# 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*

CAIMS, Kelowna, BC, Canada
June 2022

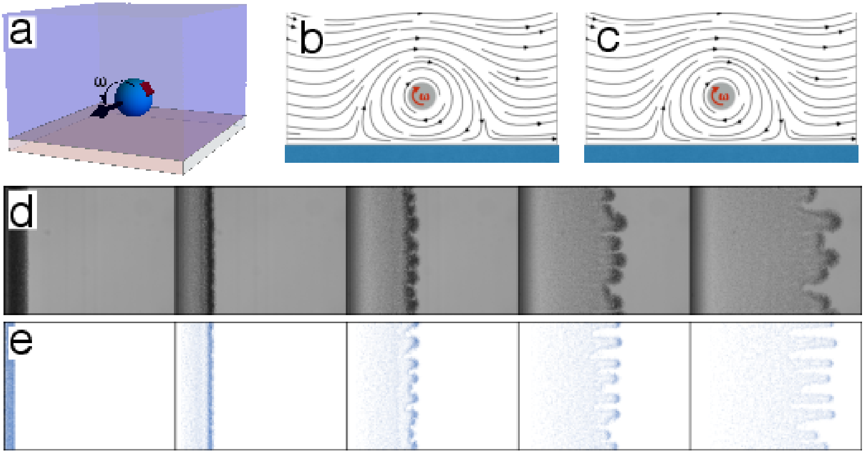
# Outline

# Outline

# Research interests

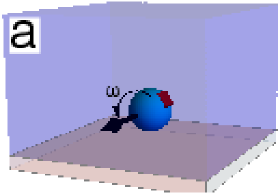
- The primary focus of my research is **fluid dynamics at small scales** (100nm-10$\mu m$), where **thermal fluctuations / Brownian motion** play an important role.
- A key approach I use and try to understand is **fluctuating hydrodynamics** (stochastic partial differential equations).
- Tools: fast 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).

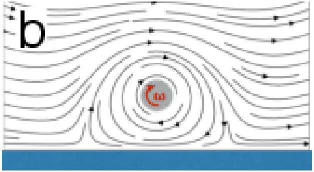
# Microrollers: Fingering Instability

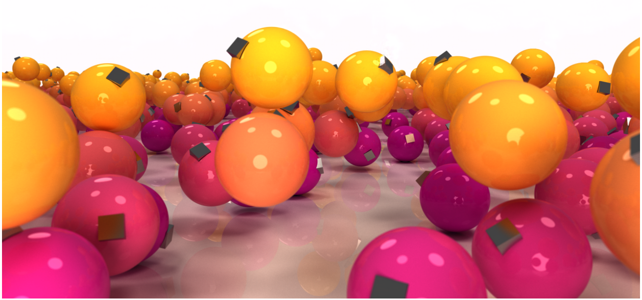



Experiments by Michelle Driscoll, simulations by **Blaise Delmotte** (was at Courant, now at LadHyX Paris), *Nature Physics* 13 (2017) [1]

# Microrollers: Uniform Monolayers

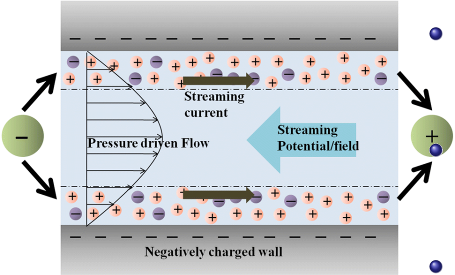


B. Sprinkle et al., *Soft Matter* 16 (2020) [**ArXiv:2005.06002**] [2]

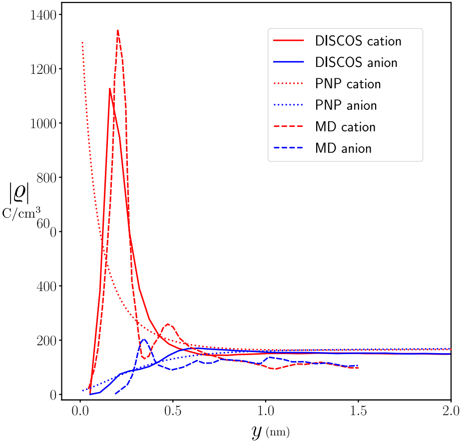
# Electrohydrodynamics

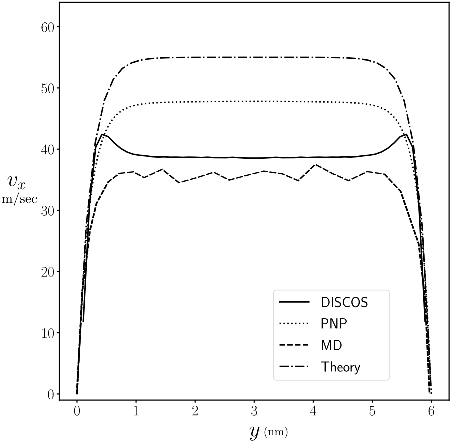



**Electro-hydrodynamic flow**
Key issue: Debye length/layer of molecular scales and continuum approach is questionable quantitatively:
*no sterics, no image charges, no fluctuations, no ion pairing*

- **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]

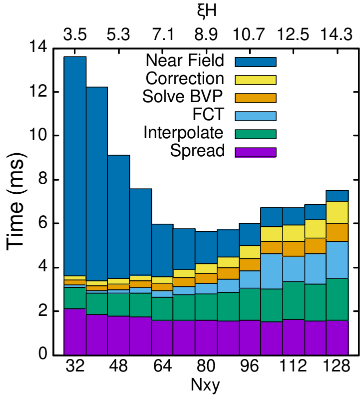
# Electroosmotic flow: MD vs BD

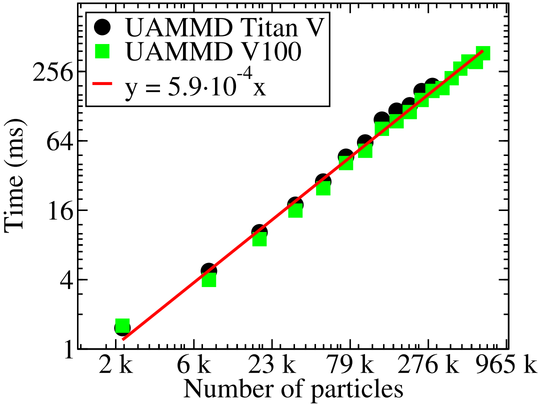



Continuing work on Courant on spectral **GPU-based** methods/codes for electrolyte BD-HI and **electrochemical applications**

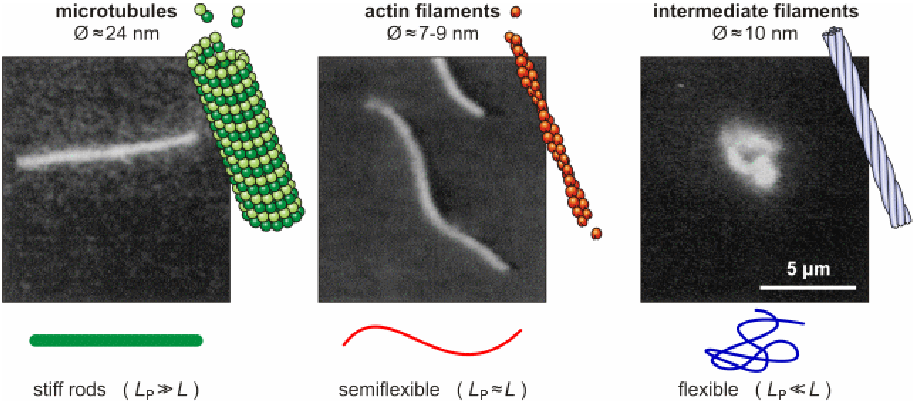
# GPU acceleration




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

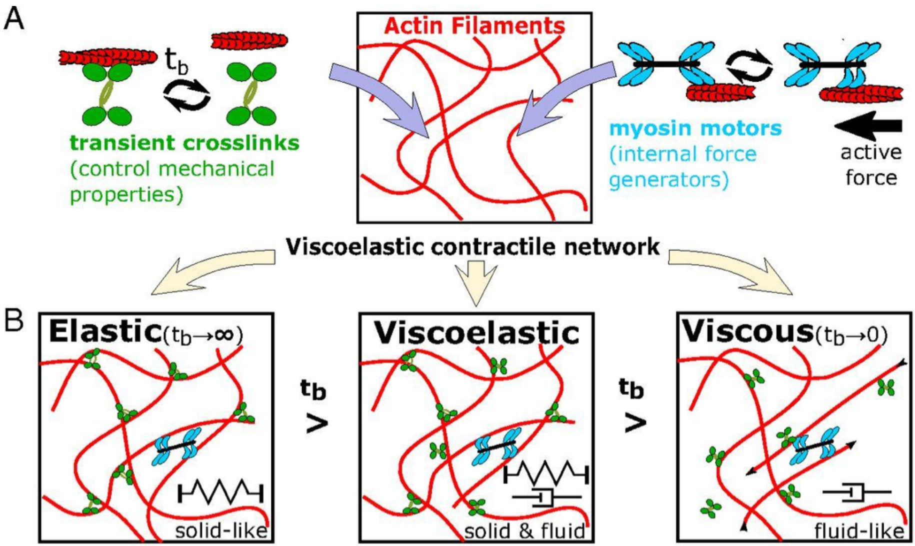
# Fibers involved in cell mechanics




Pawlizak and Käs, University of Leipzig

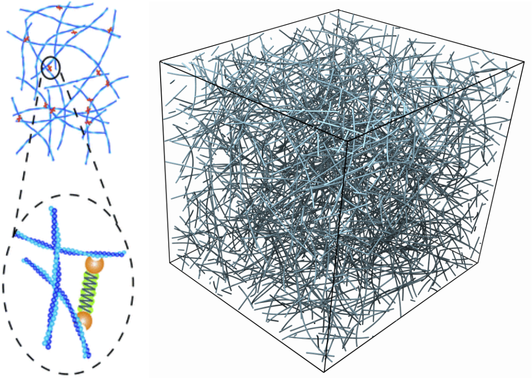
$L_p$ =persistence length, $L$ =fiber length, $a = \epsilon L$ =fiber radius, $\epsilon$ =slenderness ratio

# 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, $\mathbf{Q}(t) = \{\mathbf{q}_1(t), \ldots, \mathbf{q}_N(t)\}$:
$$d\mathbf{Q} = \boldsymbol{\mathcal{M}}\mathbf{F}dt + (2k_B T\,\boldsymbol{\mathcal{M}})^{\frac{1}{2}}\, d\boldsymbol{\mathcal{B}} + k_B T\,(\partial_{\mathbf{Q}} \cdot \boldsymbol{\mathcal{M}})\, dt,$$
where $\boldsymbol{\mathcal{B}}(t)$ is a vector of Brownian motions, and $\mathbf{F}(\mathbf{Q})$ are electrostatic+steric+external forces.
- The symmetric positive semidefinite (SPD) but dense **hydrodynamic mobility matrix** $\boldsymbol{\mathcal{M}}(\mathbf{Q})$:
$3 \times 3$ block $\mathbf{M}_{ij}$ that maps a force on particle $j$ to a velocity of particle $i$ (Stokes flow problem).

# Computational Issues in BDHI

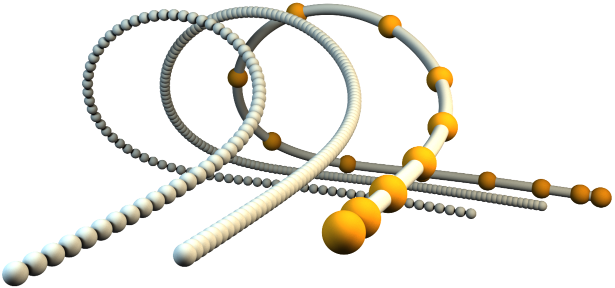
Key challenges for fast **linear-scaling** BD-HI:

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

# Outline

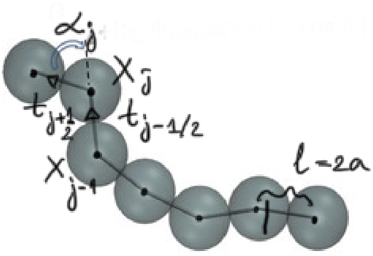
# Fiber Representation

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: $\|\mathbf{X}_{j+1} - \mathbf{X}_j\| = l \sim a$ (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 $\kappa_b$)

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

# 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**:

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

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

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

# 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
$$\nabla\pi=\eta\nabla^2\mathbf{v}+\sum_j \mathbf{F}_j\,\delta_a(\mathbf{X}_j-\mathbf{r}),$$
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
$$\mathbf{U}_j=d\mathbf{X}_j/dt=\int d\mathbf{r}\;\mathbf{v}(\mathbf{r},t)\,\delta_a(\mathbf{X}_j-\mathbf{r}).$$
- Continuum limit is obvious (without Brownian fluctuations)
$$\nabla\pi(\mathbf{r},t)=\eta\nabla^2\mathbf{v}(\mathbf{r},t)+\int_0^L ds\;\mathbf{f}(s,t)\delta_a(\mathbf{X}(s,t)-\mathbf{r})$$
$$\mathbf{U}(s,t)=\partial_t\mathbf{X}(s,t)=\int d\mathbf{r}\;\mathbf{v}(\mathbf{r},t)\,\delta_a(\mathbf{X}(s,t)-\mathbf{r})$$
$$\mathbf{f}=-\kappa_b\mathbf{X}_{ssss}+\boldsymbol{\lambda}$$

# Multiblob chains in Stokes flow

- We can (temporarily) eliminate the fluid velocity to write an equation for **fiber only**.
- Define the positive semi-definite **hydrodynamic kernel**

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

  where $\mathbb{G}$ is the Green's function for (periodic) Stokes flow.
- Define $\mathbf{M}\left(\mathbf{X}\right)\succeq\mathbf{0}$ to be the symmetric positive semidefinite (SPD) **mobility matrix** with blocks

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

- Discrete dynamics = **inextensibility** +

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

# Inextensible fibers in Stokes flow

- Define a positive semidefinite **mobility operator**

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

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

$$\mathbf{U}=\mathbf{X}_t=\mathcal{M}\left[\mathbf{X}\right]\left(-\kappa_b\mathbf{X}_{ssss}+\boldsymbol{\lambda}\right)$$

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

- Is this PDE well-posed? We have shown *numerically* that
  - Fiber **velocity converges pointwise** (strongly) up to the endpoints.
  - **Moments of $\lambda$ 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**

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

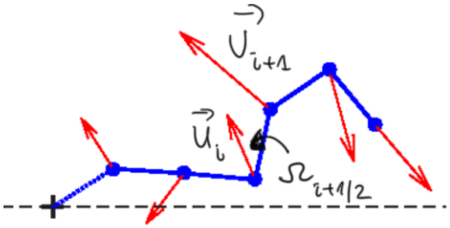
$$\mathcal{S}\left(\mathbf{r}\right) = \frac{1}{8\pi\eta r}\left(\mathbf{I} + \hat{\mathbf{r}}\hat{\mathbf{r}}^T\right) \equiv \mathbb{G}, \quad \text{and} \quad \mathcal{D}\left(\mathbf{r}\right) = \frac{1}{8\pi\eta r^3}\left(\mathbf{I} - \hat{\mathbf{r}}\hat{\mathbf{r}}^T\right)$$

# 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)
  $\left(\mathcal{M}\,\mathbf{f}\right)(s)\approx\left(\mathcal{M}_{\mathrm{SBT}}\,\mathbf{f}\right)(s)=\left(\mathcal{M}_{\mathrm{L}}\,\mathbf{f}\right)(s)+\left(\mathcal{M}_{\mathrm{NL}}\,\mathbf{f}\right)(s)=$
  $$=\frac{1}{8\pi\eta}\left(\log\left(\frac{(L-s)s}{4a^2}\right)\left(\mathbf{I}+\boldsymbol{\tau}(s)\boldsymbol{\tau}(s)^T\right)+4\mathbf{I}\right)\mathbf{f}(s)$$
  $$+\frac{1}{8\pi\eta}\int_0^L ds'\left(\mathcal{S}\left(\mathbf{X}(s)-\mathbf{X}(s')\right)\mathbf{f}\left(s'\right)-\left(\frac{\mathbf{I}+\boldsymbol{\tau}(s)\boldsymbol{\tau}(s)^T}{\left|s-s'\right|}\right)\mathbf{f}(s)\right)$$
- 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:

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

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

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

- We can express this in terms of tension

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

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

# Continuum equations

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

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

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

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

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

- 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**

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

  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**

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

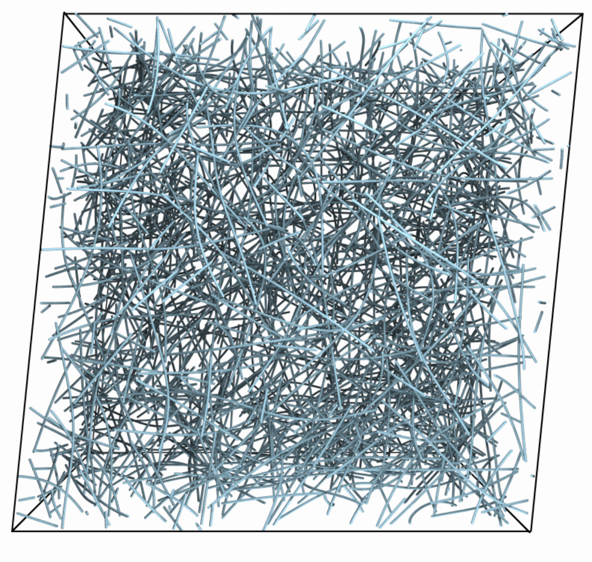
- $\mathbf{f}^n$ contains other forces such as **cross-linkers** (can be stiff). **Flow** is easy to add to the rhs.

# The gory details

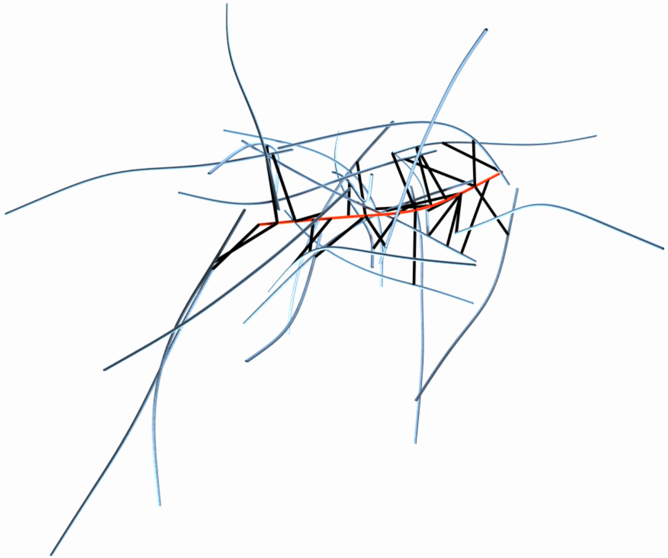
1. For dense suspensions, supplement L+NL splitting with additional **1-5 GMRES iterations** for stability.
2. Evaluate long-ranged hydrodynamic interactions between Chebyshev nodes in **linear time** using *Positively Split Ewald* (PSE) method (FFT based for triply periodic), also works for **deformed/sheared 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:

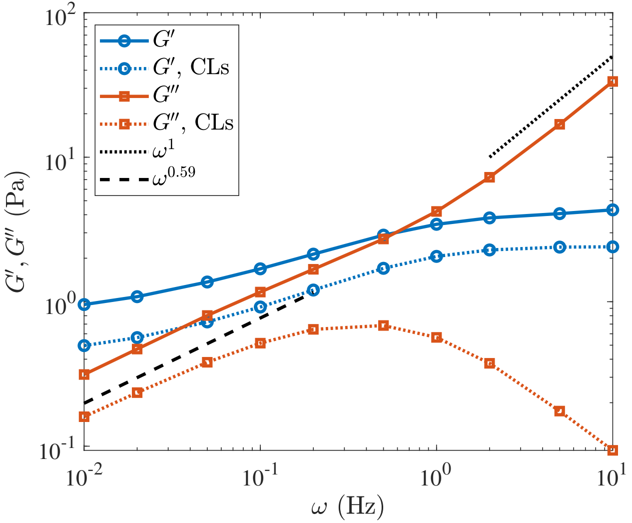
$$\boldsymbol{\sigma}^{(i)} = \frac{1}{V} \sum_{\text{fibers}} \int_0^L ds\, \mathbf{X}^i(s) \left(\mathbf{f}_b(s) + \boldsymbol{\lambda}(s)\right)^T$$

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

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

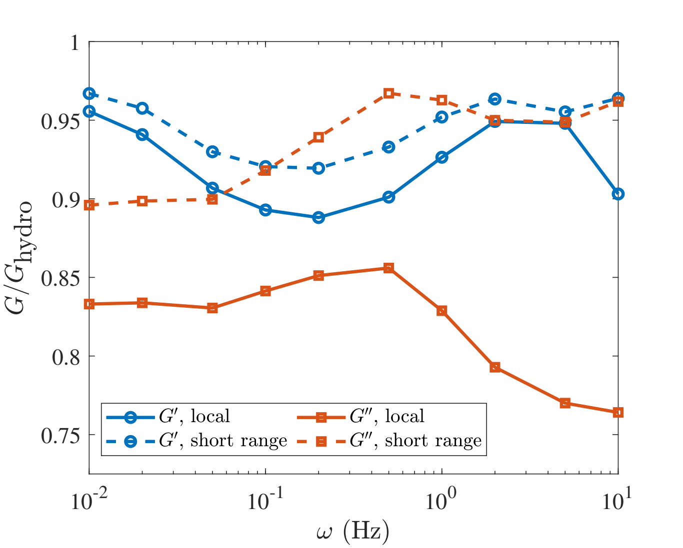
$$G' = \frac{2}{\gamma_0 T} \int_0^T \sigma_{21} \sin(\omega t)\, dt \qquad G'' = \frac{2}{\gamma_0 T} \int_0^T \sigma_{21} \cos(\omega t)\, dt.$$

# 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**.

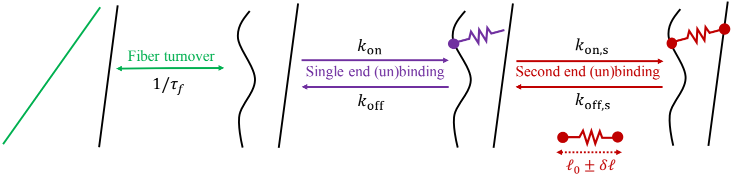
# Dynamic cross linking

**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**.

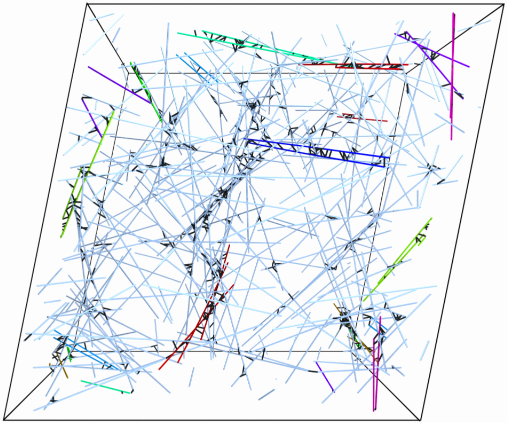
Assumptions behind linking algorithm

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

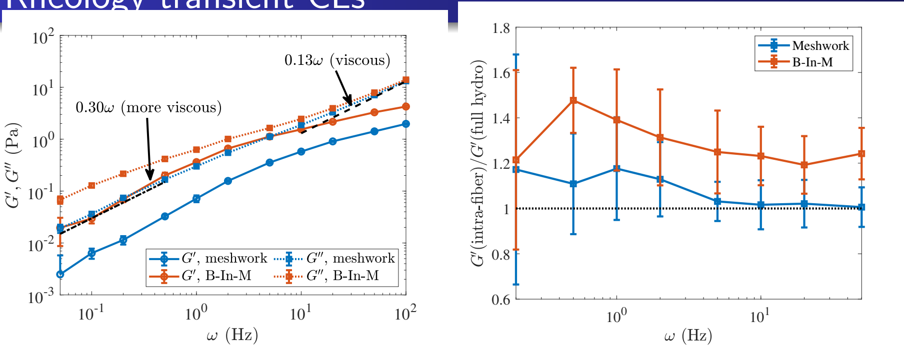



O. Maxian et al, PLOS Comp. Bio., 2021 [**bioRxiv:2021.07.07.451453**] [6]
and Biophysical J., 2022 [**bioRxiv:021.09.17.460819**] [7]

# 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)

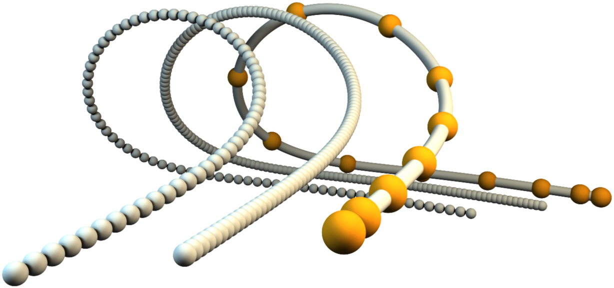
- **Rigid fibers** are "easy" though so far we have only implemented *without* inter-fiber hydro [7].
- **Fluctuating hydrodynamics** gives the fluctuating Stokes equations

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

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