Fast and accurate evaluation of close-to-touching rigid body interactions

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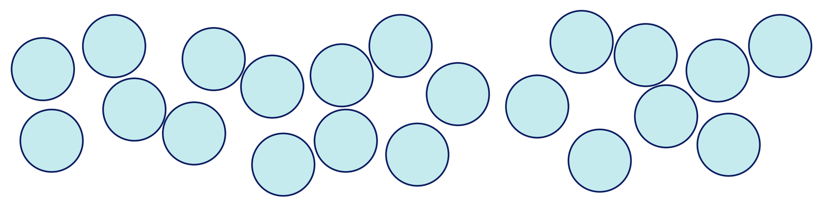
Motivation

Dense colloidal suspensions have numerous industrial and biomedical applications.

- Exhibit interesting **non-linear behaviors not fully understood.**
- Numerical simulations challenging due to **close-to-touching interactions / collision.**
- Require: **high-resolution, large iteration counts in linear solve,** and **small time-steps.**



Related work

- Collision handling: repulsion, LCP (linear complementarity problem). **Unclear** if the dynamics are physical.
- RCIP (recursively compresed inverse preconditioning), **expensive** for moving geometries.

Boundary integral equations

For N_Ω non-overlapping discs, $\Omega = \bigcup_{k=1}^{N_\Omega} \Omega_k$, the BIE formulation is:

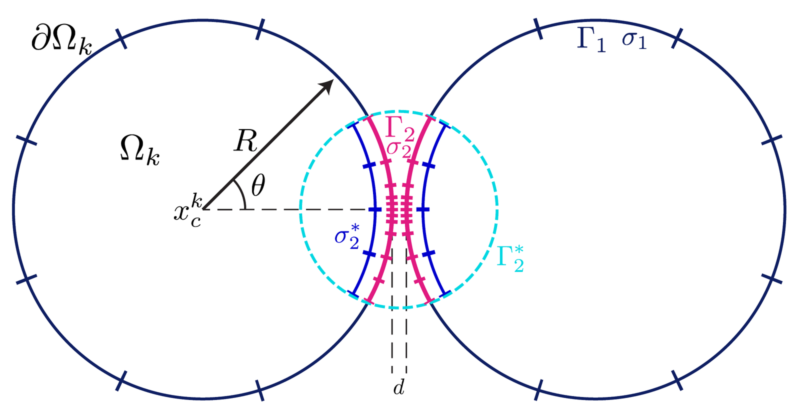
$$\mathcal{K}\sigma = g \qquad \text{on } \partial\Omega.$$

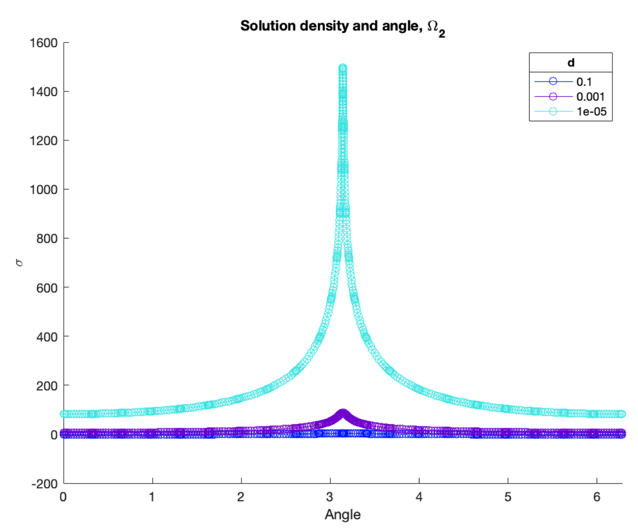
where:

- $\mathcal{K}$ is the boundary integral operator
- g are the boundary conditions

Close-to-touching interactions

When the distance d between two discs gets small, σ becomes **highly peaked**. This requires a fine discretization of the boundary in the close-to-touching region.

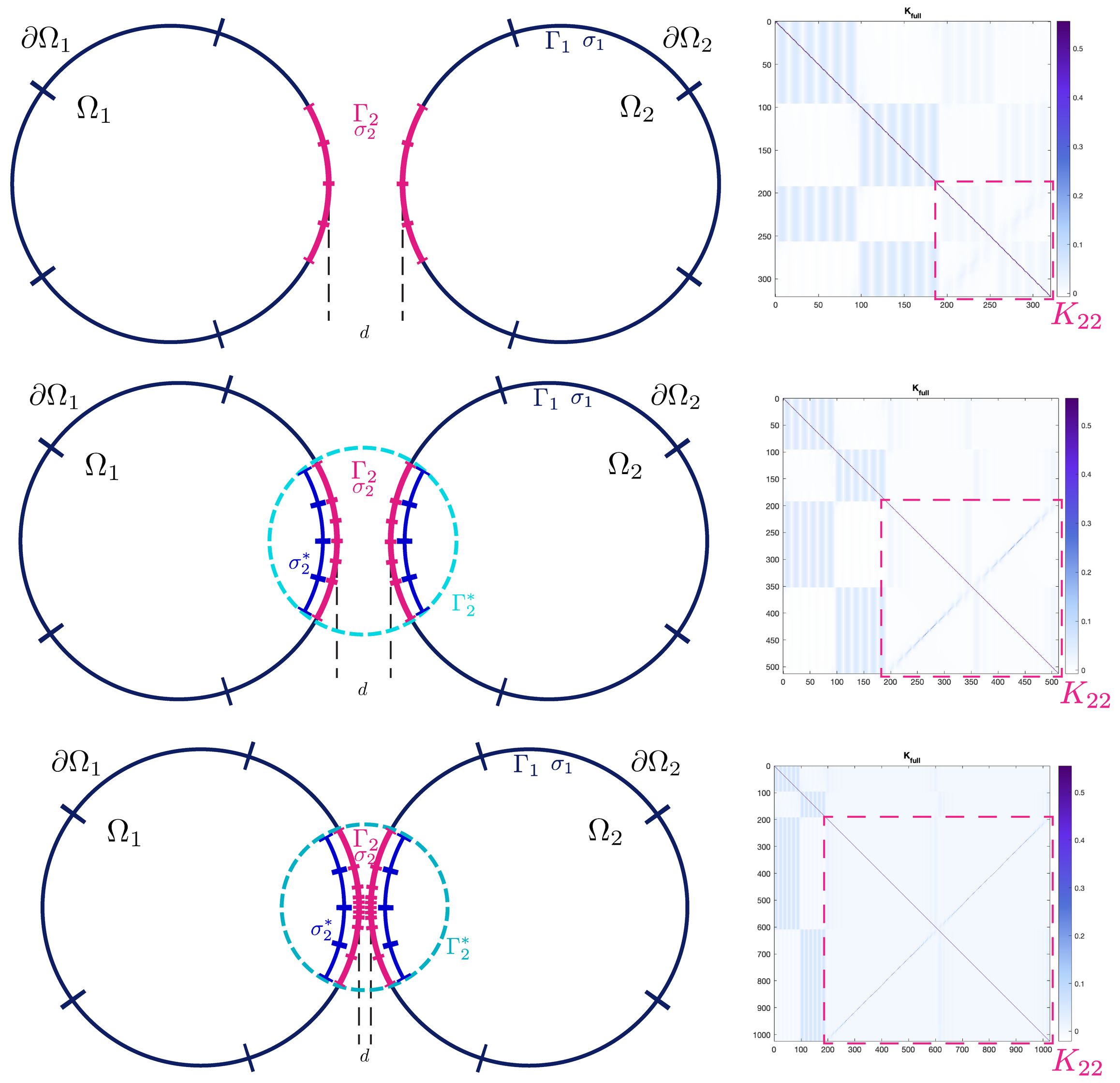




Compressing close-to-touching interactions

Let Γ_2 be the close-to-touching region and $\Gamma_1 = \partial\Omega \setminus \Gamma_2$. The BIE can be written as a block linear system,

$$\begin{pmatrix} \mathcal{K}_{11} & \mathcal{K}_{12} \\ \mathcal{K}_{21} & \mathcal{K}_{22} \end{pmatrix} \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}.$$



First we use the following **right preconditioner**:

$$\begin{pmatrix} \mathcal{I} & 0 \\ 0 & \mathcal{K}_{22}^{-1} \end{pmatrix}.$$

Then we compute an L^2 **projection** from the fine discretization to the coarse discretization with $W_c^{-1}P^TW_f$, where:

- W_c and W_f are diagonal matrices with weights for smooth integration on the coarse and fine discretizations
- P is the prolongation matrix

The discretized BIE can be written as:

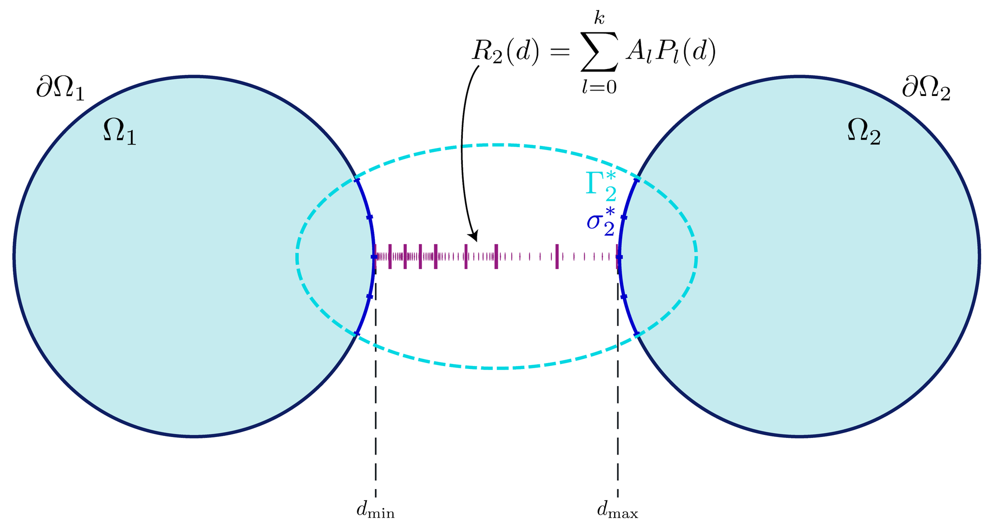
$$\left[I + \begin{pmatrix} K_{11} - I & K_{12}^c \\ K_{21}^c & 0 \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & R_2 \end{pmatrix} \right] \begin{pmatrix} \sigma_1 \\ \sigma_2^* \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2^* \end{pmatrix},$$

where $R_2 = W_c^{-1}P^TW_fK_{22}^{-1}P$. After solving this BIE formulation, we construct an **approximate solution density**:

$$\sigma = \begin{pmatrix} I & 0 \\ 0 & R_2 \end{pmatrix} \begin{pmatrix} \sigma_1 \\ \sigma_2^* \end{pmatrix}.$$

Interpolation for different distances

We **precompute** $R_2(d)$ for $d \in [d_{\min}, d_{\max}]$. Then we construct a **piecewise polynomial interpolant** for $R_2(d)$ and then interpolate to any value of d in the interval.



Capacitance and elastance problems

We test our approach with the capacitance and elastance problems, where each disc is a "perfect electrical conductor". The BIE formulation for the capacitance problem is:

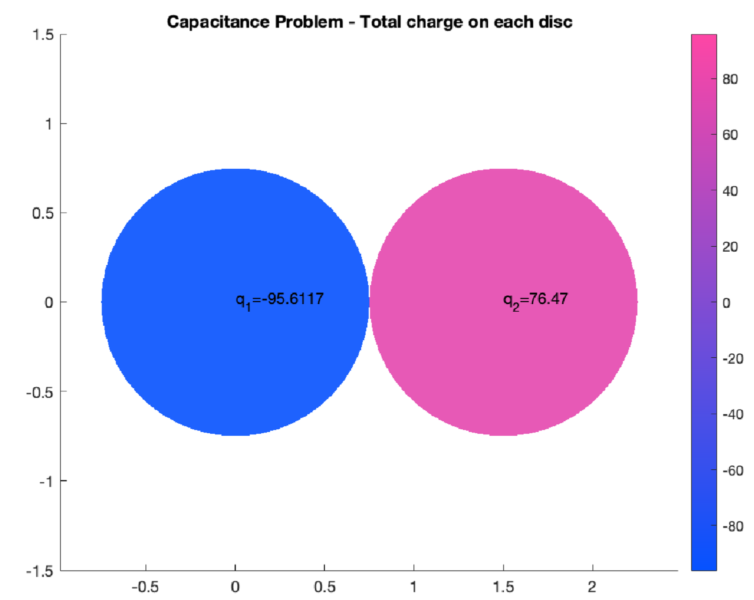
$$(\mathcal{I}/2 + \mathcal{D} + \mathcal{S})\,[\sigma] = \sum_{k=1}^{N_\Omega} u_k 1_{\partial\Omega_k} \qquad \text{on } \partial\Omega.$$

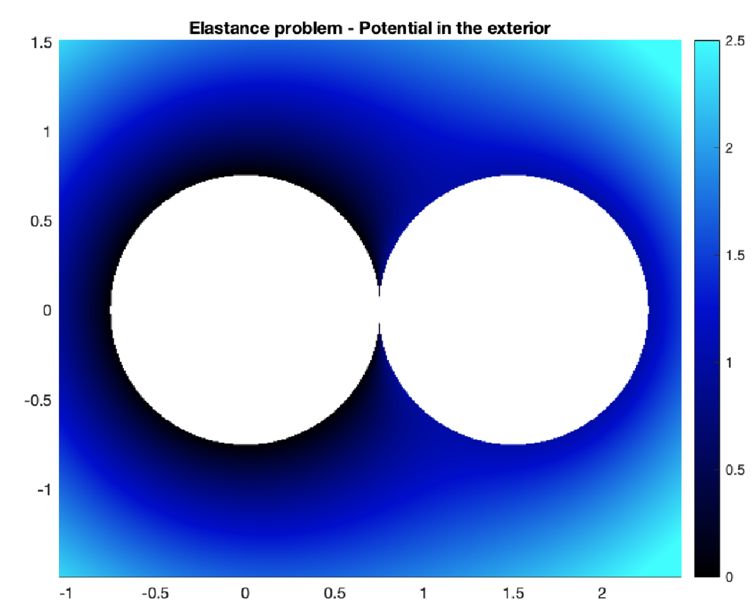
While the BIE formulation for the elastance problem is:

$$(\mathcal{I}/2 + \mathcal{D})\,[\sigma] + \sum_{k=1}^{N_\Omega} 1_{\partial\Omega_k} \int_{\partial\Omega} 1_{\partial\Omega_k}\sigma = -\mathcal{S}[\nu] \qquad \text{on } \partial\Omega,$$

where

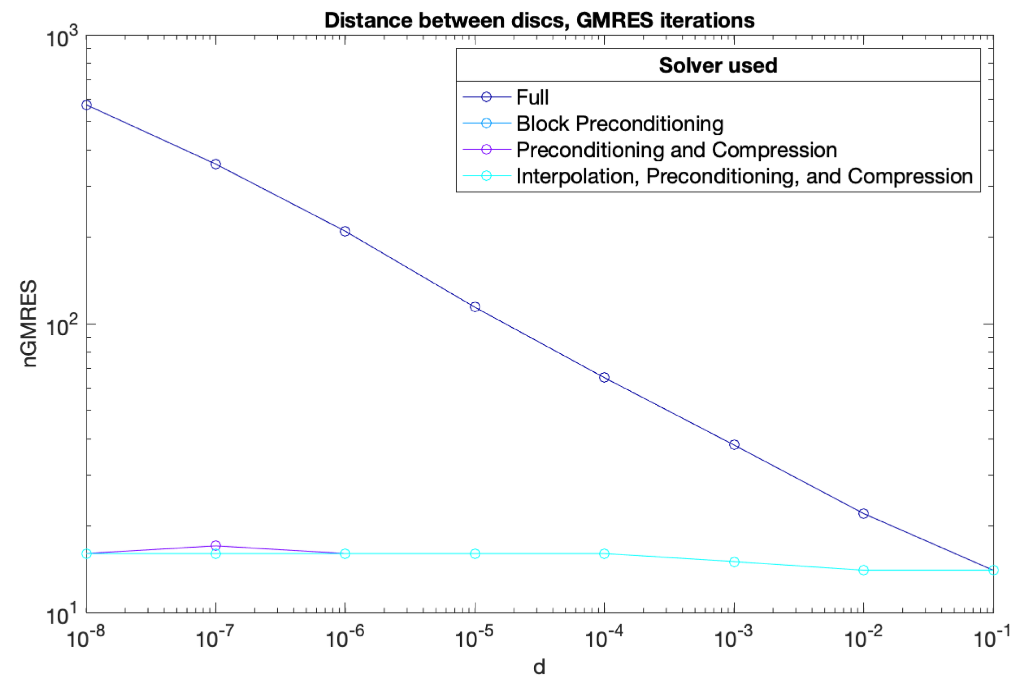
$$\nu = \sum_{k=1}^{N_\Omega} 1_{\partial\Omega_k} \frac{q_k}{|\partial\Omega_k|}.$$

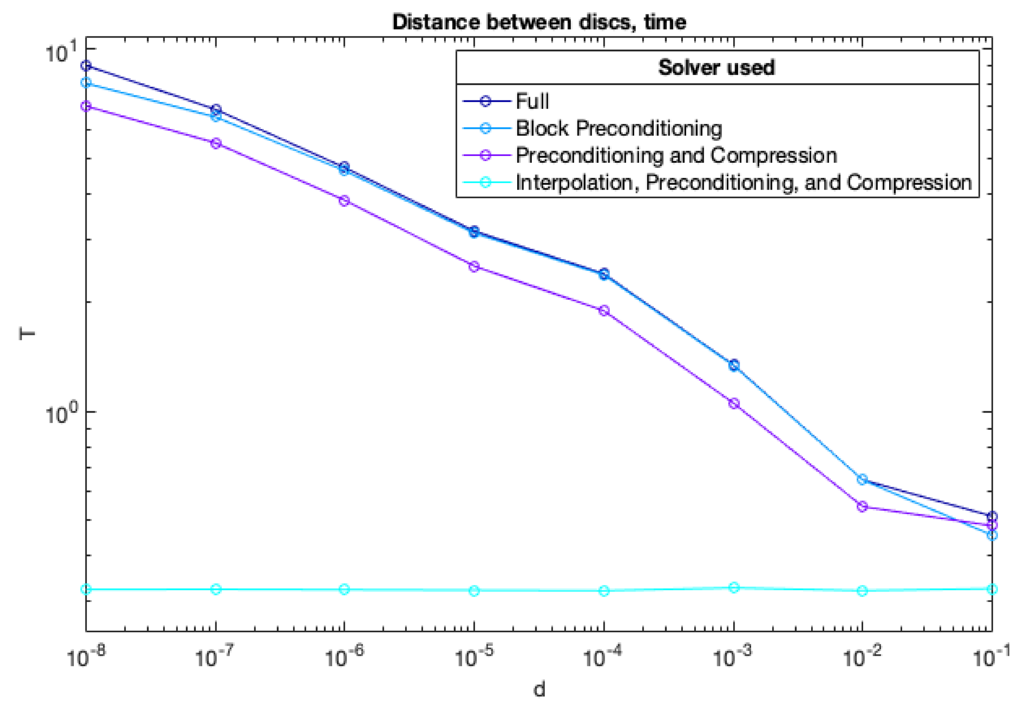




Numerical Results

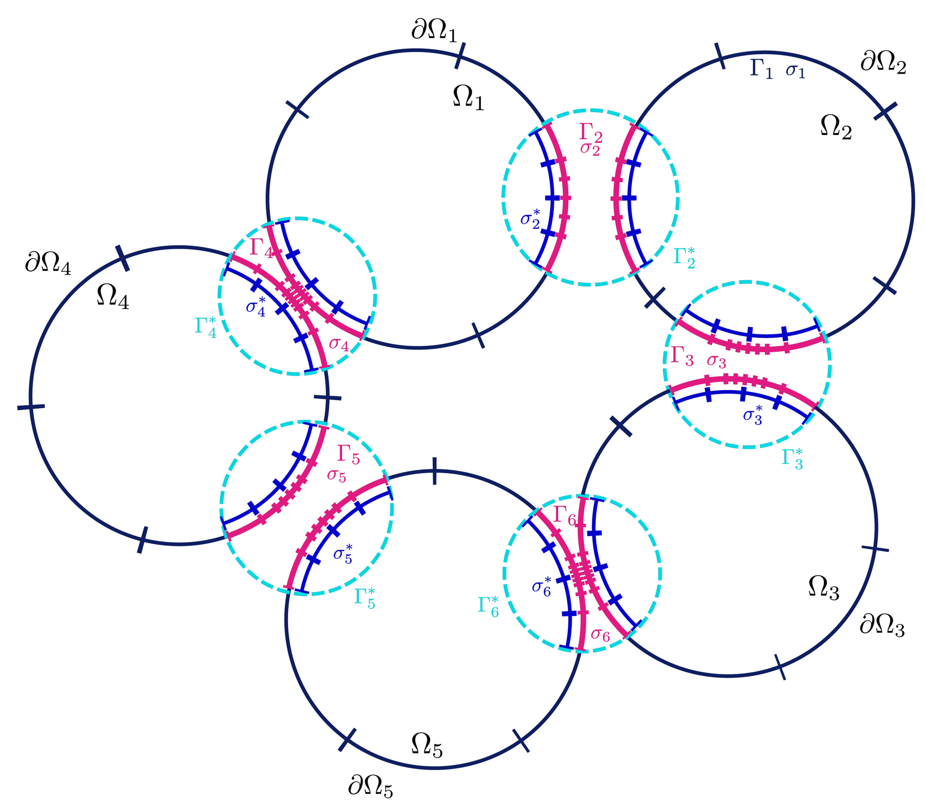
For $d = 10^{-8}$ we were able to get 6 digits of accuracy.





Future work

Consider more discs, use different interpolation nodes for distances, solve the Stokes mobility problem.



References

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[3] M. Rachh and L. Greengard, *Integral equation methods for elastance and mobility problems in two dimensions*, SIAM Journal on Numerical Analysis, 54 (2016), pp. 2889–2909.