Convergent Slender Body Theory

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

Dhairya Malhotra, Alex Barnett

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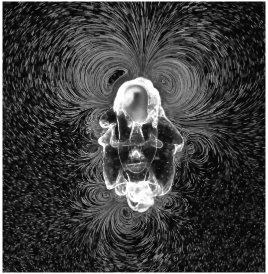
Slender Body Theory

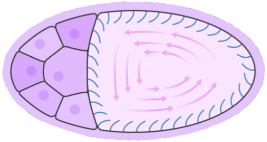
Stokes simulations with fibers are key to modeling complex fluids (suspensions, rheology, industrial, biomedical, cellular biophysics).

Slender Body Theory (SBT):

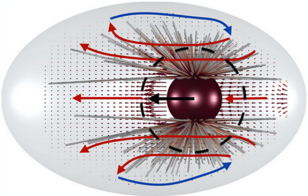
- Asymptotic expansion in radius (ε) as $\varepsilon \to 0$ (Keller-Rubinow '76).
- Doublet correction to make velocity theta-independent (Johnson '80).



Starfish larvae (Gilpin et al. 2016)



Drosophila oocyte (Stein et al. 2021)



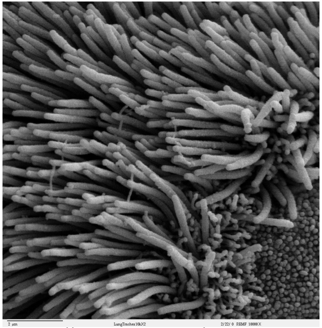
Mitotic spindle (Nazockdast et al. 2015)

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 infty-norm.



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

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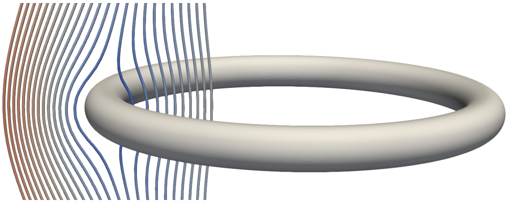
ε	$\boldsymbol{u}_{exact}$	Rel-Error
1e-1	6.14921383598 56e-2	0.5e-2
1e-2	9.09845223245 84e-2	0.1e-3
1e-3	1.20156558899 04e-1	0.2e-5
1e-4	1.49319329075 87e-1	0.2e-7
1e-5	1.78481913130 97e-1	0.3e-9



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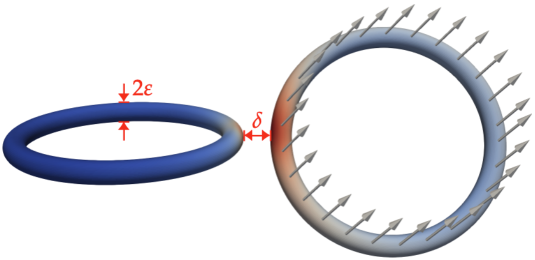

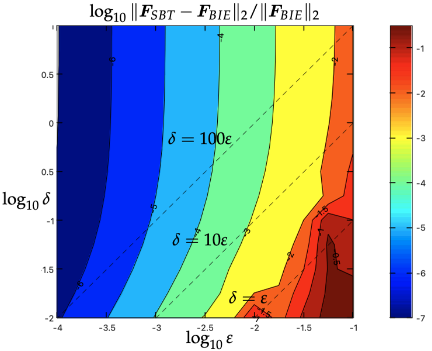

Convergent Slender Body Theory

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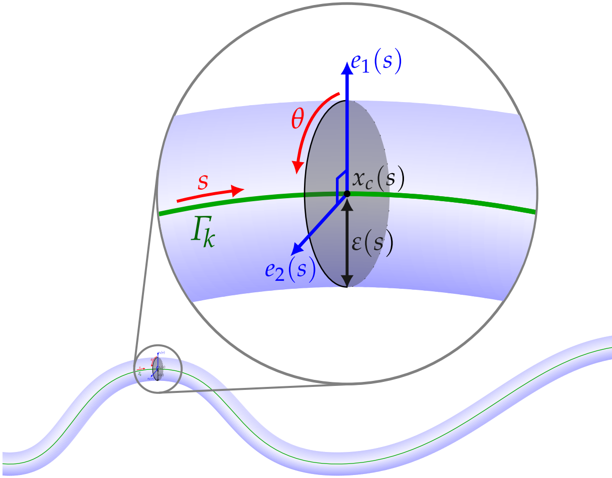
Focus on rigid fibers in this talk -- flexible fibers for future.

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 $e_1(s)$



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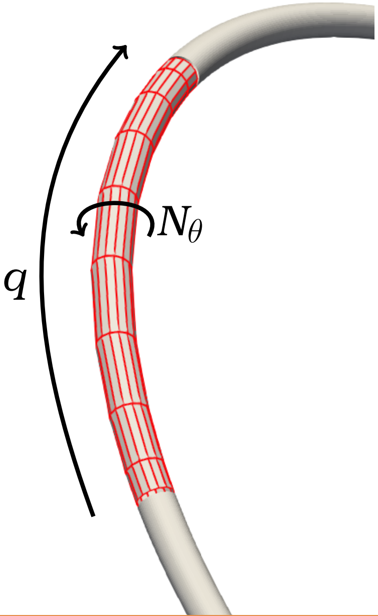
Discretization:

- 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

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

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

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$$= \underbrace{\sum_{x \notin \mathcal{N}(\Gamma_k)} \int_{\Gamma_k} \mathcal{K}(x-y)\,\sigma(y)\,da(y)}_{\text{far-field}} + \underbrace{\sum_{x \in \mathcal{N}(\Gamma_k)} \int_{\Gamma_k} \mathcal{K}(x-y)\,\sigma(y)\,da(y)}_{\text{near interactions}}$$

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Far-field

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

Near interactions

- Build special quadrature rules!

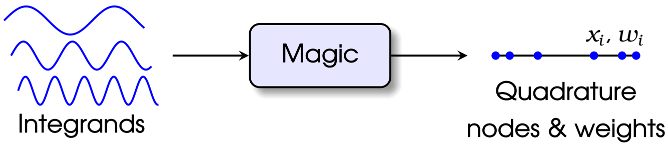
Generating Special Quadrature Rules

Integrands

Quadrature
nodes & weights

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

Generating Special Quadrature Rules



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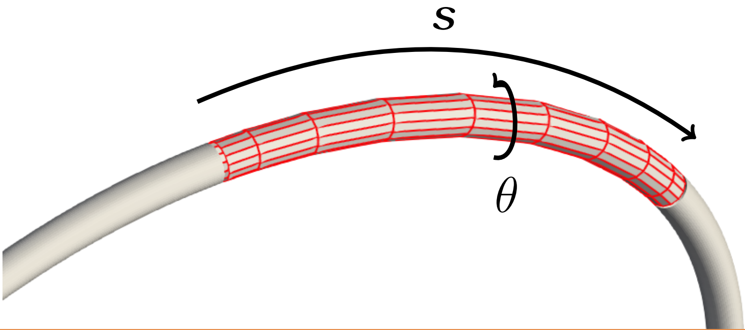
$$\int_{\Gamma_k} \mathcal{K}(x-y)\,\sigma(y)\,da(y) = \int_s \int_\theta \mathcal{K}(x-y(s,\theta))\,\sigma(s,\theta)\,J(s,\theta)\,d\theta\,ds$$



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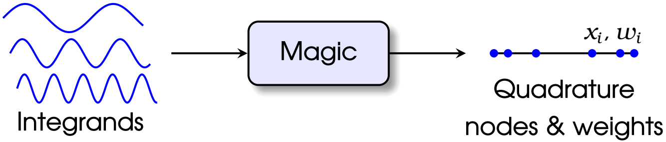

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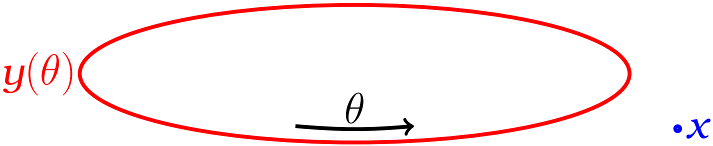

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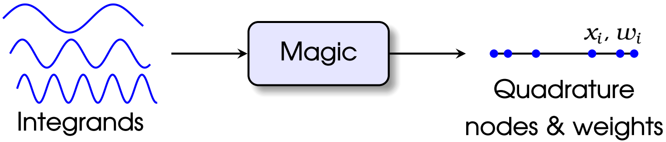

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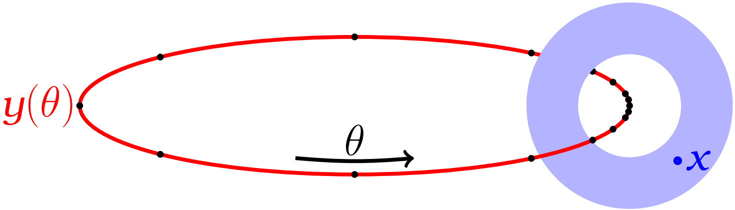
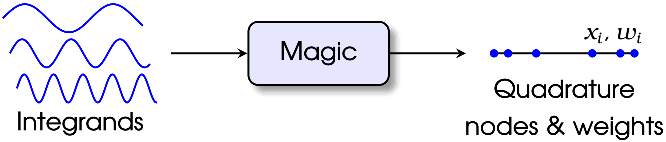


~ 48 quadrature nodes for $n_0 = 8$ and 10-digits accuracy.
$\sim 26M$ modal Green's function evaluations/sec/core (Skylake 2.4GHz)

Generating Special Quadrature Rules



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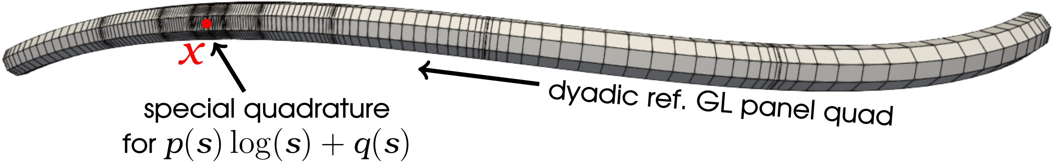

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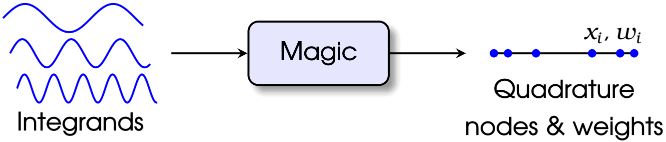

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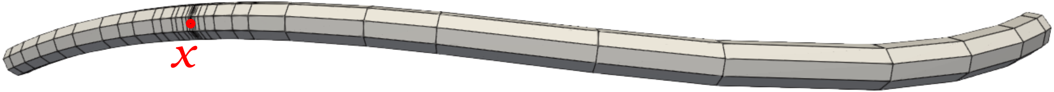
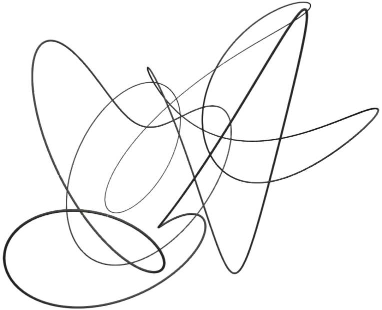
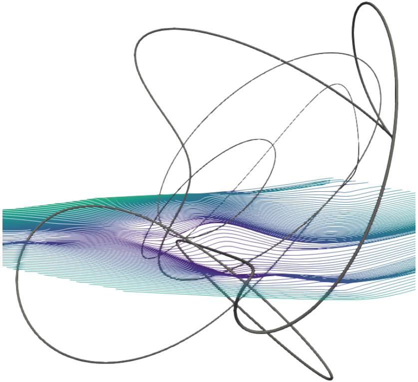


Instead build special quadrature rules!

- 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:

$$\Delta \boldsymbol{u} - \nabla p = 0, \qquad \boldsymbol{u}|_\Gamma = \boldsymbol{u}_0,$$
$$\nabla \cdot \boldsymbol{u} = 0, \qquad u(x) \to 0 \text{ as } |x| \to 0,$$

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

wire length = 16

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

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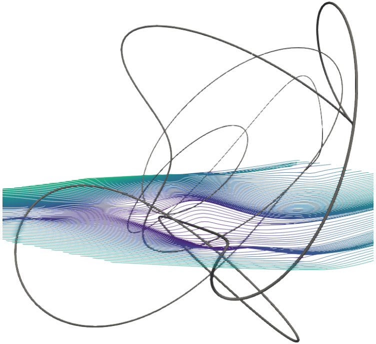
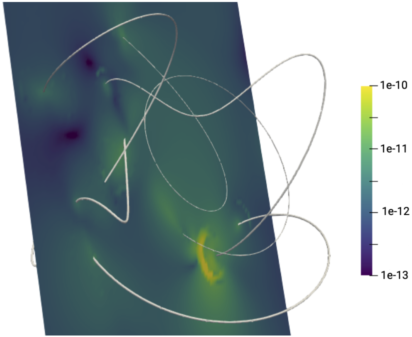
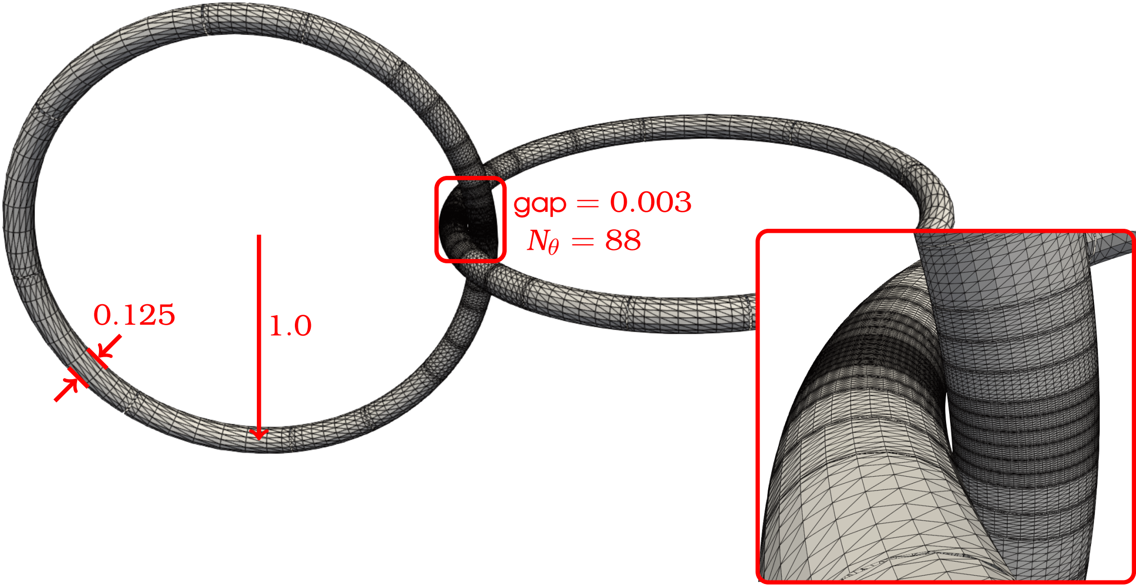




						1-core			40-cores	
N	N_{panel}	N_θ	ϵ_{GMRES}	N_{iter}	$\lVert e \rVert_\infty$	T_{setup}	(N/T_{setup})	T_{solve}	T_{setup}	T_{solve}
1.0e4	49	8	1e-02	5	3.5e-02	0.193	(5.4e4)	0.130	0.042	0.017
2.6e4	103	12	1e-05	22	5.5e-05	0.572	(4.5e4)	4.039	0.045	0.215
4.7e4	157	20	1e-07	33	6.6e-07	1.416	(3.3e4)	19.518	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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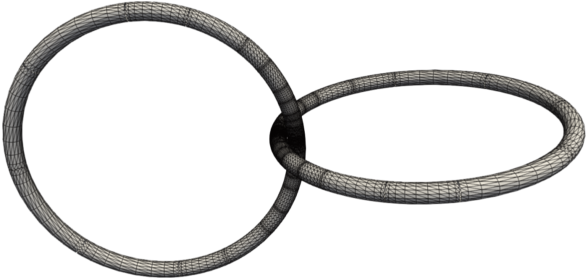

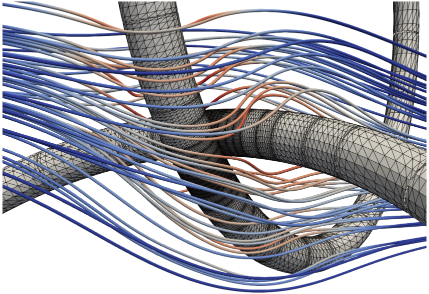

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N	ϵ_{GMRES}	N_{iter}	$\|e\|_\infty$	T_{setup}	(N/T_{setup})	T_{solve}	T_{setup}	T_{solve}
6.5e4	1e-02	4	2.1e-02	8.1	(8.0e+3)	6.5	1.28	1.4
6.5e4	1e-05	24	2.4e-03	16.8	(3.8e+3)	42.9	2.50	7.7
6.5e4	1e-07	43	2.8e-06	23.5	(2.7e+3)	81.6	3.31	12.8
6.5e4	1e-10	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 $\boldsymbol{x}_i^c$.

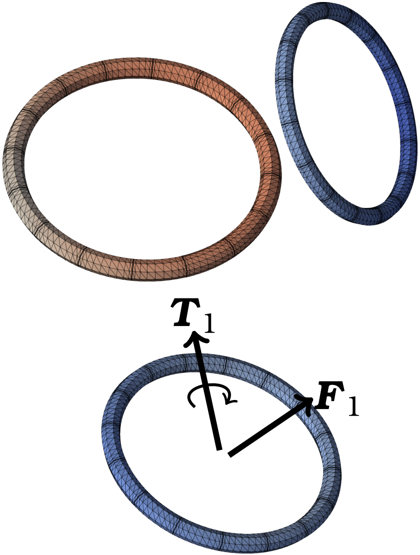
- Stokesian fluid in $\mathbb{R}^3 \setminus \Omega$

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

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

- Boundary conditions on $\partial\Omega$,

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



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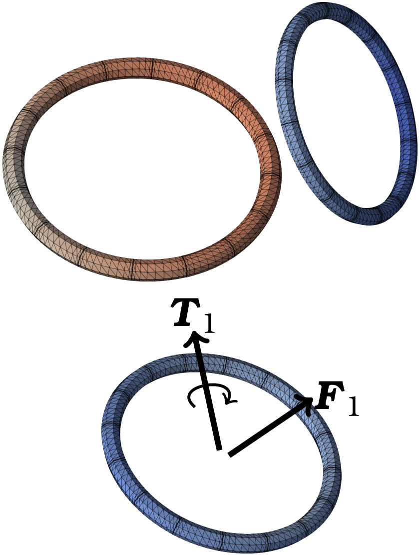
unknown: $\boldsymbol{V}(\boldsymbol{u}_i, \boldsymbol{\omega}_i)$



Mobility problem - double-layer formulation

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

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

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

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Second kind integral equation $\cdots$ but doesn't work for slender bodies!

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

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

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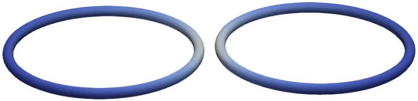
where, $\mathcal{K} = \mathcal{D} + \mathcal{S}/(2\varepsilon \log \varepsilon^{-1})$.

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



Time-stepping: 5-th order adaptive SDC

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

40 CPU cores

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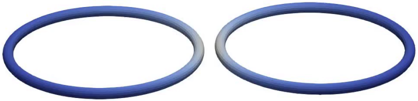

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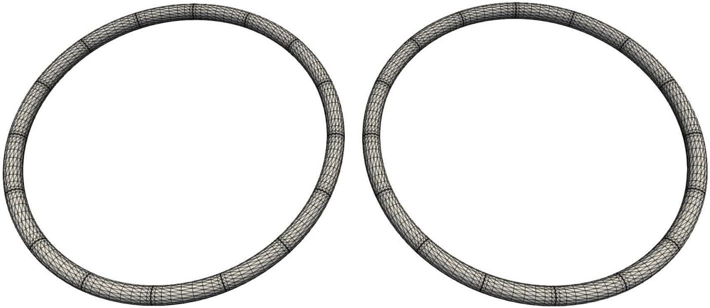
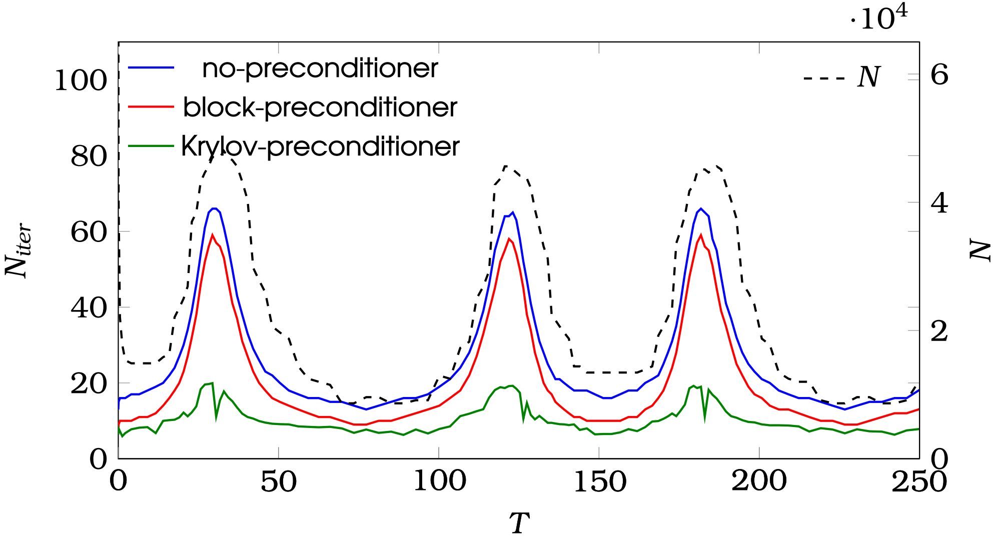


Numerical Results - Sedimentation Flow



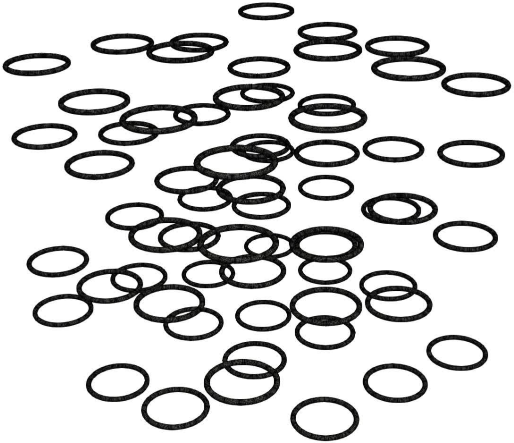
Numerical Results - Sedimentation Flow

5-th order adaptive SDC

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

0.5 million unknowns
64 rings.

160 CPU cores



CSBQ library

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>
```

CSBQ library

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Requirements: C++11 compiler with OpenMP

Build system: none (header only)

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

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

Library overview

SCTL: Scientific Computing Template Library

BoundaryIntegralOp **Kernel** **FMM** **Quadrature**

GMRES **SDC** **Profile** **Vec (SIMD)** **Comm**

Vector **Matrix** **VTUData** **Interpolation** **Tree**

Library overview

CSBQ: Convergent Slender Body Quadrature

- SlenderElemL
- RigidBodyL, Mobility
- CubeVolumeVis, Utils

SCTL: Scientific Computing Template Library

- BoundaryIntegralOp
- Kernel
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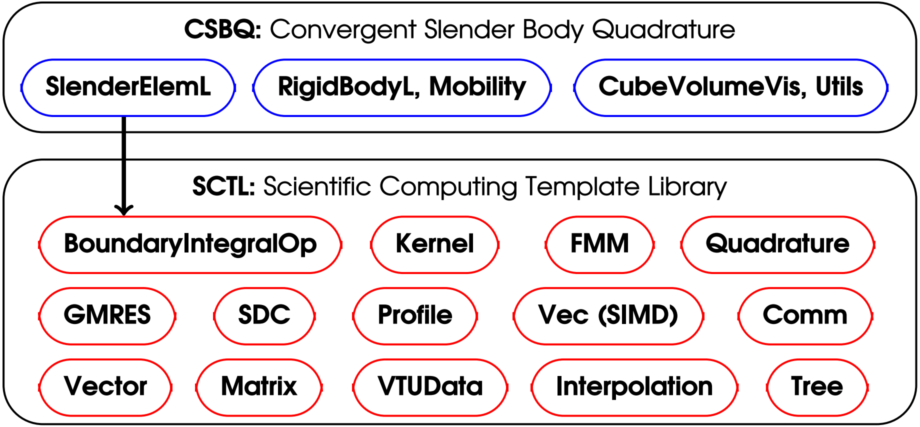
Library overview



Library overview

Applications

CSBQ: Convergent Slender Body Quadrature

- **SlenderElemL**
- **RigidBodyL, Mobility**
- **CubeVolumeVis, Utils**

SCTL: Scientific Computing Template Library

- **BoundaryIntegralOp**
- **Kernel**
- **FMM**
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- **Tree**

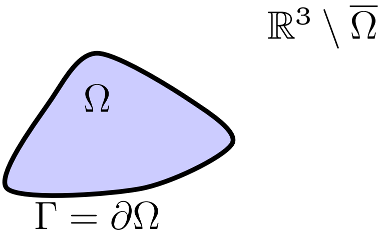
Step 1: Stokes Dirichlet boundary value problem (exterior)

- Stokes equations:

$$\begin{aligned} \Delta \mathbf{u} - \nabla p = 0 \qquad & \text{in } \mathbb{R}^3 \setminus \overline{\Omega}, \\ \nabla \cdot \mathbf{u} = 0 \qquad & \text{in } \mathbb{R}^3 \setminus \overline{\Omega}, \end{aligned}$$

- Boundary conditions:

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



Solving BIEs with CSBQ

Step 2: Integral Equation Formulation

- Boundary integral representation:

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

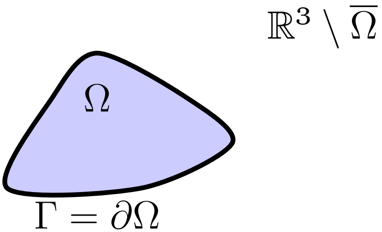
where

$$\mathcal{S}[\sigma](\mathbf{x}) := \int_\Gamma S(\mathbf{x}-\mathbf{y})\,\sigma(\mathbf{y})\,dS_{\mathbf{y}},$$
$$\mathcal{D}[\sigma](\mathbf{x}) := \int_\Gamma D(\mathbf{x}-\mathbf{y})\,\sigma(\mathbf{y})\,dS_{\mathbf{y}},$$
$$\eta = 1/(\epsilon \log \epsilon^{-1})$$

- Enforce boundary conditions:

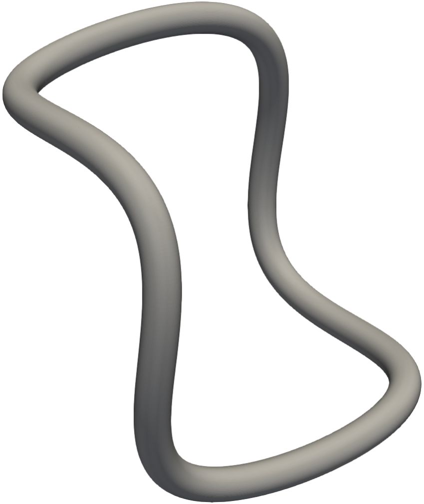
$$(I/2 + D + \eta\, S)\sigma = \mathbf{u}_0 \quad \text{on } \Gamma,$$

Solve for unknown σ



Solving BIEs with CSBQ

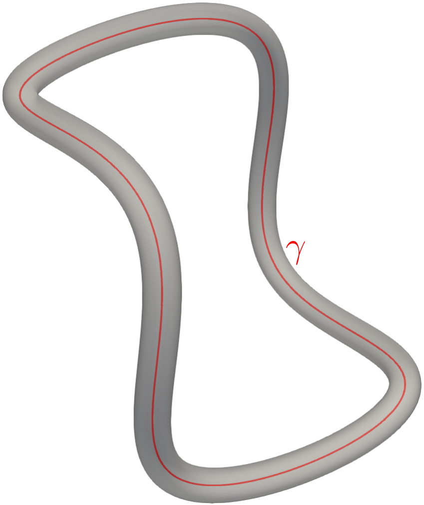
Step 3: Discretize the geometry



Solving BIEs with CSBQ

Step 3: Discretize the geometry

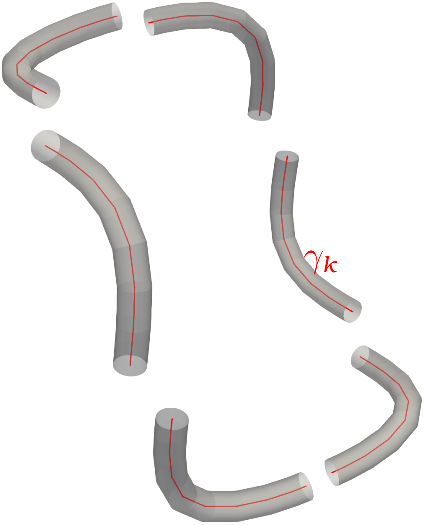
- Geometry described by centerline γ.



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

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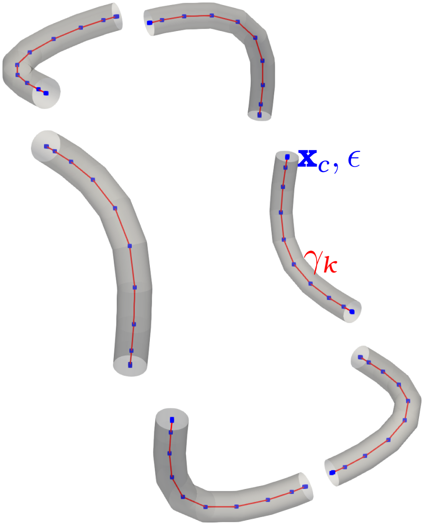


Solving BIEs with CSBQ

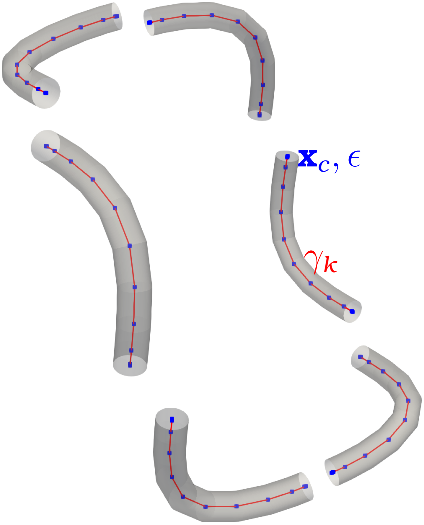
Step 3: Discretize the geometry

- 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_lst(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 ...
};
```

Solving BIEs with CSBQ

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    }
    // other member functions ...
};
```

- 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

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Step 5: Solve Integral Equation

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

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

Solving BIEs with CSBQ

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

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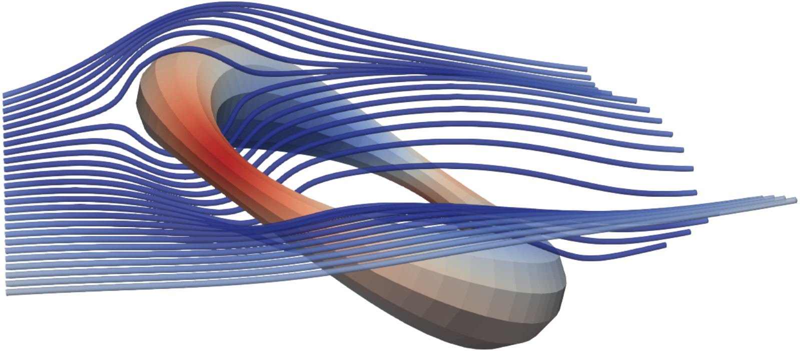

Conclusions

- 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.

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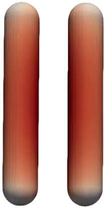
Limitations and ongoing work:

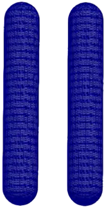
- Flexible fibers -- applications in biological fluids.

Extra

Extra

Numerical Results - Sedimentation Flow





Numerical Results - Sedimentation Flow