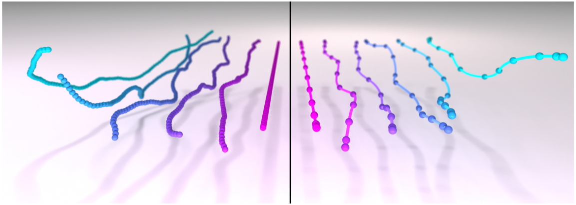
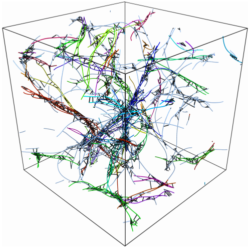
Simulations of semiflexible fiber suspensions with Brownian fluctuations, hydrodynamic interactions, and steric repulsion

Ondrej Maxian
Flatiron CTPCGI Workshop

June 13, 2024



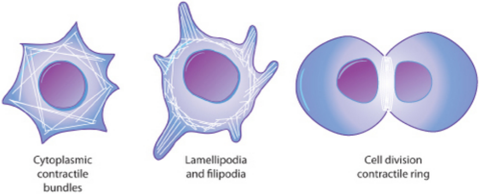


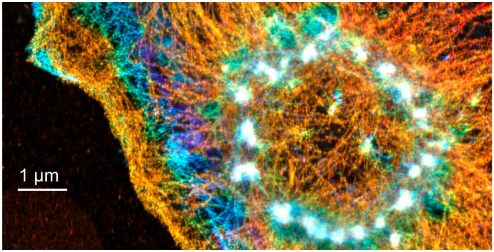
Aleksandar Donev (d. 2023)

Actin cytoskeleton

Cross-linked network of *inextensible, slender, fluctuating* filaments

- Dictate cell's shape and ability to move and divide
- Interact through the background solvent





Nature education, Herron et al. *Nat Commun.* (2022)

Deterministic evolution

Fiber shape $\mathbb{X}(s)$ associated with bending energy density ($\ell_p = \kappa/(k_B T)$)

$$\mathcal{E}^{(\kappa)}[\mathbb{X}] = \frac{\kappa}{2} \int_0^L \partial_s^2 \mathbb{X}(s) \cdot \partial_s^2 \mathbb{X}(s)\, ds$$

and associated force density

$$\mathbf{f}^{(\kappa)} = -\frac{\delta \mathcal{E}^{(\kappa)}}{\delta \mathbb{X}} = -\kappa \partial_s^4 \mathbb{X}$$

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Using mobility $\boldsymbol{\mathcal{M}}[\mathbb{X}]$ (hydrodynamics), evolution equation is

$$\partial_t \mathbb{X} = \boldsymbol{\mathcal{M}} \left(\mathbf{f}^{(\kappa)} + \boldsymbol{\lambda} + \mathbf{f}^{(\mathrm{ext})} \right)$$

Constraint force $\boldsymbol{\lambda}(s)$ enforces $\boldsymbol{\tau}(s) \cdot \boldsymbol{\tau}(s) = 1$, where $\boldsymbol{\tau} = \partial_s \mathbb{X}$.

Continuum kinematics

Differentiate constraint $\rightarrow \partial_t \boldsymbol{\tau} \cdot \boldsymbol{\tau} = 0 \rightarrow \partial_t \boldsymbol{\tau} = \boldsymbol{\Omega} \times \boldsymbol{\tau}$

$$\partial_t \mathbb{X}(s) = \mathbf{U}_{\mathrm{MP}} + \int_{L/2}^{s} \left(\boldsymbol{\Omega}\left(s'\right) \times \boldsymbol{\tau}\left(s'\right) \right) \, ds' := \left(\mathcal{K} \boldsymbol{\alpha} \right)(s),$$

where $\mathbf{U}_{\mathrm{MP}} = \mathbf{U}(s = L/2)$ and $\boldsymbol{\alpha} = \left(\boldsymbol{\Omega}(\cdot), \mathbf{U}_{\mathrm{MP}} \right)$

- Tangent vectors performing rotations on unit sphere
- We can turn into *discrete* rotations

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Principle of virtual work $\rightarrow$ closed system ($\boldsymbol{\mathcal{K}}^* = L^2$ adjoint of $\boldsymbol{\mathcal{K}}$)

$$\mathcal{P} = \langle \boldsymbol{\mathcal{K}}\boldsymbol{\alpha}, \boldsymbol{\lambda} \rangle = \int_0^L \left(\boldsymbol{\mathcal{K}}\boldsymbol{\alpha}\right)(s') \cdot \boldsymbol{\lambda}(s') \, ds' := \langle \boldsymbol{\alpha}, \boldsymbol{\mathcal{K}}^* \boldsymbol{\lambda} \rangle = 0$$

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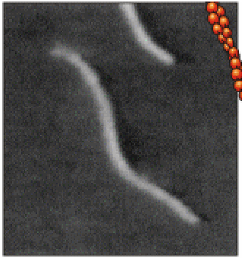
Saddle point system for $(\boldsymbol{\lambda}, \boldsymbol{\alpha})$

$$\begin{pmatrix} -\boldsymbol{\mathcal{M}} & \mathcal{K} \\ \mathcal{K}^* & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda} \\ \boldsymbol{\alpha} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mathcal{M}}(-\delta \mathcal{E}^{(\kappa)} / \delta \mathbb{X}) \\ \mathbf{0} \end{pmatrix},$$

Discretization challenges

Actin filaments are *semiflexible* $\ell_p \gtrsim L$ (smooth)

- Spectral methods desirable
- How to write overdamped Langevin dynamics? (usually discrete)
- Hydrodynamics? (want to be continuous)



$L = 5\ \mu\text{m},\ \ell_p/L \approx 3$

Pawlizak and Käs, University of Leipzig., Ward et al. (Dogic lab) *Nat. Mat. (2015)*

Discretization philosophy

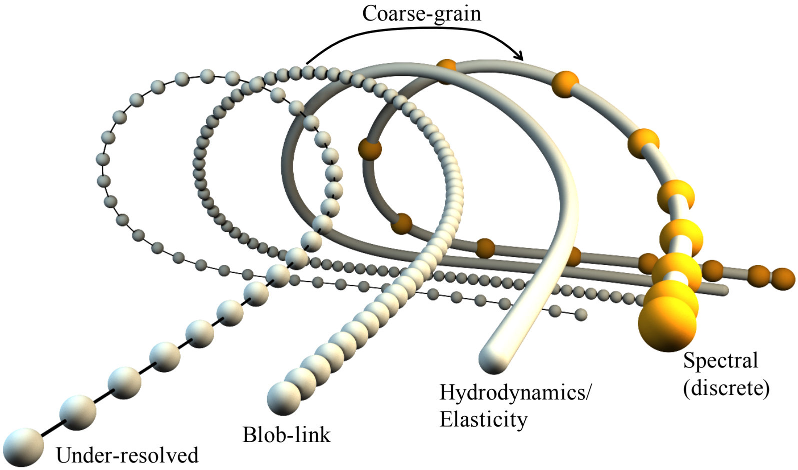
Observed fiber shapes are *smooth* $\rightarrow$ spectral methods

- Represent fiber by N_x Chebyshev collocation nodes $\mathbf{X}$
- Build polynomial *interpolant* $\mathbb{X}(s)$ from $\mathbf{X}$
- Interpolant $\rightarrow$ quadratures for hydrodynamics, bending energy
- Discrete DOFs $\rightarrow$ overdamped Langevin equation for fluctuations

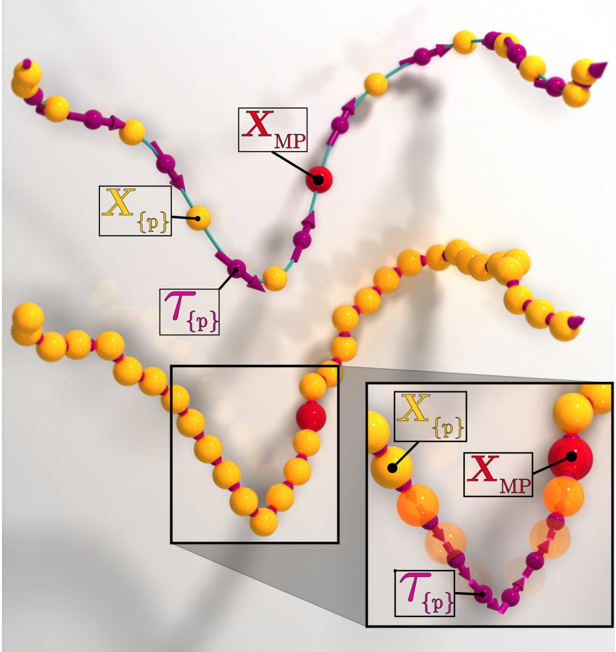
Improve on existing "blob-link" models for fluctuating hydro

- Spatial DOFs no longer tied to resolving hydro!

Big idea: mix continuum and discrete



Spectral discretization



Building spectral discretization

DOFs: $\boldsymbol{\tau}$ at N nodes of type 1 (no EPs) Chebyshev grid, $\mathbf{X}_{\mathrm{MP}}$

- Chebyshev polynomial $\boldsymbol{\tau}(s)$ constrained by $\|\boldsymbol{\tau}(s_j)\| = 1$
- Obtain $\mathbb{X}(s)$ by integrating $\boldsymbol{\tau}(s)$ on $N_x = N + 1$ point grid (type 2, with EPs). Set $\mathbf{X}_{\{i\}} = \mathbb{X}(s_i)$.
- Defines set of nodes $\mathbf{X}_{\{i\}}$ and invertible mapping

$$\mathbf{X} = \mathcal{X}\begin{pmatrix}\boldsymbol{\tau} \\ \mathbf{X}_{\mathrm{MP}}\end{pmatrix}$$

- Gives natural discretization for $\mathbf{K}$

$$\partial_t \mathbf{X} = \mathcal{X}\begin{pmatrix}\mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}\end{pmatrix}\begin{pmatrix}\boldsymbol{\Omega} \\ \mathbf{U}_{\mathrm{MP}}\end{pmatrix} := \mathcal{X}\bar{\mathbf{C}}\boldsymbol{\alpha} := \mathbf{K}\boldsymbol{\alpha}$$

Discrete saddle point system

We need an SPD mobility matrix ($\mathbb{R}^n$). How to think about this?

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Discretize L^2 inner product

$$\langle \mathbf{X}, \boldsymbol{\lambda} \rangle_{L^2} = \mathbf{X}^T \mathbf{E}_u^T \mathbf{W}_u \mathbf{E}_u \boldsymbol{\lambda} := \mathbf{X}^T \widetilde{\mathbf{W}} \boldsymbol{\lambda} := \mathbf{X}^T \underbrace{\boldsymbol{\Lambda}}_{\text{“Force”}}$$

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The work done in fluid is

$$\begin{aligned} \langle \mathbf{f}, \mathbf{U} \rangle_{L^2} &= \langle \widetilde{\mathbf{W}}^{-1} \mathbf{F}, \mathbf{M} \widetilde{\mathbf{W}}^{-1} \mathbf{F} \rangle_{L^2} \\ &= \mathbf{F}^T \widetilde{\mathbf{W}}^{-1} \widetilde{\mathbf{W}} \mathbf{M} \widetilde{\mathbf{W}}^{-1} \mathbf{F} = \mathbf{F}^T \mathbf{M} \widetilde{\mathbf{W}}^{-1} \mathbf{F} \geq 0 \end{aligned}$$

so $\widetilde{\mathbf{M}} := \mathbf{M} \widetilde{\mathbf{W}}^{-1}$ is an SPD matrix acting on force.

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Write saddle point system over force

$$\begin{pmatrix} -\widetilde{\mathbf{M}} & \mathbf{K} \\ \mathbf{K}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\Lambda} \\ \alpha \end{pmatrix} = \begin{pmatrix} -\widetilde{\mathbf{M}} \left(\partial \mathcal{E}^{(\kappa)} / \partial \mathbf{X} \right) \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} -\widetilde{\mathbf{M}} \mathbf{L} \mathbf{X} \\ \mathbf{0} \end{pmatrix}$$

Discrete Langevin equation

Saddle point system over forces

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Deterministic dynamics (eliminate $\boldsymbol{\Lambda}$)

$$\partial_t \mathbf{X} = -\widehat{\mathbf{N}}\mathbf{L}\mathbf{X}, \qquad \widehat{\mathbf{N}} = \mathbf{K}\left(\mathbf{K}^T \widetilde{\mathbf{M}}^{-1} \mathbf{K}\right)^{\dagger} \mathbf{K}^T$$

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Deterministic dynamics + time reversibility $\rightarrow$ Langevin equation

$$\partial_t \mathbf{X} = -\widehat{\mathbf{N}}\mathbf{L}\mathbf{X} + k_B T \partial_{\mathbf{X}} \cdot \widehat{\mathbf{N}} + \sqrt{2 k_B T}\,\widehat{\mathbf{N}}^{1/2}\mathcal{W}(t)$$

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Samples from equilibrium distribution

$$P_{\text{eq}}(\boldsymbol{\tau}) = Z^{-1}\exp\left(-\mathcal{E}^{(\kappa)}(\boldsymbol{\tau})/k_B T\right)\prod_{p=1}^{N}\delta\left(\boldsymbol{\tau}_{\{p\}}^T\boldsymbol{\tau}_{\{p\}} - 1\right)$$

Solving the discrete Langevin equation

Deterministic dynamics + time reversibility → Langevin equation

$$\partial_t \mathbf{X} = - \underbrace{\widehat{\mathbf{N}}\mathbf{L}\mathbf{X}}_{\text{Backward Euler}} + \underbrace{k_B T \partial_{\mathbf{X}} \cdot \widehat{\mathbf{N}}}_{\text{Midpoint integrator}} + \underbrace{\sqrt{2 k_B T} \widehat{\mathbf{N}}^{1/2}}_{\text{Saddle point solve}} \mathcal{W}(t)$$

- Drift term captured *in expectation* by midpoint scheme

Solving the discrete Langevin equation

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- Drift term captured *in expectation* by midpoint scheme
- $\widehat{\mathbf{N}}^{1/2}$ captured via saddle point solve ($\mathbf{W} \sim \mathcal{N}(0,1)$)

$$\begin{pmatrix} -\widetilde{\mathbf{M}} & \mathbf{K} \\ \mathbf{K}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{\Lambda} \\ \boldsymbol{\alpha} \end{pmatrix} = \begin{pmatrix} -\widetilde{\mathbf{M}}\mathbf{L}\mathbf{X} + \sqrt{\frac{2k_B T}{\Delta t}}\widetilde{\mathbf{M}}^{1/2}\mathbf{W} \\ \mathbf{0} \end{pmatrix}$$

$$\Rightarrow \partial_t \mathbf{X} = \text{Deterministic} + \sqrt{\frac{2k_B T}{\Delta t}}\widehat{\mathbf{N}}^{1/2}\mathbf{W}$$

- Last thing: compute actions of $\widetilde{\mathbf{M}}$ and $\widetilde{\mathbf{M}}^{1/2}$

Mobility: regularized singularities

Immersed boundary style approach

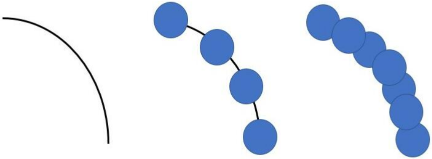
- Represent fiber as a chain of beads (blobs)
- Each bead exerts a regularized force on the fluid

$$-\nabla p(\mathbf{x}) + \mu \Delta \mathbf{u}(\mathbf{x}) = -\delta_{\hat{a}}(\mathbf{x} - \mathbf{y})$$

- Define fluid velocity at bead center as

$$\mathbf{U}(\mathbf{y}) = \int \mathbf{u}(\mathbf{x}) \delta_{\hat{a}}(\mathbf{x} - \mathbf{y}) \, d\mathbf{y}$$

- Automatically SPD



Rotne-Prager-Yamakawa (RPY) mobility

$\delta_{\hat{a}}$ is a δ function on the surface of a sphere of radius $\hat{a}$

- Solution derived analytically using Fourier techniques

$$8\pi\mu\mathbf{M}_{\mathrm{RPY}}\left(\mathbf{x},\mathbf{x}_0;\hat{a}\right)=\mathbf{S}\left(\mathbf{x}-\mathbf{x}_0\right)+\frac{2\hat{a}^2}{3}\mathbf{D}\left(\mathbf{x}-\mathbf{x}_0\right)\quad\left(R\geq 2\hat{a}\right)$$

$$\mathbf{S}\left(\mathbf{r}\right)=\frac{\mathbf{I}+\hat{\mathbf{r}}\hat{\mathbf{r}}}{r}\qquad\mathbf{D}\left(\mathbf{r}\right)=\frac{\mathbf{I}-3\hat{\mathbf{r}}\hat{\mathbf{r}}}{r^3}$$

- Correction when $R\leq 2\hat{a}$ known & simple

Rotne and Prager. *J. Chem. Phys.* (1969).

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Velocity on fiber i is given by

$$\mathbf{U}^{(i)}(s) = \sum_j \int_0^L \mathbf{M}_{\text{RPY}}\left(\mathbb{X}^{(i)}(s), \mathbb{X}^{(j)}(s'); \hat{a}\right) \mathbf{f}^{(j)}(s')\, ds'$$

- Applies for any fiber, not just self
- Equivalent to SBT for specific choice of $\hat{a} \approx 1.1204a$

Rotne and Prager. *J. Chem. Phys.* (1969).

Hydrodynamic mobility: upsampled reference

The (i, j) block of $\widetilde{\mathbf{M}}$ is the determined by the action

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- Resulting mobility matrix (and square root!)

$$\widetilde{\mathbf{M}}_{\text{ref}} = \widetilde{\mathbf{W}}^{-1}\mathbf{E}_u^T\mathbf{W}_u\widetilde{\mathbf{M}}_{\text{RPY},u}\mathbf{W}_u\mathbf{E}_u\widetilde{\mathbf{W}}^{-1}$$

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- Apply $\widetilde{\mathbf{M}}_{\mathrm{RPY},u}^{(1/2)}$ fast using positively-split Ewald method (GPU)

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$$\widetilde{\mathbf{M}}_{\text{ref}}^{1/2} = \widetilde{\mathbf{W}}^{-1}\mathbf{E}_u^T\mathbf{W}_u\widetilde{\mathbf{M}}_{\text{RPY},u}^{1/2}$$

- Apply $\widetilde{\mathbf{M}}_{\text{RPY},u}^{(1/2)}$ fast using positively-split Ewald method (GPU)
- Problem: accuracy (# oversampled) limited by self term

Fiore et al. *J. Chem. Phys.* (2017).

Replacing the self term

Make the self term more efficient through special quadrature scheme

$$\int_0^L \mathbf{M}_{\text{RPY}}\left(\mathbb{X}(s), \mathbb{X}(s')\right) \mathbf{f}(s')\, ds'$$

$$= \underbrace{\int_{|s-s'|>2\hat{a}} \left(\mathbf{S}\left(\mathbb{X}(s), \mathbb{X}(s')\right) + \frac{2\hat{a}^2}{3} \mathbf{D}\left(\mathbb{X}(s), \mathbb{X}(s')\right) \right) \mathbf{f}\left(s'\right)\, ds'}_{\text{Special quadrature (based on singularity subtraction)}}$$

$$+ \frac{1}{8\pi\mu} \underbrace{\int_{|s-s'|\leq 2\hat{a}} \left(\left(\frac{4}{3\hat{a}} - \frac{3R\left(\mathbb{X}(s), \mathbb{X}(s')\right)}{8\hat{a}^2} \right) \mathbf{I} + \frac{\mathbf{R}\widehat{\mathbf{R}}\left(\mathbb{X}(s), \mathbb{X}(s')\right)}{8\hat{a}^2} \right) \mathbf{f}(s')\, ds'.}_{\text{Gauss-Legendre quadrature}}$$

Total cost independent of ϵ

- SQ scheme independent of ϵ
- Gauss-Legendre actually requires less points as $\epsilon \to 0$
- Not guaranteed SPD; symmetrize and truncate eigs $\to \widetilde{\mathbf{M}}_{\text{SQS}}$
- Good for local mobility: $\widetilde{\mathbf{M}} = \text{BDiag}\left\{ \widetilde{\mathbf{M}}_{\text{SQS}} \right\}$

Nonlocal mobility

Two options

$$\begin{aligned} \text{(Oversamp)} \quad & \widetilde{\mathbf{M}}_{\text{ref}} = \widetilde{\mathbf{W}}^{-1} \mathbf{E}_u^T \mathbf{W}_u \widetilde{\mathbf{M}}_{\text{RPY},u} \mathbf{W}_u \mathbf{E}_u \widetilde{\mathbf{W}}^{-1} \\ \text{(SQS)} \quad & \widetilde{\mathbf{M}} = \widetilde{\mathbf{M}}_{\text{ref}} - \text{BDiag}\left\{\widetilde{\mathbf{M}}_{\text{ref}}\right\} + \text{BDiag}\left\{\widetilde{\mathbf{M}}_{\text{SQS}}\right\}, \end{aligned}$$

SQS for many fibers not guaranteed SPD

- Even for exact quadrature

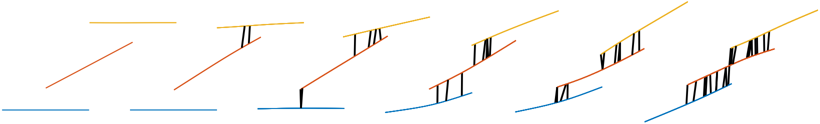
Need something more complicated

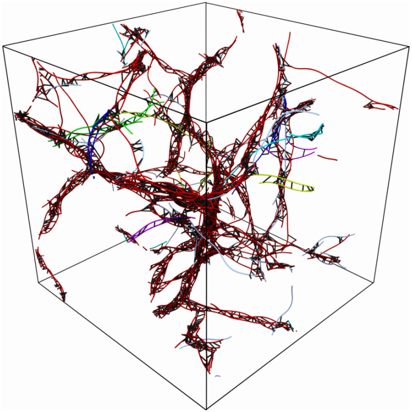
- Split into near + far field, special quad on near?

Dynamics of bundling in cross-linked actin networks

Couple the fibers to moving cross linkers (CLs, elastic springs)

- CLs bind fibers, pulling them closer together
- Ratcheting action creates bundles

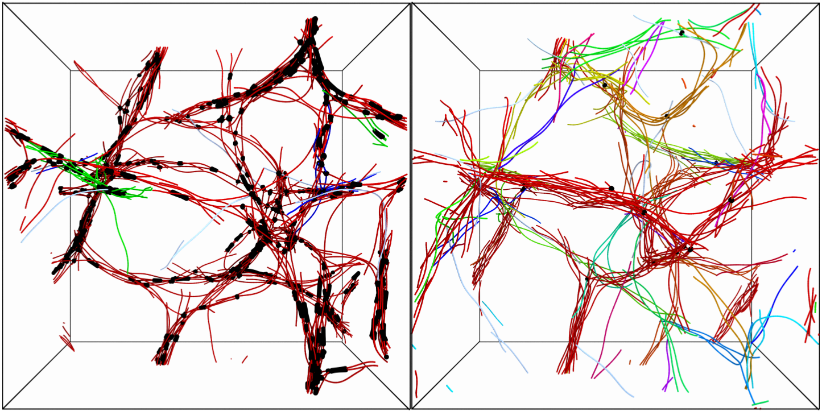




Bundling with sterics

Number of contacts reduced by 99% using "soft" erf potential (Gaussian force)

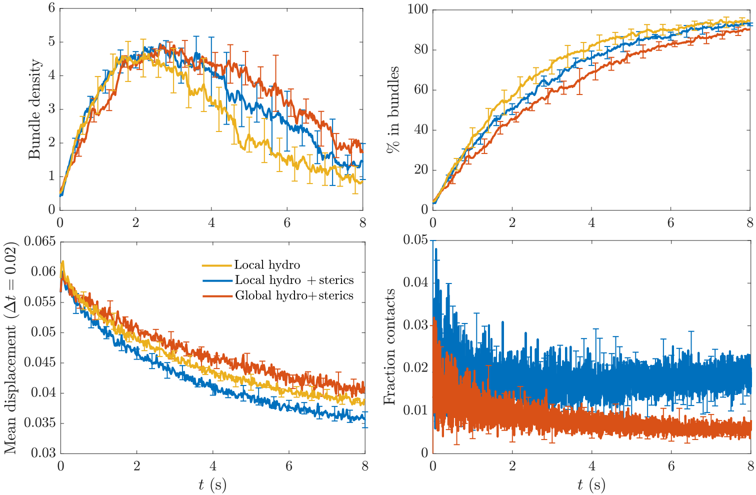
- But 5× time step reduction required



Sterics and hydrodynamics: small Δt

- Hydrodynamics reduces speed of bundling
- Reduces # of contacts

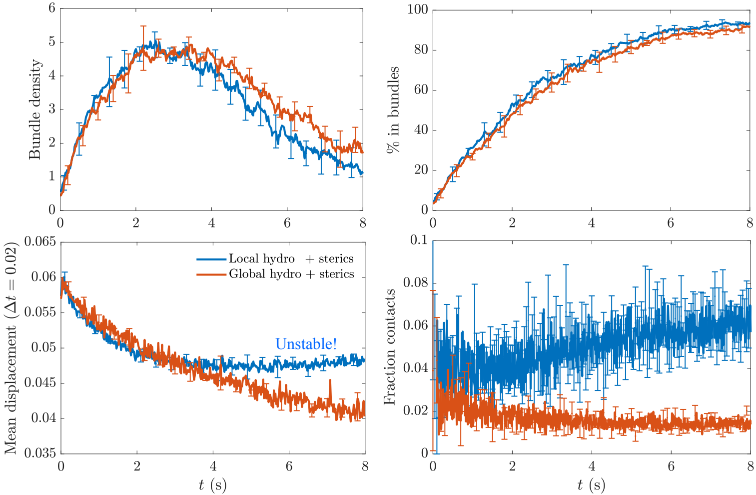
$$\Delta t = 2 \times 10^{-5}$$



Sterics and hydrodynamics: larger Δt

- Larger time step size with hydro (but more expensive)

$$\Delta t = 5 \times 10^{-5}$$



Conclusions

Developed algorithm for slender fiber simulations with

- Thermal fluctuations
- Hydrodynamic interactions
- Steric repulsion

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Future extensions

- Molecular motors
- Branched filaments

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Future extensions

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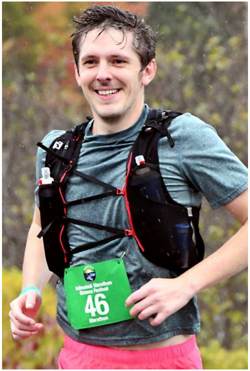
Software available

- `https://slenderbody.readthedocs.io/`

(Other) Acknowledgments



Special quadratures for Stokeslet and doublet

Factor out leading order singularity

$$\mathbf{U}^{(S)} = \int_{D(s)} \mathbf{S}\left(\mathbb{X}(s), \mathbb{X}(s')\right) \mathbf{f}\left(s'\right)\, ds'$$

$$= \frac{1}{8\pi\mu} \underbrace{\int_{D(s)} \left(\frac{\mathbf{I} + \widehat{\partial_s \mathbb{X}}(s)\widehat{\partial_s \mathbb{X}}(s)}{\|\partial_s \mathbb{X}(s)\|\, |s - s'|} \right) \mathbf{f}(s)\, ds'}_{\text{Evaluate analytically}}$$

$$+ \int_{D(s)} \left(\mathbf{S}\left(\mathbb{X}(s), \mathbb{X}(s')\right) \mathbf{f}\left(s'\right) - \frac{1}{8\pi\mu} \left(\frac{\mathbf{I} + \widehat{\partial_s \mathbb{X}}(s)\widehat{\partial_s \mathbb{X}}(s)}{|s - s'|} \right) \mathbf{f}(s) \right) ds'$$

Remaining integral can be written as $\mathbf{g}(s, s')\operatorname{sign}(s - s')$

- Expand $\mathbf{g}(s, s')$ in Chebyshev basis in s'
- Precompute $\int T_k(s')\operatorname{sign}(s - s')$ for each s
- Adjoint method can obtain integrals from values of $\mathbf{g}$

AK Tornberg. arXiv: 2012.12585.

Applying mobility

$$
\begin{tikzcd}
 & & \left(\boldsymbol{\tau}_{\{k=1,\ldots N\}}, \boldsymbol{X}_{\mathrm{MP}}\right) \arrow[d, "\boldsymbol{\mathcal{X}}"] & & \\
 & & \boldsymbol{X}_{\{k=1,\ldots N+1\}} \arrow[d, "\text{Chebyshev interpolation}"] & & \\
 & & \mathbb{X}(s) \arrow[r] \arrow[dll] & \boldsymbol{M}\left[\mathbb{X}(\cdot)\right] \arrow[dd, "\text{Special quadrature}"] & \\
\mathcal{E}_{\mathrm{bend}}\left[\mathbb{X}(\cdot)\right] \arrow[dr] & & & & \\
 & \boldsymbol{F}_{\mathrm{bend}}\left(\boldsymbol{X}\right) \arrow[rr, "\widetilde{\boldsymbol{W}}^{-1}"] & & \boldsymbol{f}_{\mathrm{bend}}\left(\boldsymbol{X}\right) \arrow[r] & \widetilde{\boldsymbol{M}}\boldsymbol{F}
\end{tikzcd}
$$

Discrete part: inextensibility

Langevin equation must be modified because of inextensibility

- $\boldsymbol{\tau}_{\{i\}}$ remains unit vector, rotates as rigid rod (ang. vel. $\boldsymbol{\Omega}_{\{i\}}$)

$$\partial_t \boldsymbol{\tau}_{\{i\}} = \boldsymbol{\Omega}_{\{i\}} \times \boldsymbol{\tau}_{\{i\}} \to \partial_t \boldsymbol{\tau} = -\mathbf{C}\boldsymbol{\Omega}$$

- Results in constrained motions for $\mathbf{X}$

$$\partial_t \mathbf{X} = \boldsymbol{\mathcal{X}} \begin{pmatrix} -\mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \boldsymbol{\Omega} \\ \mathbf{U}_{\mathrm{MP}} \end{pmatrix} := \boldsymbol{\mathcal{X}} \bar{\mathbf{C}} \boldsymbol{\alpha} := \mathbf{K} \boldsymbol{\alpha}$$

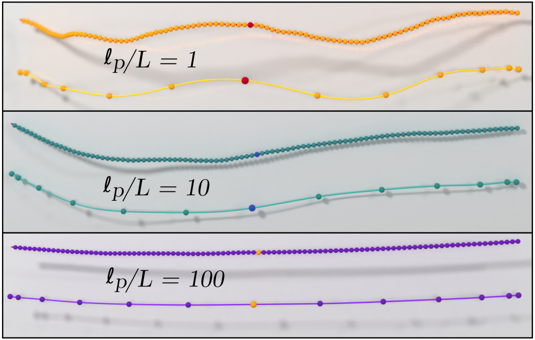
- Discrete time: solve for $\boldsymbol{\alpha} = (\boldsymbol{\Omega}, \mathbf{U}_{\mathrm{MP}})$, rotate by $\boldsymbol{\Omega} \Delta t$, update $\mathbf{X}_{\mathrm{MP}}$

Continuum part: energy

Fibers resist bending according to curvature energy *functional*

$$\mathcal{E}_{\text{bend}}\left[\mathbb{X}(\cdot)\right] = \frac{\kappa}{2}\int_0^L \partial_s^2 \mathbb{X}(s) \cdot \partial_s^2 \mathbb{X}(s)\, ds$$

- $\kappa =$ bending stiffness
- $\ell_p = \kappa/(k_B T)$ defines a "persistence length"
- Fibers bend on this length, shorter than this straight
- Hope for spectral methods when $\ell_p \simeq L$ (actin)



Discretizing force

Obtain from energy functional to ensure discrete force/torque balance

$$
\begin{aligned}
\mathcal{E}_{\text{bend}}\left[\mathbb{X}(\cdot)\right] &= \frac{\kappa}{2}\int_0^L \partial_s^2\mathbb{X}(s)\cdot\partial_s^2\mathbb{X}(s)\,ds \\
&= \frac{\kappa}{2}\left(\mathbf{E}_{N_x\to 2N_x}\mathbf{D}^2\mathbf{X}\right)^T\mathbf{W}_{2N}\left(\mathbf{E}_{N_x\to 2N_x}\mathbf{D}^2\mathbf{X}\right) \\
&= \frac{\kappa}{2}\left(\mathbf{D}^2\mathbf{X}\right)^T\widetilde{\mathbf{W}}\left(\mathbf{D}^2\mathbf{X}\right) \\
&= (1/2)\mathbf{X}^T\mathbf{L}\mathbf{X}
\end{aligned}
$$

- Upsampling to grid of size $2N_x$ to integrate *exactly*
- No aliasing
- Corresponds to L^2 inner product weights matrix $\widetilde{\mathbf{W}}$
- Force $\mathbf{F} = -\partial\mathcal{E}/\partial\mathbf{X} = -\mathbf{L}\mathbf{X}$
- Force density $\mathbf{f} = \widetilde{\mathbf{W}}^{-1}\mathbf{F}$ $\left(\langle\mathbf{X},\mathbf{f}\rangle_{L^2} = \mathbf{X}^T\mathbf{F}\right)$

Li et al. Geophys. J. Int. (2017).

Steric interactions

Consider steric interaction energy

$$\mathcal{E}^{()}ij^{(s)} = \int_0^L \int_0^L \hat{\mathcal{E}}\left(r\left(\mathbb{X}^{(i)}(s^{(i)}), \mathbb{X}^{(j)}(s^{(j)})\right)\right)\, ds^{(i)}\, ds^{(j)},$$

Use error function so force is Gaussian with $\delta \sim a$

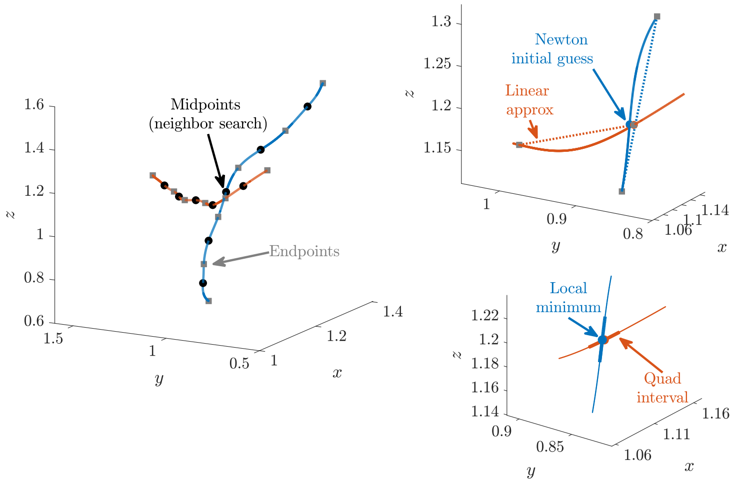
$$\hat{\mathcal{E}}(r) = \frac{\mathcal{E}_0}{a^2}\operatorname{erf}\left(r/(\delta\sqrt{2})\right)$$

$$\frac{d\hat{\mathcal{E}}}{dr} = \frac{\mathcal{E}_0}{a^2\delta}\sqrt{\frac{2}{\pi}}\exp\left(-r^2/\left(2\delta^2\right)\right)$$

Evaluate integral discretely $\rightarrow$ differentiate to get force

Evaluating integrals

Brute force way: oversample points ($N_u \sim L/\delta \sim 1/\epsilon$) to determine contacting intervals



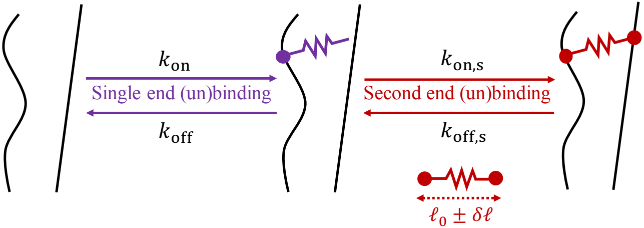
Transient cross linking

Two components to it

- Position of linker attachments / connectivity list (SSA)
- Force given connectivity list (smoothed δ function)

Assumptions behind linking algorithm

- Infinite reservoir of linkers (amount controlled by $k_{\mathrm{on}}/k_{\mathrm{off}}$)
- Diffusion is fast
- Just consider four rates
- Choose $k_{\mathrm{on,s}}$ to maintain detailed balance



Goals for bundling

Filaments move in three ways

1. Cross linking forces
2. "Rigid body" translation and rotation
3. *Semiflexible* bending fluctuations

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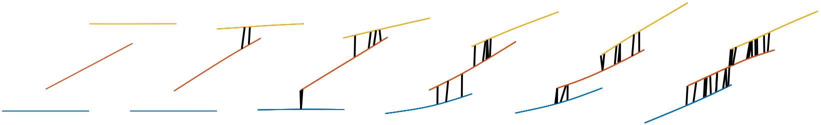
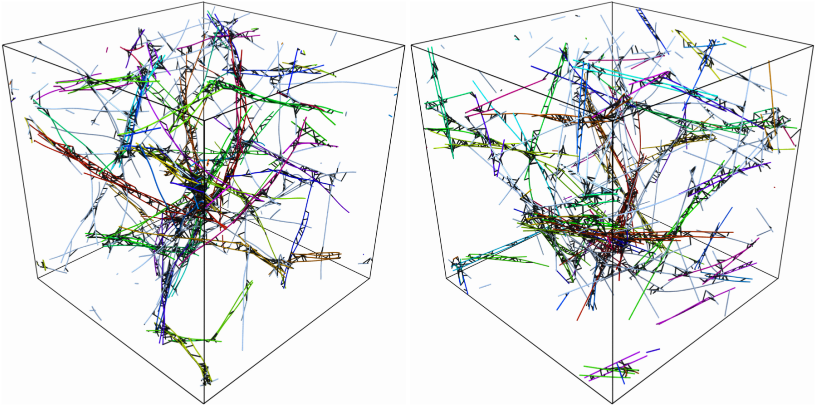
Goal is to explore the role of the bending flucts

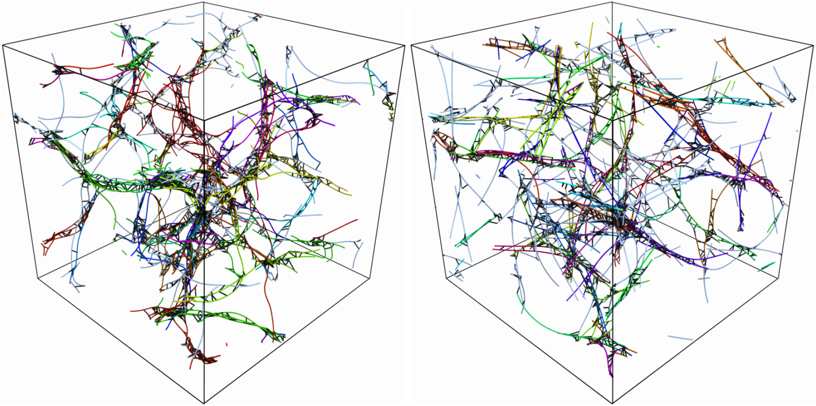
- Intuition: fluctuations increase binding frequency
- How small does ℓ_p have to be?
- Strategy: simulate fibers with #1 and #2 only, compare to fluctuating



Movie: $\ell_p/L = 10$

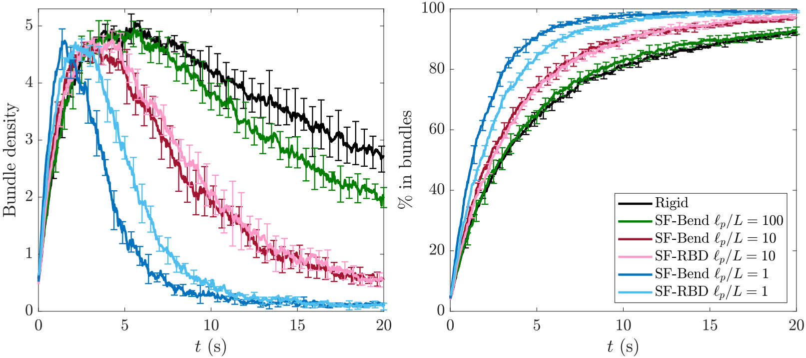


Movie: $\ell_p/L = 1$



Bundling statistics

Statistics confirm movies



- $\ell_p/L = 100$: similar to rigid
- $\ell_p/L = 10$: small difference from "RBD" filaments *without* bending fluctuations
- $\ell_p/L = 1$: speed-up due to semiflexible bending fluctuations
- Actin in vivo: $\ell_p/L \approx 30$