

Convergent Slender Body Theory

Code: <https://github.com/dmalhotra/CSBQ>

Dhairya Malhotra, Alex Barnett

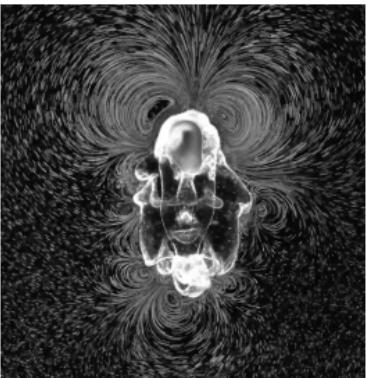
June 13, 2024

Slender Body Theory

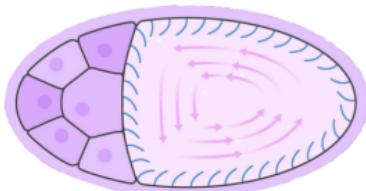
Stokes simulations with fibers are key to modeling complex fluids (suspensions, rheology, industrial, biomedical, cellular biophysics).

Slender Body Theory (SBT):

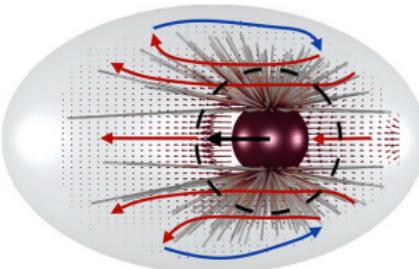
- Asymptotic expansion in radius (ε) as $\varepsilon \rightarrow 0$ (Keller-Rubinow '76).
- Doublet correction to make velocity theta-independent (Johnson '80).



Starfish larvae
(Gilpin et al. 2016)



Drosophila oocyte
(Stein et al. 2021)

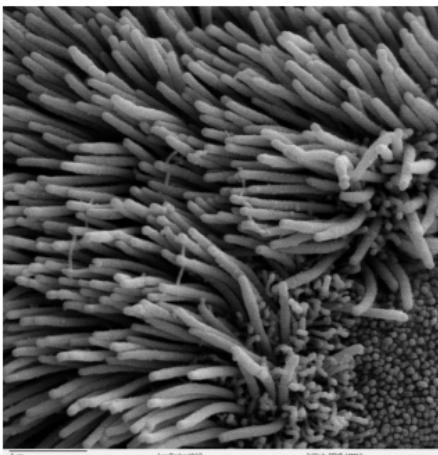


Mitotic spindle (Nazockdast et al. 2015)

Slender Body Theory Error Estimates

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 infinity-norm.



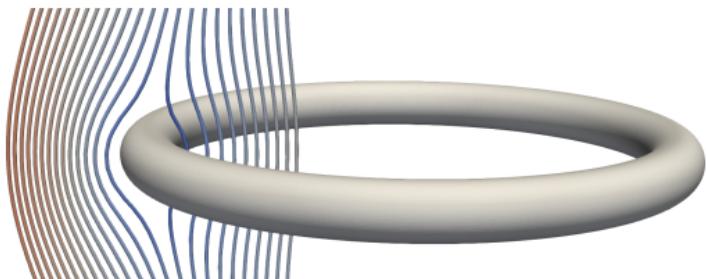
Source: <http://remf.dartmouth.edu/imagesindex.html>

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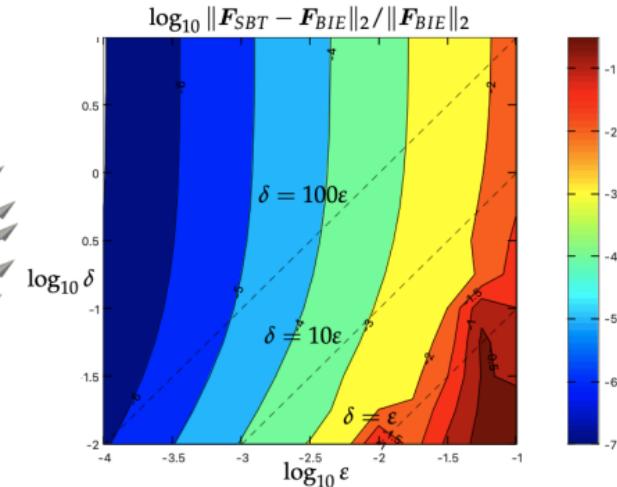
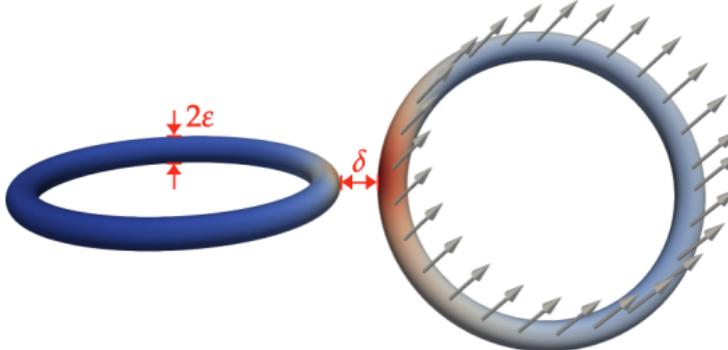
ε	\mathbf{u}_{exact}	Rel-Error
1e-1	6.1492138359856e-2	0.5e-2
1e-2	9.0984522324584e-2	0.1e-3
1e-3	1.2015655889904e-1	0.2e-5
1e-4	1.4931932907587e-1	0.2e-7
1e-5	1.7848191313097e-1	0.3e-9



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Convergent Slender Body Theory



Goals: Develop boundary integral methods to solve the slender body BVP

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

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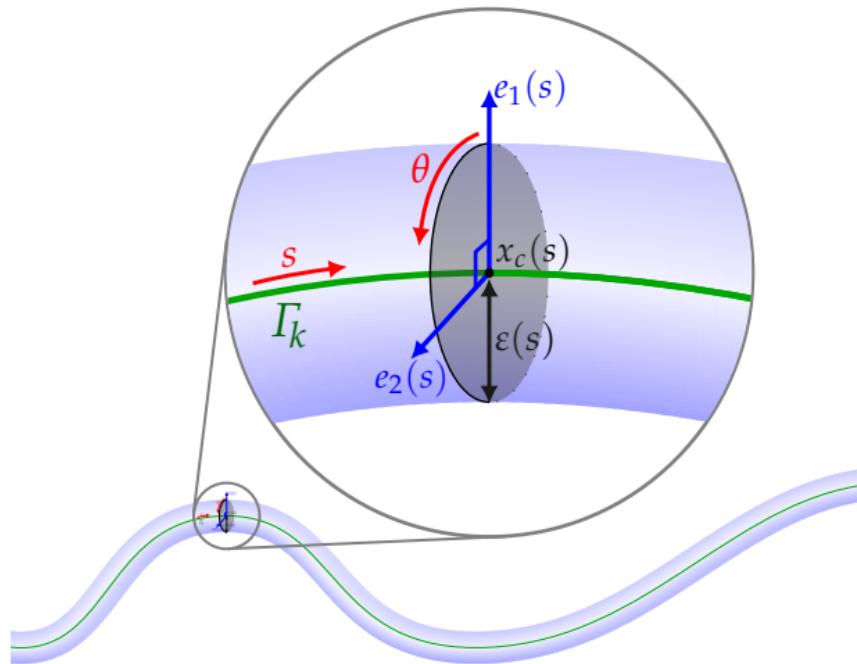
Focus on rigid fibers in this talk -- flexible fibers for future.

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

Discretization

Geometry description:

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



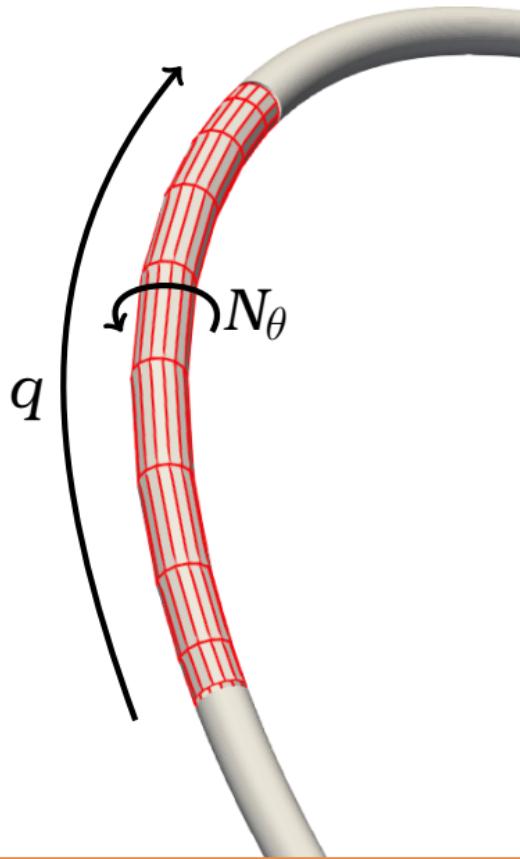
Discretization

Geometry description:

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- orientation vector $e_1(s)$

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



$$u(x) = \int_{\Gamma} \mathcal{K}(x - y) \sigma(y) da(y)$$

Boundary Quadratures



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

Boundary Quadratures

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

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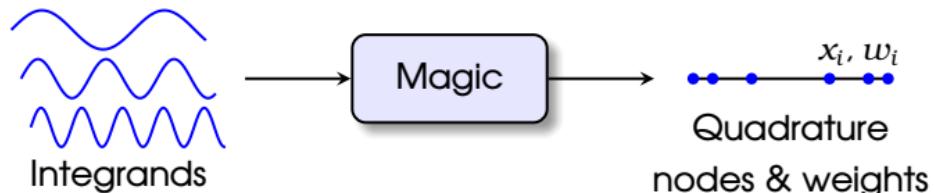
Far-field

- Tensor product quad:
Gauss-Legendre \times PTR
- Accelerate with PVFMM
 $\mathcal{O}(N^2) \rightarrow \mathcal{O}(N)$

Near interactions

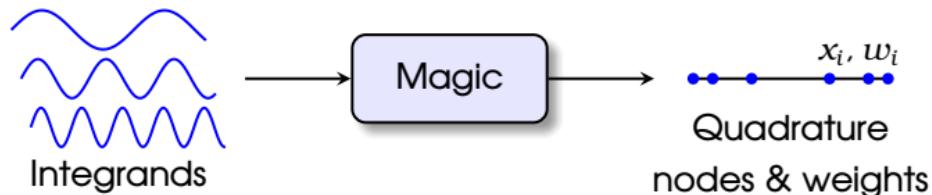
- Build special quadrature rules!

Generating Special Quadrature Rules



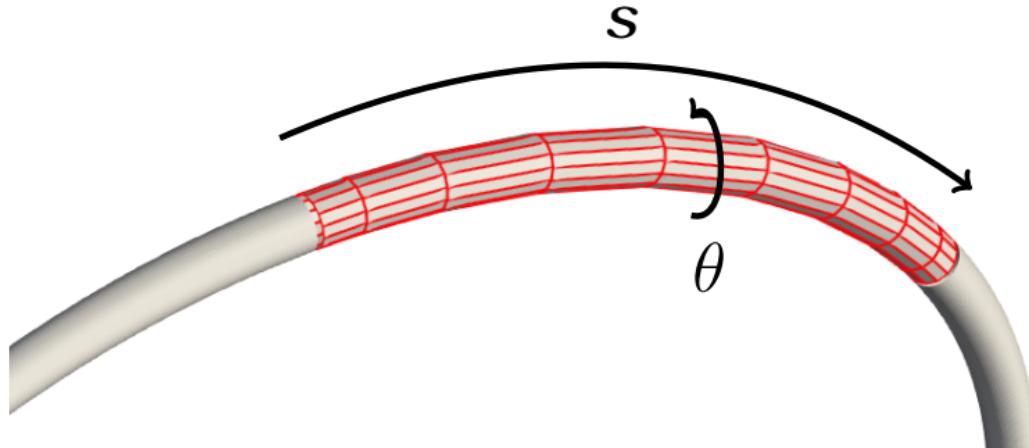
Generalized Gaussian Quad.
Bremer, Gimbutas and
Rokhlin - SISC 2010

Generating Special Quadrature Rules

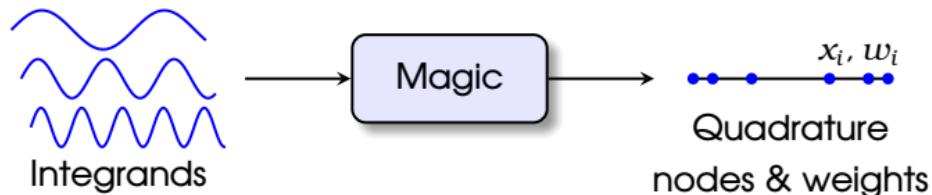


Generalized Gaussian Quad.
Bremer, Gimbutas and
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$$\int_{\Gamma_k} \mathcal{K}(x - y) \sigma(y) da(y) = \int_s \int_{\theta} \mathcal{K}(x - y(s, \theta)) \sigma(s, \theta) J(s, \theta) d\theta ds$$

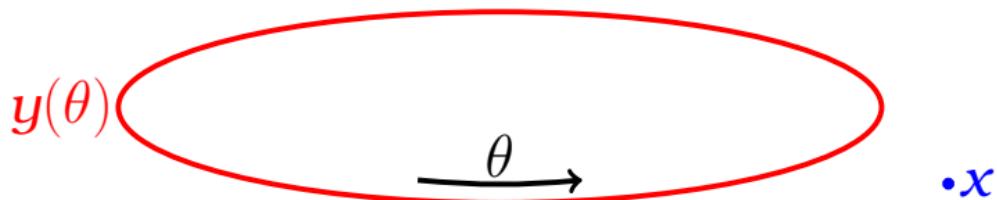


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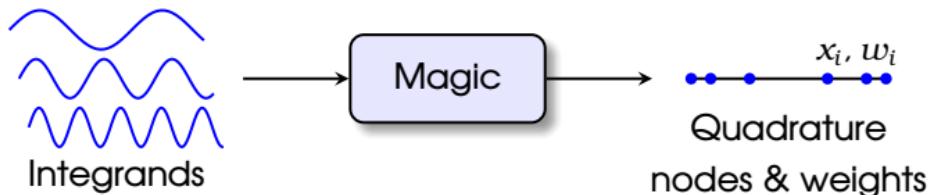


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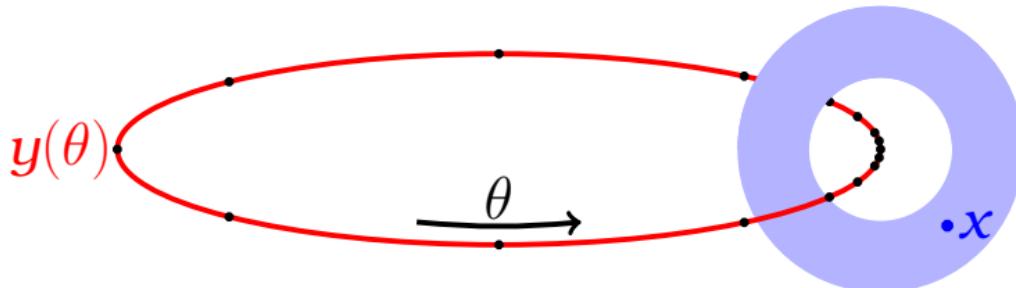


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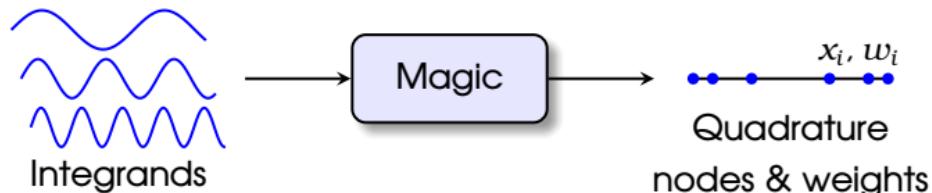
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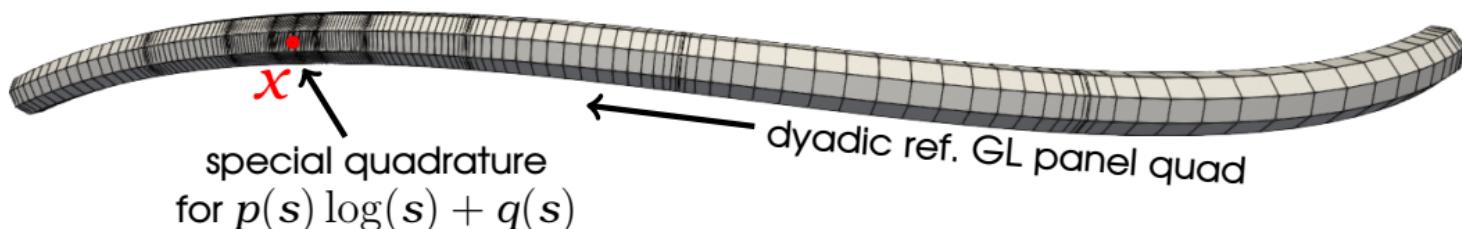
~ 48 quadrature nodes for $n_0 = 8$ and 10-digits accuracy.
~ 26M modal Green's function evaluations/sec/core (Skylake 2.4GHz)

Generating Special Quadrature Rules

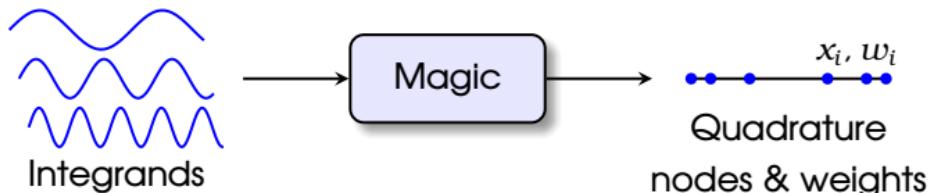


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Generating Special Quadrature Rules



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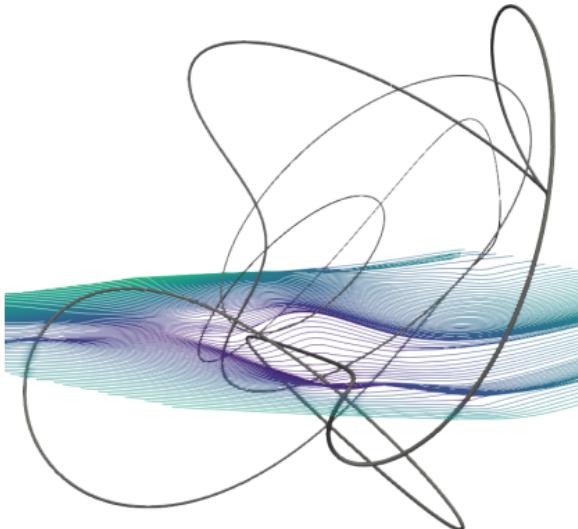
$$\int_{\Gamma_k} \mathcal{K}(x - y) \sigma(y) da(y) = \int_s \int_\theta \mathcal{K}(x - y(s, \theta)) \sigma(s, \theta) J(s, \theta) d\theta ds$$



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:

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

$$\mathbf{u}|_{\Gamma} = \mathbf{u}_0,$$

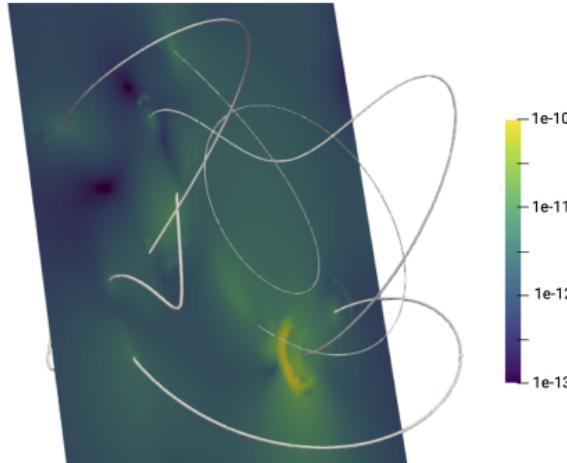
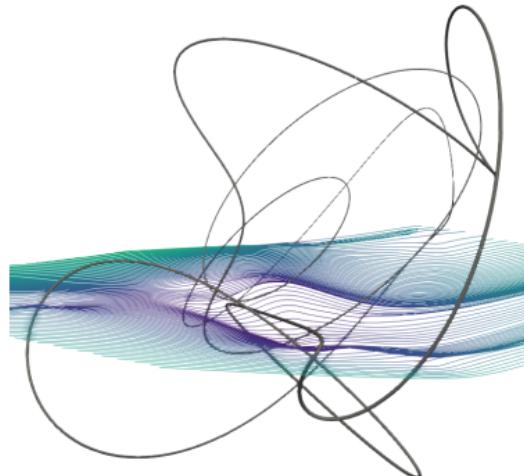
$$u(x) \rightarrow 0 \text{ as } |x| \rightarrow 0,$$

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

wire length = 16

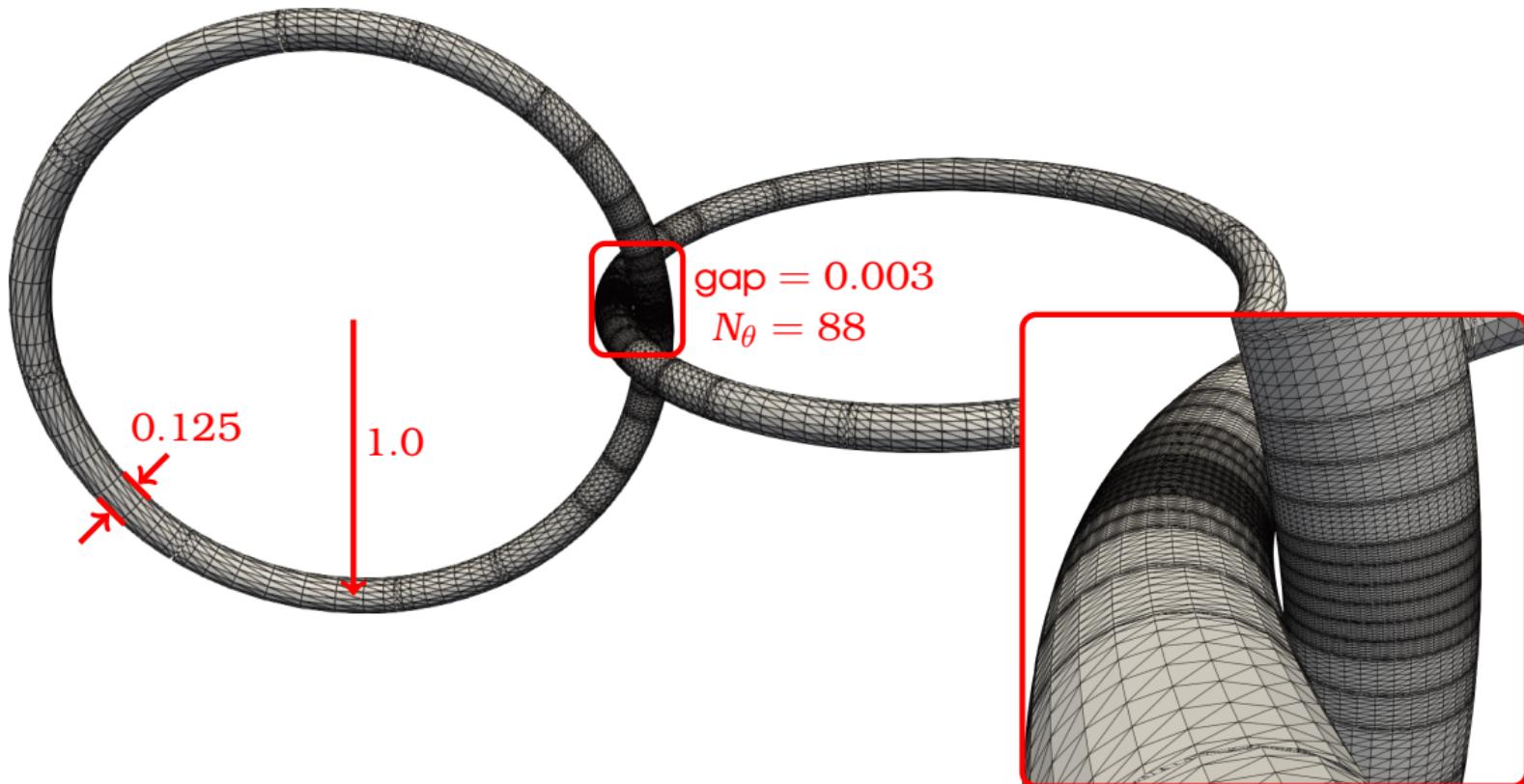
BIE formulation: $(I/2 + D + S / (2\varepsilon \log \varepsilon^{-1})) \boldsymbol{\sigma} = \mathbf{u}_0$

Numerical Results - Stokes BVP

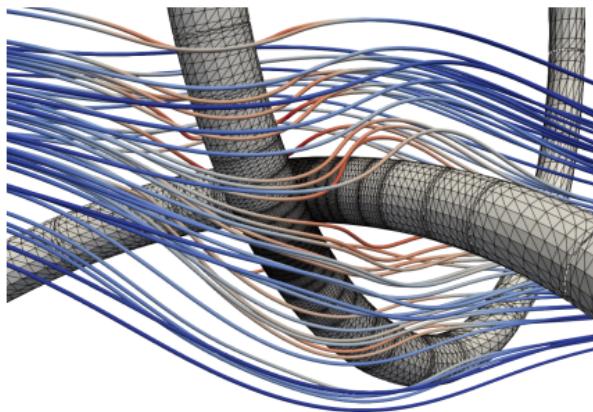
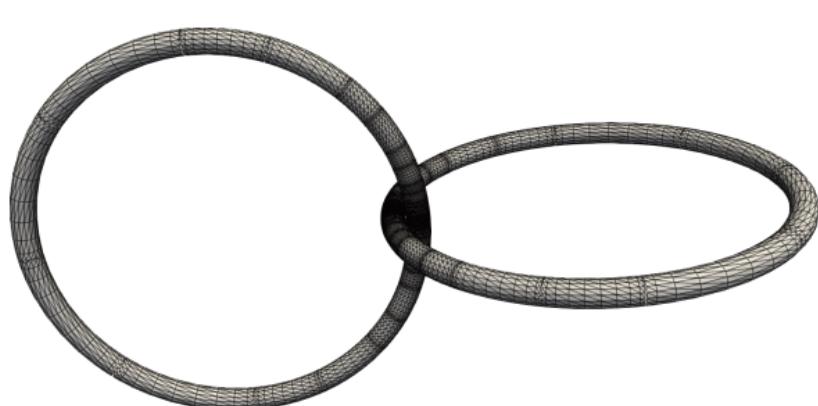


N	N_{panel}	N_θ	ϵ_{GMRES}	N_{iter}	$\ e\ _\infty$	1-core			40-cores	
						T_{setup}	(N/T_{setup})	T_{solve}	T_{setup}	T_{solve}
1.0e4	49	8	1e-02	5	3.5e-02	0.193	(5.4e4)	0.130	0.042	0.017
2.6e4	103	12	1e-05	22	5.5e-05	0.572	(4.5e4)	4.039	0.045	0.215
4.7e4	157	20	1e-07	33	6.6e-07	1.416	(3.3e4)	19.518	0.134	1.162
8.3e4	227	24	1e-08	38	4.5e-08	3.623	(2.3e4)	78.907	0.324	3.689
2.2e5	457	40	1e-10	49	2.9e-10	21.949	(1.0e4)	746.966	4.458	48.494

Numerical Results - close-to-touching



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				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

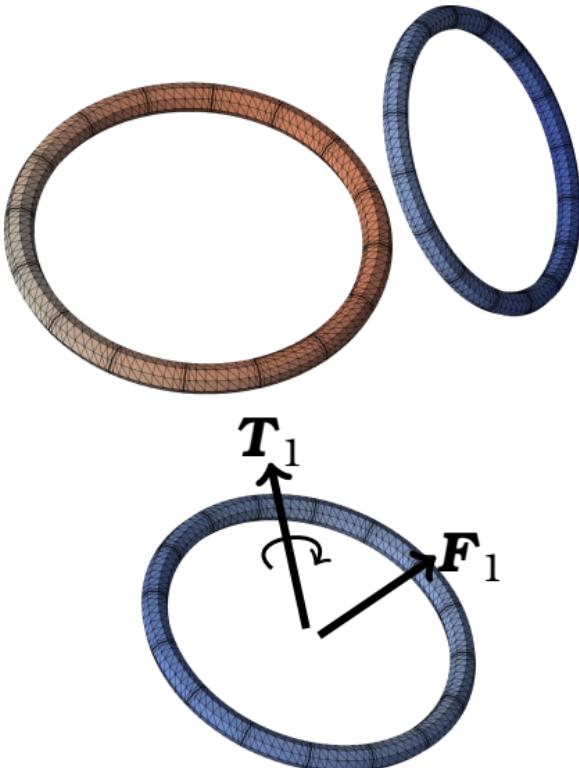
Mobility problem

- n rigid bodies $\Omega = \sum_{i=1}^n \Omega_i$
with velocities $\mathbf{V}(\mathbf{x}) = \mathbf{v}_i + \omega_i \times (\mathbf{x} - \mathbf{x}_i^c)$,
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 $\partial\Omega$,
$$\mathbf{u} = \mathbf{V} + \mathbf{u}_s.$$



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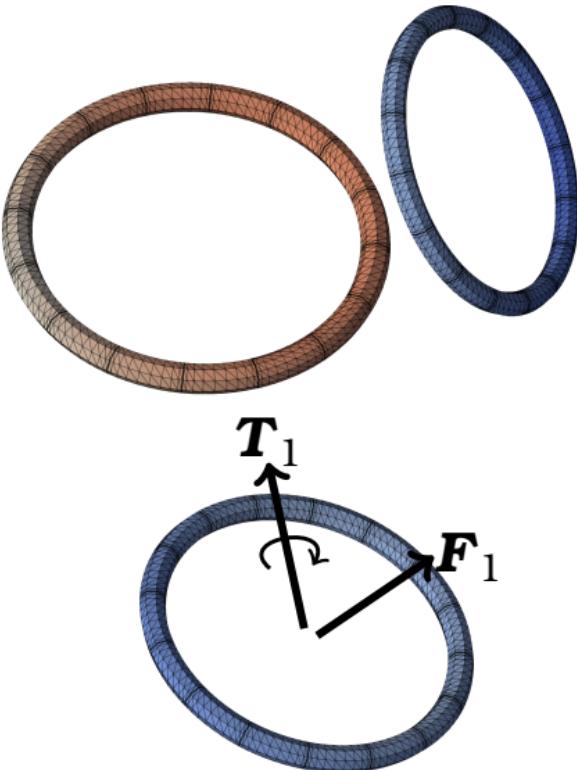
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- Boundary conditions on $\partial\Omega$,
$$\mathbf{u} = \mathbf{v} + \mathbf{u}_s.$$

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 $\partial\Omega$),

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

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

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Second kind integral equation ... but doesn't work for slender bodies!

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Second kind integral equation ... but doesn't work for slender bodies!

$$\kappa(I/2 + D) \sim 1/(\varepsilon^2 \log \varepsilon^{-1})$$

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

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

Mobility problem - combined field formulation



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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!

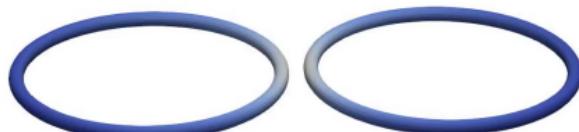
Numerical Results - Sedimentation Flow



Time-stepping: 5-th order adaptive SDC

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

40 CPU cores



Numerical Results - Sedimentation Flow



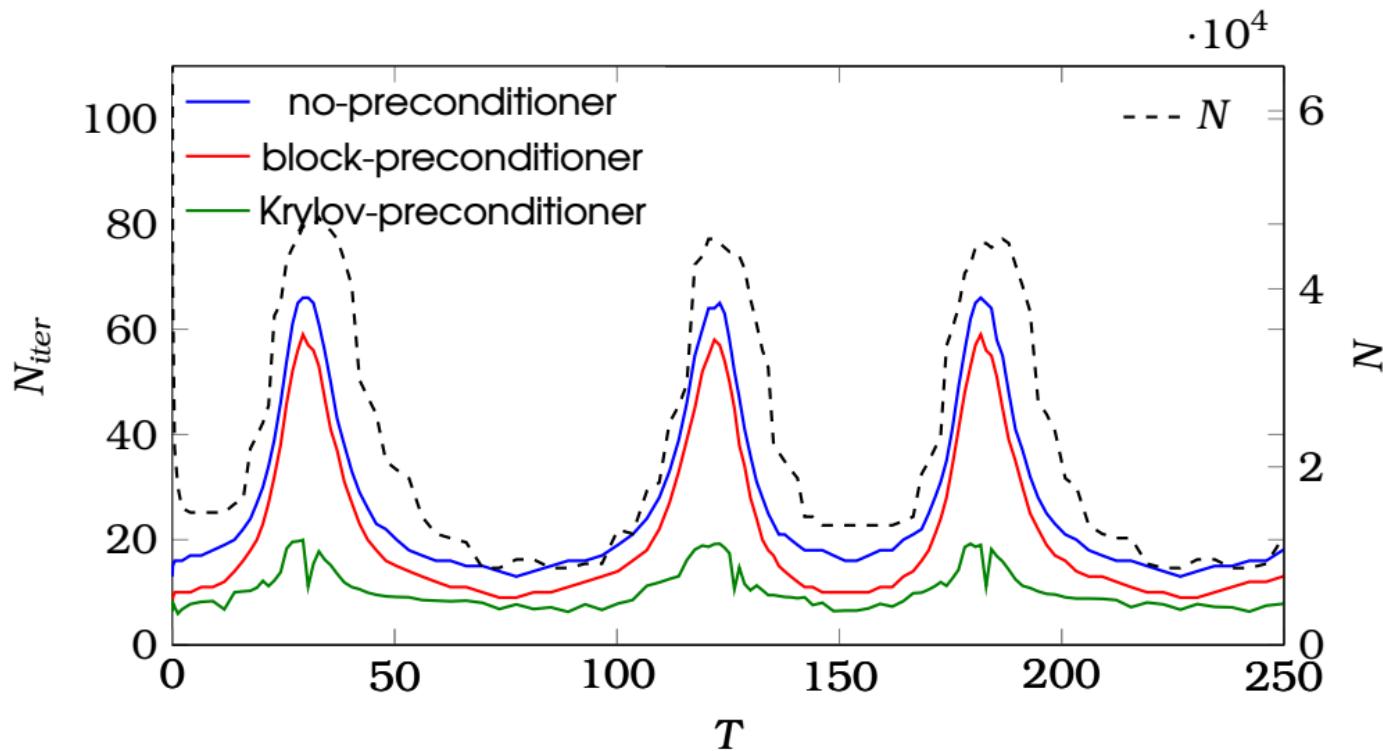
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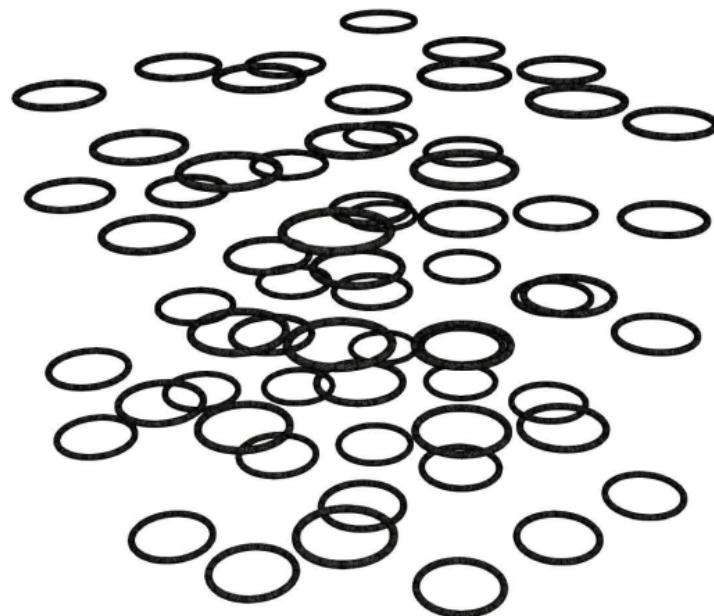
5-th order adaptive SDC

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

0.5 million unknowns

64 rings.

160 CPU cores



Code: <https://github.com/dmalhotra/CSBQ>

(remember to checkout submodule SCTL)

Requirements: C++11 compiler with OpenMP

Build system: none (header only)

```
#include <csbq.hpp>
```

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#include <csbq.hpp>
```

Optional dependencies: BLAS, LAPACK, FFTW, MPI, and PVFMM

SCTL: Scientific Computing Template Library

BoundaryIntegralOp

Kernel

FMM

Quadrature

GMRES

SDC

Profile

Vec (SIMD)

Comm

Vector

Matrix

VTUData

Interpolation

Tree

CSBQ: Convergent Slender Body Quadrature

SlenderElemL

RigidBodyL, Mobility

CubeVolumeVis, Utils

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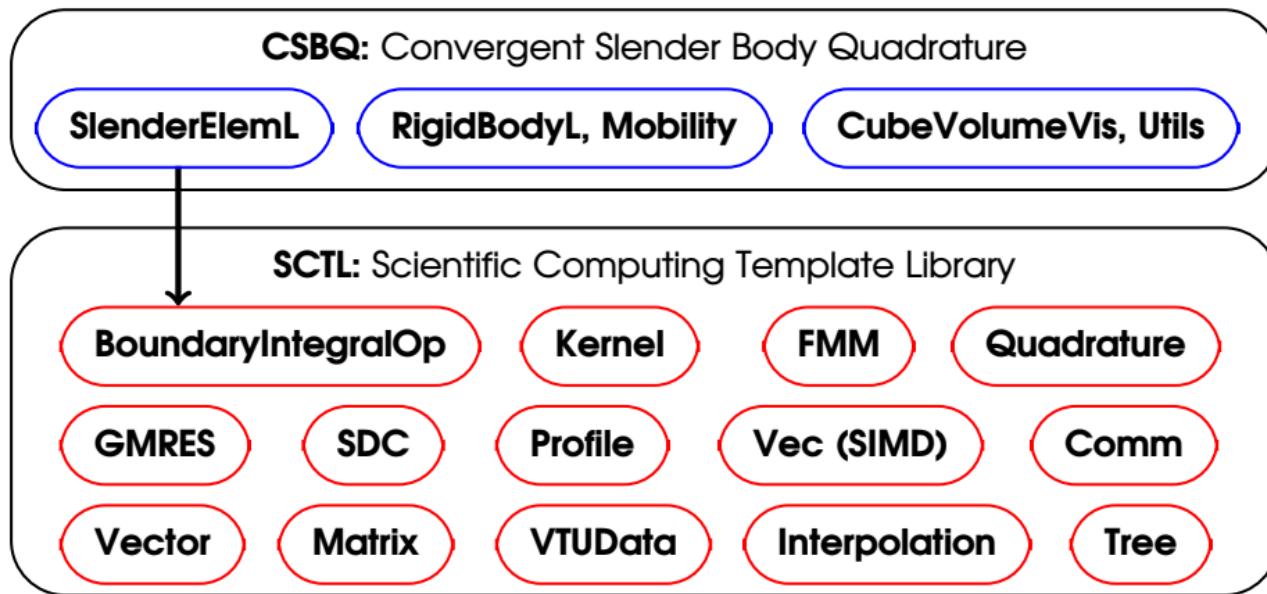
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Applications

CSBQ: Convergent Slender Body Quadrature

SlenderElemL

RigidBodyL, Mobility

CubeVolumeVis, Utils



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Kernel

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Step 1: Stokes Dirichlet boundary value problem (exterior)

- Stokes equations:

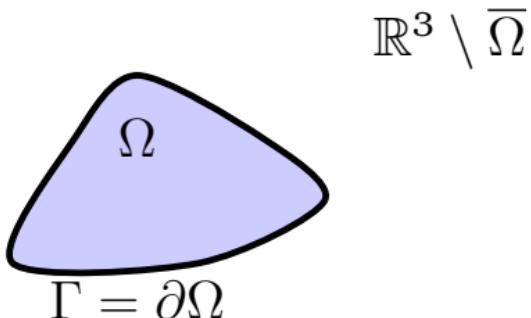
$$\Delta \mathbf{u} - \nabla p = 0 \quad \text{in } \mathbb{R}^3 \setminus \overline{\Omega},$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \mathbb{R}^3 \setminus \overline{\Omega},$$

- Boundary conditions:

$$\mathbf{u}|_{\Gamma} = \mathbf{u}_0 \quad \text{on } \Gamma,$$

$$\mathbf{u}(\mathbf{x}) \rightarrow \mathbf{0} \quad \text{as } |\mathbf{x}| \rightarrow \infty$$



Solving BIEs with CSBQ

Step 2: Integral Equation Formulation

- Boundary integral representation:

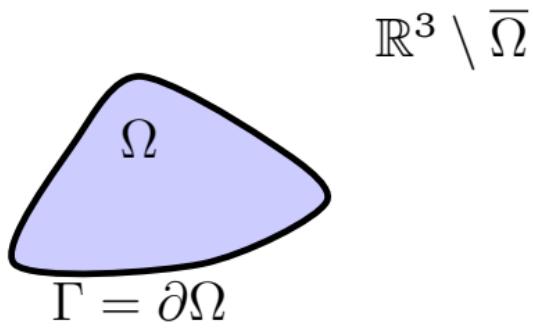
$$\mathbf{u} = \mathcal{D}[\sigma] + \eta \mathcal{S}[\sigma] \quad \text{in } \mathbb{R}^3 \setminus \overline{\Omega},$$

where

$$\mathcal{S}[\sigma](\mathbf{x}) := \int_{\Gamma} S(\mathbf{x} - \mathbf{y}) \sigma(\mathbf{y}) dS_y,$$

$$\mathcal{D}[\sigma](\mathbf{x}) := \int_{\Gamma} D(\mathbf{x} - \mathbf{y}) \sigma(\mathbf{y}) dS_y,$$

$$\eta = 1/(\epsilon \log \epsilon^{-1})$$

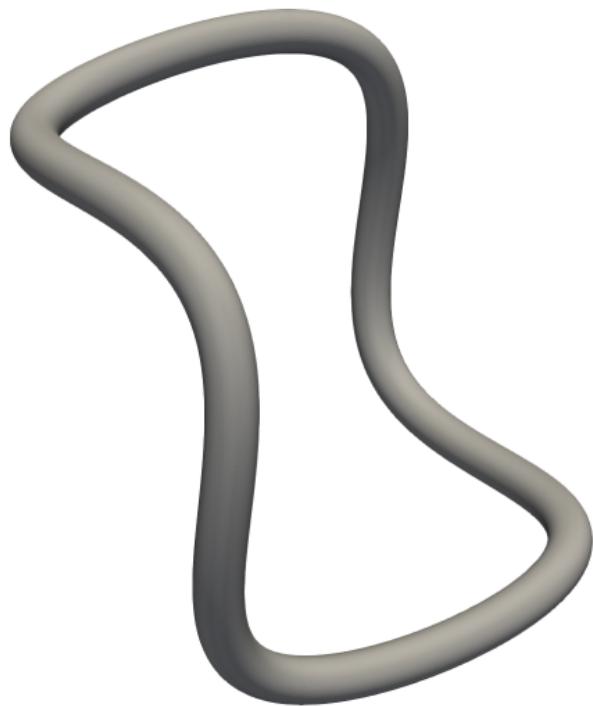


- Enforce boundary conditions:

$$(I/2 + D + \eta S)\sigma = \mathbf{u}_0 \quad \text{on } \Gamma,$$

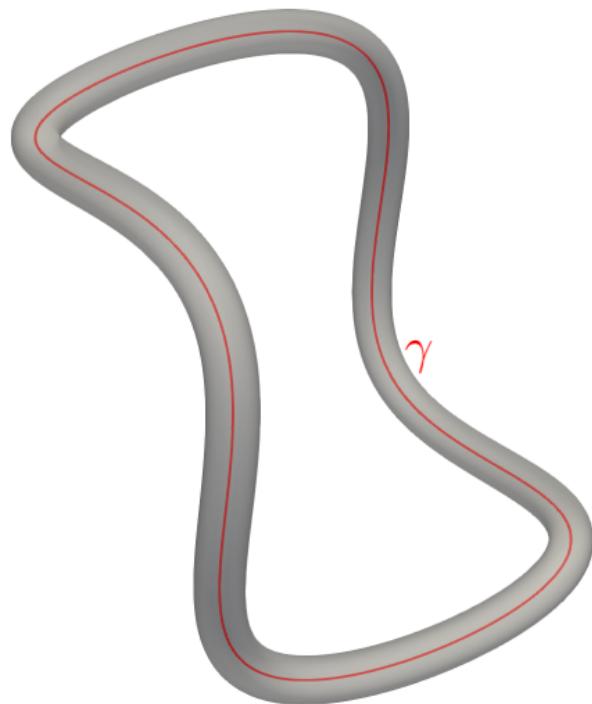
Solve for unknown σ

Step 3: Discretize the geometry



Step 3: Discretize the geometry

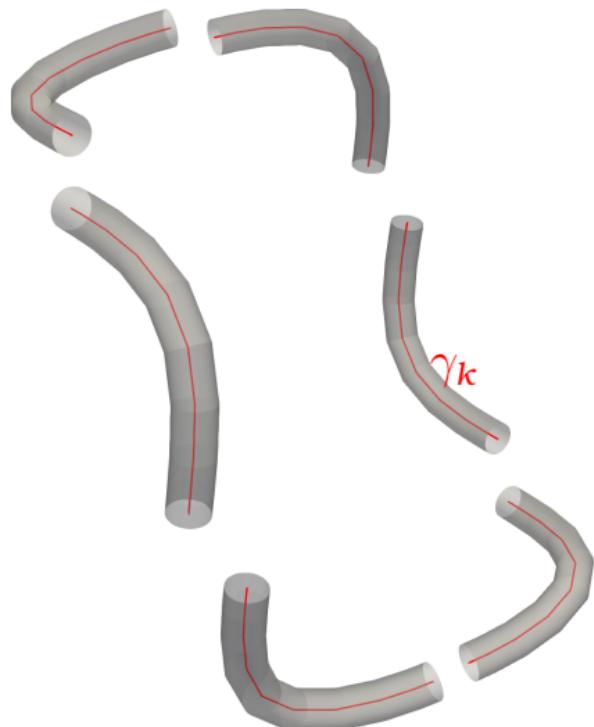
- Geometry described by centerline γ .



Solving BIEs with CSBQ

Step 3: Discretize the geometry

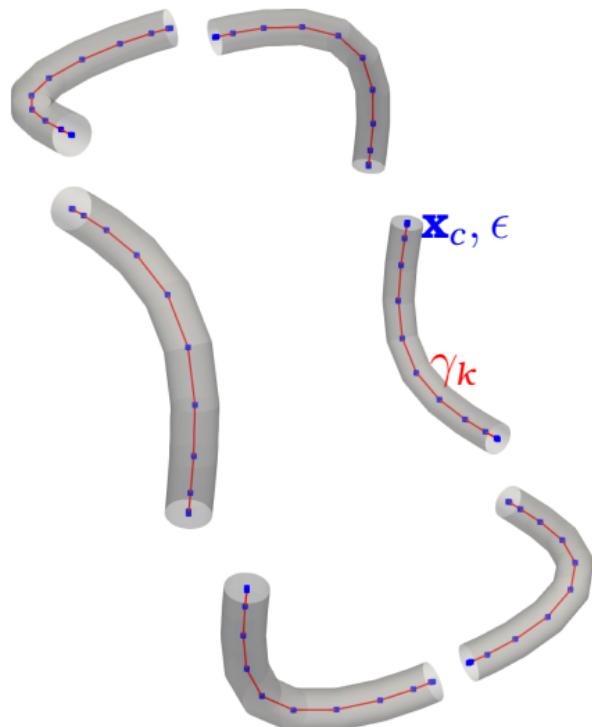
- Geometry described by centerline γ .
- Partition into panels.
 - Choose panel order and Fourier order.



Solving BIEs with CSBQ

Step 3: Discretize the geometry

- Geometry described by centerline γ .
- Partition into panels.
 - Choose panel order and Fourier order.
- Determine nodes \mathbf{x}_c and radius ϵ .



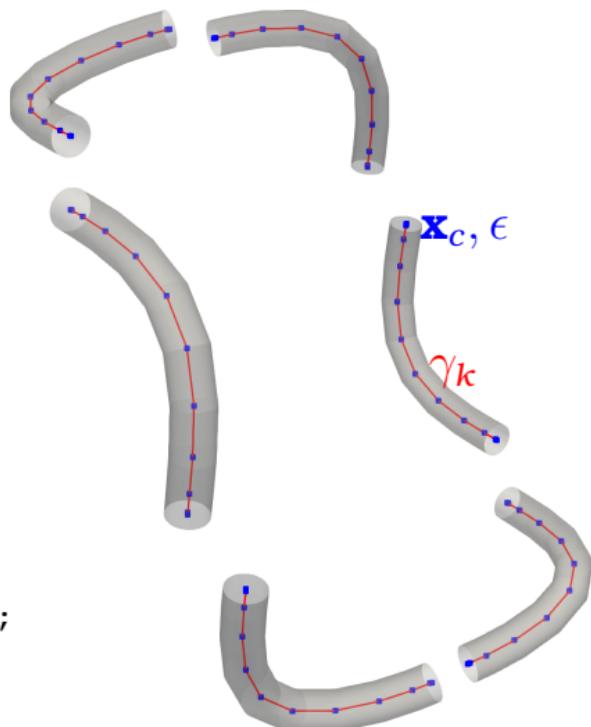
Solving BIEs with CSBQ

Step 3: Discretize the geometry

- Geometry described by centerline γ .
- Partition into panels.
 - Choose panel order and Fourier order.
- Determine nodes \mathbf{x}_c and radius ϵ .

Code:

```
Vector<Long> ElemOrder, FourierOrder;  
Vector<double> Xc, eps;  
// set vector data ...  
  
SlenderElemList<double> elem_1st(ElemOrder,  
                                    FourierOrder, Xc, eps);
```



Step 4: Discretize Integral Operator

- Stokes combined field kernel:

```
struct Stokes3D_CF_ {
    template <Integer digits, class VecType>
    static void uKerMatrix(VecType (&u)[3][3], const VecType (&r)[3],
                          const VecType (&n)[3], const void* ctx_ptr) {
        // u[i][j] = [Stokes-SL] + [Stokes-DL];
    }
    // other member functions ...
};
```

Step 4: Discretize Integral Operator

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- Boundary integral operator:

```
Stokes3D_CF ker;
BoundaryIntegralOp<double, Stokes3D_CF> LayerPotenOp(ker);
LayerPotenOp.AddElemList(elem_lst); // add geometry to operator
LayerPotenOp.SetAccuracy(tol); // set accuracy

const auto BIO = [&LayerPotenOp](Vector<double>* U,
                                const Vector<double>& sigma) {
    LayerPotenOp.ComputePotential(*U, sigma);
    (*U) += sigma * 0.5;
};
```

$$\mathbf{u}(\mathbf{x}) = (\mathcal{D} + \mathcal{S})[\sigma](\mathbf{x})$$

$$K\sigma := (I/2 + D + S)\sigma$$

Solving BIEs with CSBQ



Step 5: Solve Integral Equation

```
Vector<double> sigma, U0(LayerPotenOp.Dim(0));
// set boundary condition U0

GMRES<double> solver;
solver(&sigma, BIO, U0, tol);
```

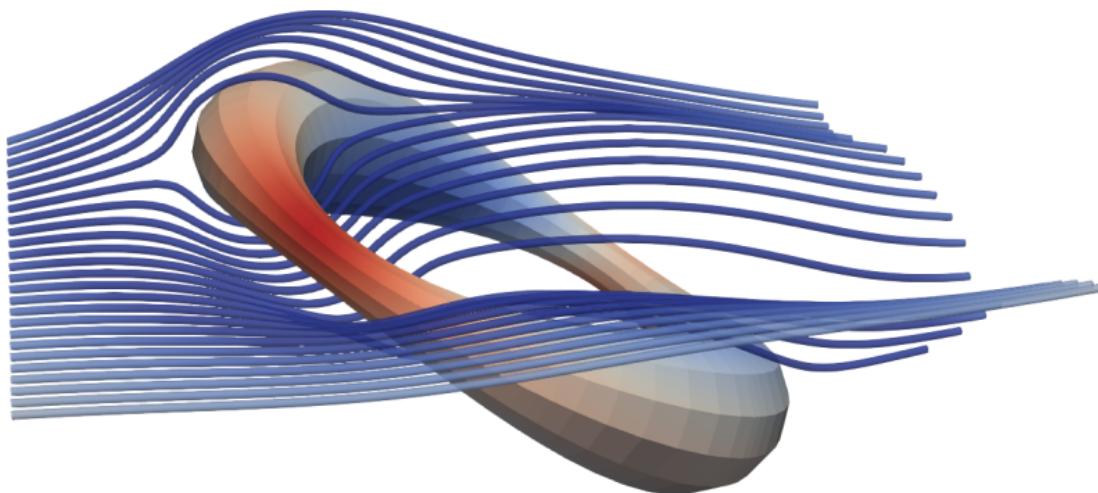
Step 6: Post-process

```
Vector<double> U;
LayerPotenOp.SetTargetCoord(Xtrg); // Set targets for LayerPotenOp
LayerPotenOp.ComputePotential(U, sigma); // Evaluate solution
//... Write to VTK file
```

Solving BIEs with CSBQ

Step 6: Post-process

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Conclusions

- Convergent boundary integral formulation for slender bodies,
 - unlike SBT, boundary conditions enforced to high accuracy.
- Special quadrature - efficient for aspect ratios as large as 10^5 .
 - quadrature setup rates $\sim 20,000$ unknowns/s/core (at 7-digits).
- Combined field BIE formulations,
 - well-conditioned for slender-body geometries.

Conclusions

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- Combined field BIE formulations,
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Limitations and ongoing work:

- Flexible fibers -- applications in biological fluids.