Efficient Convergent Boundary Integral Methods for Slender Bodies

Dhairya Malhotra, Alex Barnett

SIAM 2021 Annual Meeting

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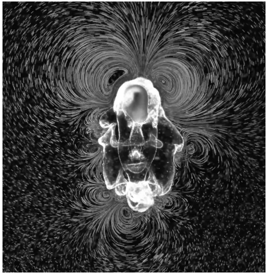
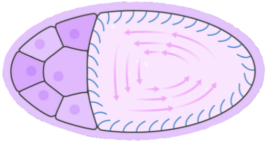
Motivations

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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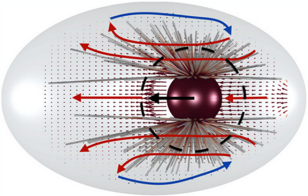

Mitotic spindle (Nazockdast et al. 2015)

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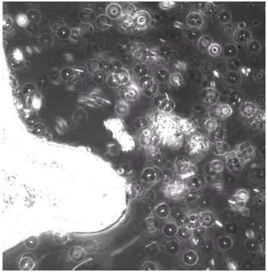
Slender Body Theory (SBT):

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



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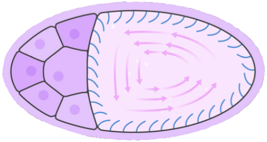

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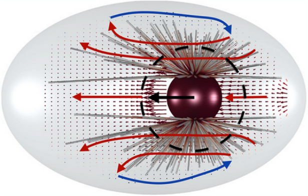

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Slender Body Theory

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

- classical asymptotics claims: $r^2 \log(r)$
- rigorous analysis: $r \log^{3/2}(r)$ (Mori-Ohm-Spirn '19)
- numerical tests: $r^{1.7}$ (Mitchell et al. '21 -- verify close-touching breakdown)

  close-to-touching with gap=10r, only 2.5-digits in the infty-norm.

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

Limitations:

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

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 varying radius.

Validate current SBT simulations.

Most existing qudaratures cannot resolve high aspect ratio geometries.

Related work: Mitchell et al, '21

- mixed-BVP corresponding to flexible fiber loop

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We focus on the static BVP for rigid fibers

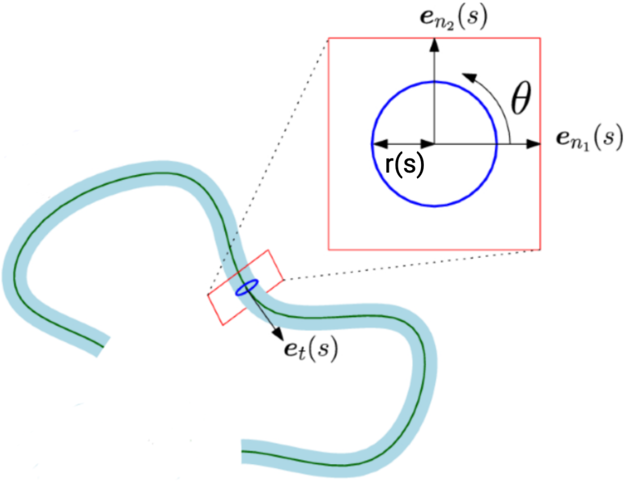
- mobility problems (rigid and flexible fiber) for future.

Only loops for now, to avoids complications with endpoint singularities.

Discretization

Geometry description:

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



Discretization

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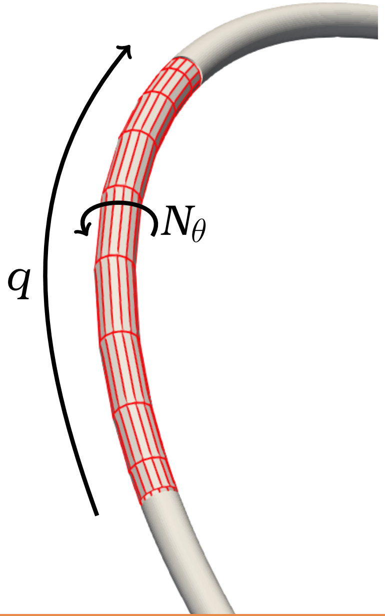
Discretization:

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



Boundary Quadratures

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

Boundary Quadratures

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

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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_θ in θ.
- given tolerance ϵ, define region $\mathcal{N}(\gamma_k)$, such that far-field is valid outside it.

Boundary Quadratures

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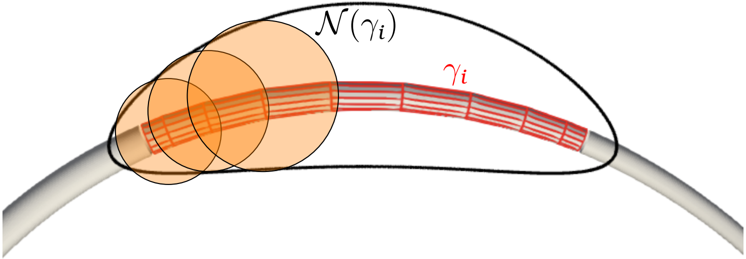

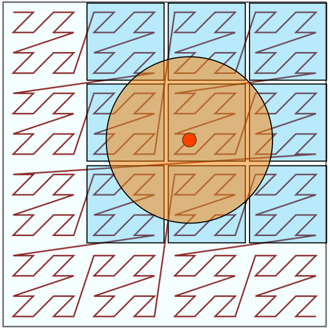

Boundary Quadratures

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

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

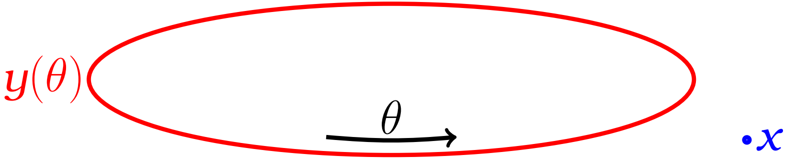
Inner integral:

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

Outer integral:

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

Fast Modal Green's Function Evaluation



$$\int_\theta \mathcal{K}(x - y(\theta))\, \sigma(\theta)\, d\theta = \sum_n \mathcal{K}_n(x)\widehat{\sigma_n}$$

where, $y(\theta)$ is a circular source loop, and $\mathcal{K}_n(x) = \int_\theta e^{-in\theta}\mathcal{K}(x - y(\theta))\, d\theta$ are the modal Green's functions.

- Periodic trapezoidal rule becomes expensive as $x \longrightarrow y$.

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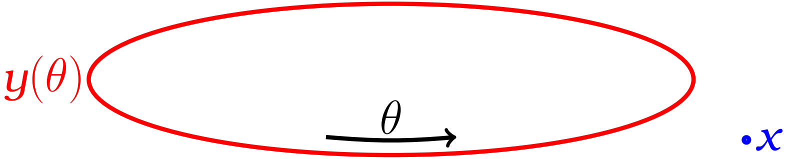

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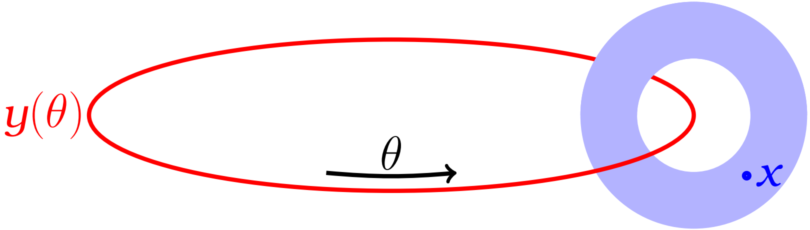
- Periodic trapezoidal rule becomes expensive as $x \longrightarrow y$.
- Fast evaluation using analytic representation in terms of special functions -- Young, Hao, Martinsson JCP-2012;
  - method of choice for axisymmetric problems; however, assumes axisymmetric normal vector.

Fast Modal Green's Function Evaluation



Build special quadrature rule (w_i, θ_i) for all $n \leq n_0$ and all targets x in the annulus:

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

- inspired by generalized Gaussian quadratures of: Bremer, Gimbutas and Rokhlin - SISC 2010.

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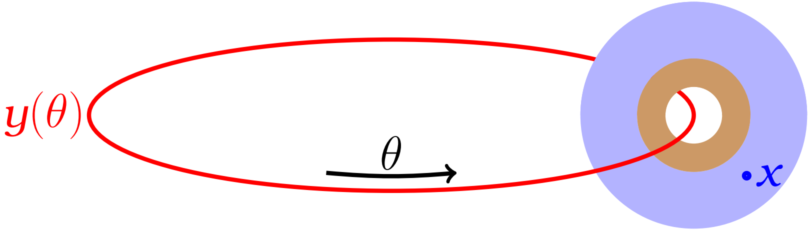

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- build quadrature rules for each nested annulus region.

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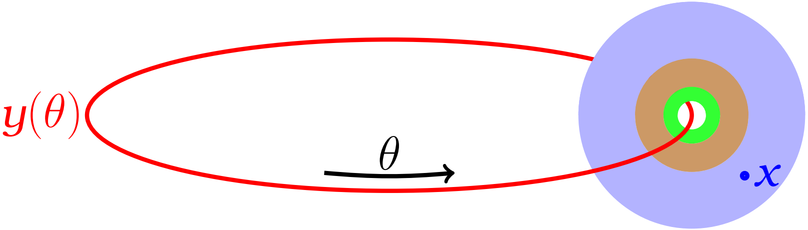

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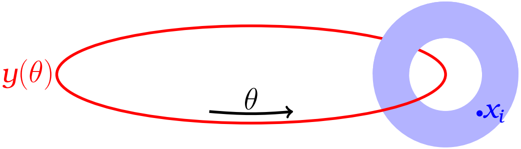
Generalized Chebyshev Quadratures

- Generate several integrands:

$$f_i(\theta) = e^{-in_i\theta}\mathcal{K}(x_i - y(\theta))$$



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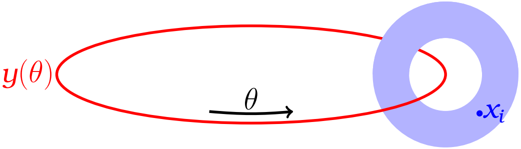

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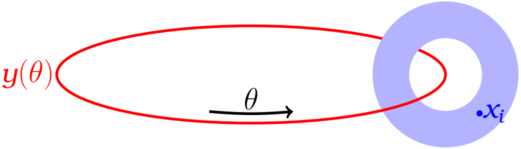

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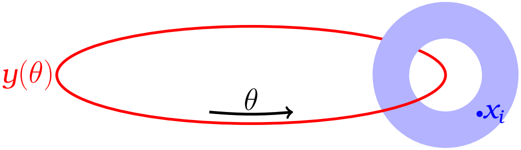

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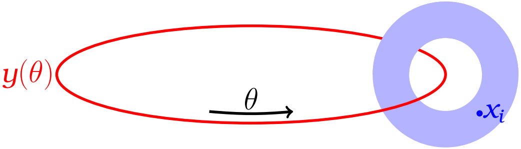

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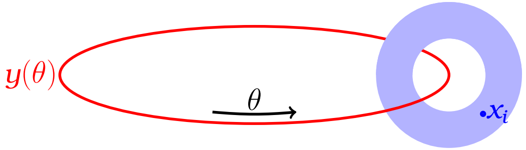

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$\approx$ 48 quadrature nodes for $n_0 = 8$ and 10-digits accuracy.
$\approx 13M$ (complex) modal Green's function evaluations/sec/core (Skylake 2.4GHz)

Quadratures for Outer Integral

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

Quadratures for Outer Integral

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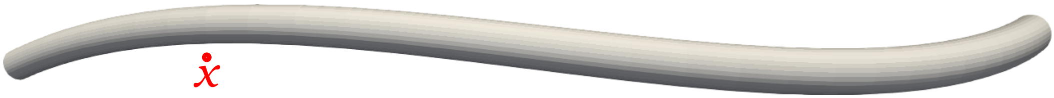
Near Interactions: x is off-surface or adjacent panel



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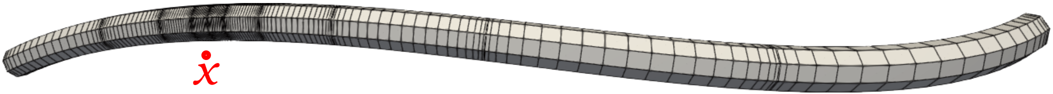

- panel (Gauss-Lengendre) quadrature with dyadic refienement.

Quadratures for Outer Integral (singular case)

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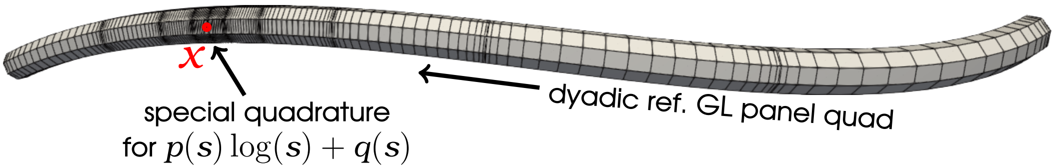

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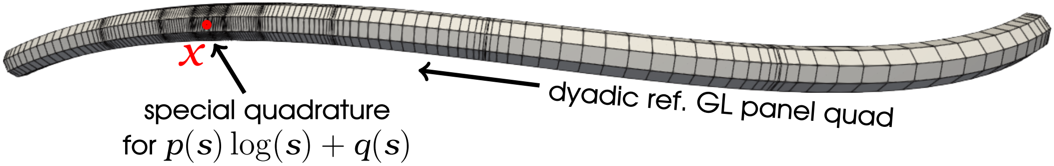

Special Quadrature Rules:

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

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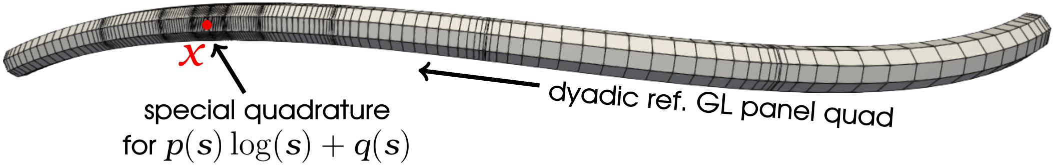

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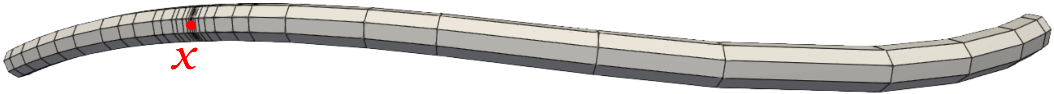

- Separate rules for different aspect ratios (1 -- 10^4 in powers of 2)

Overall Algorithm

Discretization using piecewise polynomial approximation.

Far-field interactions using standard quadratures (GL $\times$ PTR).

Near interactions

- fast scheme for modal Green's function.
- adaptive quadrature in s for non-singular case.
- generalized Chebyshev quadrature s for singular case.
- store local corrections to the far-field instead of computing on-the-fly.

Numerical Results

Numerical Results - comparison with BIEST

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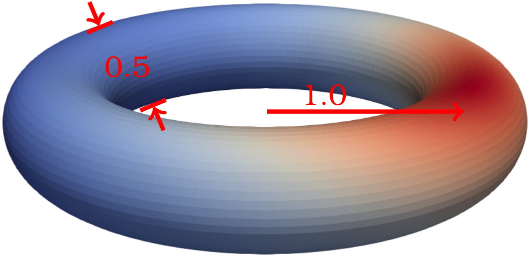
Green's identity (Laplace):

$\Delta u = 0,$ 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)

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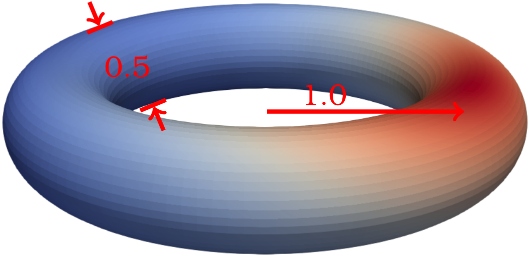

Slender-body Quadrature				BIEST*			
N	$\|\|e\|\|_\infty$	T_{setup}	T_{eval}	N	$\|\|e\|\|_\infty$	T_{setup}	T_{eval}
320	1.5e-04	0.032	0.0004	507	2.0e-03	0.1319	0.0017
720	3.5e-06	0.094	0.0013	1323	4.0e-06	1.4884	0.0042
1280	5.4e-09	0.228	0.0033	2523	4.3e-09	6.6825	0.0313
2000	2.5e-10	0.501	0.0079	4107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

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

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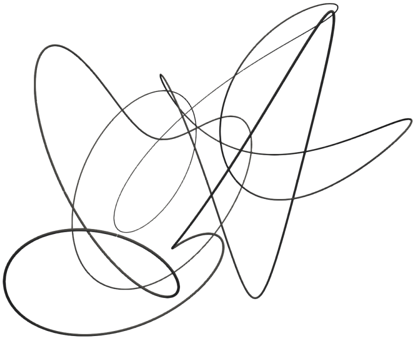

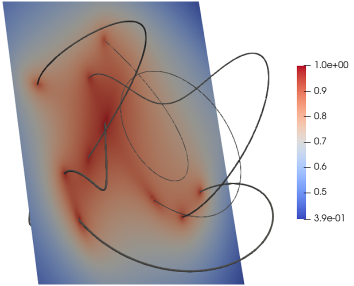

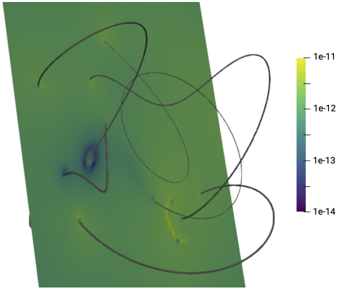

Exterior Laplace BVP:

$$\Delta u = 0, \quad u|_\Gamma = 1,$$
$$u(x) \to 0 \text{ as } |x| \to 0$$

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

wire length = 16

Numerical Results - Laplace BVP

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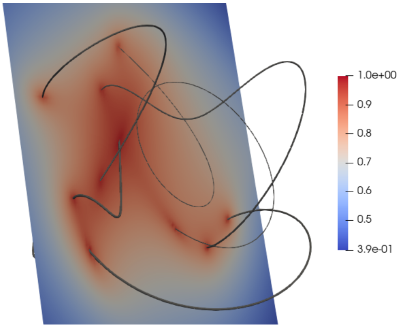
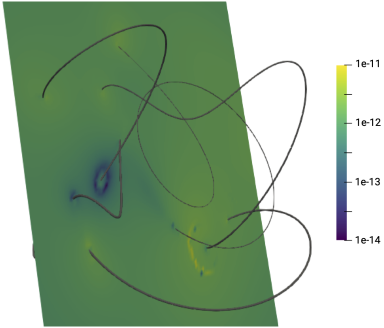
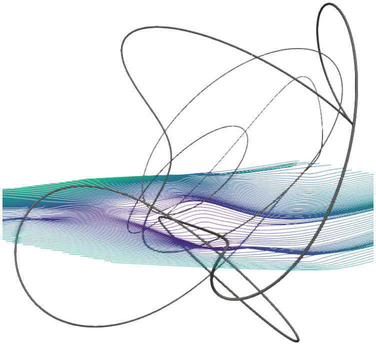
$$\Delta u = 0$$
$$u|_\Gamma = 1$$
$$u(x) \to 0$$
as $|x| \to 0$

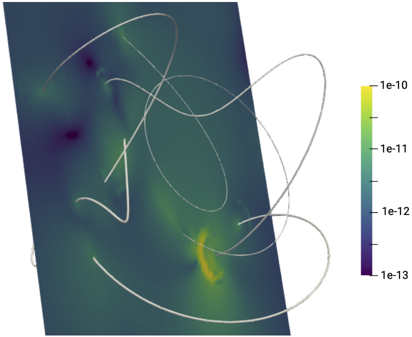




						1-core			40-cores	
N	N_{panel}	N_θ	ϵ_{GMRES}	N_{iter}	$\|e\|_\infty$	T_{setup}	(N/T_{setup})	T_{solve}	T_{setup}	T_{solve}
2.8e3	70	4	1e-02	4	4.2e-02	0.13	(2.1e4)	0.03	0.020	0.013
1.4e4	172	8	1e-04	10	1.0e-03	0.72	(1.9e4)	1.81	0.051	0.094
3.0e4	252	12	1e-05	14	3.1e-05	1.82	(1.6e4)	12.25	0.091	2.527
3.1e4	262	12	1e-07	20	2.4e-07	2.47	(1.2e4)	18.97	0.213	4.239
6.5e4	272	24	1e-09	28	1.1e-09	7.74	(8.4e3)	114.05	0.325	7.136

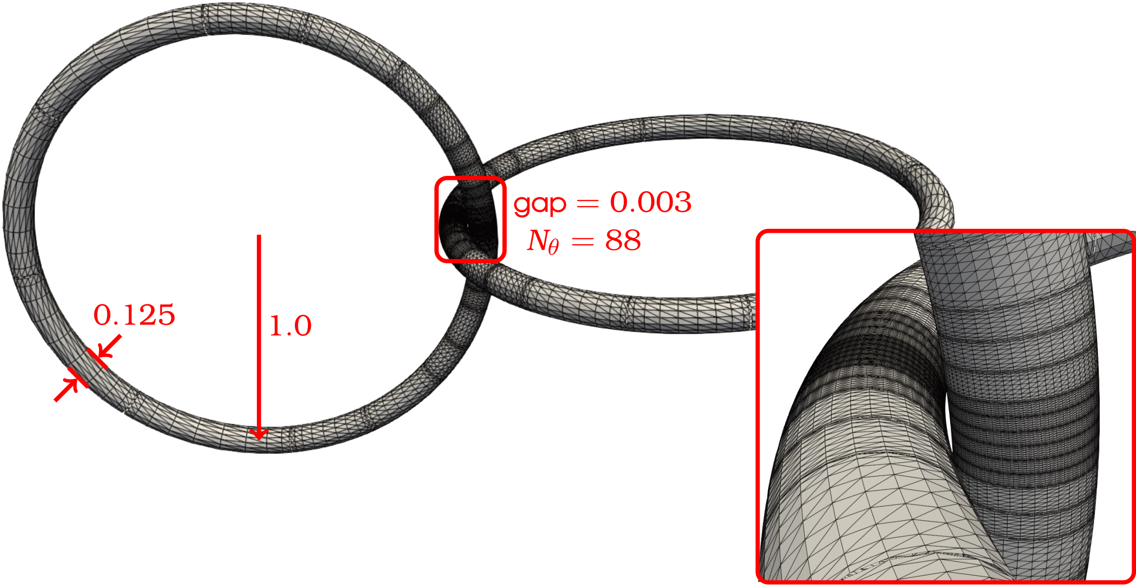
Numerical Results - Stokes BVP





						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}
4.9e3	122	4	1e-03	10	1.9e-02	0.33	(1.4e4)	0.7	0.024	0.05
3.0e4	252	12	1e-05	21	1.7e-04	3.31	(9.1e3)	61.2	0.197	5.25
3.1e4	262	12	1e-07	33	4.1e-06	4.43	(7.0e3)	104.3	0.224	7.69
6.5e4	272	24	1e-09	43	1.4e-08	17.70	(3.6e3)	586.0	0.796	22.94
7.7e4	276	28	1e-11	54	4.1e-09	27.67	(2.7e3)	1034.2	1.229	38.85

Numerical Results - close-to-touching



Numerical Results - close-to-touching

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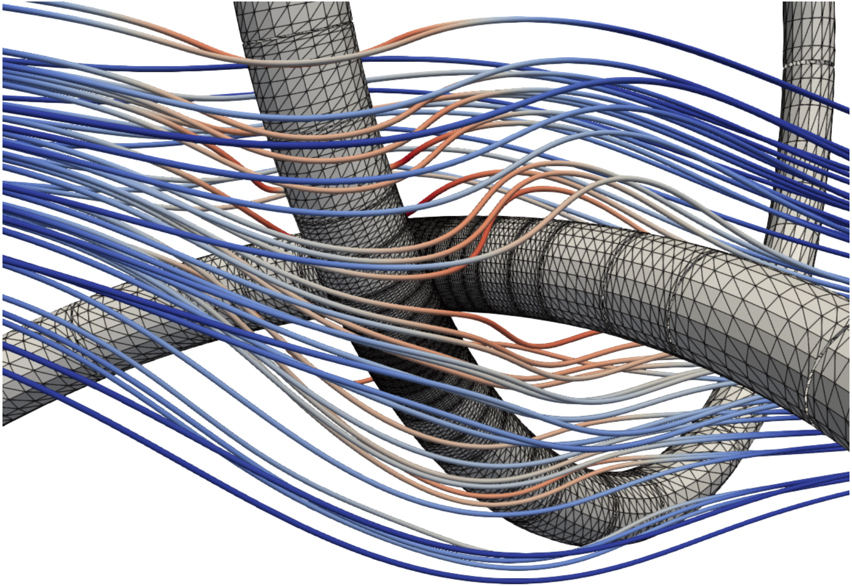

Numerical Results - close-to-touching

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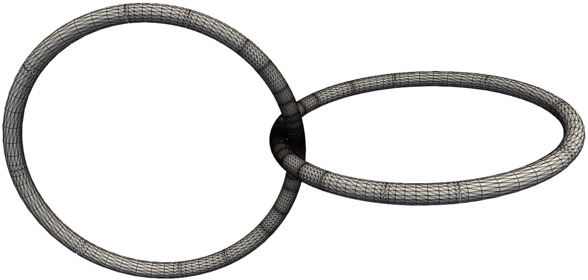

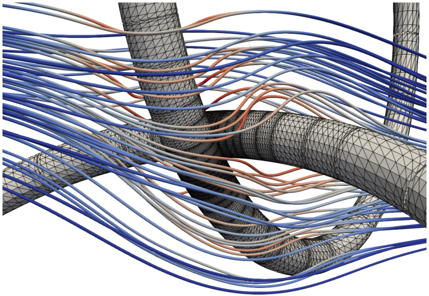

				1-core		40-cores	
N	ϵ_{GMRES}	N_{iter}	$\|\|e\|\|_\infty$	T_{setup} (N/T_{setup})	T_{solve}	T_{setup}	T_{solve}
2.2e4	1e-02	4	2.1e-02	8.1 (2.7e+3)	6.5	1.28	1.4
2.2e4	1e-05	24	2.4e-03	16.8 (1.3e+3)	42.9	2.50	7.7
2.2e4	1e-07	43	2.8e-06	23.5 (9.2e+2)	81.6	3.31	12.8
2.2e4	1e-10	59	5.4e-08	35.6 (6.0e+2)	122.9	4.06	19.2
2.2e4	1e-13	72	1.3e-10	49.9 (4.3e+2)	162.6	5.27	23.2

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 10^4.
  - fast computation of modal/toroidal Green's function.
  - special (Chebyshev) quadratues for singular integrals along length of fibers.
  - quadrature setup rates up to $20,000$ points/s/core for Laplace (comparable to FMM speeds).
  - distributed memory parallelisation (partially complete).

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Ongoing work:

- Open fibers (singularities at ends).
- Mobility problem and flexible fibers.
- Comparison w/ SBT efficiency when SBT is sufficiently accurate.