Numerical methods for inextensible slender fibers in Stokes flow

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Outline

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2. Fibers in Stokes flow
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5. Actin gels
6. Future Challenges
   - Adding twist
   - Adding Brownian motion
Motivation

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Motivation

Fibers involved in cell mechanics

- **microtubules** (Ø ≈ 24 nm)
- **actin filaments** (Ø ≈ 7-9 nm)
- **intermediate filaments** (Ø ≈ 10 nm)

**Stiff rods** \( (L_p \gg L) \)

**Semiflexible** \( (L_p \approx L) \)

**Flexible** \( (L_p \ll L) \)

\( L_p \) = persistence length, \( L \) = fiber length, \( a = \epsilon L \) = fiber radius, \( \epsilon \) = slenderness ratio

Pawlizak and Käs, University of Leipzig
Cytoskeleton rheology

Motivation

Ahmed and Betz. PNAS. (2015)

Transient crosslinks (control mechanical properties)

Myosin motors (internal force generators)

Viscoelastic contractile network

Elastic ($t_b \to \infty$)

Viscoelastic

Viscous ($t_b \to 0$)

Ahmed and Betz. PNAS. (2015)
Motivation

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**.
Motivation

Does nonlocal hydrodynamics matter?

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:
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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**


*An integral-based spectral method for inextensible slender fibers in Stokes flow* [1]
Inextensible multiblob chains

- **Inextensibility:** $\|X_{j+1} - X_j\| = l \sim a$ (e.g., $a$ or $2a$).
- **Tangent vectors:**
  $$\tau_{j+1/2} = (X_{j+1} - X_j)/l$$
- **Bending angles:**
  $$\cos \alpha_j = \tau_{j+1/2} \cdot \tau_{j-1/2}$$
- **Elastic energy (bending modulus $\kappa_b$)**
  $$E_b = \frac{2\kappa_b}{l} \sum_{j=1}^{N-1} \sin^2 \left( \frac{\alpha_j}{2} \right)$$
Persistence length due to thermal fluctuations $\xi = \frac{2\kappa_b}{k_B T} \gg l$ gives us a continuum limit, $\alpha_j \ll 1$.

Fiber centerline $X(s)$ where the arc length $0 \leq s \leq L$.

The tangent vector is $\tau = \partial X / \partial s = X_s$, and the fibers are inextensible,

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

Bending energy functional is integral of inverse curvature squared:

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

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

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

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

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

\[
\mathbf{X}_{ss}(0/L) = 0, \quad \mathbf{X}_{sss}(0/L) = 0.
\]

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

\[
\Lambda_i = T_{i+1/2} \tau_{i+1/2} - T_{i-1/2} \tau_{i-1/2} \quad \Rightarrow \quad \lambda = (T \tau)_s.
\]
For multiblob chains in **Stokes flow**, fluid velocity $v(r, t)$ satisfies $\nabla \cdot v = 0$ and

$$
\nabla \pi = \eta \nabla^2 v + \sum_j F_j \delta_a (X_j - r),
$$

where $\delta_a$ is a **regularized delta/blob function** whose width is proportional to $a$, and

$$
F = -l \kappa_b D^4 X + \Lambda
$$

Blobs/fiber are advected by fluid

$$
U_j = dX_j/dt = \int dr \ v(r, t) \delta_a (X_j - r).
$$

Continuum limit is obvious

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

$$
U (s, t) = \partial_t X (s, t) = \int dr \ v(r, t) \delta_a (X(s, t) - r)
$$

$$
f = -\kappa_b X_{ssss} + \lambda$$
We can (temporarily) eliminate the fluid velocity to write an equation for fiber only.

Define the positive semi-definite hydrodynamic kernel

\[ \mathcal{R}(r_1, r_2) = \int \delta_a (r_1 - r') \mathcal{G}(r', r'') \delta_a (r_2 - r'') \, dr' \, dr'', \]

where \( \mathcal{G} \) is the Green’s function for (periodic) Stokes flow.

Define \( \mathbf{M}(\mathbf{X}) \succeq \mathbf{0} \) to be the symmetric positive semidefinite (SPD) mobility matrix with blocks

\[ M_{ij}(X_i, X_j) = \mathcal{R}(X_i, X_j) = \mathcal{R}(X_i - X_j). \]

Discrete dynamics = inextensibility +

\[ \mathbf{U} = d\mathbf{X}/dt = \mathbf{M}(\mathbf{X}) \mathbf{F}(\mathbf{X}) = \mathbf{M} \left( -I_{\kappa_b} D^4 \mathbf{X} + \Lambda \right) \]
Inextensible fibers in Stokes flow

- Define a positive semidefinite **mobility operator**
  \[
  (\mathcal{M} [X(\cdot)] f(\cdot))(s) = \int_0^L ds' \mathcal{R}(X(s), X(s')) f(s')
  \]

- Continuum dynamics is a **non-local PDE**
  \[
  U = X_t = \mathcal{M} [X] (-\kappa_b X_{ssss} + \lambda)
  \]
  \[
  \tau(s, t) \cdot \tau(s, t) = 1 \quad \forall (s, t).
  \]

- Is this PDE well-posed (weak, strong)? Since \( \lambda \) 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.
\[ \mathcal{R} (r_1, r_2) = \int \delta_a (r_1 - r') \mathcal{G} (r', r'') \delta_a (r_2 - r'') \ dr' dr'' \]

- Taking the regularization kernel and unbounded Stokes flow
  \[ \delta_a (r) = (4\pi a^2)^{-1} \delta (r - a) \]
  gives the Rotne-Prager-Yamakawa (RPY) kernel

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

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

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

- **Matched asymptotics** gives (away from endpoints)
  \[ (\mathcal{M} \mathbf{f})(s) \approx (\mathcal{M}_{\text{SBT}} \mathbf{f})(s) = (\mathcal{M}_{\text{loc}} \mathbf{f})(s) + (\mathcal{M}_{\text{FP}} \mathbf{f})(s) = \]
  \[ = \frac{1}{8\pi\mu} \left( \log \left( \frac{(L - s)s}{4a^2} \right) \left( \mathbf{I} + \mathbf{\tau}(s)\mathbf{\tau}(s)^T \right) + 4\mathbf{I} \right) \mathbf{f}(s) \]
  \[ + \frac{1}{8\pi\mu} \int_0^L ds' \left( \mathcal{S}(\mathbf{X}(s) - \mathbf{X}(s')) \mathbf{f}(s') - \left( \frac{\mathbf{I} + \mathbf{\tau}(s)\mathbf{\tau}(s)^T}{|s - s'|} \right) \mathbf{f}(s) \right) \]

- For a special choice of blob radius \( a = (e^{3/2}/4) \epsilon L = 1.12\epsilon L \), 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).
Fibers in Stokes flow

Slender body theory

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

- SBT is great for numerics since it involves quadratures that can be computed accurately for smooth \( f \) to spectral accuracy.
- Problem 1: The local drag term is logarithmically singular at endpoints for cylindrical fibers. Many use (unphysical) ellipsoidal fibers: \( \mathcal{M}_{\text{loc}} = \mathcal{O} \left( \log \left( \frac{L}{a} \right) \right) \).
- 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** ($\delta \sim 0.05 - 0.1 \gg \epsilon$)
\( (\mathcal{M}_{\text{loc}} f)(s) \sim c(s) \left( I + \tau(s)\tau(s)^T \right) f(s), \) where \( c(s) \sim \log \left( \frac{(L - s)s}{a(s)^2} \right) \)

Note: For ellipsoidal fibers \( c(s) \) is constant (= 1 in this plot).
Velocity at $t = 0$ for fiber with $\epsilon = 10^{-3}$ relaxing due to bending elasticity.
Lack of smoothness in the solution near the endpoints – our endpoint regularization removes that problem.
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\[ \mathbf{X}_t = \mathcal{M} [\mathbf{X}] \left( -\kappa_b \mathbf{X}_{ssss} + \lambda \right) \quad \text{and} \quad \lambda = (T \tau)_s \]

- Traditional approach (Tornberg+Shelley) is to solve tension equation
  \[ \tau \cdot \tau = \mathbf{X}_s \cdot \mathbf{X}_s = 1 \quad \Rightarrow \quad (\mathbf{X}_t)_s \cdot \mathbf{X}_s = 0 \quad \text{non-local BVP} \]

- 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

\[
\frac{U_i - U_{i-1}}{\Delta s} = \Omega_{j+1/2} \times \tau_{j+1/2} \quad \Rightarrow
\]

\[
U = K\Omega^\perp = \left[ U_0, \ldots, U_0 + \Delta s \sum_{j=0}^{i-1} \Omega_{j+1/2}^\perp \times \tau_{j+1/2}, \ldots \right] \rightarrow
\]

\[
(K [X (\cdot)] \Omega^\perp (\cdot)) (s) = U (s) = U (0) + \int_0^s ds' \left( \Omega^\perp (s') \times \tau (s') \right).
\]
**Principle of virtual work:** Constraint forces should do no work for any inextensible motion of the fiber:

\[ \Lambda^T U = (K^T \Lambda)^T \Omega^\perp = 0 \quad \forall \Omega^\perp \implies K^T \Lambda = 0 \]

\[ K^T \Lambda = \left[ \sum_{j=0}^{N} \Lambda_j, \cdots, \Delta s \left( \sum_{j=i}^{N} \Lambda_j \right) \times \tau_{i+1/2}, \cdots \right] \rightarrow \]

\[ (K^* [X (\cdot)] \Lambda (\cdot))(s) = \left[ \int_0^L ds' \lambda (s') , \left( \int_s^L ds' \lambda (s') \right) \times \tau(s) \right] = 0 \forall s. \]

We can express this in terms of tension

\[ \forall s \int_s^L ds' \lambda (s') = -T(s) \tau(s) \implies \lambda = (T \tau)_s \]

but the principle of virtual work is an **integral constraint** rather than a pointwise constraint.
New **weak formulation of inextensibility** constraint:

\[
X_t = \mathcal{K}[X] \Omega^\perp = \mathcal{M}[X] (-\kappa_b X_{ssss} + \lambda)
\]

\[
\mathcal{K}^* [X] \lambda = 0
\]

\[
\partial_t \tau = \Omega^\perp \times \tau
\]

\[
X(s, t) = X(0, t) + \int_0^s ds' \tau(ds', t)
\]

**Two improvements:**

- Evolve tangent vector \( \tau \) rather than \( X \): **strictly inextensible**.
- Impose tension equation **weakly** rather than pointwise.
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Choose normal vectors $n_{1/2} \perp \tau$ (arbitrary):

$$\partial_t \tau = \Omega \perp \times \tau = g_1(s)n_1(s) + g_2(s)n_2(s)$$

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

$$g_1(s) = \sum_{j=0}^{N-1} \alpha_1 j T_j(s) \text{ kinematic vars } \alpha = \{U(0), \alpha_1 j, \alpha_2 j\}$$

Simple change of integration vars gives

$$U = \mathcal{K} [X] \alpha = U(0) + \sum_{j=0}^{N-1} \int_0^s ds' \left( \alpha_1 j T_j(s')n_1(s') + \alpha_2 j T_j(s')n_2(s') \right)$$
Chebyshev discretization contd.

- Principle of virtual work says $\forall j$
  \[ \mathcal{K}^*[X] \lambda = \left( \int_0^L \lambda(s) \, ds \right) \left( \int_0^L ds \, \lambda(s) \cdot \int_0^s ds' \, T_j(s') n_{1/2}(s') \right) := 0 \]

- **Collocation discretization** of mobility equation gives a saddle point system for $\lambda$ and $\alpha$,
  \[
  \begin{pmatrix}
  -M(X) & K(X) \\
  K^*(X) & 0
  \end{pmatrix}
  \begin{pmatrix}
  \lambda \\
  \alpha
  \end{pmatrix} =
  \begin{pmatrix}
  M(X)(-\kappa_b D_{BC}^4 X) \\
  0
  \end{pmatrix}
  \]

  but should try Galerkin in the future.

- Bending elasticity + BCs discretized using **rectangular collocation**

Temporal discretization

- Use multistep \textit{extrapolation} for nonlinear terms:
  \[
  X^{n+1/2,p} = \frac{3}{2} X^n - \frac{1}{2} X^{n-1}
  \]
  \[
  \lambda^{n+1/2,p} = 2 \lambda^{n-1/2} - \lambda^{n-3/2}.
  \]

- \textbf{Split} mobility into \textit{local and non-local} parts, \( M = M_L + M_{NL} \):
  \[
  K^{n+1/2,p} \alpha^{n+1/2} = M_L^{n+1/2,p} \left( -\frac{\kappa_b}{2} D_{BC}^4 \left( X^n + X^{n+1,*}_n \right) + \lambda^{n+1/2} \right) + M_{NL}^{n+1/2,p} \left( -\kappa_b D_{BC}^4 X^{n+1/2,p} + \lambda^{n+1/2,p} \right)
  \]
  \[
  (K^*)^{n+1/2,p} \lambda^{n+1/2} = 0,
  \]
  where \( X^{n+1,*} = X^n + \Delta t K^{n+1/2,*} \alpha^{n+1/2} \).

- Actual fiber update is \textit{strictly inextensible}
  \[
  \tau^{n+1} = \text{rotate} \left( \tau^n, \Delta t \Omega^{n+1/2,p} \right).
  \]
For dense suspensions, supplement 2nd order temporal method with additional 1-5 GMRES iterations for stability.

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.

For nearby fibers, use specialized near-singular quadrature (af Klinteberg and Barnett. BIT Num. Math. 2020 [4]) to get 2-3 digits.

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).
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Actin network/gel
Cross Linkers

- Cross linker (CL) between $X^{(i)}(s^*_i)$ and $X^{(j)}(s^*_j)$, with
  \[ R = \|X^{(i)}(s^*_i) - X^{(j)}(s^*_j)\| \]

- Model cross-linker as just a spring with **Gaussian smoothing** to preserve spectral accuracy (std= $\sigma \sim 0.1L$):
  \[
  f^{(CL,i)}(s) = -K_c \left(1 - \frac{l}{R}\right) \delta_\sigma(s - s^*_i) \int_0^L ds' \left(X^{(i)}(s) - X^{(j)}(s')\right) \delta_\sigma(s' - s^*_j)
  \]

- 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 $\sigma$, treat CL elasticity implicitly.
Rheology

Apply linear shear flow $v_0(x, y, z) = \dot{\gamma}_0 \cos(\omega t)y$ and measure the visco-elastic stress induced by the fibers and cross links:

$$\sigma^{(i)} = \frac{1}{V} \sum_{\text{fibers}} \int_0^L ds X^i(s) (f_b(s) + \lambda(s))^T$$

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

$$\frac{\sigma_{21}}{\dot{\gamma}_0} = G' \sin(\omega t) + G'' \cos(\omega t) = \text{elastic+viscous.}$$

$$G' = \frac{2}{\gamma_0 T} \int_0^T \sigma_{21} \sin(\omega t) \, dt \quad G'' = \frac{2}{\gamma_0 T} \int_0^T \sigma_{21} \cos(\omega t) \, dt.$$
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 $\tau_c \approx 0.5 - 1\text{s}$
- 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.
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For given force densities \( f(s, t) \) and **parallel torque** densities \( m(s, t) \) along the fiber centerlines,

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

\[
\Omega^\parallel(s) = \tau(s) \cdot \int dr \frac{\nabla}{2} \times v(r, t) \delta_a (X(s) - r)
\]

- 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 $\mathbf{B}(s) = [\mathbf{r}(s), \mathbf{a}(s), \mathbf{b}(s)]$ called the Bishop frame, which satisfies the no-twist condition:
  \[ \mathbf{a}_s \cdot \mathbf{b} = 0 \quad \Rightarrow \quad \partial_s \mathbf{a} = (\mathbf{r} \times \mathbf{r}_s) \times \mathbf{a} \]
- 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.
  \[ \mathbf{f} = -\kappa_b \mathbf{X}_{ssss} + \kappa_t \left( \theta_s (\mathbf{r} \times \mathbf{r}_s) \right)_s + \lambda, \]
  \[ m = \kappa \mathbf{r} \theta_{ss} \]
- Bishop frame evolves even if $\Omega^\parallel = 0$,
  \[ \partial_t \theta(s, t) = \partial_t \theta(s = 0, t) + \int_0^s ds' \Omega_s (s', t) \cdot \mathbf{r} (s', t). \]
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 ?
Fluctuating hydrodynamics gives the fluctuating Stokes equations
\[ \rho \partial_t v + \nabla \pi = \eta \nabla^2 v + \nabla \cdot \left( \sqrt{2\eta k_B T} \mathcal{W} \right) \]
\[ + \int_0^L ds \, f(s, t) \delta_a (X(s, t) - r). \]

The thermal fluctuations (Brownian motion of fiber) are driven by a white-noise stochastic stress tensor \( \mathcal{W}(r, t) \).

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?
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 \texttt{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.

Anna-Karin Tornberg and Michael J Shelley.
Simulating the dynamics and interactions of flexible fibers in stokes flows.

Rapid sampling of stochastic displacements in brownian dynamics simulations.
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.