SMAI 2021 – Juin 2021, La Grande-Motte

Fast & accurate computation of singular/nearly-singular integrals in high-order boundary elements

H. Montanelli, M. Aussal, H. Haddar

DEFI Research Team, CMAP
Inria Saclay & École Polytechnique

Sessions Parallèles – Méthodes Numériques 2

Helmholtz & integral eqns.

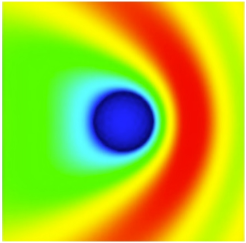
Background

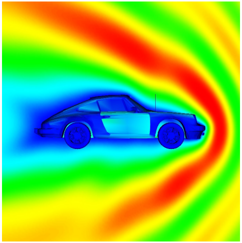
- $v = u(\boldsymbol{x})e^{-i\omega t}$ soln. to $v_{tt} = c^2 \Delta v \Rightarrow u$ soln. to $\Delta u + k^2 u = 0$ (Helmholtz)
- 3D Helmholtz may be replaced by 2D integral eqns., *e.g.*,

$$\int_\Gamma G(\boldsymbol{x}, \boldsymbol{y}) \left[\frac{\partial u}{\partial n}\right](\boldsymbol{y}) d\Gamma(\boldsymbol{y}) = f(\boldsymbol{x}), \quad G(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{4\pi} \frac{e^{ik|\boldsymbol{x}-\boldsymbol{y}|}}{|\boldsymbol{x}-\boldsymbol{y}|}$$

Challenges

- When $\boldsymbol{x}$ approaches $\boldsymbol{y}$, the integral is near-singular, and singular when $\boldsymbol{x} = \boldsymbol{y}$
- Solutions at large wavenumbers k are highly oscillatory ($N \propto k^2$)





Nyström vs. boundary elements

Integral equation

$$\int_\Gamma G(\boldsymbol{x},\boldsymbol{y})v(\boldsymbol{y})d\Gamma(\boldsymbol{y}) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma$$

Nyström methods (Alpert, Barnett, Bruno, Greengard, Rokhlin, etc.)

- Seek the numerical solution by replacing the $\int$ with a weighted sum

$$\sum_{i=1}^{n} w_i G(\boldsymbol{x}_j,\boldsymbol{y}_i)v(\boldsymbol{y}_i) = f(\boldsymbol{x}_j), \quad 1 \leq j \leq n$$

- High-order but restricted in terms of geometry

Boundary element methods (Betcke, Hackbusch, Sauter, Schwab, etc.)

- Based on a finite-element formulation of the integral equation

$$\int_\Gamma\int_\Gamma G(\boldsymbol{x},\boldsymbol{y})v(\boldsymbol{y})d\Gamma(\boldsymbol{y})u(\boldsymbol{x})d\Gamma(\boldsymbol{x}) = \int_\Gamma f(\boldsymbol{x})u(\boldsymbol{x})d\Gamma(\boldsymbol{x}), \quad \forall u \in H^s(\Gamma)$$

- Flexible with respect to geometry but often low-order

Singular/near-singular $\int$'s in BEMs (1/3)

Boundary element methods

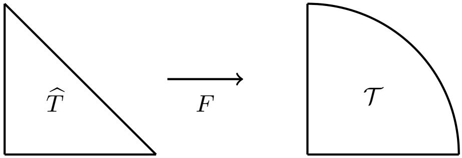
$$\int_\Gamma \int_\Gamma G(\boldsymbol{x},\boldsymbol{y}) u(\boldsymbol{x}) d\Gamma(\boldsymbol{x}) v(\boldsymbol{y}) d\Gamma(\boldsymbol{y}) = \int_\Gamma f(\boldsymbol{x}) u(\boldsymbol{x}) d\Gamma(\boldsymbol{x}), \quad \forall u \in H^s(\Gamma)$$

Setup

- Compute weakly singular/near-singular integrals of the form

$$I(\boldsymbol{x}_0) = \int_{\mathcal{T}} \frac{\hat{u}(F^{-1}(\boldsymbol{x}))}{|\boldsymbol{x} - \boldsymbol{x}_0|} dS(\boldsymbol{x})$$

- $\mathcal{T}$ is a curved triangular element defined by degree $F : \widehat{T} \mapsto \mathcal{T}$ of degree p
- $\boldsymbol{x}_0 \in \mathbb{R}^3$ is a point on/close to $\mathcal{T}$, $\hat{u}$ is a basis function of the same degree p



Singular/near-singular $\int$'s in BEMs (2/3)

A simple example

- Consider the following integral that is singular at the origin

$$I = \int_{|\boldsymbol{x}|\le 1} \frac{f(x_1, x_2)}{\sqrt{x_1^2 + x_2^2}} dx_1 dx_2$$

Singularity cancellation (Duffy, Hackbusch, Johnston, Sauter, Telles, etc.)

- Change of variables such that the Jacobian cancels the singularity

$$I = \int_0^1 \int_0^{2\pi} \frac{f(r\cos\theta, r\sin\theta)}{r} r dr d\theta = \int_0^1 \int_0^{2\pi} f(r\cos\theta, r\sin\theta) dr d\theta$$

Singularity subtraction (Aliabadi, Guiggiani, Hall, Järvenpää, etc.)

- Terms having the same asymptotic behavior at the singularity are subtracted

$$I = \int_{|\boldsymbol{x}|\le 1} \left\{ \frac{f(x_1, x_2)}{\sqrt{x_1^2 + x_2^2}} - \frac{f(0,0)}{\sqrt{x_1^2 + x_2^2}} \right\} dx_1 dx_2 + \int_{|\boldsymbol{x}|\le 1} \frac{f(0,0)}{\sqrt{x_1^2 + x_2^2}} dx_1 dx_2$$

Singular/near-singular $\int$'s in BEMs (3/3)

Continuation approach (Cormack, Rosen, Vijayakumar)

- Suppose f is homogeneous, *i.e.*, $f(\lambda \boldsymbol{x}) = \lambda^{q+1} f(\boldsymbol{x})$, then

$$I = \frac{1}{q+2} \int_{|\boldsymbol{x}|=1} \frac{f(x_1, x_2)}{\sqrt{x_1^2 + x_2^2}} dx_1 dx_2 = \frac{1}{q+2} \int_0^{2\pi} f(\cos\theta, \sin\theta) d\theta$$

A more complicated example

- Consider the following integral that is near-singular at the origin

$$I(h) = \int_{|\boldsymbol{x}|\le 1} \frac{f(x_1, x_2)}{\sqrt{x_1^2 + x_2^2 + h^2}} dx_1 dx_2$$

- Continuation approach still works and yields

$$I(h) = h^{q+2} \int_0^{2\pi} f(\cos\theta, \sin\theta) \int_h^{+\infty} \frac{du}{u^{q+3}\sqrt{1+u^2}} d\theta$$

- How do we utilize the continuation approach on curved elements?
- Existing method is expensive and has poor accuracy near the boundary

Method – Presentation

Problem

$$I(\boldsymbol{x}_0) = \int_{\mathcal{T}} \frac{\hat{u}(F^{-1}(\boldsymbol{x}))}{|\boldsymbol{x}-\boldsymbol{x}_0|} dS(\boldsymbol{x}), \quad F : \widehat{T} \mapsto \mathcal{T}$$

Method

- Step 1 – Mapping back to the reference element

$$I(\boldsymbol{x}_0) = \int_{\widehat{\mathcal{T}}} \frac{v(\hat{\boldsymbol{x}})}{|F(\hat{\boldsymbol{x}})-\boldsymbol{x}_0|} dS(\hat{\boldsymbol{x}}), \quad F : \widehat{T} \mapsto \mathcal{T}$$

- Step 2 – Locating the singularity/near-singularity via $\hat{\boldsymbol{x}}_0 = \operatorname{argmin}|F(\hat{\boldsymbol{x}})-\boldsymbol{x}_0|^2$
- Step 3 – Taylor expanding/subtracting

$$I(\boldsymbol{x}_0) = \int_{\widehat{T}} T_{-1}(\hat{\boldsymbol{x}},h) dS(\hat{\boldsymbol{x}}) + \int_{\widehat{T}} \left\{ \frac{v(\hat{\boldsymbol{x}})}{|F(\hat{\boldsymbol{x}})-\boldsymbol{x}_0|} - T_{-1}(\hat{\boldsymbol{x}},h) \right\} dS(\hat{\boldsymbol{x}})$$

- Step 4 – Integrating the Taylor term with continuation + exact 1D integration

$$I_{-1}(h) = v(\hat{\boldsymbol{x}}_0) \sum_{i=1}^{3} s_i \int_{\partial \widehat{T}_i} \frac{\sqrt{|J(\hat{\boldsymbol{x}}_0)(\hat{\boldsymbol{x}}-\hat{\boldsymbol{x}}_0)|^2+h^2}-h}{|J(\hat{\boldsymbol{x}}_0)(\hat{\boldsymbol{x}}-\hat{\boldsymbol{x}}_0)|^2} ds(\hat{\boldsymbol{x}})$$

Method – Step 2

Goal ► Locating the singularity/near-singularity via $\hat{\boldsymbol{x}}_0 = \mathrm{argmin}|F(\hat{\boldsymbol{x}}) - \boldsymbol{x}_0|^2$

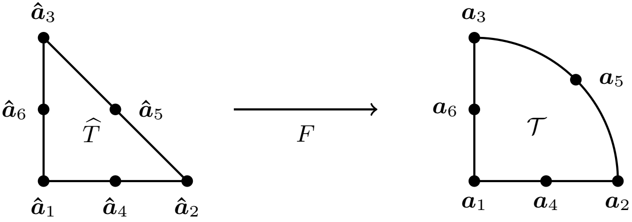
Cost function

- To compute $\hat{\boldsymbol{x}}_0$, we minimize $E(\hat{\boldsymbol{x}}) = |F(\hat{\boldsymbol{x}}) - \boldsymbol{x}_0|^2$ with, *e.g.*, for $p = 2$

$$F(\hat{\boldsymbol{x}}) = \sum_{j=1}^{6} \hat{u}_j(\hat{\boldsymbol{x}})\boldsymbol{a}_j \in \mathcal{T}$$

Numerical optimization

- Get close to a minimum with gradient descent: $\hat{\boldsymbol{x}}_0^{\text{new}} = \hat{\boldsymbol{x}}_0 - \eta \nabla E(\hat{\boldsymbol{x}}_0)$
- Improve the accuracy with Newton's method: $\hat{\boldsymbol{x}}_0^{\text{new}} = \hat{\boldsymbol{x}}_0 - \eta H(\hat{\boldsymbol{x}}_0)^{-1} \nabla E(\hat{\boldsymbol{x}}_0)$



Method – Step 3

Goal ▶ Taylor expanding/subtracting $I = \int T_{-1} + \int \left\{ vR^{-1} - T_{-1} \right\}$

First-order Taylor series

- Write $F(\hat{\boldsymbol{x}}) - \boldsymbol{x}_0 = F(\hat{\boldsymbol{x}}) - F(\hat{\boldsymbol{x}}_0) + F(\hat{\boldsymbol{x}}_0) - \boldsymbol{x}_0$ (*"on $\mathcal{T}$" + "$\perp$ to $\mathcal{T}$"*)
- First-order Taylor series in $\delta\hat{x} = |\hat{\boldsymbol{x}} - \hat{\boldsymbol{x}}_0|$

$$F(\hat{\boldsymbol{x}}) - \boldsymbol{x}_0 = J(\hat{\boldsymbol{x}}_0)(\hat{\boldsymbol{x}} - \hat{\boldsymbol{x}}_0) + F(\hat{\boldsymbol{x}}_0) - \boldsymbol{x}_0 + \mathcal{O}(\delta\hat{x}^2) \quad (\text{"on } J\text{"} + \text{"}\perp \text{ to } J\text{"})$$

- From the Taylor expansion of $R^2 = |F(\hat{\boldsymbol{x}}) - \boldsymbol{x}_0|^2$, we obtain that of vR^{-1}

$$vR^{-1} = v(\hat{\boldsymbol{x}}_0) \left[|J(\hat{\boldsymbol{x}}_0)(\hat{\boldsymbol{x}} - \hat{\boldsymbol{x}}_0)|^2 + h^2 \right]^{-\frac{1}{2}} + \mathcal{O}(\delta\hat{x}^0) = T_{-1} + \mathcal{O}(\delta\hat{x}^0)$$

Higher-order expansions

- More Taylor terms—smoother 2D integrand for faster 2D quadrature, *e.g.*,

$$T_0(\hat{\boldsymbol{x}}, h) = \frac{v_0'}{[|J_0\delta\hat{\boldsymbol{x}}|^2 + h^2]^{\frac{1}{2}}} - \frac{hv_0}{2} \sum_{j=1}^{3} a_j \frac{\delta\hat{x}_1^{3-j}\delta\hat{x}_2^{j-1}}{[|J_0\delta\hat{\boldsymbol{x}}|^2 + h^2]^{\frac{3}{2}}} - \dots$$

$$T_1(\hat{\boldsymbol{x}}, h) = \dots$$

Method – Step 4

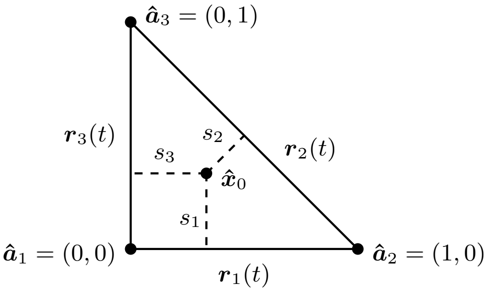
Goal ▶ Calculating $\int T_{-1}$ with continuation + exact 1D integration

Continuation appoach on triangles

- Parametrize each vertex, *e.g.*, $\boldsymbol{r}_1(t) = (t, 0)^T$ with $0 \leq t \leq 1$

$$I_{-1}(h) = v(\hat{\boldsymbol{x}}_0) \sum_{i=1}^{3} s_i \int_0^1 \frac{\sqrt{|J(\hat{\boldsymbol{x}}_0)(\boldsymbol{r}_i(t) - \hat{\boldsymbol{x}}_0)|^2 + h^2} - h}{|J(\hat{\boldsymbol{x}}_0)(\boldsymbol{r}_i(t) - \hat{\boldsymbol{x}}_0)|^2} |\boldsymbol{r}_i'(t)| dt$$

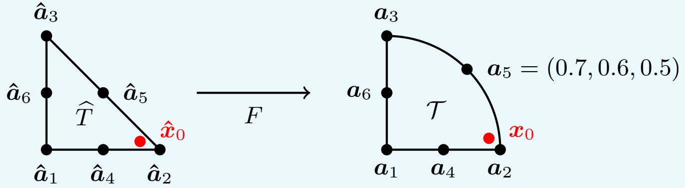
- Near-singular for small s_i's, slow ρ^{-2n} convergence ($\rho \approx 1$)—exact integration

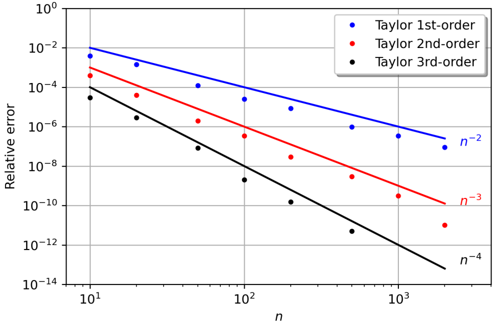


Numerical experiments (1/2)

Goal ► Computing $\int_{\mathcal{T}} |\boldsymbol{x} - \boldsymbol{x}_0|^{-1}$ for $\boldsymbol{x}_0 = F(0.99, 0.01) + 10^{-4}\boldsymbol{z}$ $(p = 2)$

Setup



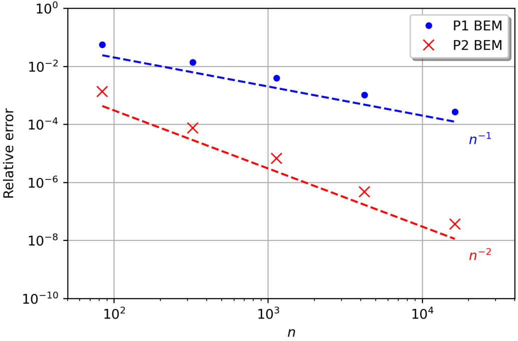


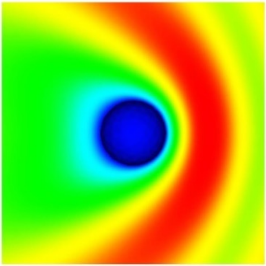
Numerical experiments (2/2)

Goal ▶ Solving 3D spherical scattering Helmholtz $\Delta u + u = 0$ $(p = 1, 2)$

Setup

- Single-layer potential formulation of the integral equation
- Relative error in the SER vs. number of elements—exact solution is known
- Implemented in C++, soon available as part of `castor` (≈ 2,000 ++)





Summary

Method

- Novel method for computing weakly singular/near-singular integrals
- Based on Taylor subtraction and the continuation approach
- Exact calculation of 1D integrals completely removes the near-singular issue

Future

- Applicable to quadrilateral elements with some tweaks
- Extension to strongly and hyper singular integrals
- Maxwell's equations, elasticity problems, etc.