+Shelley [2] use **artificial regularization** of the integrand in $\mathcal{M}_{\text{FP}}$.

Limitations of slender body theory

- Problem 1 compounds problem 2, and for fibers of slenderness $\epsilon \sim 10^{-2}$ all of SBT seems to break down.
- Problem 2 solution: One can avoid matched asymptotics entirely by constructing **special quadrature methods** for the RPY kernel (using ideas of af Klinteberg, Barnett, Tornberg).
- Problem 1 temporary "solution":
  Make fibers **tapered near the endpoints** ($\delta \sim 0.05 - 0.1 \gg \epsilon$)

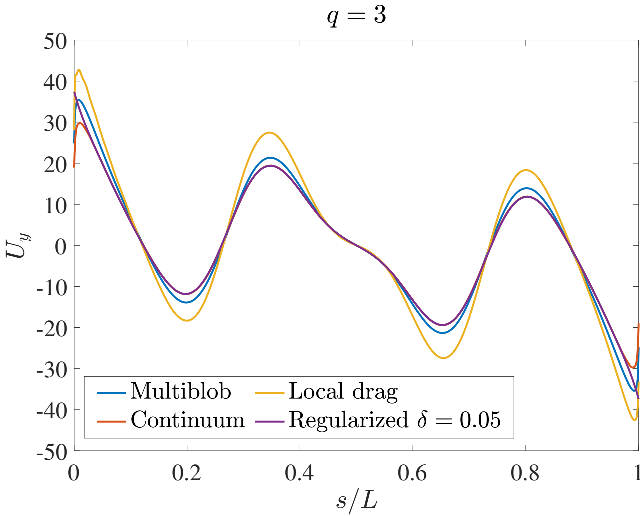
Regularization of end points

$$\left(\mathcal{M}_{\text{loc}}\,\mathbf{f}\right)(s) \sim c(s)\left(\mathbf{I} + \boldsymbol{\tau}(s)\boldsymbol{\tau}(s)^T\right)\mathbf{f}(s), \quad \text{where} \quad c(s) \sim \log\left(\frac{(L-s)s}{a(s)^2}\right)$$



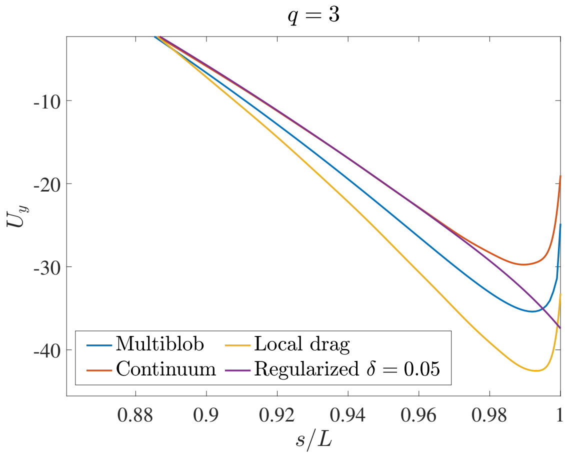
Note: For ellipsoidal fibers $c(s)$ is constant ($= 1$ in this plot).

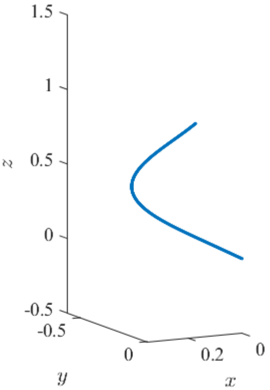
Cylindrical fibers



Velocity at $t = 0$ for fiber with $\epsilon = 10^{-3}$ relaxing due to bending elasticity.

Cylindrical endpoints





Lack of smoothness in the solution near the endpoints – our **endpoint regularization** removes that problem.

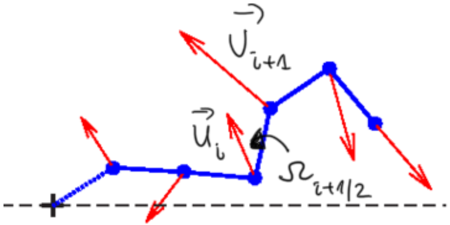
Outline

Tension equation

$$\mathbf{X}_t = \mathcal{M}[\mathbf{X}]\left(-\kappa_b \mathbf{X}_{ssss} + \boldsymbol{\lambda}\right) \quad \text{and} \quad \boldsymbol{\lambda} = \left(T\boldsymbol{\tau}\right)_s$$

- Traditional approach (Tornberg+Shelley) is to solve **tension equation**
$$\boldsymbol{\tau} \cdot \boldsymbol{\tau} = \mathbf{X}_s \cdot \mathbf{X}_s = 1 \quad \Rightarrow \quad \left(\mathbf{X}_t\right)_s \cdot \mathbf{X}_s = 0 \quad \text{non-local BVP}$$
- Tension equation is linear in $T(s)$ but very nonlinear in $\mathbf{X}$ and its derivatives, causing **aliasing issues**.
- Method does not strictly enforce inextensibility numerically, requiring adding a **penalty for stretching**.
- To solve these problems, let us first go back to multiblobs for simplicity, and then take continuum limits.

Inextensible motions



$$\frac{\mathbf{U}_i - \mathbf{U}_{i-1}}{\Delta s} = \boldsymbol{\Omega}_{j+1/2} \times \boldsymbol{\tau}_{j+1/2} \quad \Rightarrow$$

$$\mathbf{U} = \mathbf{K}\boldsymbol{\Omega}^{\perp} = \left[\mathbf{U}_0, \cdots, \mathbf{U}_0 + \Delta s \sum_{j=0}^{i-1} \boldsymbol{\Omega}^{\perp}_{j+1/2} \times \boldsymbol{\tau}_{j+1/2}, \cdots \right] \rightarrow$$

$$\left(\mathcal{K}\left[\mathbf{X}(\cdot)\right] \boldsymbol{\Omega}^{\perp}(\cdot) \right)(s) = \mathbf{U}(s) = \mathbf{U}(0) + \int_0^s ds' \left(\boldsymbol{\Omega}^{\perp}(s') \times \boldsymbol{\tau}(s') \right).$$

Principle of virtual work

- **Principle of virtual work**: Constraint forces should do no work for any inextensible motion of the fiber:

$$\boldsymbol{\Lambda}^T \mathbf{U} = \left(\mathbf{K}^T \boldsymbol{\Lambda}\right)^T \boldsymbol{\Omega}^\perp = 0 \quad \forall \boldsymbol{\Omega}^\perp \quad \Rightarrow \quad \mathbf{K}^T \boldsymbol{\Lambda} = \mathbf{0}$$

$$\mathbf{K}^T \boldsymbol{\Lambda} = \left[\sum_{j=0}^{N} \boldsymbol{\Lambda}_j, \cdots, \Delta s \left(\sum_{j=i}^{N} \boldsymbol{\Lambda}_j \right) \times \boldsymbol{\tau}_{i+1/2}, \cdots \right] \rightarrow$$

$$\left(\mathcal{K}^\star \left[\mathbf{X}(\cdot)\right] \boldsymbol{\lambda}(\cdot)\right)(s) = \left[\int_0^L ds' \, \boldsymbol{\lambda}(s'), \left(\int_s^L ds' \, \boldsymbol{\lambda}(s') \right) \times \boldsymbol{\tau}(s) \right] = 0 \, \forall s.$$

- We can express this in terms of tension

$$\forall s \quad \int_s^L ds' \, \boldsymbol{\lambda}(s') = -T(s) \boldsymbol{\tau}(s) \quad \Rightarrow \quad \boldsymbol{\lambda} = (T \boldsymbol{\tau})_s$$

but the principle of virtual work is an **integral constraint** rather than a pointwise constraint.

Continuum equations

- New **weak formulation of inextensibility** constraint:

$$\mathbf{X}_t = \mathcal{K}[\mathbf{X}]\,\mathbf{\Omega}^{\perp} = \mathcal{M}[\mathbf{X}]\,(-\kappa_b \mathbf{X}_{ssss} + \boldsymbol{\lambda})$$

$$\mathcal{K}^{\star}[\mathbf{X}]\,\boldsymbol{\lambda} = \mathbf{0}$$

$$\partial_t \boldsymbol{\tau} = \mathbf{\Omega}^{\perp} \times \boldsymbol{\tau}$$

$$\mathbf{X}(s,t) = \mathbf{X}(0,t) + \int_0^s ds'\, \boldsymbol{\tau}\,(ds',\, t)$$

- Two improvements:
  - Evolve tangent vector $\boldsymbol{\tau}$ rather than $\mathbf{X}$: **strictly inextensible**.
  - Impose tension equation **weakly** rather than pointwise.

Outline

Chebyshev discretization

- Choose normal vectors $\mathbf{n}_{1/2} \perp \boldsymbol{\tau}$ (arbitrary):

$$\partial_t \boldsymbol{\tau} = \boldsymbol{\Omega}^{\perp} \times \boldsymbol{\tau} = g_1(s)\mathbf{n}_1(s) + g_2(s)\mathbf{n}_2(s)$$

- Expand all functions into a **truncated Chebyshev series** on a grid of N nodes using $T_k(s)$ as a basis for L_2:

$$g_1(s) = \sum_{j=0}^{N-1} \alpha_{1j} T_j(s) \quad \text{kinematic vars } \boldsymbol{\alpha} = \{\mathbf{U}(0), \alpha_{1j}, \alpha_{2j}\}$$

- Simple change of integration vars gives

$$\mathbf{U} = \mathcal{K}[\mathbf{X}]\,\boldsymbol{\alpha} = \mathbf{U}(0) + \sum_{j=0}^{N-1} \int_0^s ds' \,\left(\alpha_{1j} T_j(s')\mathbf{n}_1(s') + \alpha_{2j} T_j(s')\mathbf{n}_2(s')\right)$$

Chebyshev discretization contd.

- Principle of virtual work says $\forall j$

$$\mathcal{K}^{\star}\left[\mathbf{X}\right]\boldsymbol{\lambda}=\begin{pmatrix}\int_0^L \boldsymbol{\lambda}(s)\,ds\\ \int_0^L ds\,\boldsymbol{\lambda}(s)\cdot\int_0^s ds'\,T_j(s')\mathbf{n}_{1/2}(s')\end{pmatrix}:=\mathbf{0}$$

- **Collocation discretization** of mobility equation gives a **saddle point system** for $\boldsymbol{\lambda}$ and α,

$$\begin{pmatrix}-\mathbf{M}(\mathbf{X}) & \mathbf{K}(\mathbf{X})\\ \mathbf{K}^{*}(\mathbf{X}) & \mathbf{0}\end{pmatrix}\begin{pmatrix}\boldsymbol{\lambda}\\ \alpha\end{pmatrix}=\begin{pmatrix}\mathbf{M}(\mathbf{X})(-\kappa_b\mathbf{D}_{BC}^4\mathbf{X})\\ \mathbf{0}\end{pmatrix}$$

  but should try Galerkin in the future.

- Bending elasticity+BCs discretized using **rectangular collocation**
  Driscoll and Hale. *IMA J. Numer. Anal.* (2016).

Temporal discretization

- Use multistep **extrapolation** for nonlinear terms:

$$\mathbf{X}^{n+1/2,p} = \frac{3}{2}\mathbf{X}^{n} - \frac{1}{2}\mathbf{X}^{n-1}$$
$$\boldsymbol{\lambda}^{n+1/2,p} = 2\boldsymbol{\lambda}^{n-1/2} - \boldsymbol{\lambda}^{n-3/2}.$$

- **Split** mobility into **local and non-local** parts, $\mathbf{M} = \mathbf{M}_L + \mathbf{M}_{NL}$:

$$\begin{aligned}\mathbf{K}^{n+1/2,p}\boldsymbol{\alpha}^{n+1/2} =& \mathbf{M}_L^{n+1/2,p}\left(-\frac{\kappa_b}{2}\mathbf{D}_{BC}^{4}\left(\mathbf{X}^{n} + \mathbf{X}^{n+1,\star}\right) + \boldsymbol{\lambda}^{n+1/2}\right)\\ &+\mathbf{M}_{NL}^{n+1/2,p}\left(-\kappa_b\mathbf{D}_{BC}^{4}\mathbf{X}^{n+1/2,p} + \boldsymbol{\lambda}^{n+1/2,p}\right)\\ \left(\mathbf{K}^{\star}\right)^{n+1/2,p}\boldsymbol{\lambda}^{n+1/2} =& \mathbf{0},\end{aligned}$$

where $\mathbf{X}^{n+1,\star} = \mathbf{X}^{n} + \Delta t\mathbf{K}^{n+1/2,*}\boldsymbol{\alpha}^{n+1/2}$.

- Actual fiber update is **strictly inextensible**

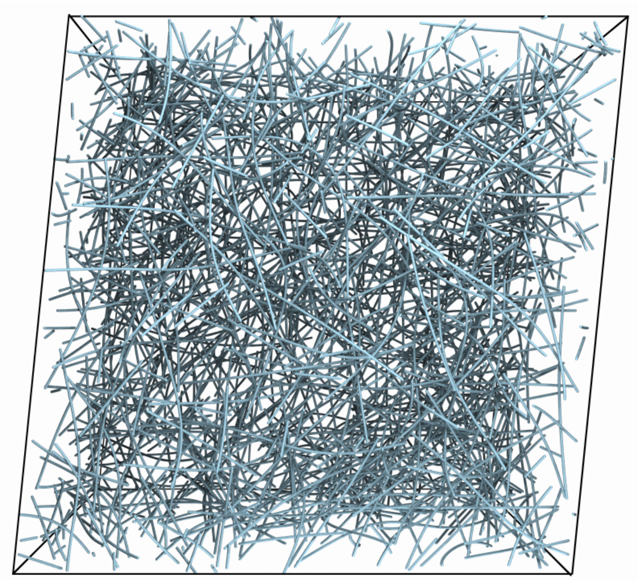
$$\boldsymbol{\tau}^{n+1} = \text{rotate}\left(\boldsymbol{\tau}^{n}, \Delta t\boldsymbol{\Omega}^{n+1/2,p}\right).$$

The gory details

1. For dense suspensions, supplement 2nd order temporal method with additional **1-5 GMRES iterations** for stability.
2. Evaluate long-ranged hydrodynamic interactions between Chebyshev nodes in linear time using **Positively Split Ewald** (PSE) method (FFT based for triply periodic), also works for **deformed/sheared unit cell** (Fiore *et al. J. Chem. Phys.* (2017) [3]).
   Future work: Ewald methods with other BCs.
3. For **nearby fibers**, use specialized **near-singular quadrature** (af Klinteberg and Barnett. BIT Num. Math. 2020 [4]) to get 2-3 digits.
4. For finite-part self interaction of one fiber with itself use specialized **quadrature with singularity-removal** by Anna Karin-Tornberg.
   Future work: Develop fast accurate quadratures for RPY kernel to *avoid* matched asymptotics (SBT).

Outline

Actin network/gel



Cross Linkers

- Cross linker (CL) between $\mathbf{X}^{(i)}(s_i^*)$ and $\mathbf{X}^{(j)}(s_j^*)$, with $R = \left\|\mathbf{X}^{(i)}(s_i^*) - \mathbf{X}^{(j)}(s_j^*)\right\|$
- Model cross-linker as just a spring with **Gaussian smoothing** to preserve spectral accuracy (std$= \sigma \sim 0.1L$):

$$\mathbf{f}^{(\mathrm{CL},i)}(s) = -K_c \left(1 - \frac{\ell}{R}\right) \delta_\sigma(s - s_i^*) \int_0^L ds' \left(\mathbf{X}^{(i)}(s) - \mathbf{X}^{(j)}(s')\right) \delta_\sigma(s' - s_j^*)$$

- Cross linker is force and torque-free.
- Randomly generated dense network of CLs (16 attachment sites per site) to give about 12 CLs per fiber (elastic network).
- Future work: Allow for dynamic binding/unbinding of CLs, reduce smoothing σ, treat CL elasticity implicitly.

Cross-linked network

Rheology

Apply linear shear flow $\mathbf{v}_0(x, y, z) = \dot{\gamma}_0 \cos(\omega t) y$ and measure the **visco-elastic stress** induced by the fibers and cross links:

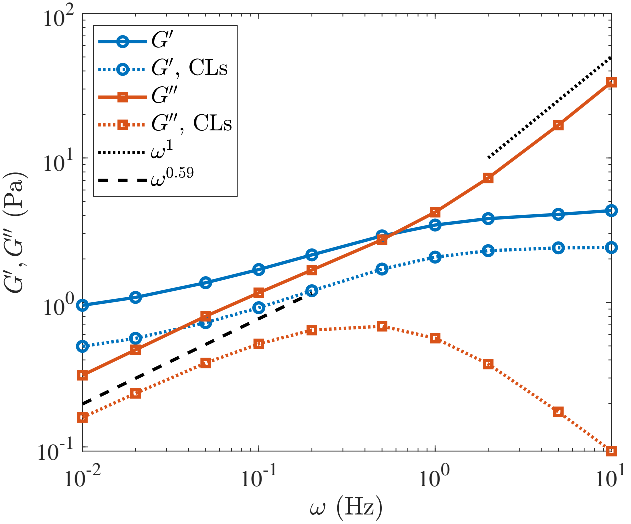
$$\boldsymbol{\sigma}^{(i)} = \frac{1}{V} \sum_{\text{fibers}} \int_0^L ds\, \mathbf{X}^i(s) \left(\mathbf{f}_b(s) + \boldsymbol{\lambda}(s)\right)^T$$

$$\boldsymbol{\sigma}^{(\text{CL})} = \frac{1}{V} \sum_{\text{CLs}=(i,j)} \int_0^L ds \left(\mathbf{X}^i(s)\mathbf{f}^{(CL,i)}(s) + \mathbf{X}^j(s)\mathbf{f}^{(CL,j)}(s)\right)$$

$$\frac{\sigma_{21}}{\gamma_0} = G' \sin(\omega t) + G'' \cos(\omega t) = \text{elastic+viscous}.$$

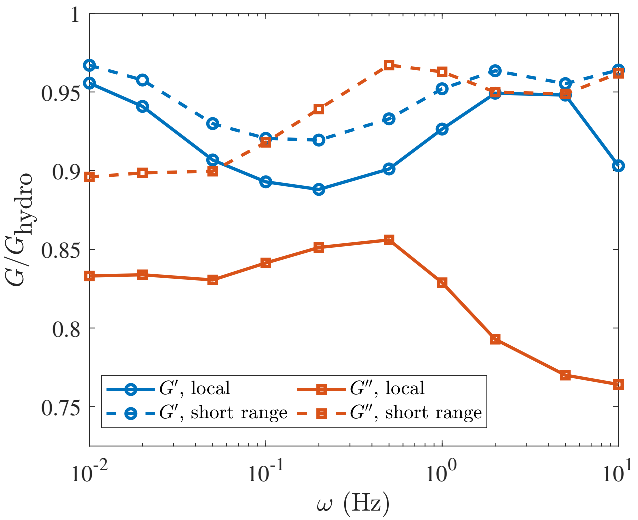
$$G' = \frac{2}{\gamma_0 T} \int_0^T \sigma_{21} \sin(\omega t)\, dt \qquad G'' = \frac{2}{\gamma_0 T} \int_0^T \sigma_{21} \cos(\omega t)\, dt.$$

Viscoelastic moduli



Elastic modulus G' and **viscous** modulus G'' for 700 fibers + 8400 CLs

Nonlocal hydrodynamics



Reduction in viscoelastic moduli with **only local drag** or **only inter-fiber nonlocal hydrodynamics**.

Rheology summary

- Network relaxation time $\tau_c \approx 0.5 - 1s$
- For $\omega^{-1} \gg \tau_c$
  - Quasi-steady; elastic solid
  - Small effect of nonlocal hydrodynamics ($\sim 10\%$)
- For $\omega^{-1} \approx \tau_c$.
  - $G'' \approx G$
  - Max change in G' due to *inter-fiber* hydro
- For $\omega^{-1} \ll \tau_c$.
  - Fibers and CLs “frozen”; network behaves like a viscous fluid
  - $G'' \gg G'$; up to 25% change due to *intra-fiber* hydro.

Outline

Twist

- For given force densities $\mathbf{f}(s,t)$ and **parallel torque** densities $m(s,t)$ along the fiber centerlines,

$$\boldsymbol{\nabla}\pi = \eta\boldsymbol{\nabla}^2\mathbf{v} + \int_0^L ds\left[\mathbf{f}(s) + m(s)\boldsymbol{\tau}(s)\frac{\boldsymbol{\nabla}}{2}\times\right]\delta_a\left(\mathbf{X}(s)-\mathbf{r}\right),$$

$$\Omega^{\parallel}(s) = \boldsymbol{\tau}(s)\cdot\int d\mathbf{r}\,\frac{\boldsymbol{\nabla}}{2}\times\mathbf{v}\left(\mathbf{r},t\right)\delta_a\left(\mathbf{X}(s)-\mathbf{r}\right)$$

- Open question: Should fiber exert **perpendicular torques** on the fluid (and vice versa)?
- Previous work using multiblob-type methods makes **m** a 3D vector (Peskin, Lim, Olson, Keaveny) and uses **Kirchhoff rod theory** (triad based) but we use scalar twist angle (inspired by work in group of Jorn Dunkel).

Bishop frame

- To each point along the fiber we attach an orthonormal triad $\mathbf{B}(s) = [\boldsymbol{\tau}(s), \mathbf{a}(s), \mathbf{b}(s)]$ called the **Bishop frame**, which satisfies the *no-twist condition*:

$$\mathbf{a}_s \cdot \mathbf{b} = 0 \quad \Rightarrow \quad \partial_s \mathbf{a} = (\boldsymbol{\tau} \times \boldsymbol{\tau}_s) \times \mathbf{a}$$

- Represent the **twist** of the *i*-th fiber by the angle $\theta(s)$ between the material frame of the cross section of the fiber and the Bishop cross section.

$$\mathbf{f} = -\kappa_b \mathbf{X}_{ssss} + \kappa_t \left(\theta_s \left(\boldsymbol{\tau} \times \boldsymbol{\tau}_s\right)\right)_s + \boldsymbol{\lambda},$$
$$m = \kappa_T \theta_{ss}$$

- Bishop frame evolves even if $\Omega^{\|} = 0$,

$$\partial_t \theta \left(s, t\right) = \partial_t \theta(s = 0, t) + \int_0^s ds' \, \boldsymbol{\Omega}_s \left(s', t\right) \cdot \boldsymbol{\tau} \left(s', t\right).$$

Why twist is hard

- Can we solve Bishop frame ODE efficiently with spectral methods?
- Temporal integration is challenging because of **extreme stiffness**: twist relaxation much faster than bend relaxation.
  Maybe twist is always in **quasi-equilibrium**?
- When **does twist matter**?
  Flagella, formins twisting growing actin filaments, macroscopic chirality in cells, and ?

Thermal fluctuations (Brownian Motion)

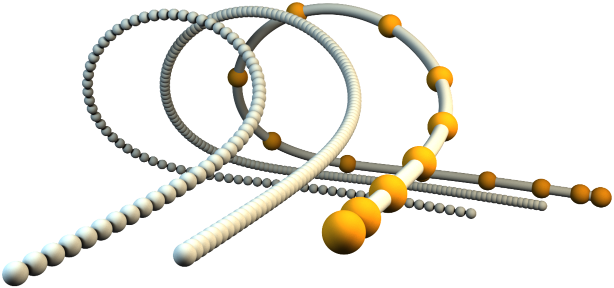
- Fluctuating hydrodynamics gives the fluctuating Stokes equations

$$\rho\partial_t \mathbf{v} + \boldsymbol{\nabla}\pi = \eta\boldsymbol{\nabla}^2\mathbf{v} + \boldsymbol{\nabla}\cdot\left(\sqrt{2\eta k_B T}\,\boldsymbol{\mathcal{W}}\right) + \int_0^L ds\, \mathbf{f}(s,t)\delta_a\left(\mathbf{X}(s,t) - \mathbf{r}\right).$$

- The **thermal fluctuations** (Brownian motion of fiber) are driven by a white-noise **stochastic stress tensor** $\boldsymbol{\mathcal{W}}(\mathbf{r}, t)$.
- Open mathematical question:
  - What is the **overdamped** limit $\eta/\rho \to \infty$ (steady Stokes)?
  - Can one even write a **multiplicative noise SPDE** for the fiber motion that makes mathematical sense?

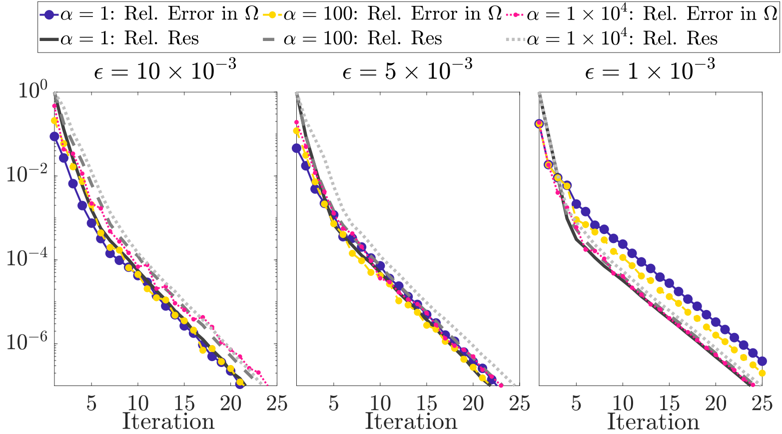
Brownian multiblob chains

For **Brownian multiblob chains** there are no mathematical issues so start there!



Multiblob chains: Linear Algebra

Since multiblobs have lots of DOFs per fiber, LA matters



GMRES convergence for implicit solver for a curved fiber, using **local-drag SBT as a preconditioner** (from B. Sprinkle).

References

Ondrej Maxian, Alex Mogilner, and Aleksandar Donev.
An integral-based spectral method for inextensible slender fibers in Stokes flow.
Submitted to Phys. Rev. F, ArXiv preprint 2007.11728, 2020.

Anna-Karin Tornberg and Michael J Shelley.
Simulating the dynamics and interactions of flexible fibers in stokes flows.
Journal of Computational Physics, 196(1):8–40, 2004.

A. M. Fiore, F. Balboa Usabiaga, A. Donev, and J. W. Swan.
Rapid sampling of stochastic displacements in brownian dynamics simulations.
J. Chem. Phys., 146(12):124116, 2017.
Software available at `https://github.com/stochasticHydroTools/PSE`.

Ludvig af Klinteberg and Alex H Barnett.
Accurate quadrature of nearly singular line integrals in two and three dimensions by singularity swapping.
BIT Numerical Mathematics, pages 1–36, 2020.