Computational methods for complex suspensions

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Outline

Outline

Donev group

Masters Sachin Natesh (now Ph.D. at Colorado Boulder)

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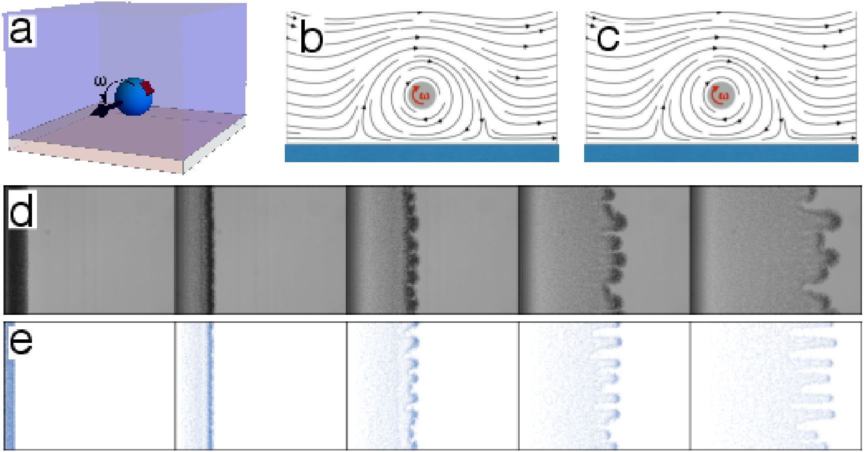
- Research currently primarily funded by **NSF** DMS (2 active grants) and CBET divisions (1 active grant).
- I lead an NSF-funded Research and Training Group (RTG) in **Modeling and Simulation**, together with Miranda Cerfon-Holmes.
- Was co-lead (with Paul Chaikin, NYU Physics) of the Interdisciplinary Research Group on **Active Matter (Soft Condensed Matter Physics)** in the NSF NYU **Materials Research** Center (MRSEC) until Aug 2020.

Research interests

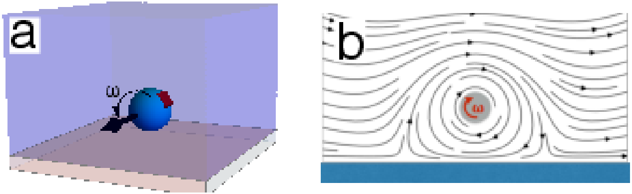
- The primary focus of my research is **fluid dynamics at small scales** (100nm-10μm), where **thermal fluctuations / Brownian motion** play an important role.
- A key approach I use and try to understand is **fluctuating hydrodynamics** (stochastic partial differential equations).
- Tools: fast methods, fast algorithms, computational fluid dynamics, applied stochastic analysis.
- Physical systems of current interest:
  suspensions of **colloids** (soft matter, Chem E) and **fibers** (comp bio), **electrolytes** (ionic solutions).

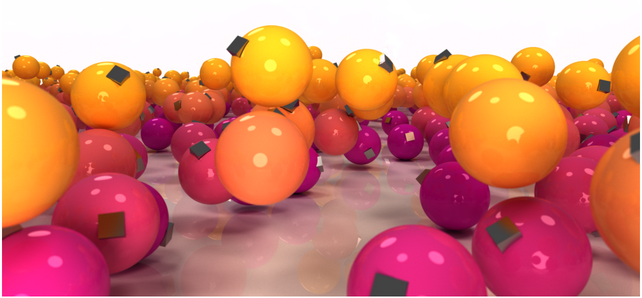
Microrollers: Fingering Instability



Experiments by Michelle Driscoll, simulations by **Blaise Delmotte** (was at Courant, now at LadHyX Paris), *Nature Physics* 13 (2017) [1]

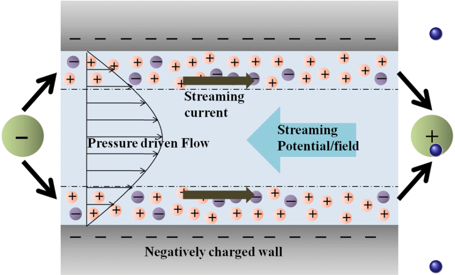
Microrollers: Uniform Monolayers





B. Sprinkle et al., *Soft Matter* 16 (2020) [**ArXiv:2005.06002**] [2]

Electrohydrodynamics

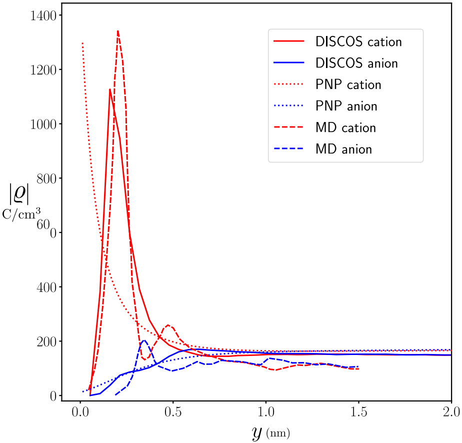


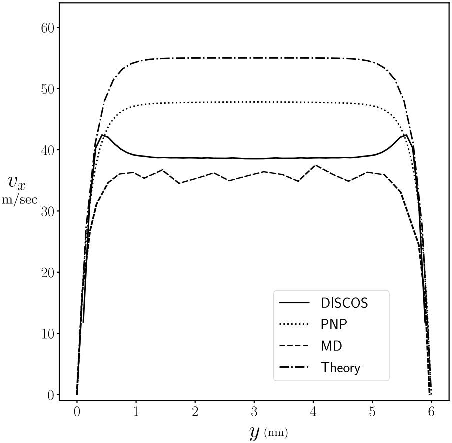
Electro-hydrodynamic flow
Key issue: Debye length/layer of molecular scales and continuum approach is questionable quantitatively: *no sterics, no image charges, no fluctuations, no ion pairing*

- **Electrolyte (ion) solutions** are important for batteries, ion-selective membranes, biology, etc.
- Past work with LBNL on **fluctuating Poisson-Nernst-Planck-Stokes** SPDE solvers.
- Semi-discrete approach: **Brownian HydroDynamics** (BD-HI) with discrete ions including both **electrostatic and hydrodynamic interactions**.

  Ladiges et al., *Phys. Rev. Fluids* 6 (2021) and **ArXiv:2204.14167** (2022) [3]

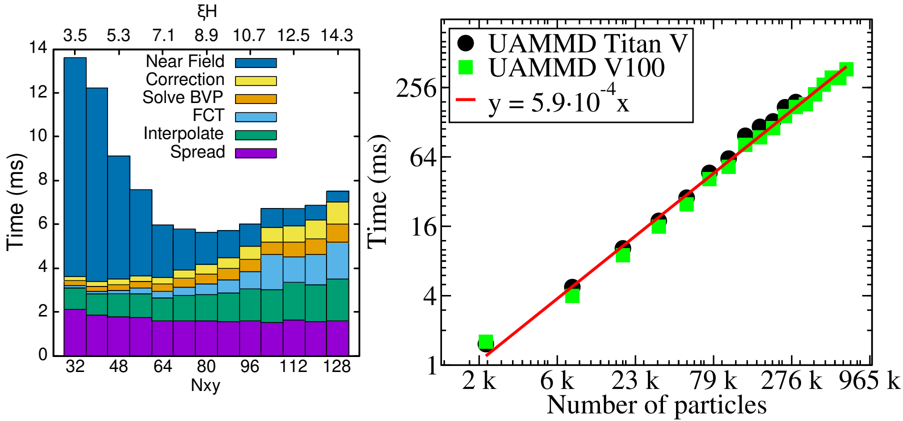
Electroosmotic flow: MD vs BD





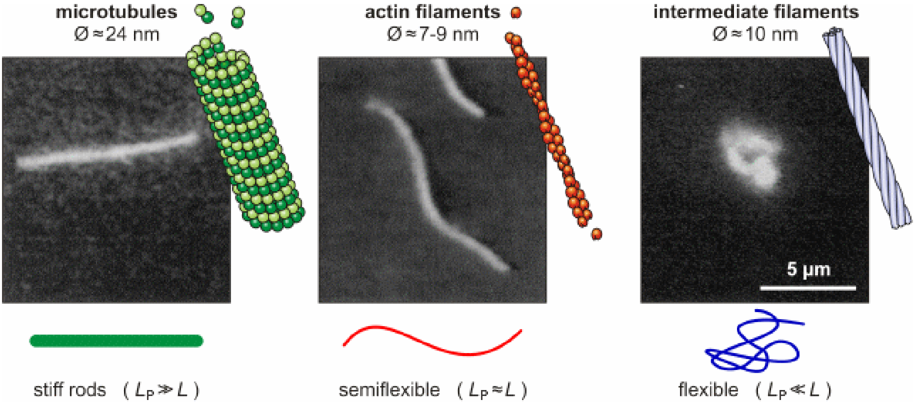
Continuing work on Courant on spectral **GPU-based** methods/codes for electrolyte BD-HI and **electrochemical applications**

GPU acceleration



(Left) **Electrostatics**: Spectral Ewald splitting (6ms for 20K charges). (Right) **Hydrodynamics** in slit channel using Fourier-Chebyshev spectral methods for *doubly-periodic geometry* (ongoing).

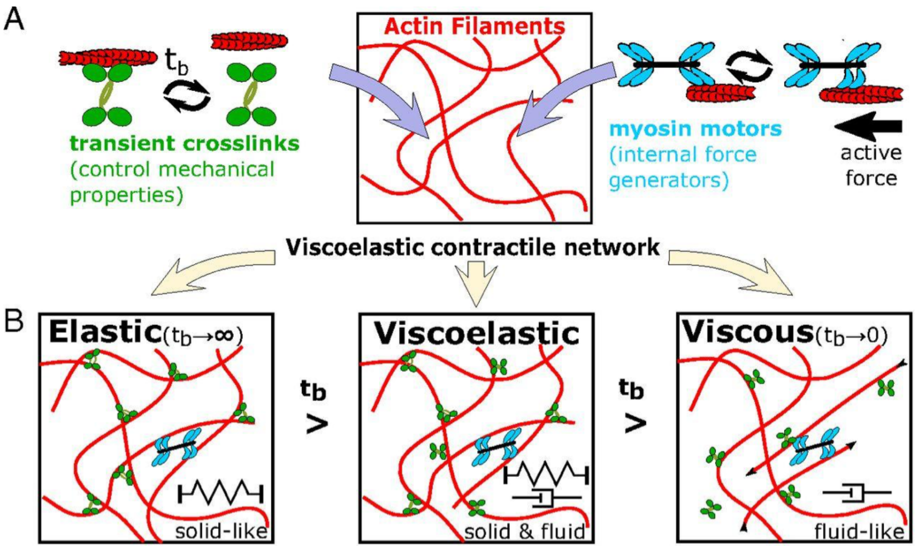
Fibers involved in cell mechanics



Pawlizak and Käs, University of Leipzig

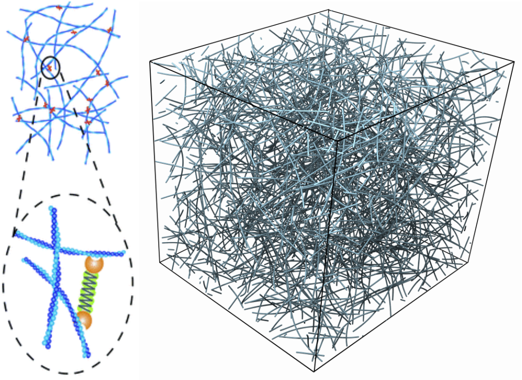
L_p =persistence length, L =fiber length, $a = \epsilon L$ =fiber radius, ϵ =slenderness ratio

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?

- Sometimes flows created by individual fibers add up constructively to produce **large-scale flows**, which advect network.
- For example, cytoplasmic streaming of a myosin-actin gels (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.
- Importance/role of **Brownian bending fluctuations** of fibers on rheology also not fully clear.

Dynamics of Flexible Fibers in Viscous Flows and Fluids, Ann. Rev. Fluid Mech. 51:539, du Roure, Lindner, Nazockdast, Shelley

Outline

Quick intro to BD-HI

- The Ito equations of **Brownian HydroDynamics** for the (correlated) positions of the N particles (ions, colloids, blobs) in fluid, $\mathbf{Q}(t) = \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t)\}$:
$$d\mathbf{Q} = \boldsymbol{\mathcal{M}}\mathbf{F}dt + (2k_BT\,\boldsymbol{\mathcal{M}})^{\frac{1}{2}}\,d\boldsymbol{\mathcal{B}} + k_BT\,(\partial_{\mathbf{Q}}\cdot\boldsymbol{\mathcal{M}})\,dt,$$
where $\boldsymbol{\mathcal{B}}(t)$ is a vector of Brownian motions, and $\mathbf{F}(\mathbf{Q})$ are electrostatic+steric+external forces.
- The symmetric positive semidefinite (SPD) but dense **hydrodynamic mobility matrix** $\boldsymbol{\mathcal{M}}(\mathbf{Q})$:
3×3 block $\mathbf{M}_{ij}$ that maps a force on particle j to a velocity of particle i (Stokes flow problem).

Computational Issues in BDHI

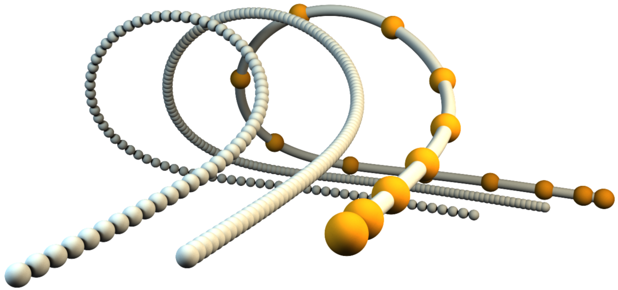
Key challenges for fast **linear-scaling** BD-HI:

- How to compute **deterministic velocities $\mathcal{M}\mathbf{F}$** (and electrostatic forces) efficiently? (Poisson and Stokes solvers)
  Green's functions, immersed boundary finite-difference approaches, Fourier(-Chebyshev) spectral methods
- Generating **Brownian displacements** $\mathcal{N}\left(\mathbf{0}, 2k_B T \Delta t\, \mathcal{M}\right)$:
  Use Fluctuating Hydrodynamics (FHD) to generate noise on fluid instead of ions with single Stokes solve!
- Generating **stochastic drift** $\sim \partial_{\mathbf{Q}} \cdot \mathcal{M}$
  Design specialized temporal integrators based on Random Finite Differences (RFDs)

Outline

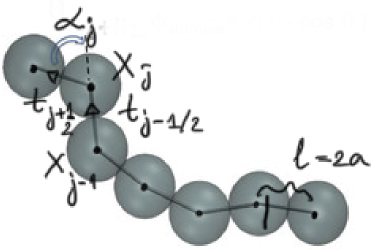
Fiber Representation

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 et al. **ArXiv:2201.04187**
PRF 2021 [4]and now with twist in *PRF 2022* [5]

Inextensible multiblob chains



Worm-like polymer chain

- Inextensibility: $\left\| \mathbf{X}_{j+1} - \mathbf{X}_j \right\| = l \sim a$ (e.g., a or $2a$).
- Tangent vectors: $\boldsymbol{\tau}_{j+1/2} = \left(\mathbf{X}_{j+1} - \mathbf{X}_j \right) / l$
- 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** $0 \le s \le L$.
- 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 curvature squared:

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

Bending elasticity

- Bending force $\mathbf{F}_j^{(b)}$ on interior blob j gives us **elastic force density**

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

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

- 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 of an immersed fiber

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

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

where $\delta_a(\mathbf{r})$ is a **blob kernel** of width $\sim a$, and

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

- Blobs/fiber are advected by fluid

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

- Continuum limit is obvious (without Brownian fluctuations)

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

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

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

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**

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

  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

$$\mathbf{M}_{ij}\left(\mathbf{X}_i, \mathbf{X}_j\right) = \boldsymbol{\mathcal{R}}\left(\mathbf{X}_i, \mathbf{X}_j\right) = \boldsymbol{\mathcal{R}}\left(\mathbf{X}_i - \mathbf{X}_j\right).$$

- Discrete dynamics = **inextensibility** +

$$\mathbf{U} = d\mathbf{X}/dt = \mathbf{M}\left(\mathbf{X}\right)\mathbf{F}\left(\mathbf{X}\right) = \mathbf{M}\left(-l\kappa_b\,\mathbf{D}^4\mathbf{X} + \boldsymbol{\Lambda}\right)$$

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? We have shown *numerically* that
  - Fiber **velocity converges pointwise** (strongly) up to the endpoints.
  - **Moments of λ converge**, e.g., stress tensor (weak convergence).

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**

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

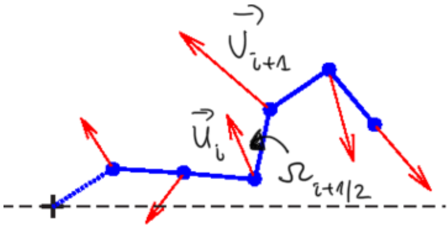
$$\mathcal{S}\left(\mathbf{r}\right)=\frac{1}{8\pi\eta r}\left(\mathbf{I}+\hat{\mathbf{r}}\hat{\mathbf{r}}^T\right)\equiv\mathbb{G},\quad\text{and}\quad\mathcal{D}\left(\mathbf{r}\right)=\frac{1}{8\pi\eta r^3}\left(\mathbf{I}-\hat{\mathbf{r}}\hat{\mathbf{r}}^T\right)$$

Slender Body Theory

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

- **Matched asymptotics** gives (away from endpoints)
  $\left(\mathcal{M}\,\mathbf{f}\right)(s)\approx\left(\mathcal{M}_{\mathrm{SBT}}\,\mathbf{f}\right)(s)=\left(\mathcal{M}_{\mathrm{L}}\,\mathbf{f}\right)(s)+\left(\mathcal{M}_{\mathrm{NL}}\,\mathbf{f}\right)(s)=$
  $$=\frac{1}{8\pi\eta}\left(\log\left(\frac{(L-s)s}{4a^2}\right)\left(\mathbf{I}+\boldsymbol{\tau}(s)\boldsymbol{\tau}(s)^T\right)+4\mathbf{I}\right)\mathbf{f}(s)$$
  $$+\frac{1}{8\pi\eta}\int_0^L ds'\left(\mathcal{S}\left(\mathbf{X}(s)-\mathbf{X}(s')\right)\mathbf{f}\left(s'\right)-\left(\frac{\mathbf{I}+\boldsymbol{\tau}(s)\boldsymbol{\tau}(s)^T}{|s-s'|}\right)\mathbf{f}(s)\right)$$
- 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** and also **ensures an SPD mobility operator**.

Inextensible motions



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

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

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

Principle of virtual work

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

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

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

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

- We can express this in terms of tension

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

but the principle of virtual work is an **integral constraint**.

Continuum equations

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

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

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

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

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

- Two improvements:
  - Evolve tangent vector $\boldsymbol{\tau}$ rather than $\mathbf{X}$: **strictly inextensible**.
  - Expose **saddle-point structure** of problem (generalized gradient descent for elastic energy).

Outline

Spatial Discretization

- We develop a **spectral discretization** in space, based on representing all functions using **Chebyshev polynomials**, with **anti-aliasing**.
- **Collocation discretization** of mobility equation gives a **saddle-point system**

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

  which we solve iteratively using a **block-diagonal preconditioner**.
- We only use $O(16-32)$ Chebyshev points per fiber so doing **dense LA for individual fibers** is OK.

Temporal discretization

- **Backward Euler** is the most stable since it ensures strict energy dissipation; also for *dense* suspensions.
- **Split** mobility into **local** (e.g., intra-fiber) and **non-local** (e.g., inter-fiber) parts, $\mathbf{M} = \mathbf{M}_L + \mathbf{M}_{NL}$:

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

  where $\mathbf{X}^{n+1,\star} = \mathbf{X}^n + \Delta t \mathbf{K}^{n+1/2,*} \boldsymbol{\Omega}^{n+1/2}$.
- Actual fiber update is **strictly inextensible**

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

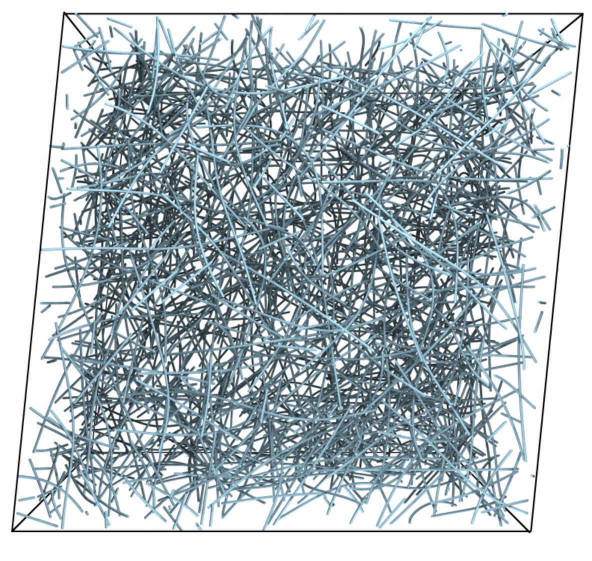
- $\mathbf{f}^n$ contains other forces such as **cross-linkers** (can be stiff). **Flow** is easy to add to the rhs.

The gory details

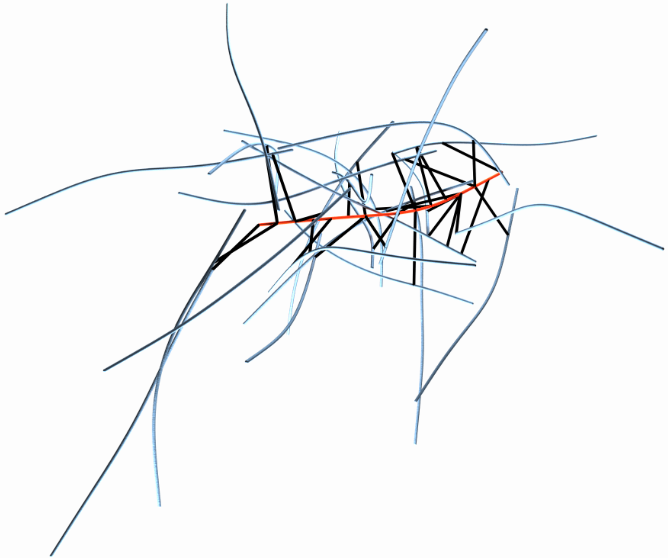
1. For dense suspensions, supplement L+NL splitting with additional **1-5 GMRES iterations** for stability.
2. Evaluate long-ranged hydrodynamic interactions between Chebyshev nodes in **linear time** using *Positively Split Ewald* (PSE) method (FFT based for triply periodic), also works for **deformed/sheared unit cell** (Fiore *et al. J. Chem. Phys.* (2017)).
3. For intra-fiber hydro we replaced slender body *theory* with superior **slender body quadrature** (singularity subtraction).
4. For **nearby fibers**, use specialized **near-singular quadrature** to get 2-3 digits.

Outline

Actin network/gel



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:

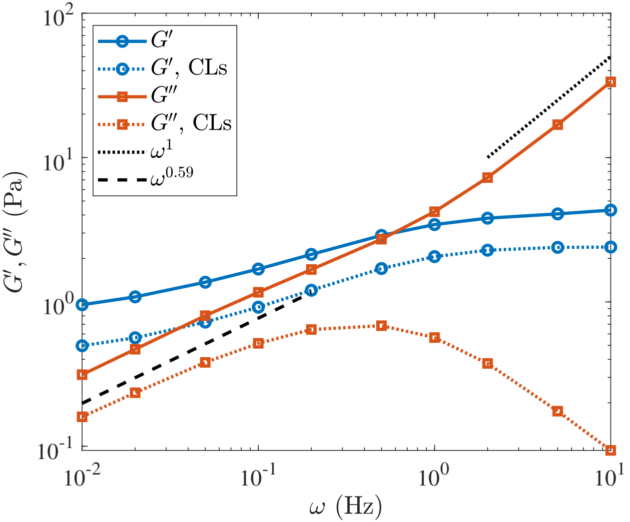
$$\boldsymbol{\sigma}^{(i)} = \frac{1}{V} \sum_{\text{fibers}} \int_0^L ds \, \mathbf{X}^i(s) \left(\mathbf{f}_b(s) + \boldsymbol{\lambda}(s) \right)^T$$

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

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

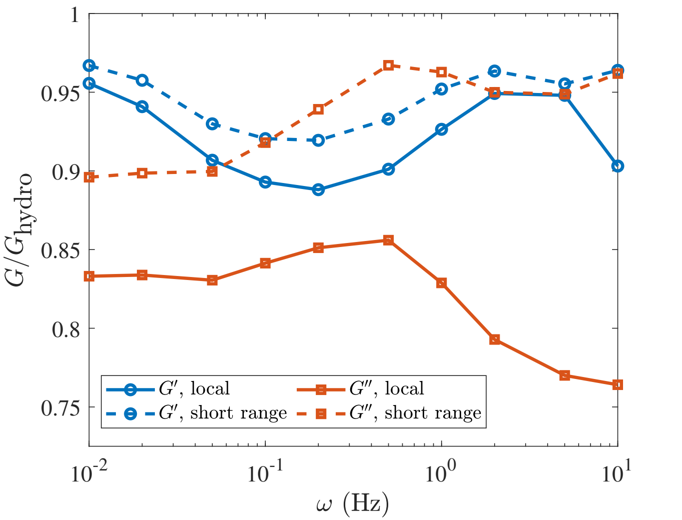
$$G' = \frac{2}{\gamma_0 T} \int_0^T \sigma_{21} \sin(\omega t) \, dt \qquad G'' = \frac{2}{\gamma_0 T} \int_0^T \sigma_{21} \cos(\omega t) \, dt.$$

Viscoelastic moduli: Maxwell fluid



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**.

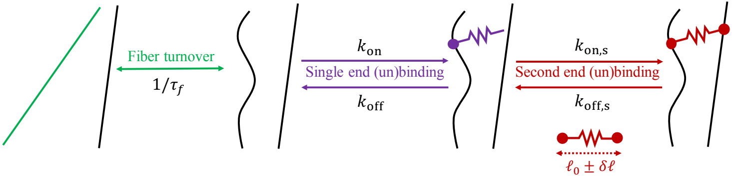
Dynamic cross linking

Kinetic Monte Carlo algorithm for cross linking:

- Discrete set of binding sites on each fiber (for efficiency).
- Doubly-bound CLs act as simple **elastic springs**.

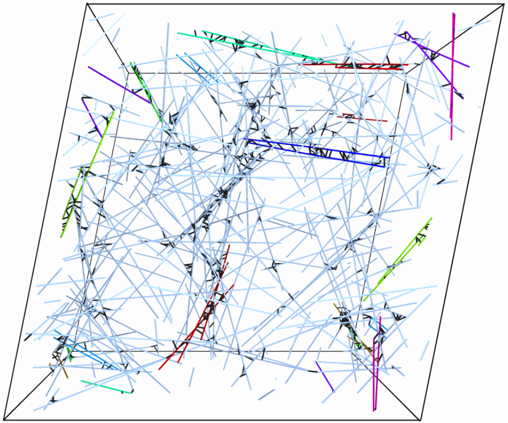
Assumptions behind linking algorithm

- Diffusion of cross-linkers is fast (**diffusion-limited binding**)
- Four reactions between fibers and CL reservoir obey **detailed balance**

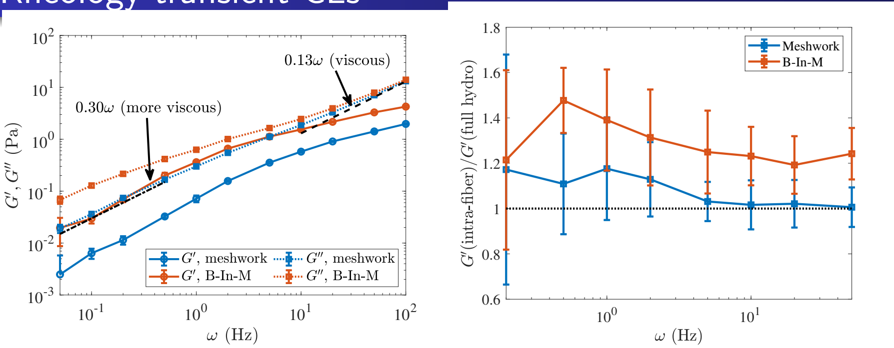


O. Maxian et al, PLOS Comp. Bio., 2021 [**bioRxiv:2021.07.07.451453**] [6] and Biophysical J., 2022 [**bioRxiv:021.09.17.460819**] [7]

Dynamically cross-linked network



Rheology transient CLs



- Measured viscoelastic moduli of dynamically cross-linked networks **without** Brownian motion.
- For bundled networks, elastic modulus overestimated by $\approx 50\%$ without inter-fiber hydro, esp. long timescales.
- Fibers in bundles closer together: stress is reduced because **entrainment flows in bundle** make straining easier.

Outline

Thermal fluctuations (Brownian Motion)

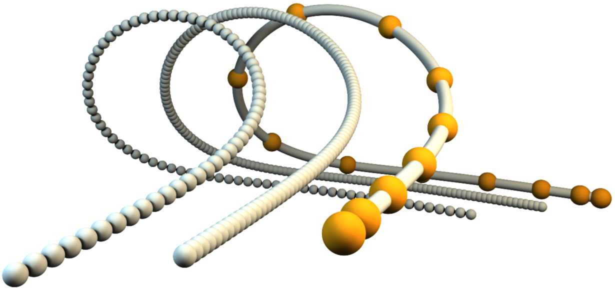
- **Rigid fibers** are "easy" though so far we have only implemented *without* inter-fiber hydro [7].
- **Fluctuating hydrodynamics** gives the fluctuating Stokes equations

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

- The **thermal fluctuations** (Brownian motion of fiber) are driven by a white-noise **stochastic stress tensor** $\mathcal{W}(\mathbf{r}, t)$.
- Must first answer deep mathematical questions:
  - Can one make sense of the (multiplicative noise) **overdamped SPDE** for a Brownian curve?
  - Does the **Brownian stress** of the fiber converge in the continuum limit? (bending energy does not)

Brownian multiblob chains

For **Brownian blob-link chains** there are no mathematical issues so start there!



Fast constrained BD-HI for blob-link chains based on rotating unit link vectors including Brownian stress (Brennan Sprinkle, in progress)

References

Michelle Driscoll, Blaise Delmotte, Mena Youssef, Stefano Sacanna, Aleksandar Donev, and Paul Chaikin.
Unstable fronts and motile structures formed by microrollers.
Nature Physics, 13:375–379, 2017.

Brennan Sprinkle, Ernest B. van der Wee, Yixiang Luo, Michelle Driscoll, and Aleksandar Donev.
Driven dynamics in dense suspensions of microrollers.
Soft Matter, 16:7982 – 8001, 2020.

D. R. Ladiges, J. G. Wang, I. Srivastava, S. P. Carney, A. Nonaka, A. L. Garcia, A. Donev, and J. B. Bell.
Modeling electrokinetic flows with the discrete ion stochastic continuum overdamped solvent algorithm.
2022.
Submitted to Phys. Rev. E, ArXiv:2204.14167.

Ondrej Maxian, Alex Mogilner, and Aleksandar Donev.
Integral-based spectral method for inextensible slender fibers in stokes flow.
Phys. Rev. Fluids, 6:014102, 2021.

Ondrej Maxian, Brennan Sprinkle, Charles S. Peskin, and Aleksandar Donev.
The hydrodynamics of a twisting, bending, inextensible fiber in stokes flow.
To appear in Phys. Rev. Fluids, ArXiv:2201.04187, 2022.

Ondrej Maxian, Raul Perez Peláez, Alex Mogilner, and Aleksandar Donev.
Simulations of dynamically cross-linked actin networks: Morphology, rheology, and hydrodynamic interactions.
PLOS Computational Biology, 17(12):e1009240, 2021.

Ondrej Maxian, Aleksandar Donev, and Alex Mogilner.
Interplay between brownian motion and cross-linking controls bundling dynamics in actin networks.
Biophysical Journal, 121(7):1230–1245, 2022.