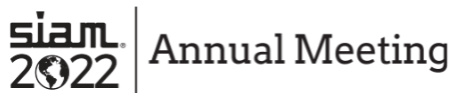


# A Fast Convergent Boundary Integral Framework for Slender Bodies

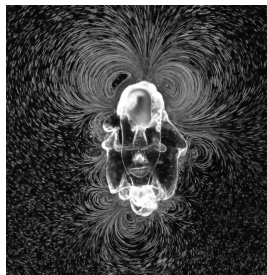
Dhairya Malhotra, Alex Barnett



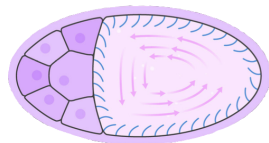
July 14, 2022

# Motivations

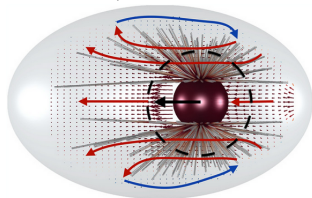
Stokes simulations with fibers are key to modeling complex fluids (suspensions, rheology, industrial, biomedical, cellular biophysics).



Starfish larvae  
(Gilpin et al. 2016)



Drosophila oocyte  
(Stein et al. 2021)



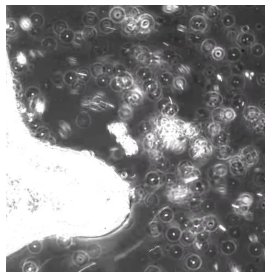
Mitotic spindle (Nazockdast et al. 2015)



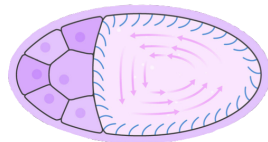
Stokes simulations with fibers are key to modeling complex fluids (suspensions, rheology, industrial, biomedical, cellular biophysics).

## Slender Body Theory (SBT):

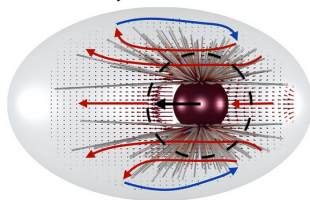
- Asymptotic expansion in radius ( $\varepsilon$ ) as  $\varepsilon \rightarrow 0$  (Keller-Rubinow '76).
- Doublet correction to make velocity theta-independent (Johnson '80).



Starfish larvae  
(Gilpin et al. 2016)



Drosophila oocyte  
(Stein et al. 2021)

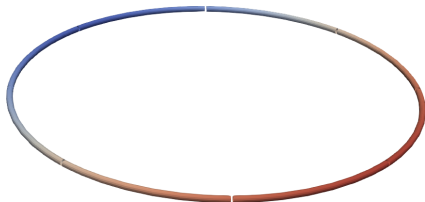


Mitotic spindle (Nazockdast et al. 2015)

**Error estimates:** Rigorous analysis difficult (few very recent studies)

- classical asymptotics claims:  $\varepsilon^2 \log(\varepsilon)$
- rigorous analysis:  $\varepsilon \log^{3/2}(\varepsilon)$  (Mori-Ohm-Spirn '19)
- numerical tests:  $\varepsilon^{1.7}$  (Mitchell et al. '21 -- verify close-touching breakdown)  
close-to-touching with gap of  $10\varepsilon$ , only 2.5-digits in the infy-norm.  
 $\varepsilon=1\text{e-}2$  only 1-2 digits achievable by SBT.

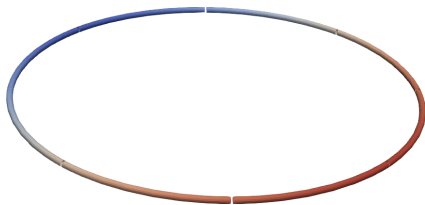
Sedimentation velocity of ellipse  
of thickness  $\varepsilon$  in a Stokesian fluid.



**Error estimates:** Rigorous analysis difficult (few very recent studies)

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 $\varepsilon=1\text{e-}2$  only 1-2 digits achievable by SBT.

| $\varepsilon$ | $\mathbf{u}_0$ | Error    |
|---------------|----------------|----------|
| 0.1           | 0.0518         | $0.7e-2$ |
| 0.01          | 0.0736         | $0.2e-3$ |
| 0.001         | 0.0950         | $0.3e-5$ |
| 0.0001        | 0.1163         | $0.4e-7$ |



**Error estimates:** Rigorous analysis difficult (few very recent studies)

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close-to-touching with gap of  $10\varepsilon$ , only 2.5-digits in the infy-norm.  
 $\varepsilon=1\text{e-}2$  only 1-2 digits achievable by SBT.

**Limitations:**

- no convergence analysis for fibers of given nonzero radius.
- uncontrolled errors when fibers close  $O(\varepsilon)$ .

Efficient convergent BIE method needed, allowing adaptivity for close interactions.

Solve the slender body BVP

- in a convergent way.
- adaptively when fibers become close.
- efficiently with effort independent of varying radius.

Validate current SBT simulations.

Most existing quadratures cannot resolve high aspect ratio geometries.

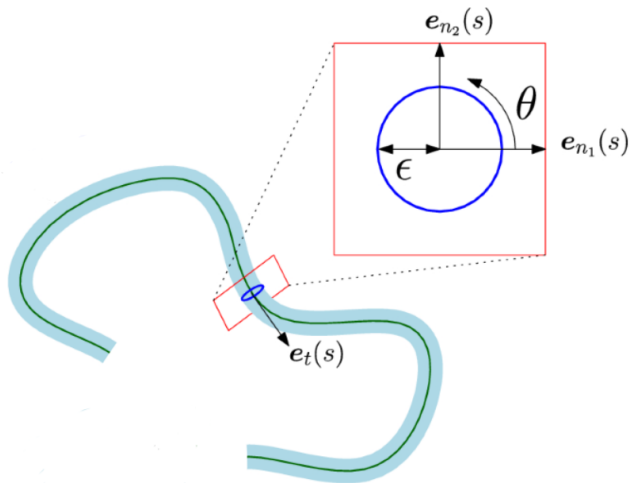
Focus on rigid fibers in this talk -- flexible fibers for future.

*Related work:* Mitchell et al, '21 (mixed-BVP corresponding to flexible fiber loop)

# Discretization

## Geometry description:

- parameterization  $s$  along fiber length
- coordinates  $x(s)$  of centerline curve
- circular cross-section with radius  $\varepsilon(s)$
- orientation vector  $e_{n_1}(s)$

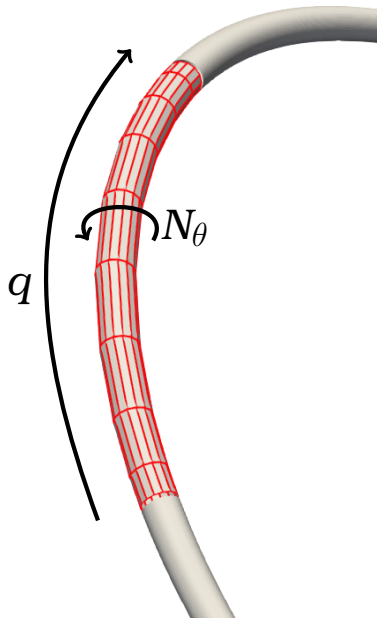


## Geometry description:

- parameterization  $s$  along fiber length
- coordinates  $x(s)$  of centerline curve
- circular cross-section with radius  $\varepsilon(s)$
- orientation vector  $e_{n_1}(s)$

## Discretization:

- piecewise Chebyshev (order  $q$ ) discretization in  $s$  for  $x(s)$ ,  $\varepsilon(s)$  and  $e_{n_1}(s)$
- Collocation nodes: tensor product of Chebyshev and Fourier discretization in angle with order  $N_\theta$ .



$$u(x) = \int_{\Gamma} \mathcal{K}(x - y) \sigma(y) da(y) = \sum_{k=1}^{N_{panel}} \int_{\gamma_k} \mathcal{K}(x - y) \sigma(y) da(y)$$



$$\begin{aligned} u(x) &= \int_{\Gamma} \mathcal{K}(x-y) \sigma(y) da(y) = \sum_{k=1}^{N_{panel}} \int_{\gamma_k} \mathcal{K}(x-y) \sigma(y) da(y) \\ &= \underbrace{\sum_{x \notin \mathcal{N}(\gamma_k)} \int_{\gamma_k} \mathcal{K}(x-y) \sigma(y) da(y)}_{\text{far-field}} + \underbrace{\sum_{x \in \mathcal{N}(\gamma_k)} \int_{\gamma_k} \mathcal{K}(x-y) \sigma(y) da(y)}_{\text{near interactions}} \end{aligned}$$

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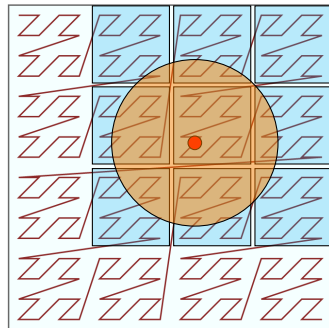
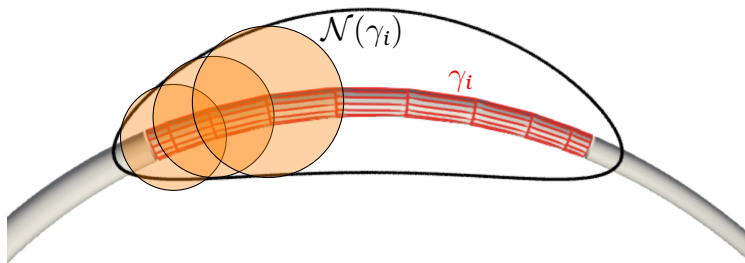
**Far field approximation:**

$$\int_{\gamma_k} \mathcal{K}(x-y) \sigma(y) da(y) \approx \sum_{i,j} \frac{2\pi w_i}{N_{\theta}} \mathcal{K}(x-y(s_i, \theta_j)) \sigma(s_i, \theta_j) J(s_i, \theta_j)$$

- Gauss-Legendre quadrature  $(s_i, w_i)$  of order  $q$ .
- periodic trapezoidal quadrature of order  $N_{\theta}$  in  $\theta$ .
- given a tolerance, define region  $\mathcal{N}(\gamma_k)$ , such that far-field is valid outside it.

# Boundary Quadratures

$$\begin{aligned}
 u(x) &= \int_{\Gamma} \mathcal{K}(x-y) \sigma(y) da(y) = \sum_{k=1}^{N_{panel}} \int_{\gamma_k} \mathcal{K}(x-y) \sigma(y) da(y) \\
 &= \underbrace{\sum_{x \notin \mathcal{N}(\gamma_k)} \int_{\gamma_k} \mathcal{K}(x-y) \sigma(y) da(y)}_{\text{far-field}} + \underbrace{\sum_{x \in \mathcal{N}(\gamma_k)} \int_{\gamma_k} \mathcal{K}(x-y) \sigma(y) da(y)}_{\text{near interactions}}
 \end{aligned}$$



**Near interactions:** for  $x \in \mathcal{N}(\gamma_k)$

$$\int_{\gamma_k} \mathcal{K}(x - y) \sigma(y) da(y) = \int_s \int_{\theta} \mathcal{K}(x - y(s, \theta)) \sigma(s, \theta) J(s, \theta) d\theta ds$$

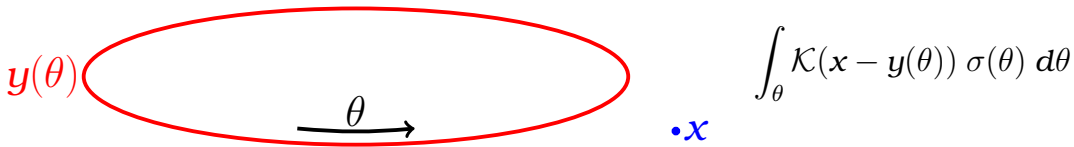
Inner integral:

- potential from a ring source (modal or toroidal Green's function).
- can be nearly singular as  $s \rightarrow s_0$ .

Outer integral:

- singular if  $x \in \gamma_k$  with logarithmic singularity at  $s = s_0$ .
- $1/s^\alpha$  decay as  $|s - s_0| \rightarrow \infty$

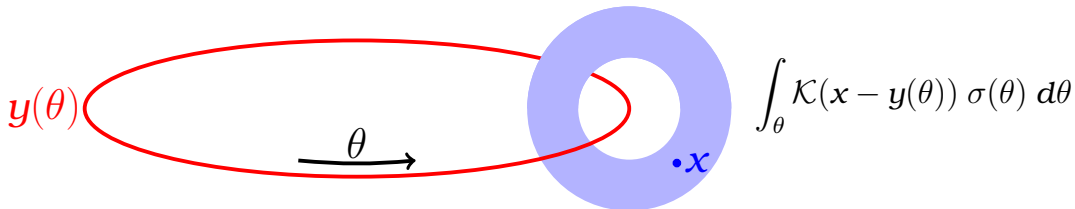
# Fast Modal Green's Function Evaluation



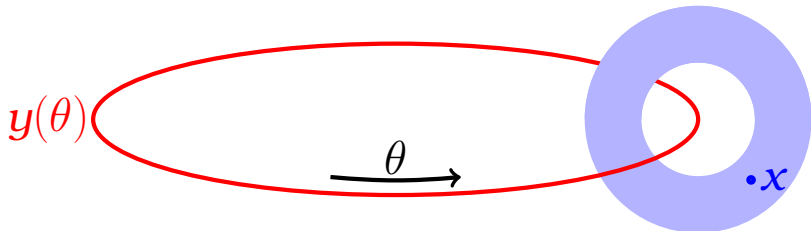
The diagram illustrates the integral equation for the Green's function evaluation. On the left, the term  $y(\theta)$  is written in red. To its right is a large red oval. Inside the oval, there is a horizontal arrow pointing to the right, with the Greek letter  $\theta$  written above it. To the right of the oval is a blue dot followed by the variable  $x$ . Further to the right is the integral expression  $\int_{\theta} \mathcal{K}(x - y(\theta)) \sigma(\theta) d\theta$ .

$$y(\theta) \int_{\theta} \mathcal{K}(x - y(\theta)) \sigma(\theta) d\theta$$

- Periodic trapezoidal rule becomes expensive as  $x \longrightarrow y$ .
- Analytic representation in special functions - Young, Hao, Martinsson JCP-2012
  - modal Green's functions -- method of choice for axisymmetric problems.



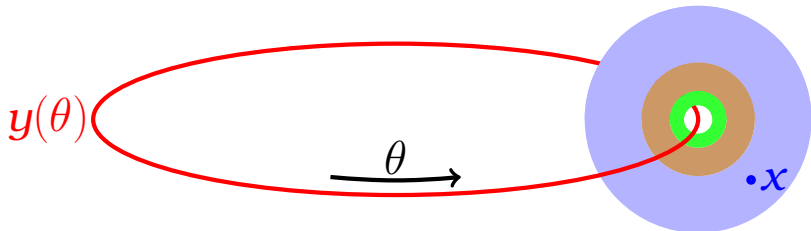
- Periodic trapezoidal rule becomes expensive as  $x \rightarrow y$ .
- Analytic representation in special functions - Young, Hao, Martinsson JCP-2012
  - modal Green's functions – method of choice for axisymmetric problems.
- Build special quadrature rules!
  - e.g. generalized Gaussian quadratures: Bremer, Gimbutas and Rokhlin - SISC 2010.



- Build special quadrature rule  $(w_i, \theta_i)$  such that,

$$\int_{\theta} e^{-in\theta} \mathcal{K}(x - y(\theta)) d\theta \approx \sum_i w_i e^{-in\theta_i} \mathcal{K}(x - y(\theta_i))$$

for all Fourier modes  $(n \leq n_0)$  and all targets  $x$  in the annulus.



- Build special quadrature rule  $(w_i, \theta_i)$  such that,

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for all Fourier modes  $(n \leq n_0)$  and all targets  $x$  in the annulus.

- Different rule for each nested annular region (up to  $10^{-6}$  from source).

$\sim 48$  quadrature nodes for  $n_0 = 8$  and 10-digits accuracy.

$\sim 26M$  modal Green's function evaluations/sec/core (Skylake 2.4GHz)



# Quadratures for Outer Integral

$$\int_{\gamma_k} \mathcal{K}(x - y) \sigma(y) da(y) = \int_s \left( \int_{\theta} \mathcal{K}(x - y(s, \theta)) \sigma(s, \theta) J(s, \theta) d\theta \right) ds$$

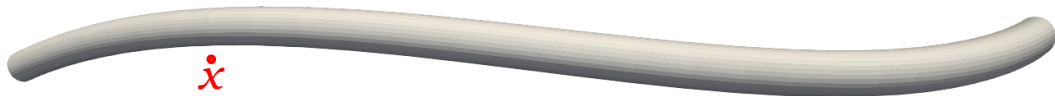
# Quadratures for Outer Integral

$$\int_{\gamma_k} \mathcal{K}(x - y) \sigma(y) da(y) = \int_s \left( \sum_{n=0}^{N_\theta/2-1} \mathcal{K}_n(x - y(s)) \widehat{\sigma}_n \right) ds$$

# Quadratures for Outer Integral

$$\int_{\gamma_k} \mathcal{K}(x - y) \sigma(y) da(y) = \int_s \left( \sum_{n=0}^{N_\theta/2-1} \mathcal{K}_n(x - y(s)) \widehat{\sigma}_n \right) ds$$

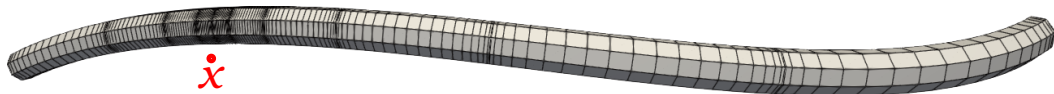
**Near Interactions:**  $x$  is off-surface or adjacent panel



# Quadratures for Outer Integral

$$\int_{\gamma_k} \mathcal{K}(x - y) \sigma(y) da(y) = \int_s \left( \sum_{n=0}^{N_\theta/2-1} \mathcal{K}_n(x - y(s)) \widehat{\sigma}_n \right) ds$$

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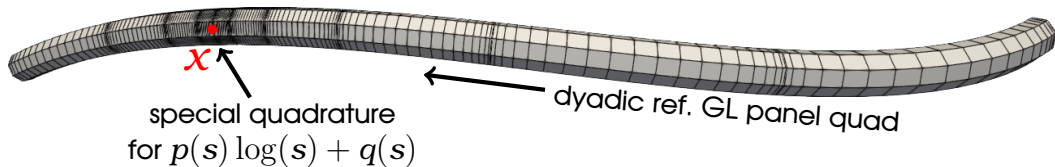


- panel (Gauss-Legendre) quadrature with dyadic refinement.

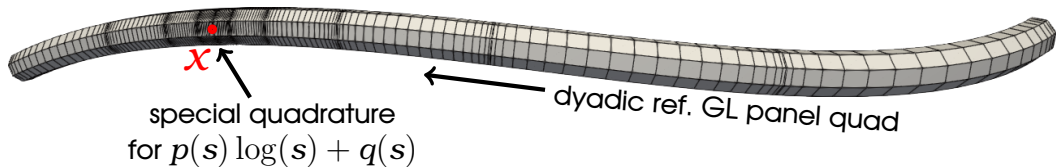
# Quadratures for Outer Integral (singular case)



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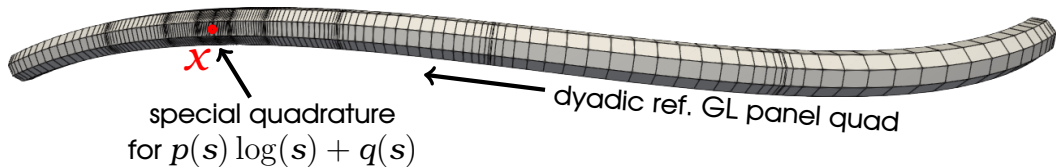
# Quadratures for Outer Integral (singular case)



## Special Quadrature Rules:

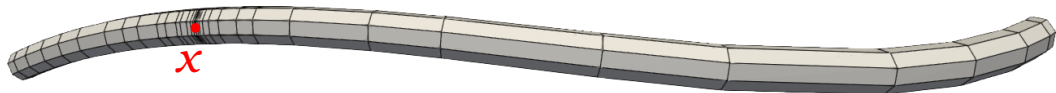
- replace composite panel quadratures with a single quadrature.
- integrand doesn't have closed form expression, but we can still generate quadrature rules!

# Quadratures for Outer Integral (singular case)



## Special Quadrature Rules:

- replace composite panel quadratures with a single quadrature.
- integrand doesn't have closed form expression, but we can still generate quadrature rules!



- Separate rules for different aspect ratios ( $1 - 10^4$  in powers of 2)



# Overall Algorithm

**Discretization:** piecewise polynomial  $\times$  Fourier.

**Far-field interactions:** standard quadratures (GL  $\times$  PTR) + FMM

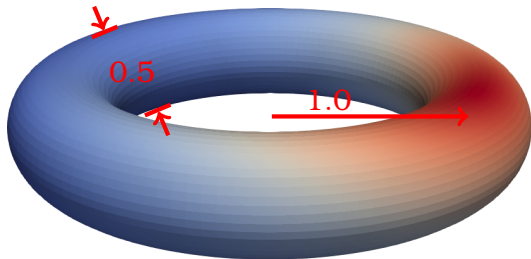
**Near interactions:**

- special quadratures for modal Green's function and singular integral in  $s$ .
- dyadic refined Gauss-Legendre quadrature in  $s$  for non-singular case.
- build local correction matrix instead of computing on-the-fly.

## Green's identity (Laplace):

$\Delta u = 0$ , then for  $x \in \Gamma$ ,

$$u(x) = \frac{u(x)}{2} + \mathcal{S}[\partial_n u](x) - \mathcal{D}[u](x)$$



## Boundary Integral Equation Solver for Taylor States (BIEST)\*

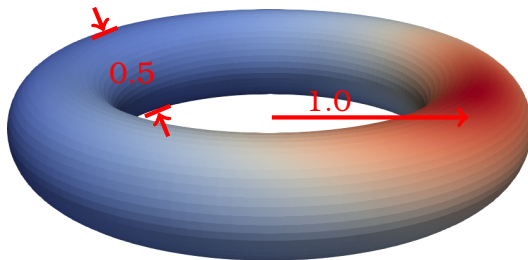
- quadrature for general toroidal surfaces with uniform grid.
- partition-of-unity to separate singular part of boundary integral.
- polar coordinate transform for singular integral.

\*JCP 2019 - Malhotra, Cerfon, Imbert-Gérard, O'Neil (<https://github.com/dmalhotra/BIEST>)

## Green's identity (Laplace):

$\Delta u = 0$ , then for  $x \in \Gamma$ ,

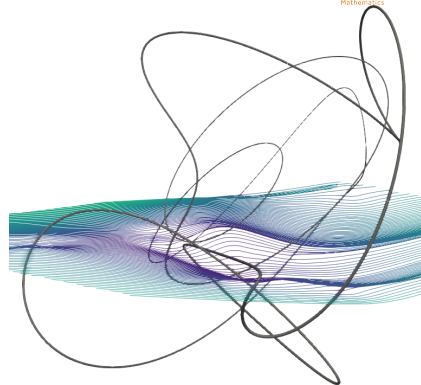
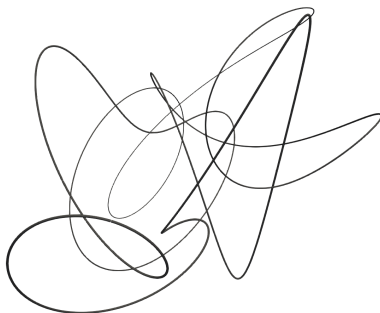
$$u(x) = \frac{u(x)}{2} + \mathcal{S}[\partial_n u](x) - \mathcal{D}[u](x)$$



| Slender-body Quadrature |                |             |            | BIEST* |                |             |            |
|-------------------------|----------------|-------------|------------|--------|----------------|-------------|------------|
| $N$                     | $\ e\ _\infty$ | $T_{setup}$ | $T_{eval}$ | $N$    | $\ e\ _\infty$ | $T_{setup}$ | $T_{eval}$ |
| 320                     | 1.5e-04        | 0.032       | 0.0004     | 507    | 2.0e-03        | 0.1319      | 0.0017     |
| 720                     | 3.5e-06        | 0.094       | 0.0013     | 1323   | 4.0e-06        | 1.4884      | 0.0042     |
| 1280                    | 5.4e-09        | 0.228       | 0.0033     | 2523   | 4.3e-09        | 6.6825      | 0.0313     |
| 2000                    | 2.5e-10        | 0.501       | 0.0079     | 4107   | 3.5e-10        | 15.4711     | 0.0862     |

\*JCP 2019 - Malhotra, Cerfon, Imbert-Gérard, O'Neil (<https://github.com/dmalhotra/BIEST>)

# Numerical Results - Stokes BVP



## Exterior Stokes

### Dirichlet BVP:

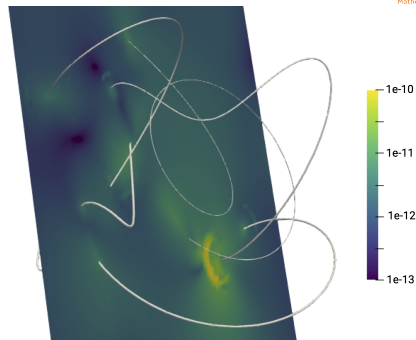
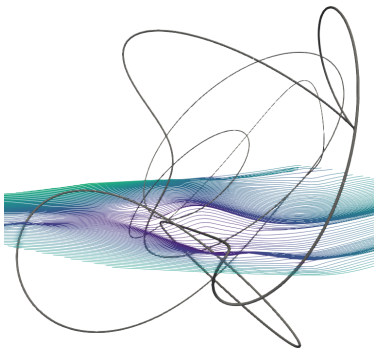
$$\begin{aligned}\Delta \mathbf{u} - \nabla p &= 0, \\ \nabla \cdot \mathbf{u} &= 0,\end{aligned}$$

$$\begin{aligned}\mathbf{u}|_{\Gamma} &= \mathbf{u}_0, \\ u(\mathbf{x}) &\rightarrow 0 \text{ as } |\mathbf{x}| \rightarrow 0,\end{aligned}$$

wire radius =  $1.5\text{e-}3$  to  $4\text{e-}3$   
wire length = 16

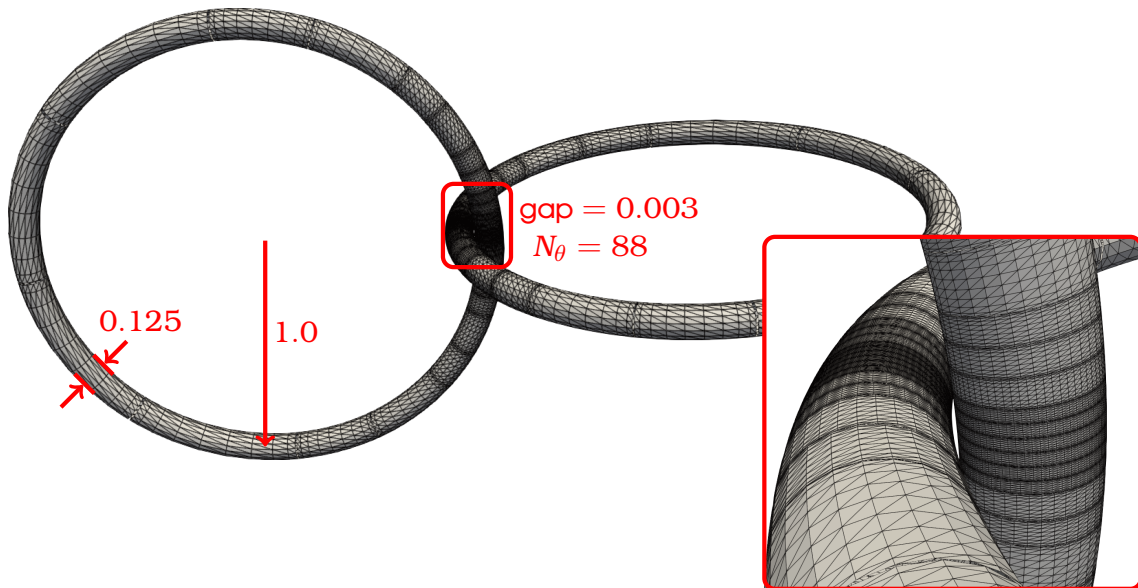
**BIE formulation:**  $(\mathcal{I}/2 + \mathcal{D} + \mathcal{S} / (2\varepsilon \log \varepsilon^{-1}))[\boldsymbol{\sigma}] = \mathbf{u}_0$

# Numerical Results - Stokes BVP

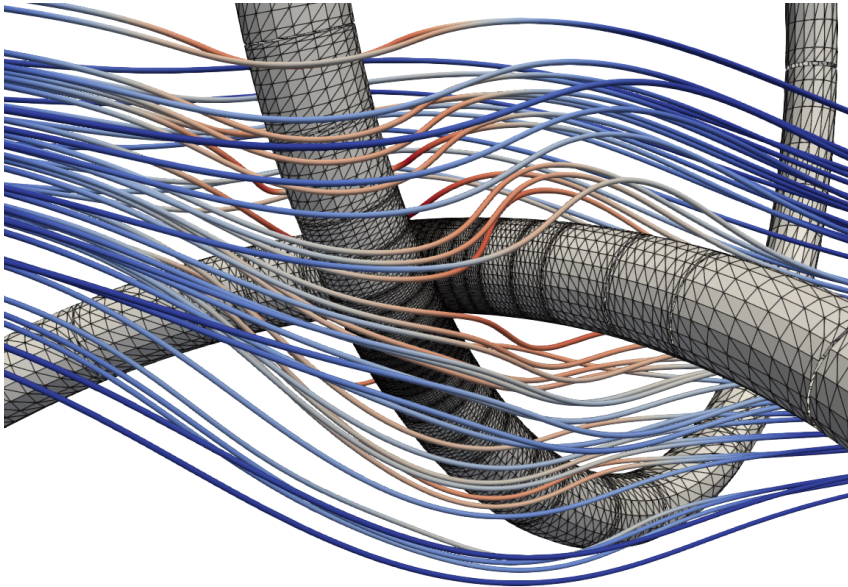


| $N$   | $N_{panel}$ | $N_{\theta}$ | $\epsilon_{GMRES}$ | $N_{iter}$ | $\ e\ _{\infty}$ | 1-core      |                 |             | 40-cores    |             |
|-------|-------------|--------------|--------------------|------------|------------------|-------------|-----------------|-------------|-------------|-------------|
|       |             |              |                    |            |                  | $T_{setup}$ | $(N/T_{setup})$ | $T_{solve}$ | $T_{setup}$ | $T_{solve}$ |
| 1.5e4 | 122         | 4            | 1e-03              | 10         | 1.9e-02          | 0.33        | (4.4e4)         | 0.7         | 0.024       | 0.05        |
| 9.1e4 | 252         | 12           | 1e-05              | 21         | 1.7e-04          | 3.31        | (2.7e4)         | 61.2        | 0.197       | 5.25        |
| 9.4e4 | 262         | 12           | 1e-07              | 33         | 4.1e-06          | 4.43        | (2.1e4)         | 104.3       | 0.224       | 7.69        |
| 2.0e5 | 272         | 24           | 1e-09              | 43         | 1.4e-08          | 17.70       | (1.1e4)         | 586.0       | 0.796       | 22.94       |
| 2.3e5 | 276         | 28           | 1e-11              | 54         | 4.1e-09          | 27.67       | (8.4e3)         | 1034.2      | 1.229       | 38.85       |

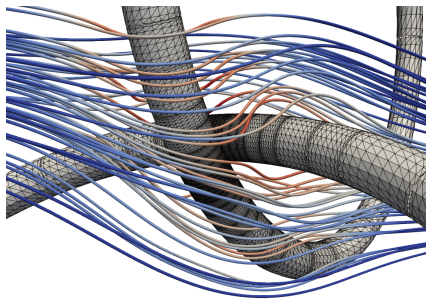
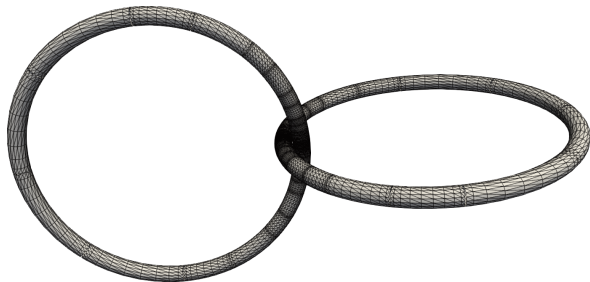
# Numerical Results - close-to-touching



# Numerical Results - close-to-touching



# Numerical Results - close-to-touching



| $N$   | $\epsilon_{GMRES}$ | $N_{iter}$ | $\ e\ _{\infty}$ | 1-core      |                 | 40-cores    |             |             |
|-------|--------------------|------------|------------------|-------------|-----------------|-------------|-------------|-------------|
|       |                    |            |                  | $T_{setup}$ | $(N/T_{setup})$ | $T_{solve}$ | $T_{setup}$ | $T_{solve}$ |
| 6.5e4 | 1e-02              | 4          | 2.1e-02          | 8.1         | (8.0e+3)        | 6.5         | 1.28        | 1.4         |
| 6.5e4 | 1e-05              | 24         | 2.4e-03          | 16.8        | (3.8e+3)        | 42.9        | 2.50        | 7.7         |
| 6.5e4 | 1e-07              | 43         | 2.8e-06          | 23.5        | (2.7e+3)        | 81.6        | 3.31        | 12.8        |
| 6.5e4 | 1e-10              | 59         | 5.4e-08          | 35.6        | (1.8e+3)        | 122.9       | 4.06        | 19.2        |
| 6.5e4 | 1e-13              | 72         | 1.3e-10          | 49.9        | (1.3e+3)        | 162.6       | 5.27        | 23.2        |

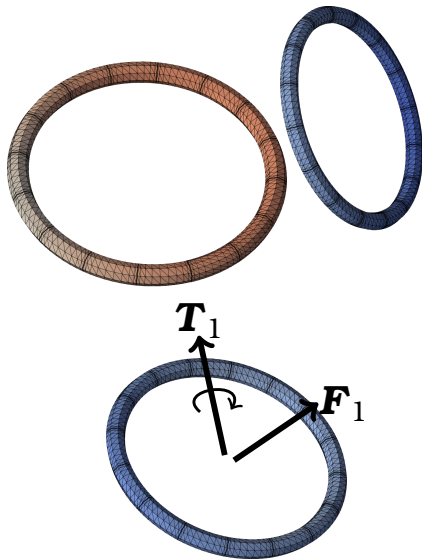


# Mobility problem

- $n$  rigid bodies  $\Omega = \sum_{i=1}^n \Omega_i$   
with velocities  $\mathbf{V}(\mathbf{x}) = \mathbf{v}_i + \boldsymbol{\omega}_i \times (\mathbf{x} - \mathbf{x}_i^c)$ ,  
and given forces  $\mathbf{F}_i$ , torques  $\mathbf{T}_i$  about  $\mathbf{x}_i^c$ .

- Stokesian fluid in  $\mathbb{R}^3 \setminus \Omega$   
$$\Delta \mathbf{u} - \nabla p = 0, \quad \nabla \cdot \mathbf{u} = 0,$$
  
$$\mathbf{u} \rightarrow 0 \text{ as } \mathbf{x} \rightarrow \infty.$$

- Boundary conditions on  $\partial\Omega$ ,  
$$\mathbf{u} = \mathbf{V} + \mathbf{u}_s.$$



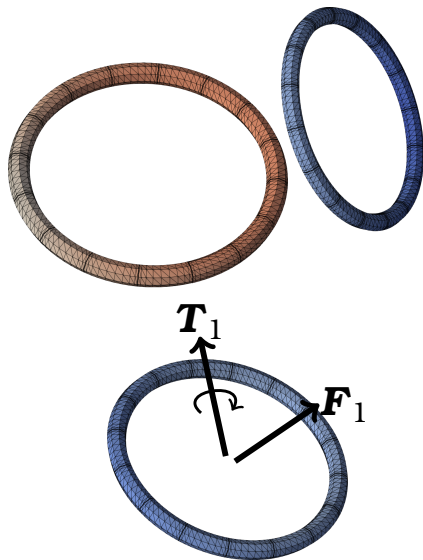
# Mobility problem

- $n$  rigid bodies  $\Omega = \sum_{i=1}^n \Omega_i$   
with velocities  $\mathbf{V}(\mathbf{x}) = \mathbf{v}_i + \boldsymbol{\omega}_i \times (\mathbf{x} - \mathbf{x}_i^c)$ ,  
and given forces  $\mathbf{F}_i$ , torques  $\mathbf{T}_i$  about  $\mathbf{x}_i^c$ .

- Stokesian fluid in  $\mathbb{R}^3 \setminus \Omega$   
$$\Delta \mathbf{u} - \nabla p = 0, \quad \nabla \cdot \mathbf{u} = 0,$$
$$\mathbf{u} \rightarrow 0 \text{ as } \mathbf{x} \rightarrow \infty.$$

- Boundary conditions on  $\partial\Omega$ ,  
$$\mathbf{u} = \mathbf{V} + \mathbf{u}_s.$$

unknown:  $\mathbf{V}(\mathbf{u}_i, \boldsymbol{\omega}_i)$



# Mobility problem - double-layer formulation

Represent fluid velocity:  $\mathbf{u} = \mathcal{S}[\boldsymbol{\nu}(\mathbf{F}_i, \mathbf{T}_i)] + \mathcal{D}[\boldsymbol{\sigma}]$

and rigid body velocity:  $\mathbf{V} = - \sum_{i=1}^{6n} \mathbf{v}_i \mathbf{v}_i^T \boldsymbol{\sigma}$

Applying boundary conditions ( $\mathbf{u} = \mathbf{V} + \mathbf{u}_s$  on  $\partial\Omega$ ),

$$(\mathcal{I}/2 + \mathcal{D})[\boldsymbol{\sigma}] + \sum_{i=1}^{6n} \mathbf{v}_i \mathbf{v}_i^T \boldsymbol{\sigma} = \mathbf{u}_s - \mathcal{S}[\boldsymbol{\nu}]$$

*(Pozrikidis - Boundary Integral and Singularity Methods for Linearized Viscous Flow)*

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Second kind integral equation, should be well-conditioned.

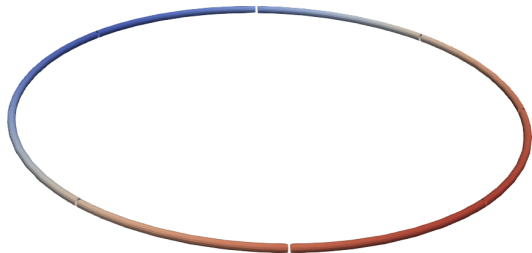
What can possibly go wrong?

# Conditioning of layer-potential operators

$$\kappa(\mathcal{S}) \quad \sim 2.6e6$$

$$\kappa(\mathcal{I}/2 + \mathcal{D}) \quad \sim 4.3e6$$

$$\kappa(\mathcal{I}/2 + \mathcal{D} + 16\mathcal{S}) \quad \sim 80$$



- For infinite cylinder (Laplace case):  $\kappa(\mathcal{I}/2 + \mathcal{D}) \sim \varepsilon^{-2} \log^{-1} \varepsilon^{-1}$
- Combined field operator well-conditioned:  $\mathcal{I}/2 + \mathcal{D} + \mathcal{S} / (2\varepsilon \log \varepsilon^{-1})$

# Mobility problem - combined field formulation

Represent fluid velocity:  $\mathbf{u} = \mathcal{S}[\nu(\mathbf{F}_i, \mathbf{T}_i)] + \mathcal{K}[\boldsymbol{\sigma}]$

and rigid body velocity:  $\mathbf{V} = - \sum_{i=1}^{6n} \mathbf{v}_i \mathbf{v}_i^T \boldsymbol{\sigma}$

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Applying boundary conditions,

$$(\mathcal{I}/2 + \mathcal{K})[\boldsymbol{\sigma} - \sum_{i=1}^{6n} \mathbf{v}_i \mathbf{v}_i^T \boldsymbol{\sigma}] + \sum_{i=1}^{6n} \mathbf{v}_i \mathbf{v}_i^T \boldsymbol{\sigma} = \mathbf{u}_s - \mathcal{S}[\boldsymbol{\nu}]$$

Second kind integral equation and well-conditioned!

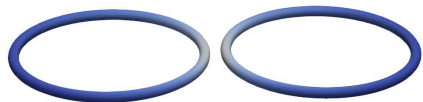


# Numerical Results - Sedimentation Flow

**Time-stepping:** 5-th order adaptive SDC

**8-digits accuracy** in quadratures, GMRES solve,  
and time-stepping.

**40 CPU cores**

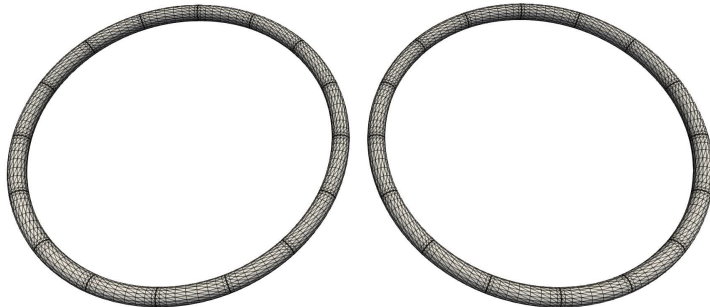
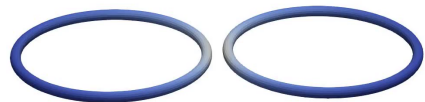


# Numerical Results - Sedimentation Flow

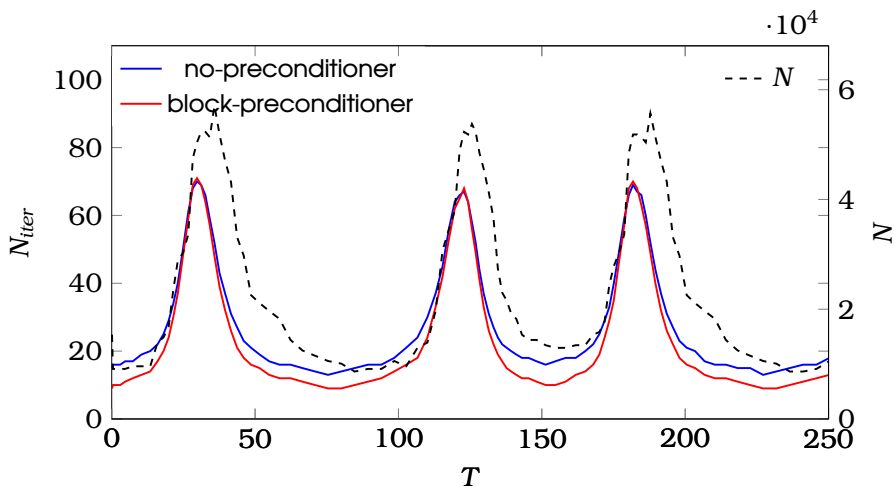
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# Numerical Results - Sedimentation Flow



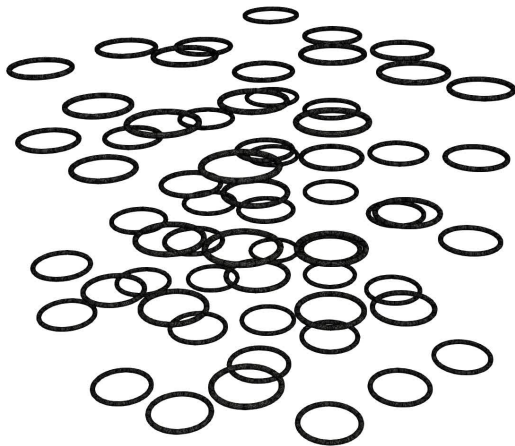
**Close-to-touching:** smaller time-steps, more unknowns ( $N$ ),  
high GMRES iteration count (block preconditioner doesn't help).

**5-th order adaptive SDC**

**8-digits accuracy** in  
quadratures, GMRES solve,  
and time-stepping.

**0.5 million unknowns**  
64 rings.

**160 CPU cores**



- Convergent boundary integral formulation for slender bodies.
  - unlike SBT, boundary conditions are actually enforced to high accuracy.
- Special quadratures - efficient for aspect ratios as large as  $10^5$ .
  - quadrature setup rates up to 20,000 unknowns/s/core (comparable to FMM speeds).
- Stokes mobility problem - combined field BIE formulation.
  - well-conditioned formulation for slender-body geometries.
  - high-order time stepping (SDC), block-diagonal preconditioner.

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## Limitations and ongoing work:

- Open problems: collisions, better preconditions / fast direct solvers.
- Open ended and flexible fibers -- applications in biological fluids.