The University of Texas at Austin
Oden Institute for Computational Engineering and Sciences

Integration of singular functions over deformable surfaces

Corrected quadratures, regularized quadratures, and rational approximation quadratures

Joar Bagge*[1], Bowei Wu[2], George Biros[1], Per-Gunnar Martinsson[1], Anna-Karin Tornberg[3], Pritpal Matharu[3]

[1]The University of Texas at Austin, Oden Institute; [2]University of Massachusetts, Lowell; [3]KTH Royal Institute of Technology, Stockholm, Sweden

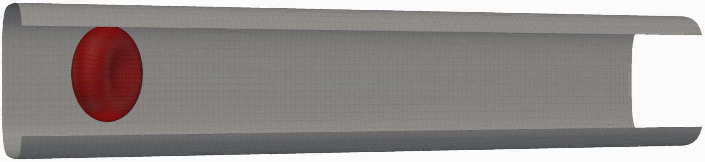
SIAM CSE25, March 3–7, 2025

* Email: joar.bagge@austin.utexas.edu

Outline

Outline

Deformable capsules in Stokes flow – Introduction



- Simulation of a **capsule** flowing through a **fluid-filled** **pipe** (diameter 11.3 µm) at around 1.93 mm/s.
  - A **capsule** is an elastic membrane filled with fluid, and can be used to model e.g. **red blood cells**. [Agarwal & Biros, Phys Rev Fluids, 2022]
  - The flow can be modeled as **Stokes flow** (due to low Reynolds number).
  - Question: How does membrane stiffness influence the capsule dynamics (e.g. shape stability, lateral drift, ...)?

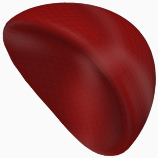
Deformable capsules in Stokes flow – Formulation

- The capsule membrane follows the local **flow field**

$$\boldsymbol{u}(\boldsymbol{x}) = \underbrace{\boldsymbol{u}_\infty(\boldsymbol{x})}_{\text{Background flow}} + \underbrace{\boldsymbol{u}_{\text{wall}}(\boldsymbol{x})}_{\text{Wall contribution}} + \underbrace{\mathcal{S}[\boldsymbol{f}](\boldsymbol{x})}_{\text{Capsule contribution}}$$

where the Stokes single layer potential is given by

$$\mathcal{S}[\boldsymbol{f}](\boldsymbol{x}) = \int_\gamma \boldsymbol{G}(\boldsymbol{x}-\boldsymbol{y})\,\boldsymbol{f}(\boldsymbol{y})\,\mathrm{d}S(\boldsymbol{y})$$



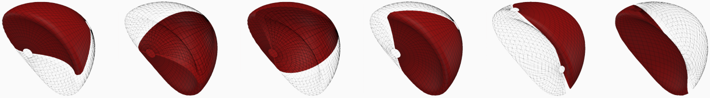
γ

and the **stokeslet** by

$$\boldsymbol{G}(\boldsymbol{r}) = \frac{1}{8\pi}\left(\frac{\boldsymbol{I}}{\|\boldsymbol{r}\|} + \frac{\boldsymbol{r}\otimes\boldsymbol{r}}{\|\boldsymbol{r}\|^3}\right)$$

- The **interfacial force *f*** is computed from the local surface deformation gradient [Skalak et al., Biophys J, 1973]

- The **capsule** is represented using a partition of unity with 6 overlapping patches



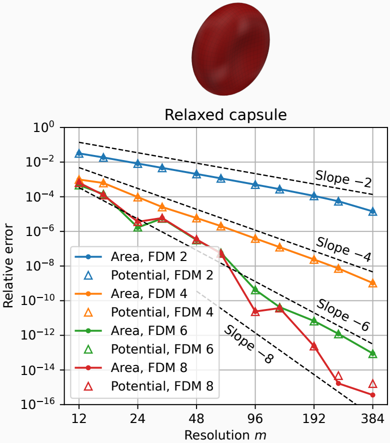
- Each patch P_i is associated with a partition of unity function $\psi_i(\boldsymbol{x})$
- A smooth integral on γ is computed as follows:

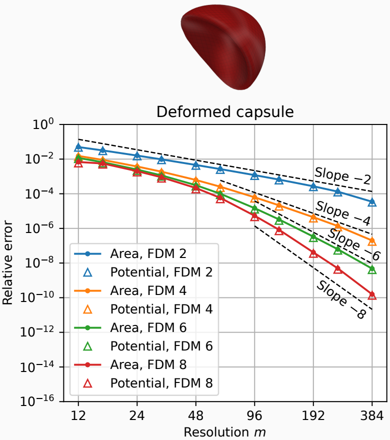
$$\int_{\gamma} g(\boldsymbol{x})\,\mathrm{d}S = \sum_{i=1}^{6} \int_{P_i} \psi_i(\boldsymbol{x}) g(\boldsymbol{x})\,\mathrm{d}S \approx \sum_{i=1}^{6} \sum_{j} \psi_i(\boldsymbol{x}_{ij}) g(\boldsymbol{x}_{ij}) W_{ij},$$

  where $W_{ij} = J_\gamma(\boldsymbol{x}_{ij}) w_{ij}$, J_γ is a Jacobian determinant and w_{ij} quadrature weights.
- We use the **trapezoidal rule** on each patch P_i and compute J_γ using standard finite differences (FD). Use $m \times m$ subintervals per patch.

Deformable capsules in Stokes flow – Smooth integration

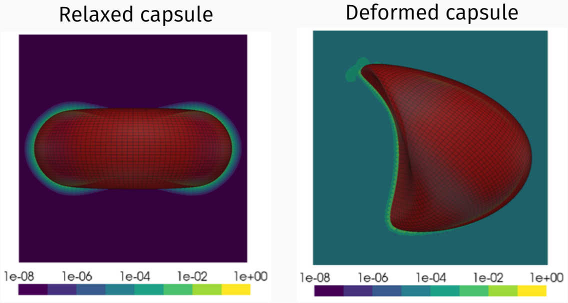
- Computing **surface area** and **faraway offsurface Stokes potential** follows the selected FDM order.





($m \times m$ subintervals per patch)

- The stokeslet is **nearly singular** close to the surface, and **singular** on the surface. **Quadrature error:**



$$\mathcal{S}[\boldsymbol{f}](\boldsymbol{x}) = \int_{\gamma} \boldsymbol{G}(\boldsymbol{x}-\boldsymbol{y})\,\boldsymbol{f}(\boldsymbol{y})\,\mathrm{d}S(\boldsymbol{y}), \qquad \boldsymbol{G}(\boldsymbol{r}) = \frac{1}{8\pi}\left(\frac{\boldsymbol{I}}{\|\boldsymbol{r}\|} + \frac{\boldsymbol{r}\otimes\boldsymbol{r}}{\|\boldsymbol{r}\|^3}\right)$$

- Mathematically, the integral is well-defined even for $\boldsymbol{x} \in \gamma$.
- We will focus on the on-surface (singular) case.

joar.bagge@austin.utexas.edu

Outline

Regularized quadrature

- Replace the stokeslet $\boldsymbol{G}(\boldsymbol{r})$ by the **regularized stokeslet**

$$\boldsymbol{G}_\delta(\boldsymbol{r}) = \frac{1}{8\pi}\left(\frac{\boldsymbol{I}}{\|\boldsymbol{r}\|}s_1^{\#}\left(\frac{\|\boldsymbol{r}\|}{\delta}\right) + \frac{\boldsymbol{r}\otimes\boldsymbol{r}}{\|\boldsymbol{r}\|^3}s_2^{\#}\left(\frac{\|\boldsymbol{r}\|}{\delta}\right)\right), \qquad \delta > 0,$$

where

$$s_1^{\#}(t) = \mathrm{erf}(t) - \frac{2}{3}t(2t^2-5)\frac{e^{-t^2}}{\sqrt{\pi}}, \qquad s_2^{\#}(t) = \mathrm{erf}(t) - \frac{2}{3}t(4t^4-14t^2+3)\frac{e^{-t^2}}{\sqrt{\pi}},$$

[Tlupova & Beale, J Comput Phys, 2019]

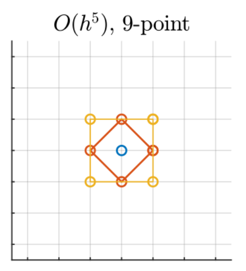
- $\boldsymbol{G}_\delta$ is smooth; integrate using regular quadrature (trapezoidal)
- The parameter δ is selected to balance the **regularization error** ($\sim \delta^5$) and **quadrature error** ($\sim h e^{-c_0(\delta/h)^2}$).
    - We let δ depend on the source ($\boldsymbol{y}$) and set $\delta \sim h$, where h is a measure of the local mesh spacing.
- Note: this scheme is a **local modification** since $s_k^{\#}(t) \to 1$ quickly as $t \to \infty$. For instance, for $t \geq 5$, both $s_k^{\#}(t) < 10^{-7}$.

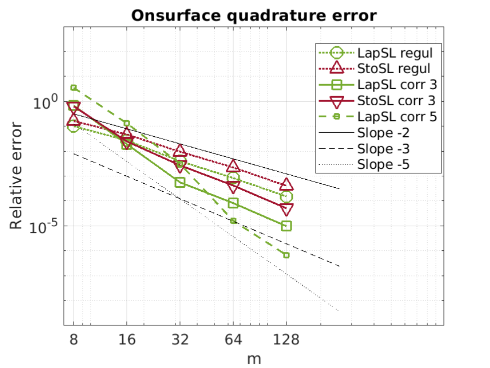
- **Locally correct** the weights of the (punctured) trapezoidal rule:

$$\sum_{j \neq i} \boldsymbol{G}(\boldsymbol{x}_i - \boldsymbol{y}_j)\boldsymbol{f}(\boldsymbol{y}_j)W_j + \sum_{j \in Z_i} \boldsymbol{C}(\boldsymbol{f}(\boldsymbol{y}_j))$$

[Wu & Martinsson, Numer Math, 2021] [Wu & Martinsson, SIAM J Numer Anal, 2023]

Stencil Z_i





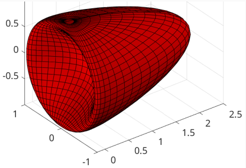
- The corrected quadrature seems better when m is large enough.

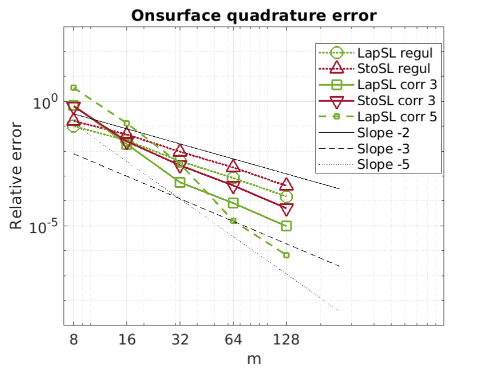
Corrected trapezoidal quadrature

- **Locally correct** the weights of the (punctured) trapezoidal rule:

$$\sum_{j \neq i} \boldsymbol{G}(\boldsymbol{x}_i - \boldsymbol{y}_j)\boldsymbol{f}(\boldsymbol{y}_j)W_j + \sum_{j \in Z_i} \boldsymbol{C}(\boldsymbol{f}(\boldsymbol{y}_j))$$

[Wu & Martinsson, Numer Math, 2021] [Wu & Martinsson, SIAM J Numer Anal, 2023]

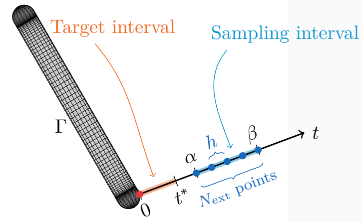




- The corrected quadrature seems better when m is large enough.

Interpolatory (approximation-based) quadrature

- Sample the field, $\mathcal{S}[\boldsymbol{f}](\boldsymbol{x})$ in N points along a line: $\mathcal{S}[\boldsymbol{f}](\boldsymbol{x}_n) = \boldsymbol{g}(t_n)$



- Construct an approximant $\widehat{\boldsymbol{g}}(t) \approx \boldsymbol{g}(t)$, and evaluate $\widehat{\boldsymbol{g}}(t)$ in the region of interest.
- Note: $\widehat{\boldsymbol{g}}(t)$ could be any kind of approximant, as long as it is fast to construct and evaluate, since the above needs to be done **many times**.
  - Polynomial approximation – tried and tested [Ying et al., J Comput Phys, 2006]
  - Rational approximation could be an alternative?

Outline

Why rational approximation?

A rational function is a ratio of two polynomials, $r(t) = \frac{p(t)}{q(t)}$

- **Rational approximation** on barycentric form (similar to AAA):

$$r(t) = \sum_{m=1}^{M} \frac{w_m f(\tau_m)}{t - \tau_m} \Big/ \sum_{m=1}^{M} \frac{w_m}{t - \tau_m}$$

  [Nakatsukasa et al., SIAM J Sci Comput, 2018]

- Half of the sample points are used as support points $\{\tau_m\}$, the other half is used to determine the weights $\{w_m\}$

Advantages over polynomials:

- **Wider class** of functions (polynomials $\subset$ rationals)
- Some functions may be **better approximated** by rationals (is the layer potential such a function?)
- Rational interpolation seems **more stable** than polynomial interpolation as $N \to \infty$ (even for equidistant sample points)

Two main error contributions:

- Quadrature error when sampling $\boldsymbol{g}(t)$: $\tilde{\boldsymbol{g}}(t) = \boldsymbol{g}(t) + \boldsymbol{\varepsilon}(t)$
- Approximation error: $\boldsymbol{g}(t) - \mathcal{R}\boldsymbol{g}(t)$,
  where $\mathcal{R}$ is the rational approximation operator.

Thus, if $\mathcal{R}$ is linear

$$\boldsymbol{g} - \mathcal{R}\tilde{\boldsymbol{g}} = \boldsymbol{g} - \mathcal{R}\boldsymbol{g} + \mathcal{R}(\boldsymbol{g} - \tilde{\boldsymbol{g}}) = (\boldsymbol{g} - \mathcal{R}\boldsymbol{g}) - \mathcal{R}\boldsymbol{\varepsilon}$$

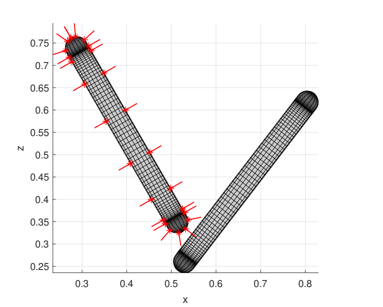
(However, $\mathcal{R}$ is not always linear!)

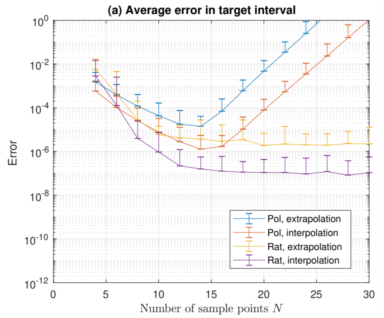
Note:

- The $(\boldsymbol{g} - \mathcal{R}\boldsymbol{g})$ term could potentially be estimated using the Hermite integral formula.
- The $\mathcal{R}\boldsymbol{\varepsilon}$ term is a bit unfortunate – what if rationals are better than polynomials at approximating $\boldsymbol{\varepsilon}$?

Rational approximation – Observed accuracy

- Computing the average error along 26 lines as the number of sample points N is varied:





- Rational approximation is stable as $N \to \infty$, unlike polynomials.
- (This is a test where ε is very small due to upsampling the grid.)

Outline

Closing remarks and conclusions

- The partition of unity representation should be able to handle **local refinement** well (not part of this talk).
- **Regularized vs corrected** quadrature
  - At low resolutions, regularized was better.
  - As the resolution increases, the corrected quadrature can have a higher order of accuracy.
- **Polynomial vs rational approximation** in interpolatory quadrature
  - Rational approximation seems better when the sampling error ε is small.
  - They tend to have more similar errors when ε is larger (not shown here).

joar.bagge@austin.utexas.edu

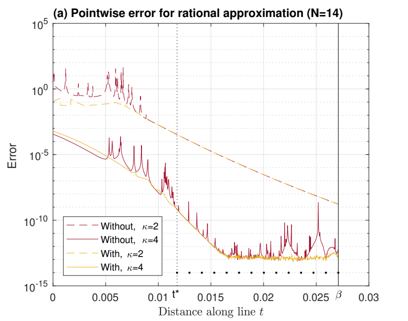
Thank you for your attention!

References

- D. Agarwal & G. Biros, Shape dynamics of a red blood cell in Poiseuille flow, *Phys Rev Fluids* **7**:093602, 2022. [link]
- D. Agarwal & G. Biros, Numerical simulation of an extensible capsule using regularized Stokes kernels and overset finite differences, *J Comput Phys* **509**:113042, 2024. [link]
- R. Skalak, A. Tozeren, R. P. Zarda & S. Chien, Strain energy function of red blood cell membranes, *Biophys J* **13**(3):245–264, 1973. [link]
- S. Tlupova & J. T. Beale, Regularized single and double layer integrals in 3D Stokes flow, *J Comput Phys* **386**:568–584, 2019. [link]
- L. Ying, G. Biros & D. Zorin, A high-order 3D boundary integral equation solver for elliptic PDEs in smooth domains, *J Comput Phys* **219**:247–275, 2006. [link]
- B. Wu & P.-G. Martinsson, Corrected trapezoidal rules for boundary integral equations in three dimensions, *Numer Math* **149**:1025–1071, 2021. [link]
- B. Wu & P.-G. Martinsson, A unified trapezoidal quadrature method for singular and hypersingular boundary integral operators on curved surfaces, *SIAM J Numer Anal* **61**:2182–2208, 2023. [link]

Handling of spurious poles

- As mentioned, spurious poles can end up in the target interval. They are avoided/handled in two ways:
  1. A small imaginary perturbation is added to $f(t)$, to make poles on the real axis less likely.
  2. A contour integration is used to cancel any poles that still end up in the target interval.



- Fixed parameters: $N = 14$, $\alpha = t^* = 0.0118$, $h = \alpha/10$, $\kappa = 2, 4$.