High-Order Boundary Integral Methods for Slender Bodies

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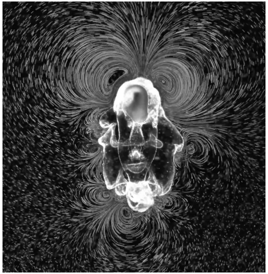
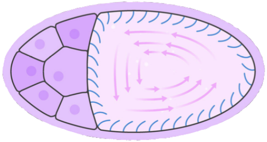
Motivations

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



Starfish larvae (Gilpin et al. 2016)



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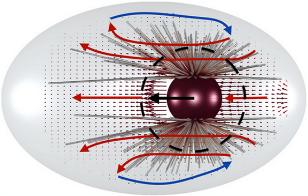


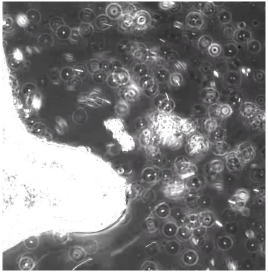
Mitotic spindle (Nazockdast et al. 2015)

Motivations

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

Slender Body Theory (SBT):

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



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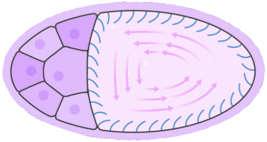

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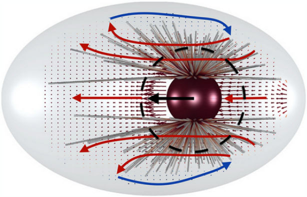

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Slender Body Theory

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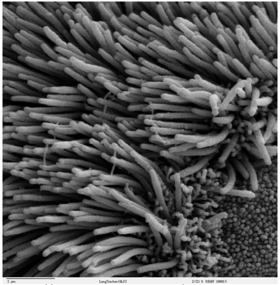
Error estimates: Rigorous analysis difficult (few very recent studies)

- 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 10ε, only 2.5-digits in the infty-norm.

  ε=1e-2 only 1-2 digits achievable by SBT.



Source: http://remf.dartmouth.edu/imagesindex.html

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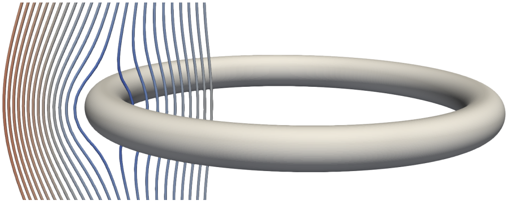
ε	$\boldsymbol{u}_{exact}$	Rel-Error
1e-1	6.1492138359856e-2	0.5e-2
1e-2	9.0984522324584e-2	0.1e-3
1e-3	1.2015655889904e-1	0.2e-5
1e-4	1.4931932907587e-1	0.2e-7
1e-5	1.7848191313097e-1	0.3e-9



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Limitations of SBT:

- 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.

Goals

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Solve the slender body BVP

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

Validate current SBT simulations.

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

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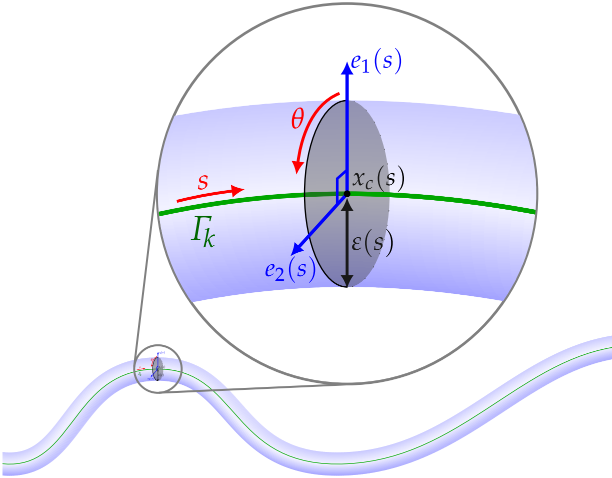
Geometry description:

- parameterization s along fiber length
- coordinates $x_c(s)$ of centerline curve
- circular cross-section with radius $\varepsilon(s)$
- orientation vector $e_1(s)$



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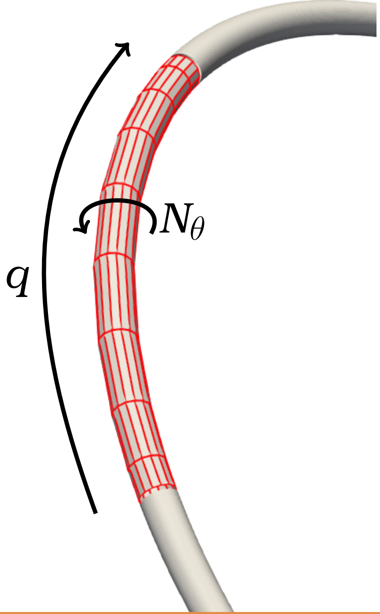
Discretization:

- piecewise Chebyshev (order q) discretization in s for $x_c(s)$, $\varepsilon(s)$, $e_1(s)$
- Collocation nodes: tensor product of Chebyshev and Fourier discretization in angle with order N_θ.



Boundary Quadratures

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

Boundary Quadratures

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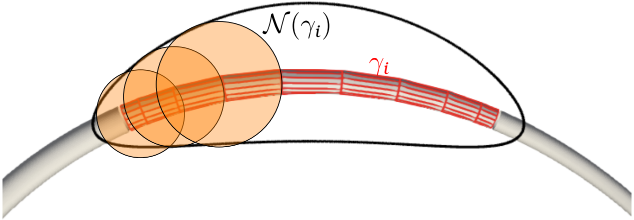
Far field approximation:

- Gauss-Legendre quadrature in s.
- periodic trapezoidal rule in θ.
- determine $\mathcal{N}(\gamma_k)$ using standard error estimates



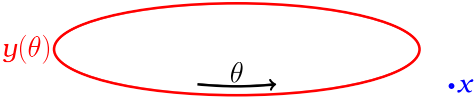
Boundary Quadratures

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

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

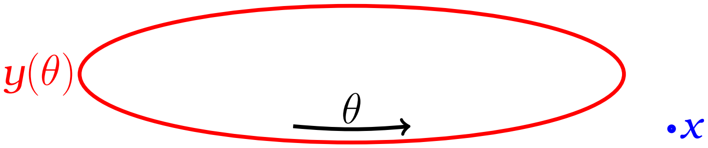
Inner integral in θ:

- potential from a ring source
  -- modal Green's function.
- can be nearly singular as $x \longrightarrow \gamma_k$.



Outer integral in s:

Fast Modal Green's Function Evaluation



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

- Analytic representation in special functions - Young, Hao, Martinsson JCP-2012
  - modal Green's functions -- method of choice for axisymmetric problems.

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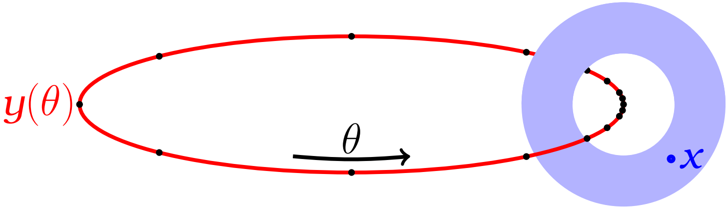

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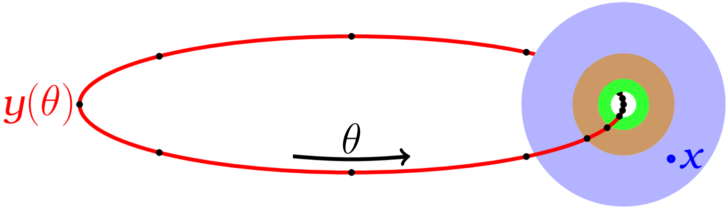
- Build special quadrature rules!
  - e.g. generalized Gaussian quadratures: Bremer, Gimbutas and Rokhlin - SISC 2010.

Fast Modal Green´s Function Evaluation



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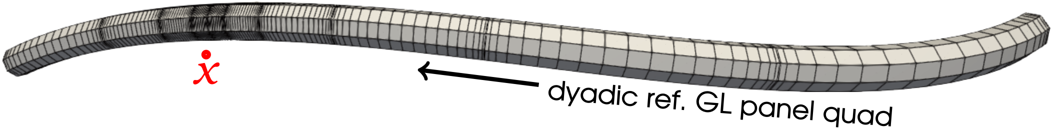
- Build special quadrature rules!
  - e.g. generalized Gaussian quadratures: Bremer, Gimbutas and Rokhlin - SISC 2010.
  - Different rule for each nested annular region (up to 10^{-6} from source).

~ 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

Near Interactions: x is off-surface or adjacent panel

- panel (Gauss-Lengendre) quadrature with dyadic refienement.



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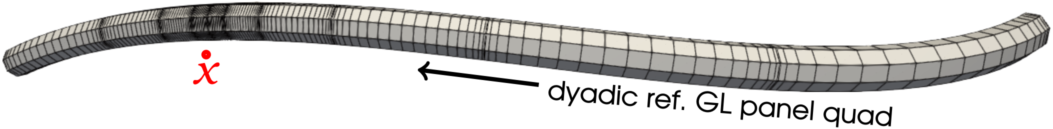
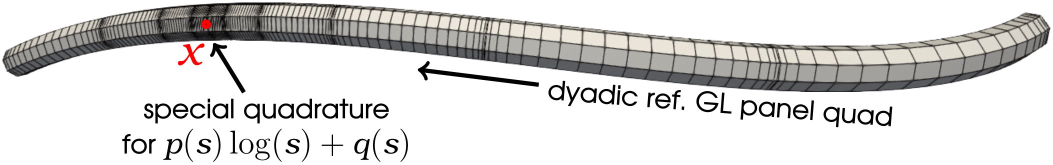


Singular Interactions: x is on-surface



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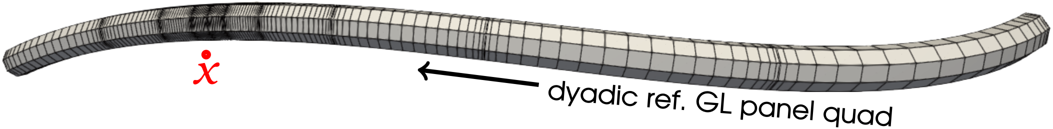

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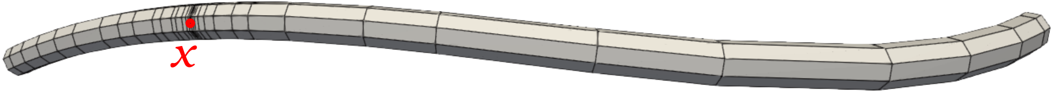
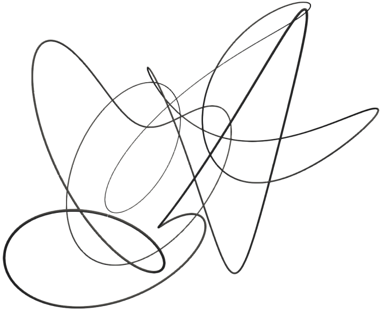
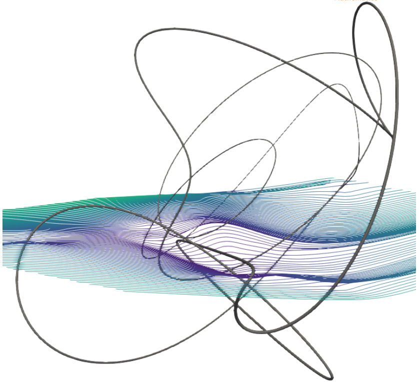


Instead build special quadrature rules!

- replace composite panel quadratures with a single quadrature.
- Separate rules for different aspect ratios (1 -- 10^4 in powers of 2)

Numerical Results - Stokes BVP





Exterior Stokes Dirichlet BVP:

$$\Delta \boldsymbol{u} - \nabla p = 0,$$
$$\nabla \cdot \boldsymbol{u} = 0,$$

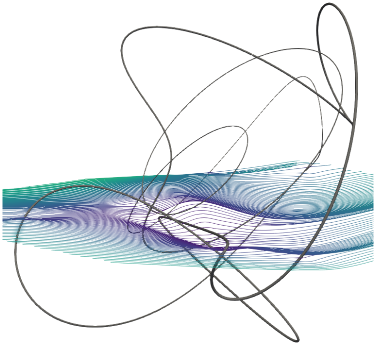
$$\boldsymbol{u}|_\Gamma = \boldsymbol{u}_0,$$
$$u(x) \to 0 \text{ as } |x| \to 0,$$

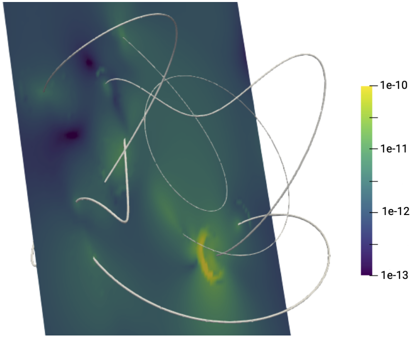
wire radius = 1.5e-3 to 4e-3

wire length = 16

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

Numerical Results - Stokes BVP





						1-core			40-cores	
N	N_{panel}	N_θ	ϵ_{GMRES}	N_{iter}	$\|\|e\|\|_\infty$	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

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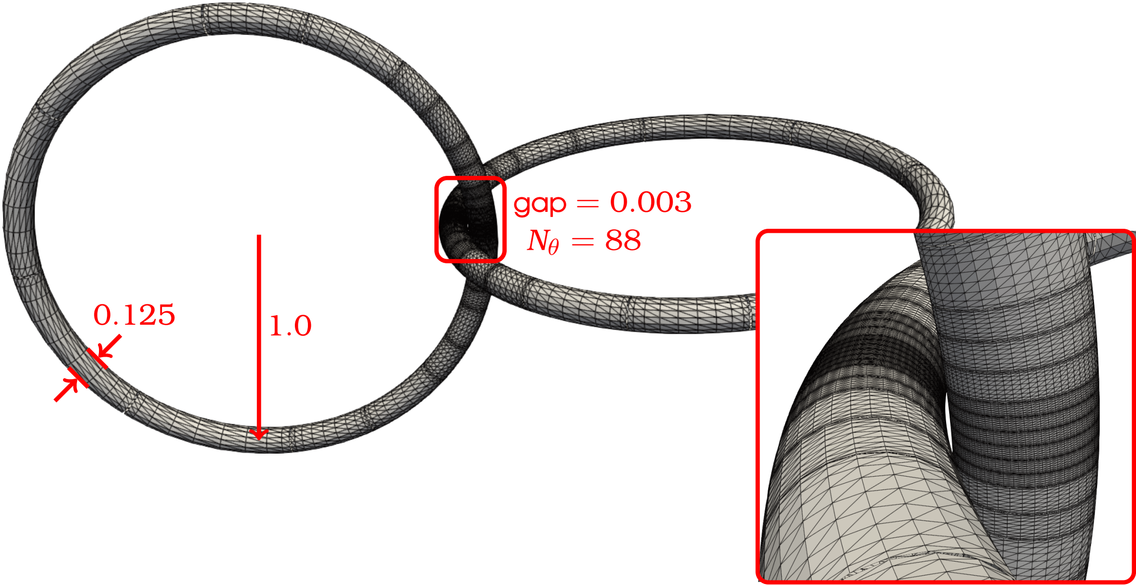

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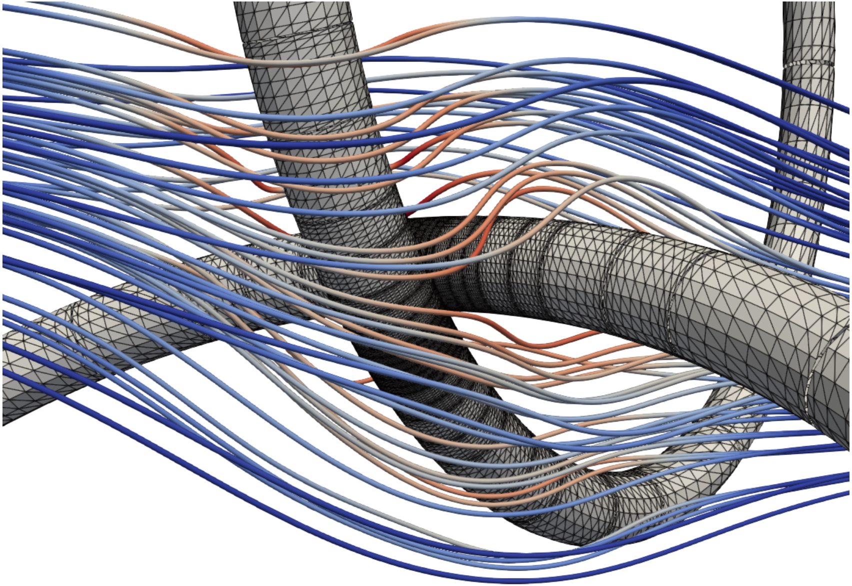

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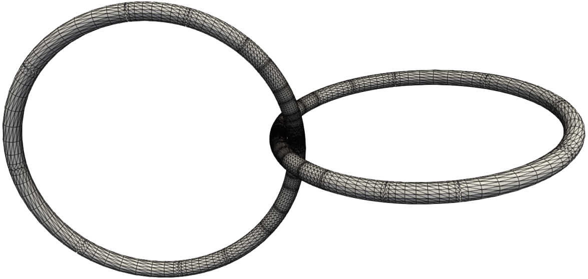
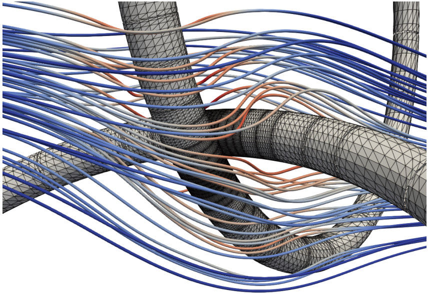




				1-core		40-cores	
N	ϵ_{GMRES}	N_{iter}	$\|\|e\|\|_\infty$	T_{setup} (N/T_{setup})	T_{solve}	T_{setup}	T_{solve}
6.5e4	1e-02	4	2.1e-02	8.1 (8.0e+3)	6.5	1.28	1.4
6.5e4	1e-05	24	2.4e-03	16.8 (3.8e+3)	42.9	2.50	7.7
6.5e4	1e-07	43	2.8e-06	23.5 (2.7e+3)	81.6	3.31	12.8
6.5e4	1e-10	59	5.4e-08	35.6 (1.8e+3)	122.9	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 $\boldsymbol{V}(\boldsymbol{x}) = \boldsymbol{v}_i + \boldsymbol{\omega}_i \times (\boldsymbol{x} - \boldsymbol{x}_i^c)$,

  and given forces $\boldsymbol{F}_i$, torques $\boldsymbol{T}_i$ abount $\boldsymbol{x}_i^c$.

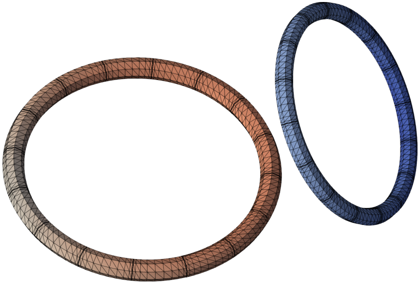
- Stokesian fluid in $\mathbb{R}^3 \setminus \Omega$

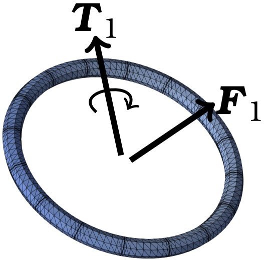
$$\Delta \boldsymbol{u} - \nabla p = 0, \quad \nabla \cdot \boldsymbol{u} = 0,$$

$$\boldsymbol{u} \to 0 \text{ as } \boldsymbol{x} \to \infty.$$

- Boundary conditions on $\partial\Omega$,

$$\boldsymbol{u} = \boldsymbol{V} + \boldsymbol{u}_s.$$





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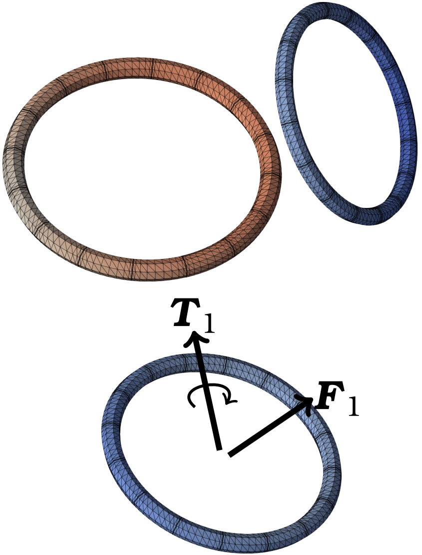
unknown: $\boldsymbol{V}(\boldsymbol{u}_i, \boldsymbol{\omega}_i)$



Mobility problem - double-layer formulation

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

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

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

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

(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

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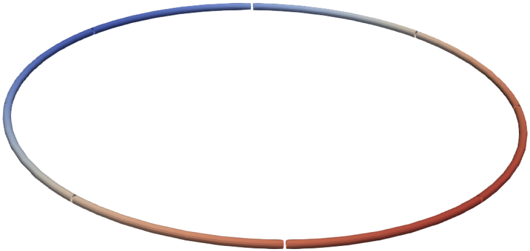
$$\kappa(\mathcal{S}) \sim 2.6e6$$

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

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



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

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where, $\mathcal{K} = \mathcal{D} + \mathcal{S}/(2\varepsilon \log \varepsilon^{-1})$.

Mobility problem - combined field formulation

Represent fluid velocity: $\boldsymbol{u} = \mathcal{S}[\boldsymbol{\nu}(\boldsymbol{F}_i, \boldsymbol{T}_i)] + \mathcal{K}[\boldsymbol{\sigma} - \sum_{i=1}^{6n} \mathfrak{v}_i \mathfrak{v}_i^T \boldsymbol{\sigma}]$

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

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where, $\mathcal{K} = \mathcal{D} + \mathcal{S}/(2\varepsilon \log \varepsilon^{-1})$.

Applying boundary conditions,

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

Second kind integral equation and well-conditioned!

Numerical Results - Sedimentation Flow

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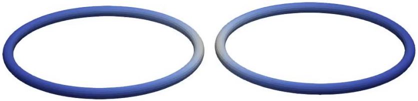

Time-stepping: 5-th order adaptive SDC

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

40 CPU cores

Numerical Results - Sedimentation Flow

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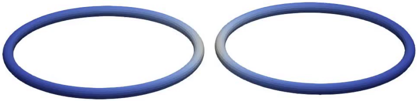

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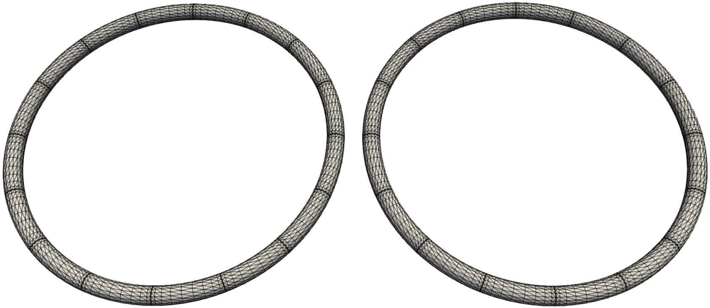
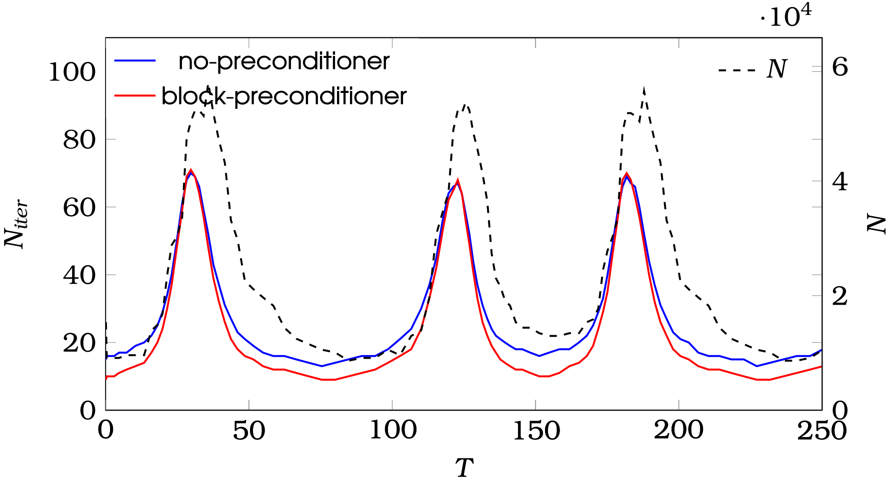


Numerical Results - Sedimentation Flow



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

$\sim 125\times$ more expensive!

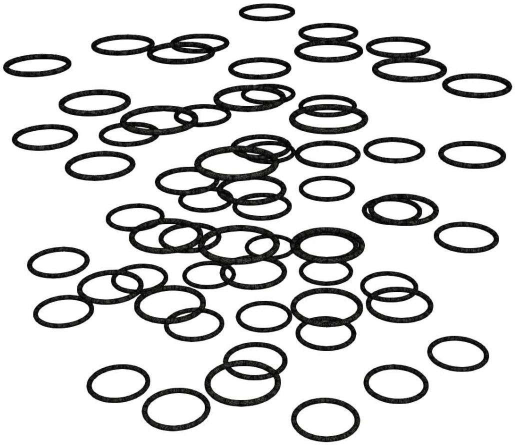
Numerical Results - Sedimentation Flow

5-th order adaptive SDC

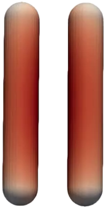
8-digits accuracy in quadratures, GMRES solve, and time-stepping.

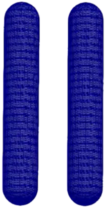
0.5 million unknowns
64 rings.

160 CPU cores



Numerical Results - Sedimentation Flow





Numerical Results - Sedimentation Flow

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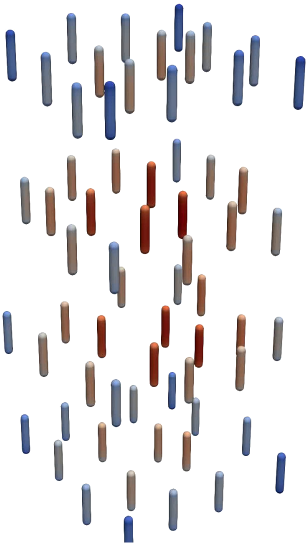

Conclusions

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- 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.
- Flexible fibers -- applications in biological fluids.