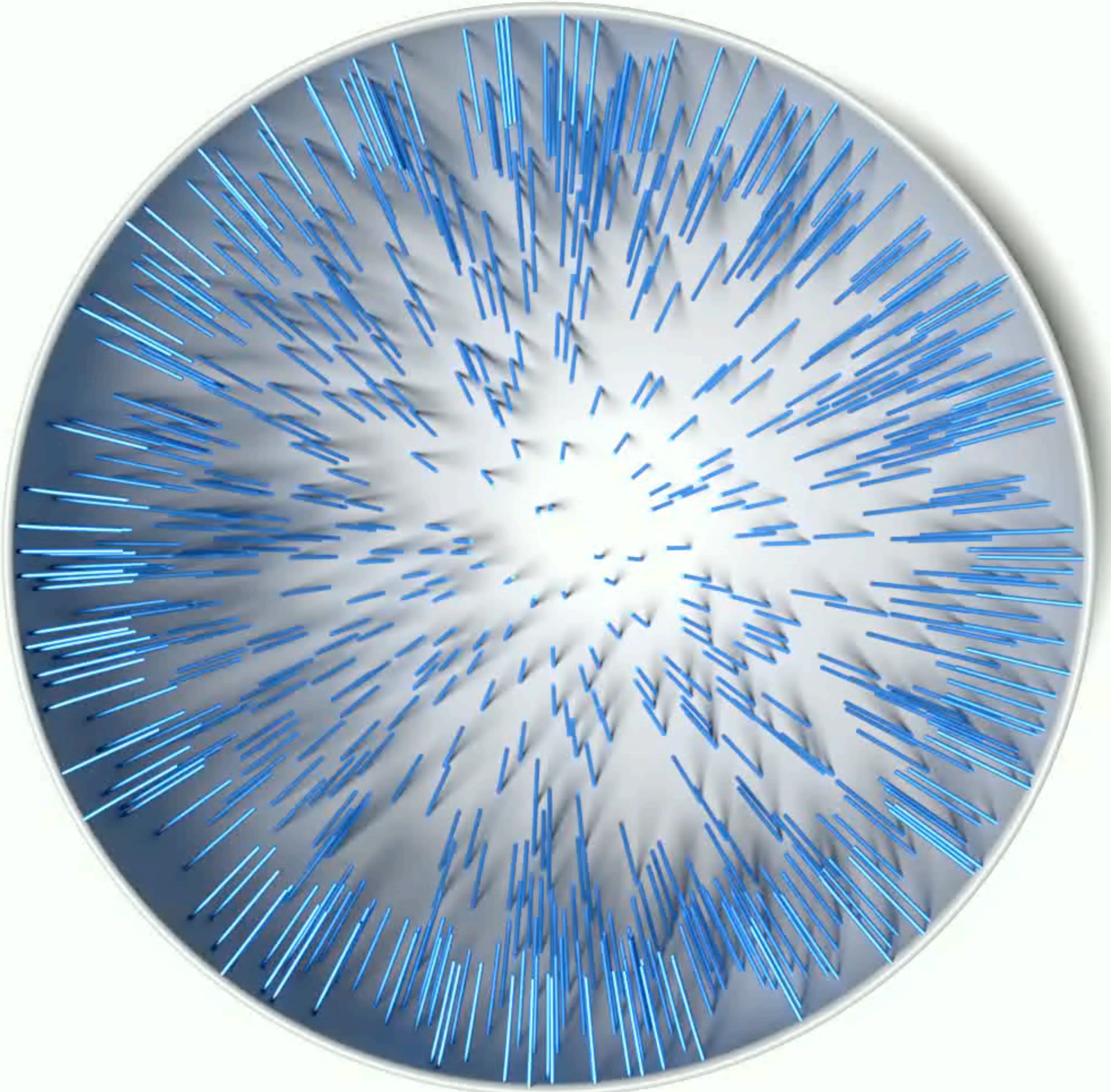
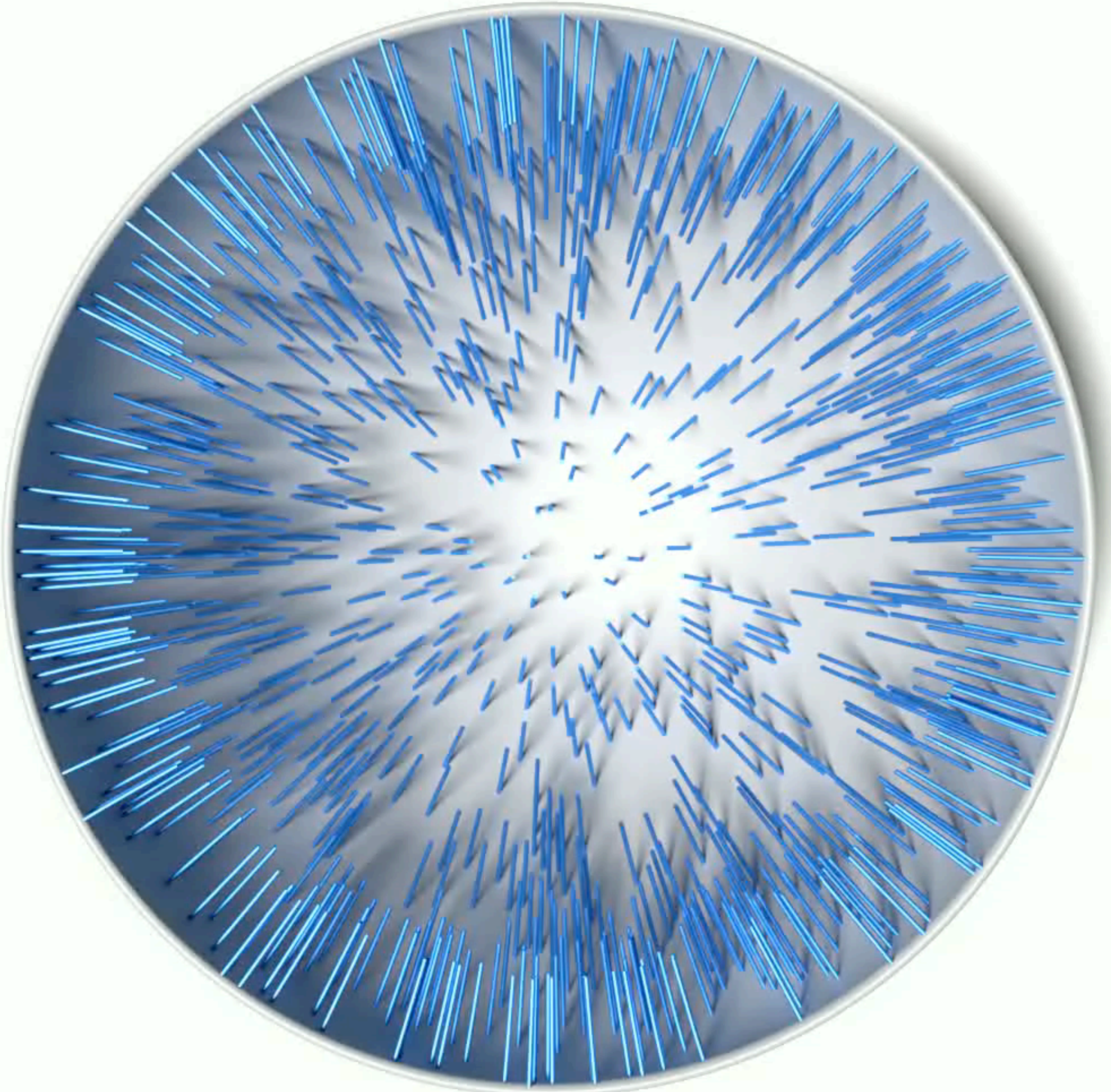
SkellySim — Computational Methods

David Stein
June 8, 2023

With 1250 microtubules



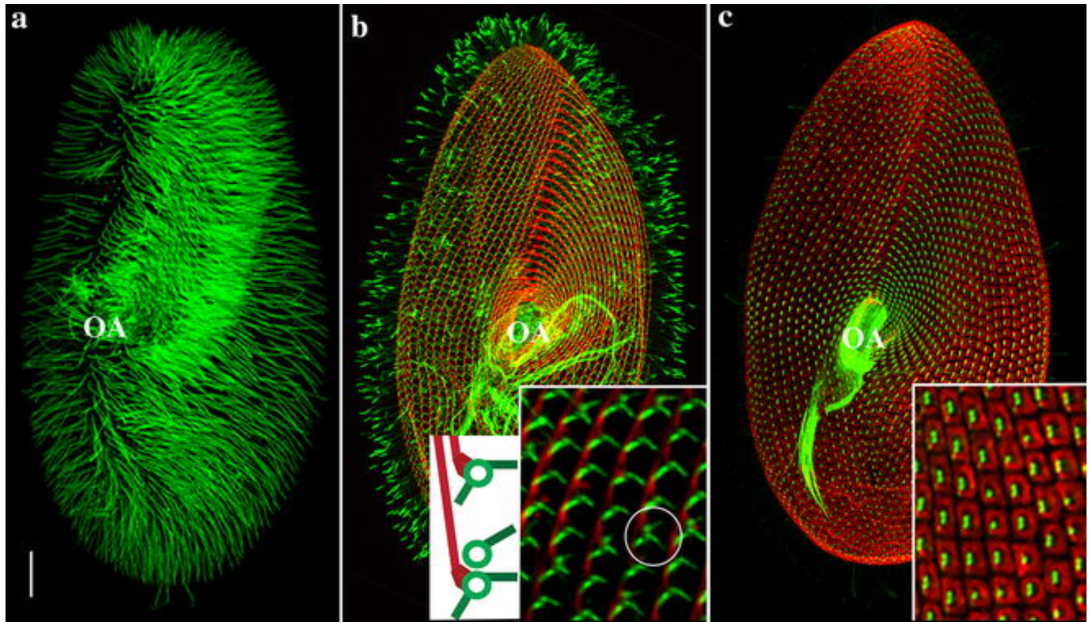
With 1500 microtubules



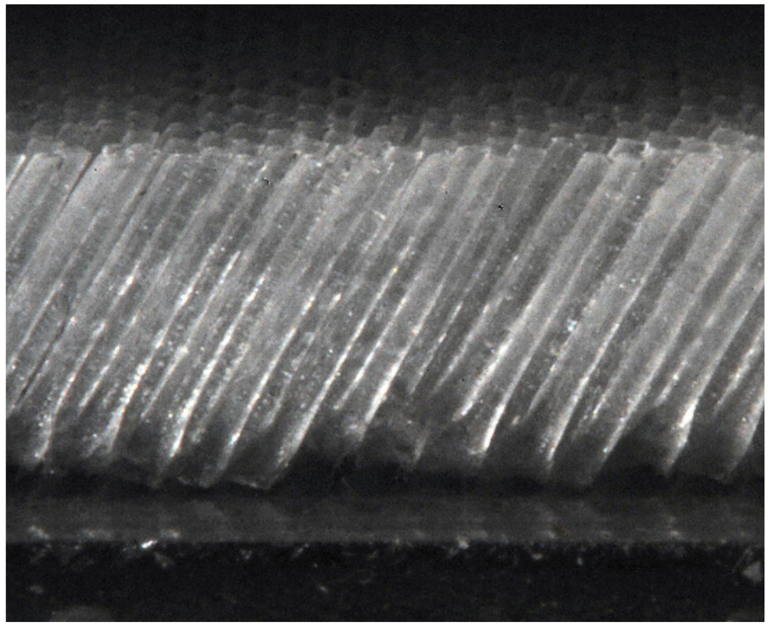
What is SkellySim?

- Large scale simulations of many long, slender, flexible filaments immersed in a fluid

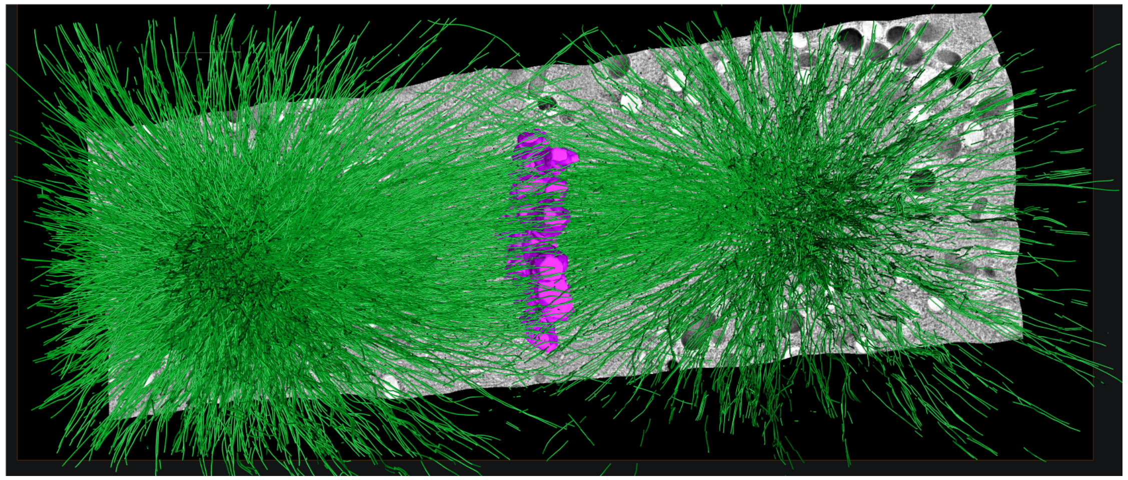
Paramecium, [Tassin et al, 2015]



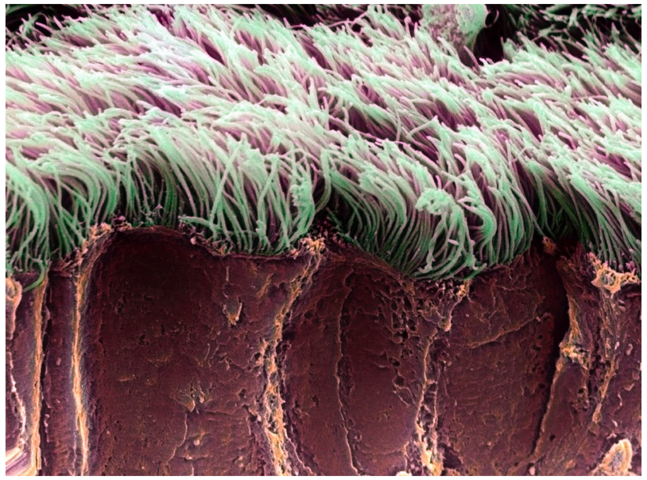
Soft Rectifier, [Alvarado et al, 2017]



Mitotic Spindle, [Redemann et al, 2017]



Bronchial Cilia [Google Images]



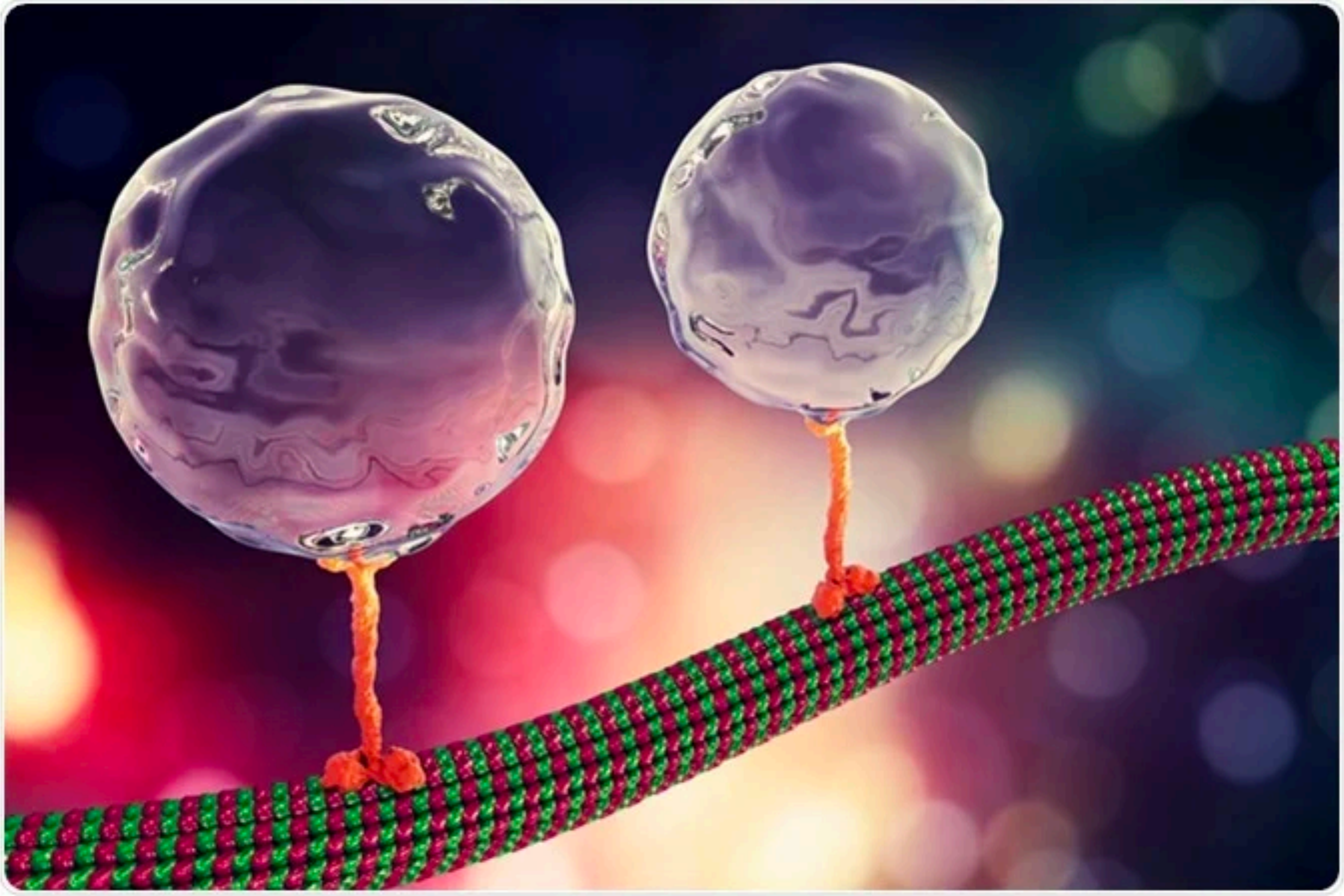
What is SkellySim?

- Large scale simulations of many long, slender, flexible filaments immersed in a fluid

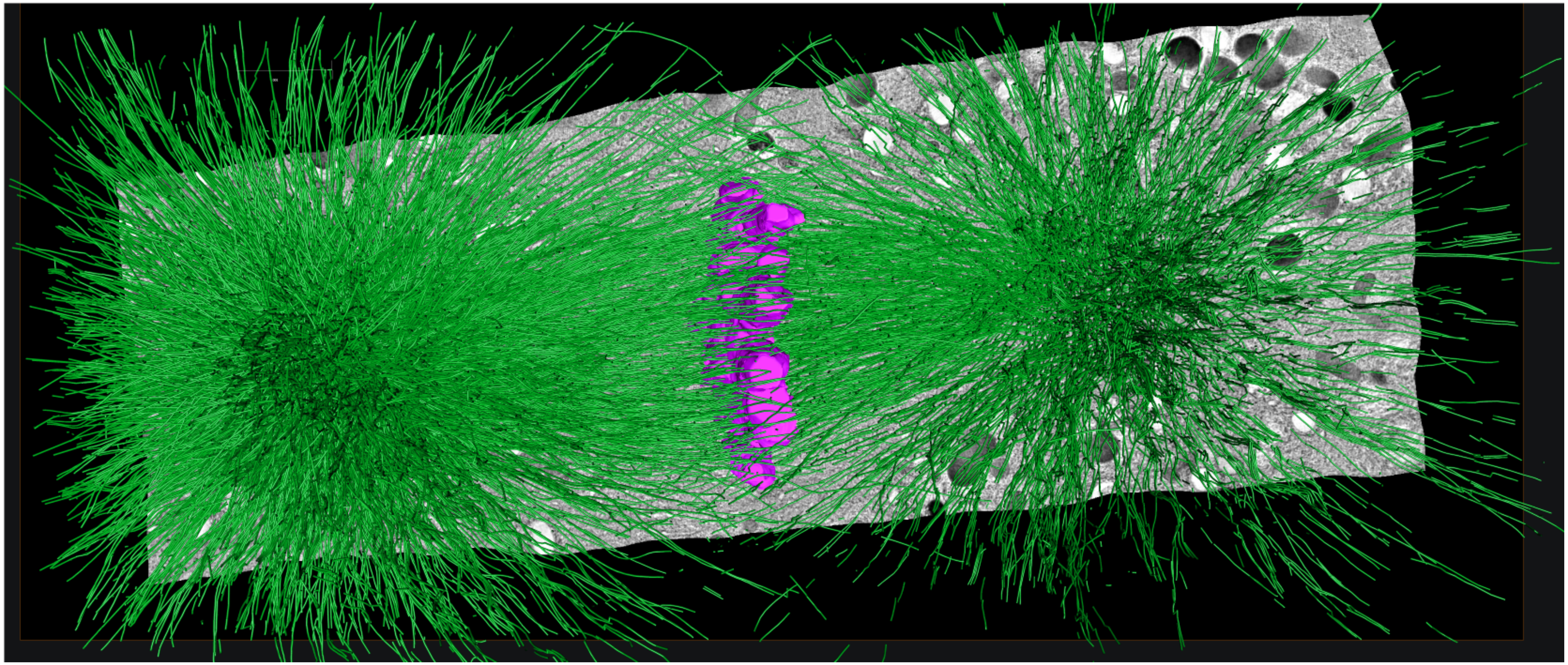
Challenges -

- Slender filaments are inherently multi-scale
- The equations of motion that govern them are *extremely stiff*
- The immersing fluid strongly couples all degrees of freedom together (and there are many degrees of freedom when there are many fibers)

Slender filaments are inherently multiscale



Slender filaments are inherently multiscale



Slender filaments are inherently multiscale

Reduce the description to the fibers *centerline* - a 1D object, rather than the full fiber (a 3D object)

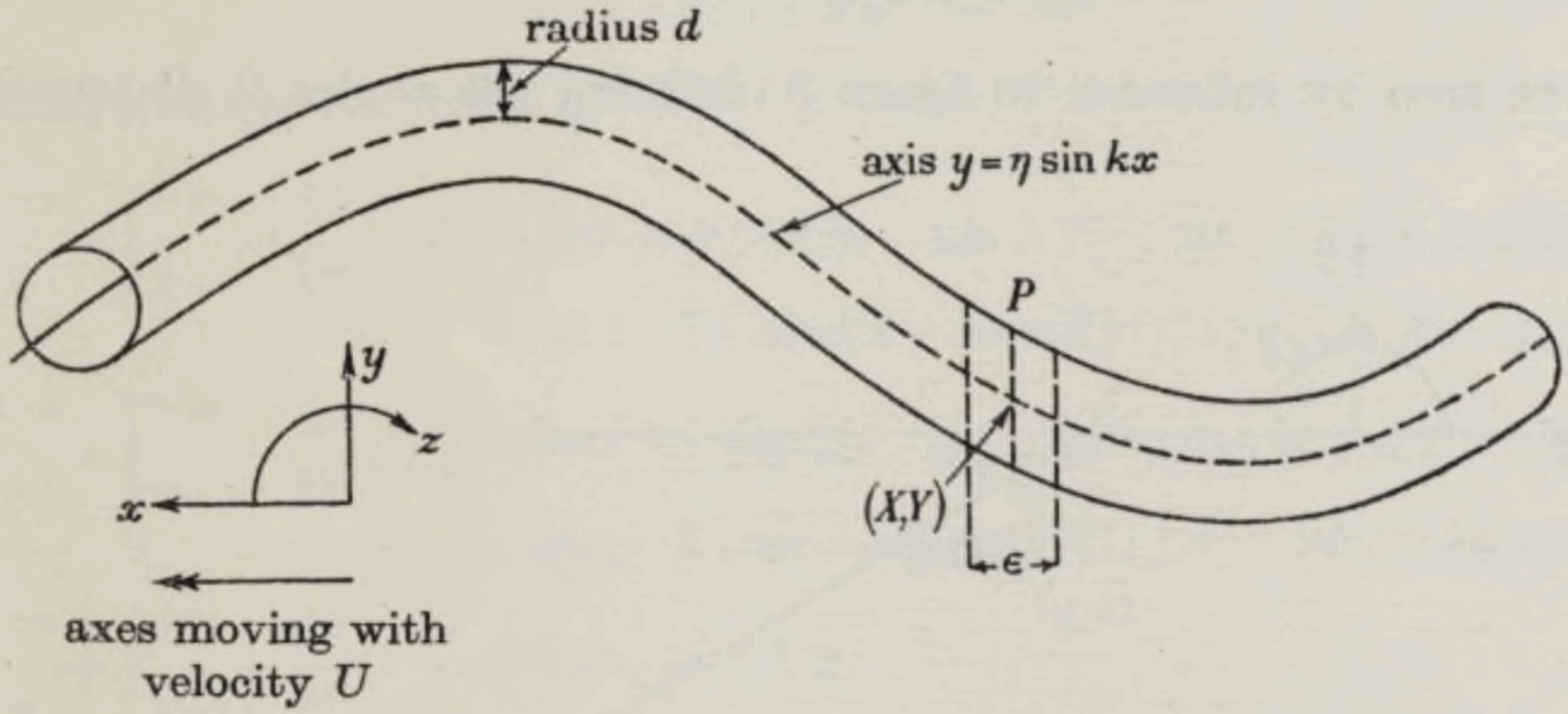


FIGURE 2. Oscillating filament referred to moving axes.

Slender filaments are inherently multiscale

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Simulating the dynamics and interactions of flexible fibers in Stokes flows

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J. Fluid Mech. (1976), *vol.* 75, *part* 4, *pp.* 705–714 705

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Slender-body theory for slow viscous flow

By JOSEPH B. KELLER

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Graduate School of Medical Sciences, Cornell University, New York 10021

(Received 15 October 1975 and in revised form 1 April 1976)

The self-propulsion of microscopic organisms through liquids

By G. J. Hancock

Department of Mathematics, Manchester University

(*Communicated by M. H. A. Newman, F.R.S.—Received* 16 *October* 1952—*Revised* 16 *December* 1952)

NATIONAL ADVISORY COMMITTEE FOR AERONAUTICS

REPORT No. 184

THE AERODYNAMIC FORCES ON AIRSHIP HULLS

By MAX M. MUNK

WASHINGTON
GOVERNMENT PRINTING OFFICE
1924

Slender filaments are inherently multiscale

Motion of a single fiber in a background flow $\mathbf{U}_0$

$$8\pi\mu\left(\frac{\partial \mathbf{x}(s,t)}{\partial t} - \mathbf{U}_0(\mathbf{x}(s,t),t)\right) = -\Lambda[\mathbf{f}](s) - \mathbf{K}[\mathbf{f}](s)$$

Local:

$$\Lambda[\mathbf{f}](s) = [-c(\mathbf{I} + \hat{\mathbf{s}}\hat{\mathbf{s}}(s)) + 2(\mathbf{I} - \hat{\mathbf{s}}\hat{\mathbf{s}}(s))]\mathbf{f}(s)$$

Nonlocal Integral Operator:

$$\mathbf{K}[\mathbf{f}](s) = \int_0^L \left(\frac{\mathbf{I} + \hat{\mathbf{R}}(s,s')\hat{\mathbf{R}}(s,s')}{|\mathbf{R}(s,s')|}\mathbf{f}(s') - \frac{\mathbf{I} + \hat{\mathbf{s}}(s)\hat{\mathbf{s}}(s)}{|s-s'|}\mathbf{f}(s)\right)\mathrm{d}s'$$

Slender filaments are inherently multiscale

$$\frac{8\pi\mu}{c}\left(\mathbf{X}_t(s) - \mathbf{U}(\mathbf{X}(s))\right) = \left(\mathbb{I} + \mathbf{X}_s(s)\mathbf{X}_s(s)\right)\mathbf{f}(s)$$

For $s \in [0, L]$, where *s* is an arc-length parameter.

μ is fluid viscosity, ε the *slenderness* of the filament:

$$c = -\ln(e\epsilon^2) \qquad \epsilon = r/L$$

and $\mathbf{X}_s = \partial_s \mathbf{X}$ is the tangent vector to the filament

The forces are those arising from the deformed filament:

$$\mathbf{f}(s) = -E\mathbf{X}_{ssss} + (T\mathbf{X}_s)_s$$

E is a *bending modulus,* and T is a *tension* (enforcing strict inextensibility)

Challenges

- ~~Slender filaments are inherently multi-scale~~
    - Use slender body theory to reduce dynamics to 1D PDEs

$$\frac{8\pi\mu}{c}\left(\mathbf{X}_t - \mathbf{U}\right) = \left(\mathbb{I} + \mathbf{X}_s\mathbf{X}_s\right)\left(-E\mathbf{X}_{ssss} + \left(T\mathbf{X}_s\right)_s\right)$$

- The equations of motion that govern them are *extremely stiff*
- The immersing fluid strongly couples all degrees of freedom together (and there are many degrees of freedom when there are many fibers)

The equations of motion are stiff

$$\frac{8\pi\mu}{c}\left(\mathbf{X}_t - \mathbf{U}\right) = \left(\mathbb{I} + \mathbf{X}_s\mathbf{X}_s\right)\left(-E\mathbf{X}_{ssss} + (T\mathbf{X}_s)_s\right)$$

Simple model problem:

$$X_t = -X_{ssss}$$

Discretize in time using Forward-Euler:

$$\frac{X(t+\Delta t) - X(t)}{\Delta t} = -X_{ssss}(t)$$

Or, upon rearrangement:

$$X(t+\Delta t) = X(t) - \Delta t X_{ssss}(t)$$

The equations of motion are stiff

$$X(t+\Delta t) = X(t) - \Delta t X_{ssss}(t)$$

Taking the Fourier Transform:

$$\hat{X}^k(t+\Delta t) = \hat{X}^k(t) - \Delta t \widehat{X_{ssss}}^k(t)$$

$$\hat{X}^k(t+\Delta t) = \hat{X}^k(t) - \Delta t (ik)^4 \hat{X}^k(t)$$

$$\hat{X}^k(t+\Delta t) = \left(1 - \Delta t k^4\right) \hat{X}^k(t)$$

Imposes a timestep restriction:

$$\Delta t k^4 < 1$$

$$\Delta t \lesssim \frac{8\pi\mu}{cEk^4}$$

The equations of motion are stiff

Simple model problem:

$$X_t = -X_{ssss}$$

Discretize in time using Backward-Euler:

$$\frac{X(t+\Delta t) - X(t)}{\Delta t} = -X_{ssss}(t+\Delta t)$$

Or, upon rearranging and taking Fourier Transform:

$$\hat{X}^k(t+\Delta t) = \frac{\hat{X}_k}{1+\Delta t k^4}$$

The equations of motion are stiff

Forward-Euler:

$$X(t+\Delta t) = X(t) - \Delta t X_{ssss}(t)$$

Backward-Euler:

$$X(t+\Delta t) = X(t) - \Delta t X_{ssss}(t+\Delta t)$$

Now, for the full equations:

$$\frac{8\pi\mu}{c}\left(\mathbf{X}_t - \mathbf{U}\right) = \left(\mathbb{I} + \mathbf{X}_s\mathbf{X}_s\right)\left(-E\mathbf{X}_{ssss} + (T\mathbf{X}_s)_s\right)$$

Full Backward-Euler:

$$\frac{8\pi\mu}{c}\left(\mathbf{X}^+ - \mathbf{X} - \Delta t\mathbf{U}^+\right) = \Delta t\left(\mathbb{I} + \mathbf{X}_s^+\mathbf{X}_s^+\right)\left(-E\mathbf{X}_{ssss}^+ + (T^+\mathbf{X}_s^+)_s\right)$$

IMEX-Scheme:

$$\frac{8\pi\mu}{c}\left(\mathbf{X}^+ - \mathbf{X} - \Delta t\mathbf{U}^+\right) = \Delta t\left(\mathbb{I} + \mathbf{X}_s\mathbf{X}_s\right)\left(-E\mathbf{X}_{ssss}^+ + (T^+\mathbf{X}_s)_s\right)$$

Provides a linear equation that must be solved at each timestep to evolve the system.

Challenges

- ~~Slender filaments are inherently multi-scale~~
  - Use slender body theory to reduce dynamics to 1D PDEs

$$\frac{8\pi\mu}{c}\left(\mathbf{X}_t - \mathbf{U}\right) = \left(\mathbb{I} + \mathbf{X}_s\mathbf{X}_s\right)\left(-E\mathbf{X}_{ssss} + (T\mathbf{X}_s)_s\right)$$

- ~~The equations of motion that govern them are *extremely stiff*~~
  - Use an Implicit-Explicit timestepping scheme
- The immersing fluid strongly couples all degrees of freedom together (and there are many degrees of freedom when there are many fibers)

The immersing fluid

What flow does a deforming fiber create in the fluid?

$$\mathbf{u}(\mathbf{x}) = \int_0^L G(\mathbf{x} - \mathbf{X}(s))\, \mathbf{f}(s)\, ds + \mathcal{O}(\epsilon^2)$$

Where G is the Stokeslet Kernel:

$$G(\mathbf{r}) = \frac{1}{8\pi\mu} \frac{\mathbb{I} - \widehat{\mathbf{r}}\widehat{\mathbf{r}}}{|\mathbf{r}|} \qquad \widehat{\mathbf{r}} = \mathbf{r}/|\mathbf{r}|$$

So the evolution equation for each fiber is:

$$\frac{8\pi\mu}{c}\left(\mathbf{X}_t^k - \underbrace{\sum_{i\neq k} \int_0^{L^i} G(\mathbf{X}^k - \mathbf{X}^i(s))\mathbf{f}^i(s)\, ds}_{\text{Fibers coupling through the fluid}}\right) = \left(\mathbb{I} + \mathbf{X}_s^k \mathbf{X}_s^k\right) \mathbf{f}^k$$

The immersing fluid

Upon discretization in space and time:

$$\tilde{\mathbf{X}}^k(s_j) - \Delta t \sum_{i \neq k} \sum_{l=1}^{N_i} G(\mathbf{X}^k(s_j) - \mathbf{X}^i(s_l))\tilde{\mathbf{f}}^i(s_l)w_l^i - C\Delta t \left(\mathbb{I} + \mathbf{X}_s^k(s_j)\mathbf{X}_s^k(s_j)\right)\tilde{\mathbf{f}}^k(s_j) = \mathbf{X}^k(s_j)$$

$$\tilde{\mathbf{f}} = -E\tilde{\mathbf{X}}_{ssss} + (\tilde{T}\mathbf{X}_s)_s$$

This is a dense linear system of equations for:

$$(\tilde{\mathbf{X}}^k(s_j), \tilde{T}^k(s_j))$$

If we have 5000 fibers with 100 discretization points each, then this system is equivalent to a 2,000,000 x 2,000,000 matrix.

N	100	1,000	10,000	100,000	1,000,000
Time	51 µs	6.5 ms	1.8 s	16 min	*
Memory	80 kB	8 MB	800 MB	80 GB	8 TB

The immersing fluid

A.N. Krylov: a short biography

A.N.Krylov

Alexei Nikolaevich Krylov was born on August 3, 1863 in a village of the Simbirsk Region in Russia. The name A.N. Krylov is probably one of the most widely known and recognized in Russia among outstanding scientists in the 20th century. Although his research interests were incredibly broad (at least for a scientist of the 20th century), his professional activity could apparently be best characterized by saying that he was a very good Maritime Engineer. This should necessarily mean that he was a very good Applied Mathematician too.

Note that in the word "Krylov" the second syllable is stressed and that "y" should be pronounced in the same way as in "Chebyshev". Another possible spelling of "Krylov" is "Kriloff".

At the age of 15, Krylov entered a Naval College in 1878 and finished it with distinction in 1884. After spending several years at the Main Hydrographic Administration and at a shipbuilding plant, in 1888 he continued his study in the Naval Academy in Saint-Petersburg. He was a talented and promising student and after ahead-of-schedule graduation from the Academy in 1890 he could stay there as Mathematics and Ship-theory lecturer.

The fame came to him in the 1890s, when his pioneering "Theory of oscillating motions of the ship", significantly extending R.E. Froude's rolling theory, became internationally known. This was the first comprehensive theoretical study in the field. In 1898 Krylov received a Gold Medal from the Royal Institution of Naval Architects (it was the first time the prize was awarded to a foreigner).

After 1900 Krylov actively collaborated with S.O. Makarov, admiral and maritime scientist, working on the ship floodability problem. The results of this work soon became classic, they are widely used nowadays over the world. Many years later, Krylov wrote about one of the early ideas of Makarov to fight the heel of a sinking ship by flooding its undamaged compartments: "This appeared to be such a great nonsense [to the naval officials] that it took 35 years ...to convince [them] that the ideas of the 22-years-old Makarov are of great practical value".
Krylov knew what he was writing about: his own ideas were often equally "welcome". To promote his innovations, he often had to fight against stagnation and rigid views of the top officials. Once, giving a speech at an important meeting before a large audience, Krylov addressed naval officers asking them for their support in his "fight against the rut in the shipbuilding". Being a naval officer at that time, he got an official reprimand for this speech.
Another incident also quite remarkably illustrates Krylov's personality: on a sitting of a high-rank technical committee Krylov once took with him several technicians directly from the ships so that they could support his opinion in the debates.

Krylov wrote about 300 papers and books. They span a wide range of topics, including shipbuilding, magnetism, artillery, mathematics, astronomy, and geodesy. His "floodability tables" have been used worldwide.
In 1904 he built the first machine in Russia for integrating ODEs.

In 1931 he published a paper on what is now called the "Krylov subspace". The title of this paper is not always translated correctly; this is the case, for instance, in B. Parlett's "The Symmetric Eigenvalue Problem". The title of the paper should be:
"On the numerical solution of the equation by which, in technical matters, frequencies of small oscillations of material systems are determined".
The paper deals with eigenvalue problems, namely, with computation of the characteristic polynomial coefficients of a given matrix. In his book, Parlett calls this an "unfortunate goal". However, they were not so unfortunate in that time. Krylov, very much restricted by the computational possibilities in 1931, was interested in problems of size approx. 6 only. Ill-conditioning does not play such a big role for these small systems.
"It is clear", wrote Krylov, "that, if for k=2 and k=3 it is easy to compose this [secular] equation, then for k=4 the laying-out becomes cumbersome, and for values k more than 5 this is completely un-realizable in a direct way. Therefore one should use methods where the full development of the determinant is avoided."
He continues, "The aim of the paper... is to present simple methods of composition of the secular equation in the developed form, after which, its solution, i.e. numerical computation of its roots, does not present any difficulty".

At the age of 15, Krylov entered a Naval College in 1878 and finished it with distinction in 1884. After spending several years at the Main Hydrographic Administration and at a shipbuilding plant…

1931: “On the numerical solution of the equation by which, in technical matters, frequencies of small oscillations of material systems are determined”.

The immersing fluid

Krylov Methods - convert inverting a linear operator A into a black-box method requiring only being able to apply the operator A

```
using LinearAlgebra
using Krylov
using LinearOperators

N = 1000;
A = I(N) + 0.01*rand(N, N);
b = rand(N);
u1 = A\b;
AOP = LinearOperator(A);
u2 = gmres(AOP, b);
```

```
[julia> @btime $A\$b;
  11.722 ms (4 allocations: 7.64 MiB)

[julia> @btime gmres($AOP, $b);
  471.605 μs (35 allocations: 177.81 KiB)
```

9 iterations!

```
using LinearAlgebra
using Krylov
using LinearOperators

N = 1000;
A = I(N) + rand(N, N);
b = rand(N);
u1 = A\b;
AOP = LinearOperator(A);
u2 = gmres(AOP, b);
```

```
[julia> @btime $A\$b;
  13.891 ms (4 allocations: 7.64 MiB)

[julia> @btime gmres($AOP, $b);
  202.292 ms (1040 allocations: 13.27 MiB)
```

1000 iterations!

The immersing fluid?

Is this well conditioned?

$$\tilde{\mathbf{X}}^k(s_j) - \Delta t \sum_{i \neq k} \sum_{l=1}^{N_i} G(\mathbf{X}^k(s_j) - \mathbf{X}^i(s_l))\tilde{\mathbf{f}}^i(s_l) w_l^i - C\Delta t \left(\mathbb{I} + \mathbf{X}_s^k(s_j)\mathbf{X}_s^k(s_j)\right) \tilde{\mathbf{f}}^k(s_j) = \mathbf{X}^k(s_j)$$

$$\tilde{\mathbf{f}} = -E\tilde{\mathbf{X}}_{ssss} + (\tilde{T}\mathbf{X}_s)_s$$

Answer: Need a preconditioner.

```
using LinearAlgebra
using Krylov
using LinearOperators
using IncompleteLU

N = 1000;
A = I(N) + rand(N, N);
b = rand(N);
u1 = A\b;
AOP = LinearOperator(A);
ILU = ilu(SparseMatrixCSC(A), τ=0.1);
u2 = gmres(AOP, b, N=ILU, ldiv=true);
```

Now 19 iterations, 27ms.

But, ILU is expensive - here 390ms.

The immersing fluid?

Is this well conditioned?

$$\tilde{\mathbf{X}}^k(s_j) - \Delta t \sum_{i \neq k} \sum_{l=1}^{N_i} \xcancel{G(\mathbf{X}^k(s_j) - \mathbf{X}^i(s_l))} \tilde{\mathbf{f}}^i(s_l) w_l^i - C\Delta t \left(\mathbb{I} + \mathbf{X}_s^k(s_j)\mathbf{X}_s^k(s_j)\right) \tilde{\mathbf{f}}^k(s_j) = \mathbf{X}^k(s_j)$$

$$\tilde{\mathbf{f}} = -E\tilde{\mathbf{X}}_{ssss} + (\tilde{T}\mathbf{X}_s)_s$$

This system of equations is decoupled: each fiber is independent! We can form a block diagonal preconditioner for the decoupled problem.

The immersing fluid?

So, we're good, right?

Krylov Methods - convert inverting a linear operator A into a black-box method requiring only being able to apply the operator A

$$\tilde{\mathbf{X}}^k(s_j) - \Delta t \sum_{i \neq k} \sum_{l=1}^{N_i} G(\mathbf{X}^k(s_j) - \mathbf{X}^i(s_l))\tilde{\mathbf{f}}^i(s_l) w_l^i - C\Delta t \left(\mathbb{I} + \mathbf{X}_s^k(s_j)\mathbf{X}_s^k(s_j)\right) \tilde{\mathbf{f}}^k(s_j) = \mathbf{X}^k(s_j)$$

$$\tilde{\mathbf{f}} = -E\tilde{\mathbf{X}}_{ssss} + (\tilde{T}\mathbf{X}_s)_s$$

Problem: this double sum is *still* expensive.

N	100	1,000	10,000	100,000	1,000,000
Time	< 0.00 ms	0.19 ms	18 ms	1.8 s	3 min

The immersing fluid?

So, we're good, right?

Krylov Methods - convert inverting a linear operator A into a black-box method requiring only being able to apply the operator A

$$\tilde{\mathbf{X}}^k(s_j) - \Delta t \sum_{i \neq k} \sum_{l=1}^{N_i} G(\mathbf{X}^k(s_j) - \mathbf{X}^i(s_l))\tilde{\mathbf{f}}^i(s_l)w_l^i - C\Delta t \left(\mathbb{I} + \mathbf{X}_s^k(s_j)\mathbf{X}_s^k(s_j)\right) \tilde{\mathbf{f}}^k(s_j) = \mathbf{X}^k(s_j)$$

$$\tilde{\mathbf{f}} = -E\tilde{\mathbf{X}}_{ssss} + (\tilde{T}\mathbf{X}_s)_s$$

Problem: this double sum is *still* extremely expensive.

N	100	x 10	1,000	x 10	10,000	x 10	100,000	x 10	1,000,000
Time	< 0.00 ms		0.19 ms	x 100	18 ms	x 100	1.8 s	x 100	3 min

The immersing fluid?

The fast multipole method:

$$\Delta t \sum_{i=1}^{N_{\text{fibers}}} \sum_{l=1}^{N_i} G(\mathbf{X}^k(s_j) - \mathbf{X}^i(s_l))\tilde{\mathbf{f}}^i(s_l)w_l^i$$

FMM reduces the quadratic scaling to linear scaling. SkellySim uses PVFMM, which parallelizes well to many cores / nodes.

N	100	1,000	10,000	100,000	1,000,000	8,000,000
Direct	< 0.00	0.19 ms	18 ms	1.8 s	3 min	
FMM, 6e-4					0.4 s	3.4 s
FMM, 4e-6					0.8 s	6.7 s
FMM, 6e-10					6.8 s	56 s

Challenges

- ~~Slender filaments are inherently multi-scale~~
    - Use slender body theory to reduce dynamics to 1D PDEs

$$\frac{8\pi\mu}{c}\left(\mathbf{X}_t - \mathbf{U}\right) = \left(\mathbb{I} + \mathbf{X}_s\mathbf{X}_s\right)\left(-E\mathbf{X}_{ssss} + (T\mathbf{X}_s)_s\right)$$

- ~~The equations of motion that govern them are *extremely stiff*~~
    - Use an Implicit-Explicit timestepping scheme
- ~~The immersing fluid strongly couples all degrees of freedom together (and there are many degrees of freedom when there are many fibers)~~
    - Solve linear system using preconditioned Krylov method with system applies accelerated by fast-multipole method

Some takeaways

Fundamentally, SkellySim is a large-scale slender-body theory code with full hydrodynamics.

- Slender-body theory is pretty okay when fiber-fiber distances > r/L
- Each timestep involves solving a stiff, dense system of equations
- These are solved via block-diagonal preconditioned GMRES
- Evaluating the full hydrodynamics requires fast algorithms (FMM)
- The preconditioner is effective when fibers are relatively far apart - convergence may stagnate when fibers are very close