Computational methods for complex suspensions

Aleksandar Donev
Ondrej Maxian, Brennan Sprinkle, Alex Mogilner (Courant)
Daniel Ladiges, John Bell, and Alejandro Garcia (LBNL)

Courant Institute, *New York University*

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Outline

1. Complex suspensions
   - Colloidal Suspensions
   - Electrolyte Solutions
2. Brownian Dynamics
3. Inextensible Fibers in Stokes Flow
   - Elasticity
   - Hydrodynamics
   - Inextensibility
4. Numerical Methods
5. Actin gels
6. Adding Brownian motion

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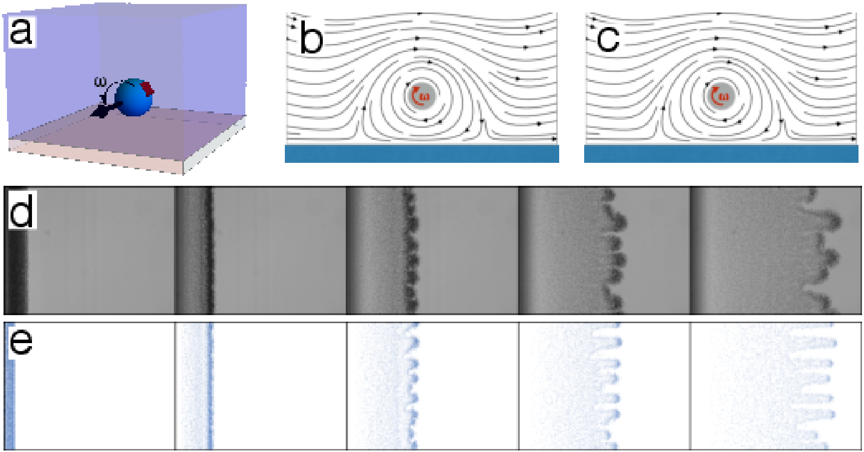
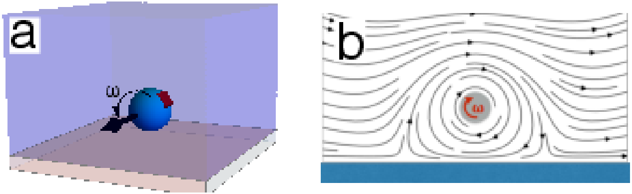
- Tools: fast methods, fast algorithms, computational fluid dynamics, applied stochastic analysis.
- Physical systems of current interest:
  suspensions of **colloids** (soft matter, Chem E) and **fibers** (comp bio), **electrolytes** (ionic solutions).

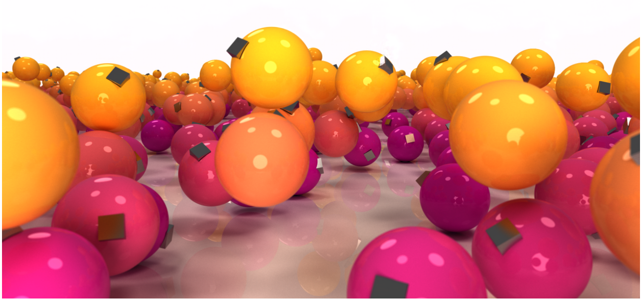
Microrollers: Fingering Instability



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

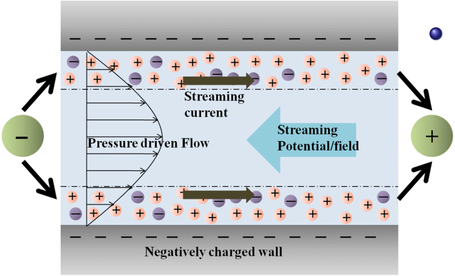
Microrollers: Uniform Monolayers





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*

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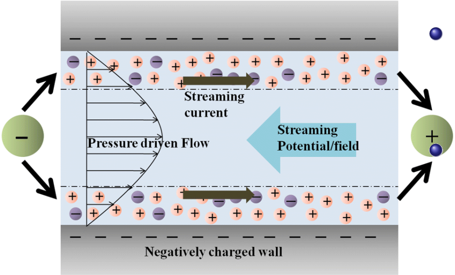

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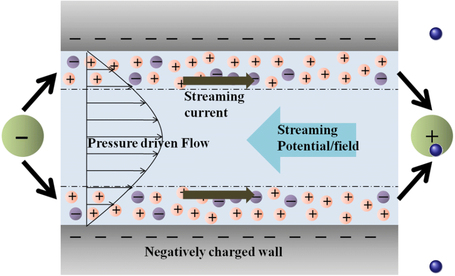

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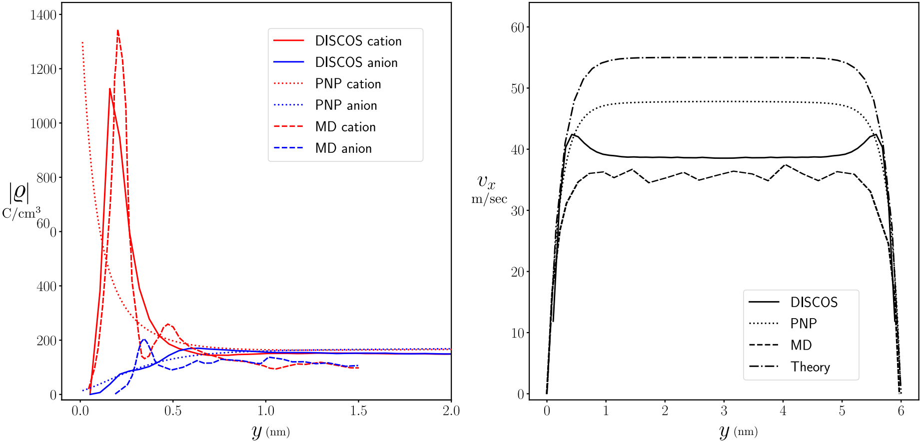
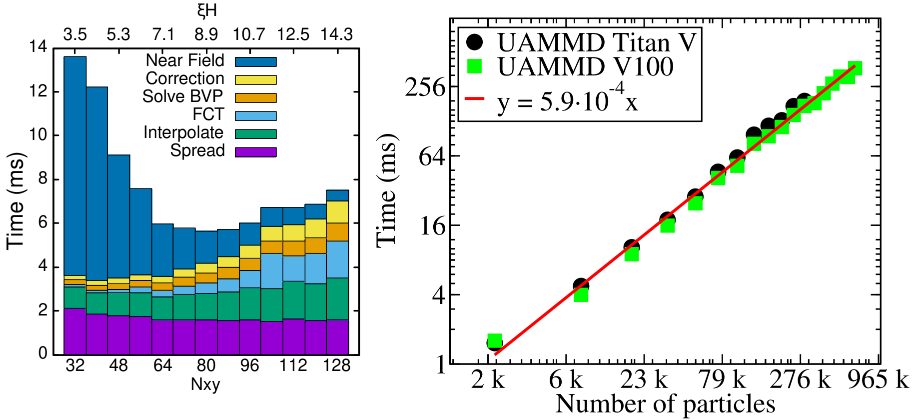
- Past work with LBNL on **fluctuating Poisson-Nernst-Planck-Stokes** SPDE solvers.
- Semi-discrete approach: **Brownian HydroDynamics** (BD-HI) with discrete ions including both **electrostatic and hydrodynamic interactions**.
  Ladiges et al., *Phys. Rev. Fluids* 6 (2021) and **ArXiv:2204.14167** (2022) [3]

Electroosmotic flow: MD vs BD



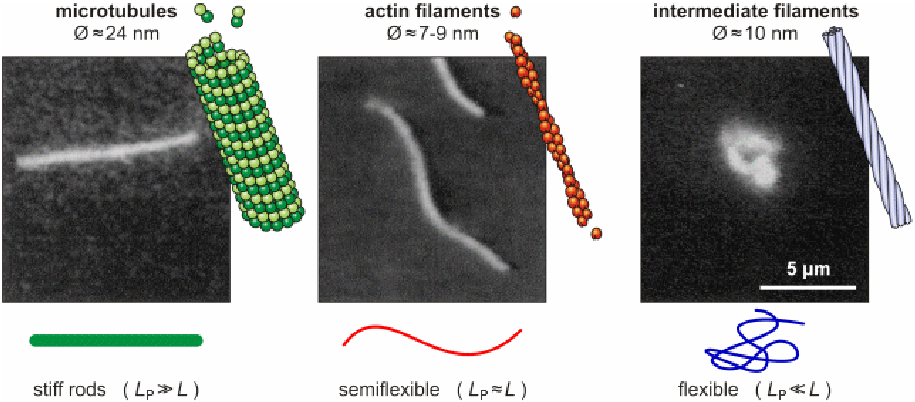
Continuing work on Courant on spectral **GPU-based** methods/codes for electrolyte BD-HI and **electrochemical applications**

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).

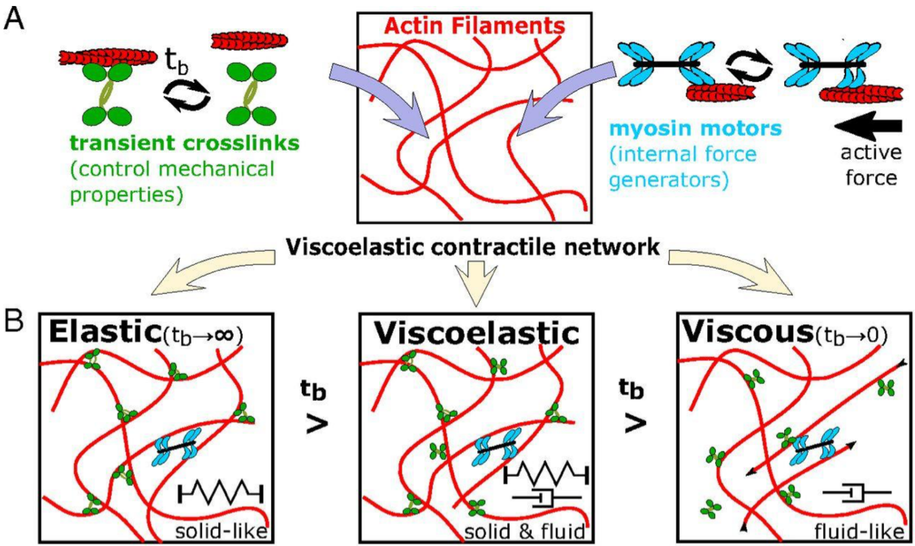
Fibers involved in cell mechanics



Pawlizak and Käs, University of Leipzig

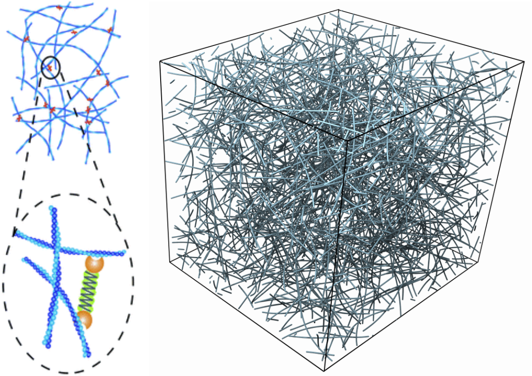
L_p =persistence length, L =fiber length, $a = \epsilon L$ =fiber radius, ϵ =slenderness ratio

Cytoskeleton rheology



Ahmed and Betz. *PNAS*. (2015)

Cross-linked actin gels



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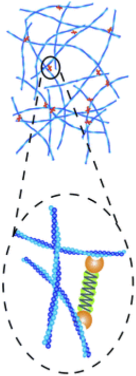

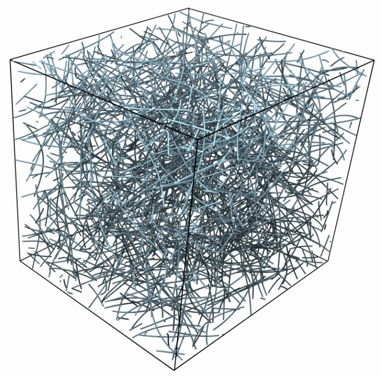

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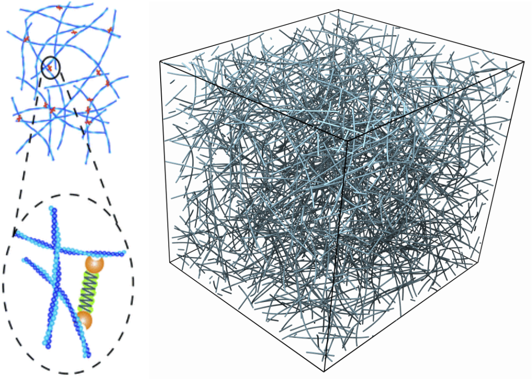

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- **Periodic cyclically sheared** unit cell: **viscoelastic moduli**.

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- 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

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Quick intro to BD-HI

- The Ito equations of **Brownian HydroDynamics** for the (correlated) positions of the N particles (ions, colloids, blobs) in fluid, $\mathbf{Q}(t) = \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t)\}$:

$$d\mathbf{Q} = \boldsymbol{\mathcal{M}}\mathbf{F}dt + (2k_B T\,\boldsymbol{\mathcal{M}})^{\frac{1}{2}}\,d\boldsymbol{\mathcal{B}} + k_B T\,(\partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{M}})\,dt,$$

where $\boldsymbol{\mathcal{B}}(t)$ is a vector of Brownian motions, and $\mathbf{F}(\mathbf{Q})$ are electrostatic+steric+external forces.

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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

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- Generating **Brownian displacements** $\mathcal{N}\left(\mathbf{0}, 2k_B T \Delta t \, \boldsymbol{\mathcal{M}}\right)$:
  Use Fluctuating Hydrodynamics (FHD) to generate noise on fluid instead of ions with single Stokes solve!

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- Generating **stochastic drift** $\sim \partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{M}}$
  Design specialized temporal integrators based on Random Finite Differences (RFDs)

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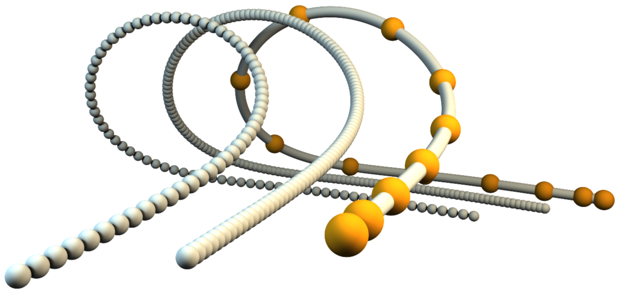
Fiber Representation

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



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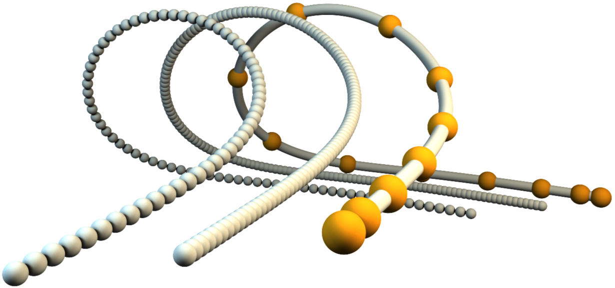
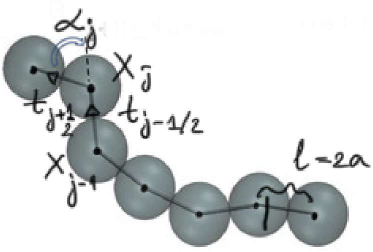


More efficient approach is to represent a fibers as **continuum curve**
O. Maxian et al. **ArXiv:2201.04187**
PRF 2021 [4]and now with twist in *PRF 2022* [5]

Inextensible multiblob chains



Worm-like polymer chain

- Inextensibility: $\|\mathbf{X}_{j+1} - \mathbf{X}_j\| = l \sim a$ (e.g., a or $2a$).

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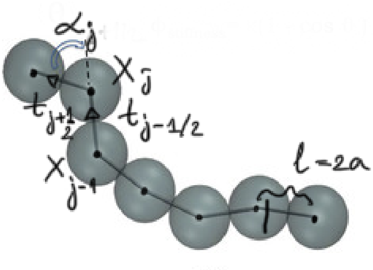

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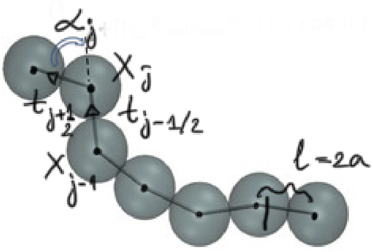

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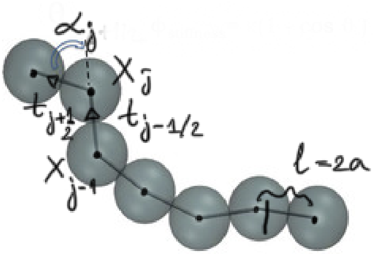

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- Elastic energy (bending modulus κ_b)

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

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- 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**

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

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

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- **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

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

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

- Continuum limit is obvious (without Brownian fluctuations)

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

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

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

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

  where $\mathbb{G}$ is the Green's function for (periodic) Stokes flow.

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

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

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**

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

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- 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**

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

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

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  - **Moments of $\boldsymbol{\lambda}$ converge**, e.g., stress tensor (weak convergence).

Rotne-Prager-Yamakawa kernel

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

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

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

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

Slender Body Theory

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

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

- **Matched asymptotics** gives (away from endpoints) $(\mathcal{M}\,\mathbf{f})(s) \approx (\mathcal{M}_{\mathrm{SBT}}\,\mathbf{f})(s) = (\mathcal{M}_{\mathrm{L}}\,\mathbf{f})(s) + (\mathcal{M}_{\mathrm{NL}}\,\mathbf{f})(s) =$

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

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

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- 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).

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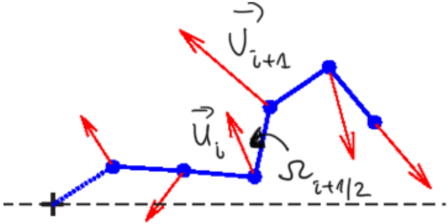
- For a special choice of blob radius $a=\left(e^{3/2}/4\right)\epsilon L=1.12\epsilon L$, this formula matches the widely-used **Slender Body Theory** (SBT).
- Our approach automatically works for **multiple fibers**, and also gives us a natural **regularization of the endpoints** and also **ensures an SPD mobility operator**.

Inextensible motions



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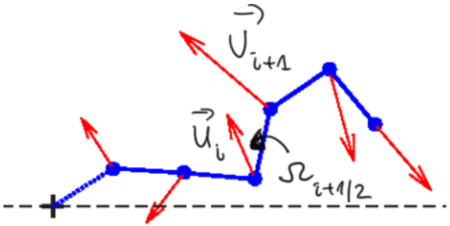

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$$\mathbf{U} = \mathbf{K}\boldsymbol{\Omega}^{\perp} = \left[\mathbf{U}_0, \cdots, \mathbf{U}_0 + \Delta s \sum_{j=0}^{i-1} \boldsymbol{\Omega}^{\perp}_{j+1/2} \times \boldsymbol{\tau}_{j+1/2}, \cdots \right] \rightarrow$$

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

Principle of virtual work

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

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

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- We can express this in terms of tension

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

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

Continuum equations

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

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  - Expose **saddle-point structure** of problem (generalized gradient descent for elastic energy).

Outline

1. Complex suspensions
   - Colloidal Suspensions
   - Electrolyte Solutions
2. Brownian Dynamics
3. Inextensible Fibers in Stokes Flow
   - Elasticity
   - Hydrodynamics
   - Inextensibility
4. Numerical Methods
5. Actin gels
6. Adding Brownian motion

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- We only use $O(16-32)$ Chebyshev points per fiber so doing **dense LA for individual fibers** is OK.

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- $\mathbf{f}^n$ contains other forces such as **cross-linkers** (can be stiff).

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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.

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4. For **nearby fibers**, use specialized **near-singular quadrature** to get 2-3 digits.

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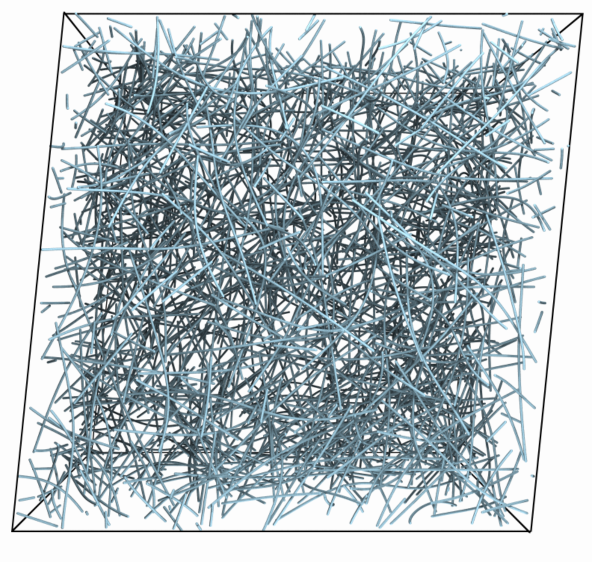
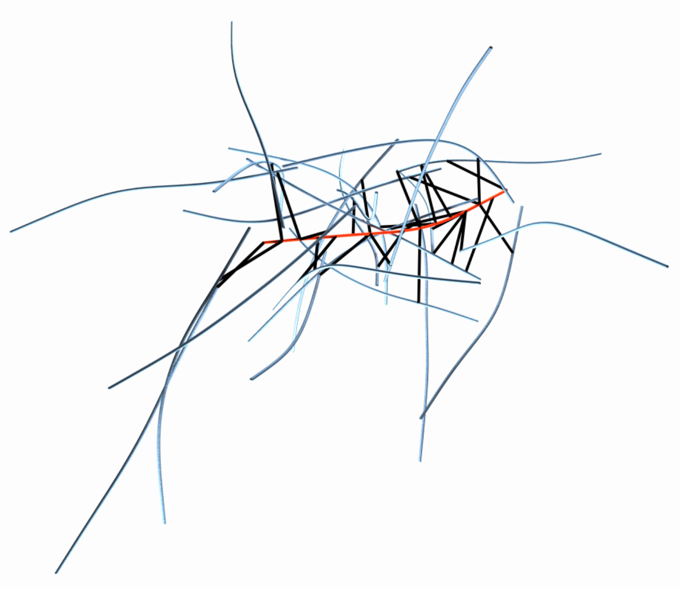
Actin network/gel



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:

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

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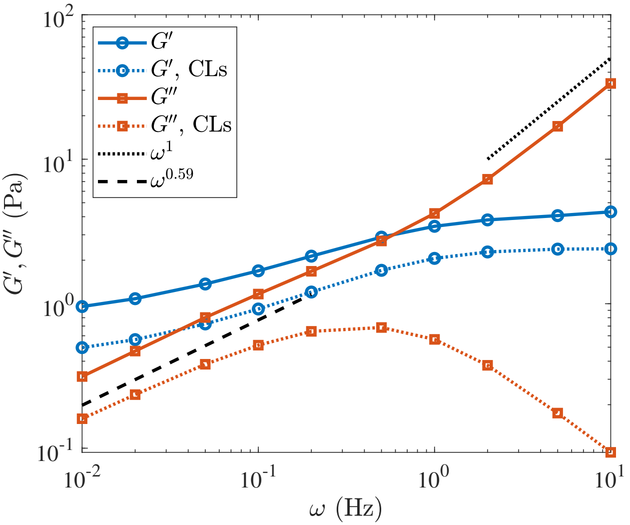
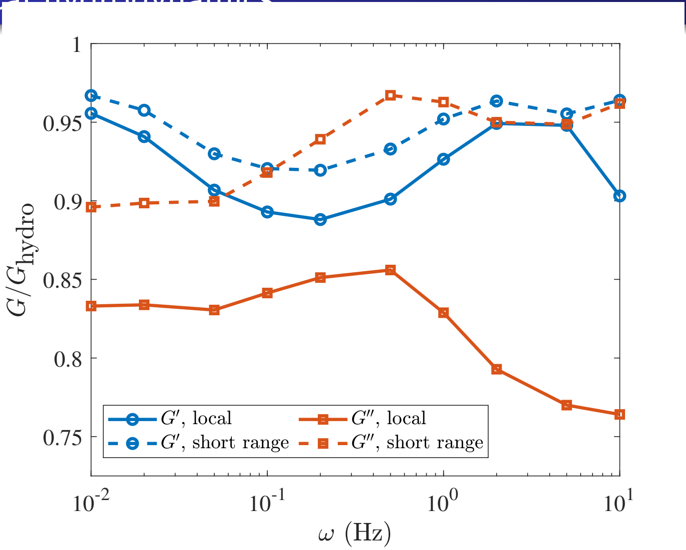
$$G' = \frac{2}{\gamma_0 T} \int_0^T \sigma_{21} \sin(\omega t)\, dt \qquad G'' = \frac{2}{\gamma_0 T} \int_0^T \sigma_{21} \cos(\omega t)\, dt.$$

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:

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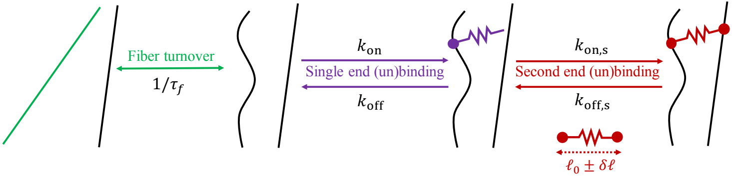
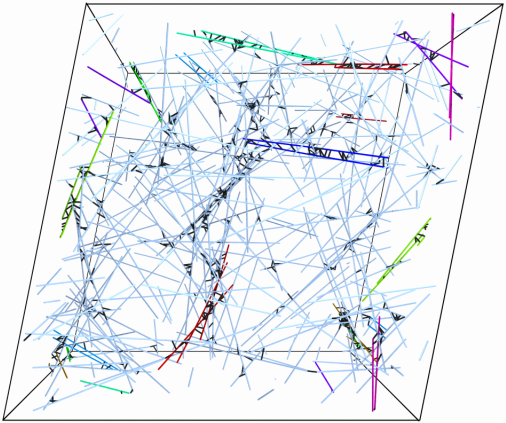
- Four reactions between fibers and CL reservoir obey **detailed balance**

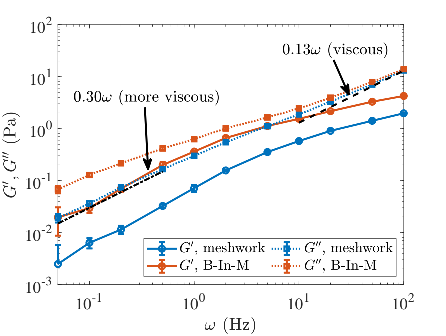


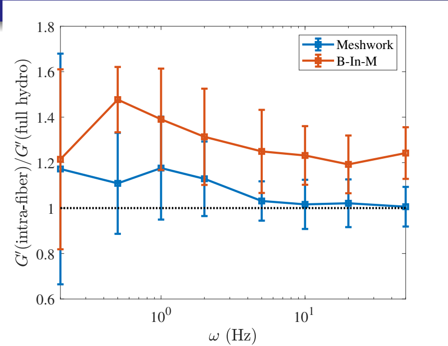
O. Maxian et al, PLOS Comp. Bio., 2021 [**bioRxiv:2021.07.07.451453**] [6]
and Biophysical J., 2022 [**bioRxiv:021.09.17.460819**] [7]

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.

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

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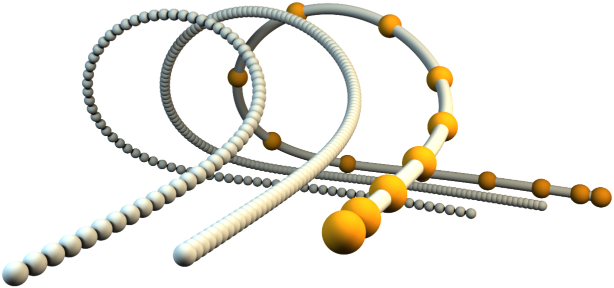
  - Does the **Brownian stress** of the fiber converge in the continuum limit? (bending energy does not)

Brownian multiblob chains

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



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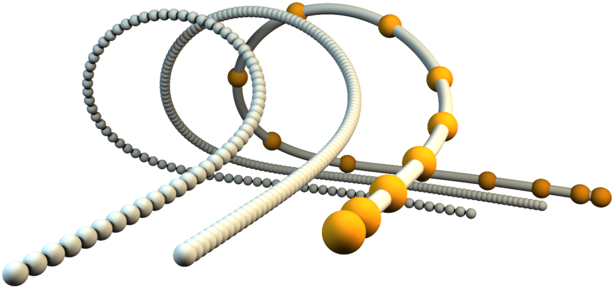

Fast constrained BD-HI for blob-link chains based on rotating unit link vectors including Brownian stress (Brennan Sprinkle, in progress)

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