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

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Helmholtz equation & integral representations

Background

- Consider the Helmhotz equation $\Delta u + k^2 u = 0$ in $\mathbb{R}^3 \setminus \overline{\Omega}$ with $u = u_D$ on $\Gamma = \partial\Omega$
- The 3D PDE may be replaced by a 2D integral equation, *e.g.*,

$$\frac{1}{4\pi}\int_\Gamma \frac{e^{ik|\boldsymbol{x}-\boldsymbol{y}|}}{|\boldsymbol{x}-\boldsymbol{y}|} q(\boldsymbol{y}) d\Gamma(\boldsymbol{y}) = u_D(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma$$

- Once the equation is solved for q, the function u is given by the LHS for all $\boldsymbol{x} \in \mathbb{R}^3 \setminus \Omega$

Challenges

- The integral becomes near-singular when $\boldsymbol{x}$ approaches $\boldsymbol{y}$
  - analytic integration
  - carefully-derived quadrature
- Solutions at large wavenumbers k are highly oscillatory
  - high-order numerical methods
- Resulting linear systems after discretization are dense
  - fast multipole method
  - hierarchical matrices

Nyström vs. boundary elements

Integral equation

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

Nyström methods (Barnett, Bruno, Bonnet, Faria, Greengard, Rokhlin, etc.)

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

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

- High-order but restricted in terms of geometry

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

- Based on a variational formulation of the integral equation

$$\int_\Gamma \int_\Gamma G(\boldsymbol{x},\boldsymbol{y})q(\boldsymbol{y})q'(\boldsymbol{x})d\Gamma(\boldsymbol{y})d\Gamma(\boldsymbol{x}) = \int_\Gamma u_D(\boldsymbol{x})q'(\boldsymbol{x})d\Gamma(\boldsymbol{x}), \quad \forall q' \in H^s(\Gamma)$$

- Flexible with respect to geometry but often low-order

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

Boundary element methods

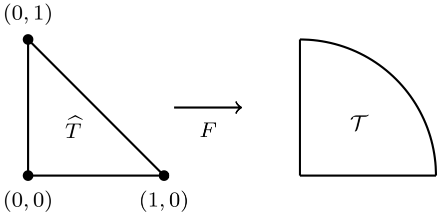
$$\int_\Gamma \int_\Gamma G(\boldsymbol{x}, \boldsymbol{y}) q(\boldsymbol{y}) q'(\boldsymbol{x}) d\Gamma(\boldsymbol{y}) d\Gamma(\boldsymbol{x}) = \int_\Gamma u_D(\boldsymbol{x}) q'(\boldsymbol{x}) d\Gamma(\boldsymbol{x}), \quad \forall q' \in H^s(\Gamma)$$

Setup

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

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

- $\mathcal{T}$ is a curved triangular element defined by $F : \widehat{T} \mapsto \mathcal{T}$ of degree d_F
- q is a basis function of degree d_q and $\boldsymbol{x}_0 \in \mathbb{R}^3$ is a point on/close to $\mathcal{T}$



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

A simple example

- Consider the following integral that is singular at the origin

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

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

- Change of variables such that the Jacobian cancels the singularity

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

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

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

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

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

Continuation approach (Cormack, Lenoir, Rosen, Salles, Vijayakumar)

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

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

A more complicated example

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

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

- Continuation approach still works and yields

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

- How do we utilize the continuation approach on curved elements?
- Our method combines singularity subtraction with the continuation approach

Method – Presentation

Problem

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

Method

- Step 1 – Mapping back to the reference element

$$I(\boldsymbol{x}_0) = \int_{\widehat{\mathcal{T}}} \frac{\hat{q}(\hat{\boldsymbol{x}})}{|F(\hat{\boldsymbol{x}}) - \boldsymbol{x}_0|} dS(\hat{\boldsymbol{x}}), \quad \hat{q}(\hat{\boldsymbol{x}}) = q(\hat{\boldsymbol{x}})|J_1(\hat{\boldsymbol{x}}) \times J_2(\hat{\boldsymbol{x}})|$$

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

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

- Step 4 – Integrating T_{-1} with continuation & transplanted Gauss quadrature

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

Method – Step 2

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

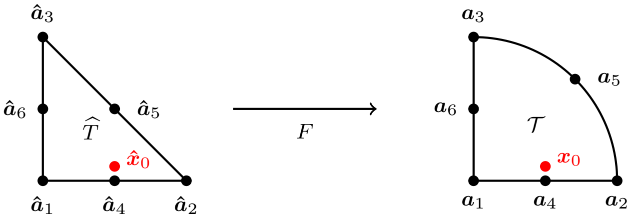
Cost function

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

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

Numerical optimization

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



Method – Step 3

Goal ▶ Taylor expanding & subtracting $I = \int T_{-1} + \int \left\{ \hat{q}R^{-1} - T_{-1} \right\}$

First-order Taylor series

- We want to calculate the asymptotic expansion of $\hat{q}(\hat{\boldsymbol{x}})R^{-1} = \hat{q}(\hat{\boldsymbol{x}})/|F(\hat{\boldsymbol{x}}) - \boldsymbol{x}_0|$
- First-order Taylor series in $\delta\hat{x} = |\hat{\boldsymbol{x}} - \hat{\boldsymbol{x}}_0|$

$$F(\hat{\boldsymbol{x}}) - \boldsymbol{x}_0 = J(\hat{\boldsymbol{x}}_0)(\hat{\boldsymbol{x}} - \hat{\boldsymbol{x}}_0) + F(\hat{\boldsymbol{x}}_0) - \boldsymbol{x}_0 + \mathcal{O}(\delta\hat{x}^2)$$

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

$$\hat{q}R^{-1} = \frac{\hat{q}(\hat{\boldsymbol{x}}_0)}{\sqrt{|J(\hat{\boldsymbol{x}}_0)(\hat{\boldsymbol{x}} - \hat{\boldsymbol{x}}_0)|^2 + h^2}} + \mathcal{O}(\delta\hat{x}^0) = T_{-1} + \mathcal{O}(\delta\hat{x}^0)$$

Higher-order expansions

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

$$T_0(\hat{\boldsymbol{x}}, h) = \frac{v_0'}{[|J(\hat{\boldsymbol{x}}_0)\delta\hat{\boldsymbol{x}}|^2 + h^2]^{\frac{1}{2}}} - \frac{hv_0}{2}\sum_{j=1}^{3} a_j \frac{\delta\hat{x}_1^{3-j}\delta\hat{x}_2^{j-1}}{[|J(\hat{\boldsymbol{x}}_0)\delta\hat{\boldsymbol{x}}|^2 + h^2]^{\frac{3}{2}}} - \dots$$

Method – Step 4 (1/2)

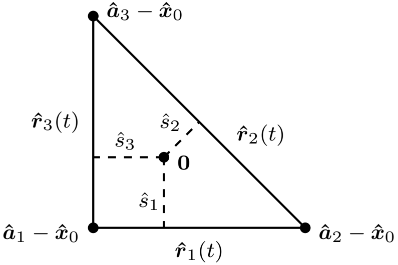
Goal ▶ Integrating T_{-1} with continuation & transplanted Gauss quadrature

Continuation approach (Lenoir, Salles)

- Transforms a 2D integral into a sum of 1D integrals along the sides of $\widehat{T} - \hat{\boldsymbol{x}}_0$

$$\int_{\widehat{T}-\hat{\boldsymbol{x}}_0} \frac{\hat{q}(\hat{\boldsymbol{x}}_0)dS(\hat{\boldsymbol{x}})}{\sqrt{|J(\hat{\boldsymbol{x}}_0)\hat{\boldsymbol{x}}|^2 + h^2}} = \hat{q}(\hat{\boldsymbol{x}}_0)\sum_{j=1}^{3} \hat{s}_j \int_{-1}^{1} \frac{\sqrt{|J(\hat{\boldsymbol{x}}_0)\hat{\boldsymbol{r}}_j(t)|^2 + h^2} - h}{|J(\hat{\boldsymbol{x}}_0)\hat{\boldsymbol{r}}_j(t)|^2} |\hat{\boldsymbol{r}}_j'(t)|dt$$

- When the origin is far from a side (close to), the integrand is analytic (but near-singular)
  - convergence with Gauss quadrature is exponential (but slow)



Method – Step 4 (2/2)

Goal ▶ Integrating T_{-1} with continuation & transplanted Gauss quadrature

Gauss quadrature

- The integral on $\hat{\boldsymbol{r}}_1$ is of the form

$$I(\epsilon) = \int_{-1}^{1} f_\epsilon(t)dt = \int_{-1}^{1} \frac{dt}{\sqrt{t^2+\epsilon^2}} \approx \sum_{k=1}^{n} w_k f_\epsilon(t_k)$$

- Because of the singularities at $t = \pm i\epsilon$, slow convergence at the rate $(1+\epsilon)^{-2n}$

Transplanted Gauss quadrature (Hale, Olver, Slevinsky, Trefethen, etc.)

- Pick conformal map g_ϵ such that $g_\epsilon(\pm 1) = \pm 1$, *e.g.*, $g_\epsilon(z) = \epsilon \sinh\left[\operatorname{arcsinh}\left(\frac{1}{\epsilon}\right) z\right]$

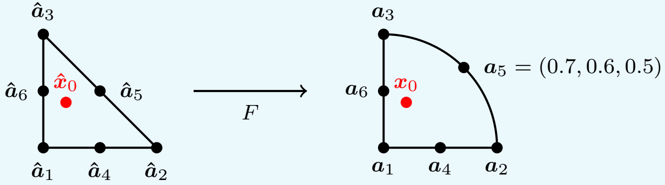
$$I(\epsilon) = \int_{-1}^{1} g_\epsilon'(t) f_\epsilon(g_\epsilon(t))dt \approx \sum_{k=1}^{n} w_k g_\epsilon'(t_k) f_\epsilon(g_\epsilon(t_k))$$

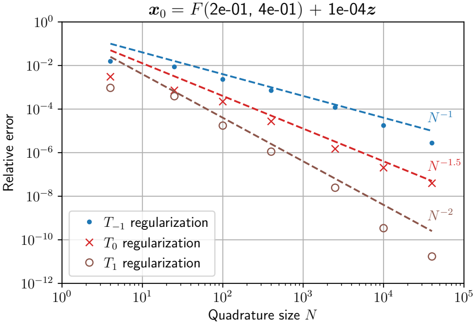
- Integrates f_ϵ exactly with a single quadrature point/weight
- Faster convergence $(1+\pi/[2\log(1/\epsilon)])^{-2n}$ for $f_\epsilon^\ell \times g$ for any smooth g and integer ℓ

Numerical experiments (1/4)

Goal ► Computing $\int_{\mathcal{T}} |\boldsymbol{x} - \boldsymbol{x}_0|^{-1}$ for $\boldsymbol{x}_0 = F(0.2, 0.4) + 10^{-4}\boldsymbol{z}$

Setup

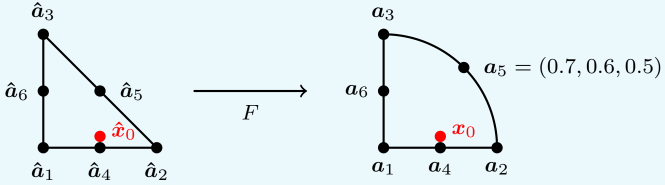


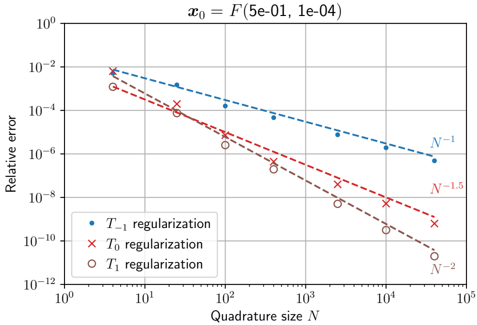


Numerical experiments (2/4)

Goal ▶ Computing $\int_{\mathcal{T}} |\boldsymbol{x} - \boldsymbol{x}_0|^{-1}$ for $\boldsymbol{x}_0 = F(0.5, 10^{-4})$

Setup





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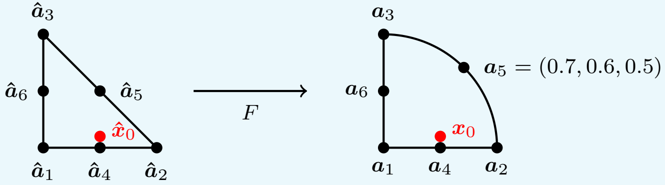
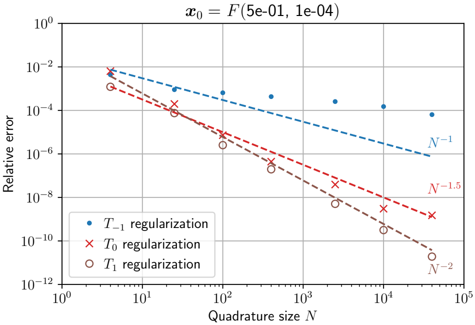




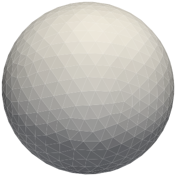
Numerical experiments (3/4)

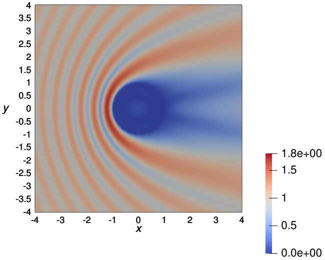
Goal ► Solving 3D Helmholtz (exterior, Dirichlet, unit sphere)

Setup

- Find u^s such that $u^i + u^s = 0$ on Γ for $u^i(r,\theta) = e^{ikr\cos\theta}$
- Single-layer potential formulation of the integral equation $\mathcal{S}_h q_h = -u^i$
- Solve for q_h then evaluate u_h at "infinity" (far-field)
- Convergence of the numerical far-field u_h to the exact far-field u as mesh size $h \to 0$

$$|u(\boldsymbol{x}) - u_h(\boldsymbol{x})| \leq c\left(h^{2d_F}\|q\|_{L_2(\Gamma)} + h^{2d_q+3}\|q\|_{H^{d_q+1}(\Gamma)}\right)$$





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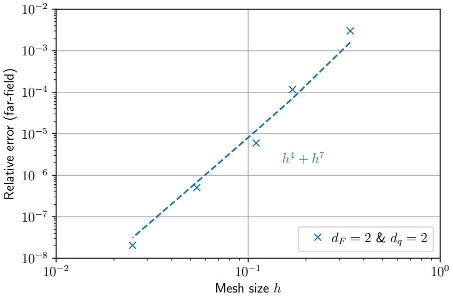


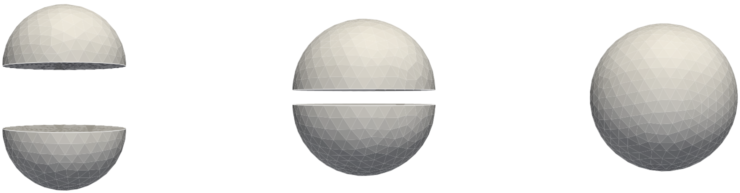
Numerical experiments (4/4)

Goal ▶ Solving 3D Helmholtz (exterior, Dirichlet, two half-spheres at $(0,0,\pm\delta)$)

Setup

- Find u_δ^s such that $u^i + u_\delta^s = 0$ on Γ_δ for $u^i(r,\theta) = e^{ikr\cos\theta}$
- Single-layer potential formulation of the integral equation $\mathcal{S}_\delta q_\delta = -u^i$
- Solve for q_δ then evaluate u_δ at "infinity" with $h = \mathcal{O}(\delta)$
- Convergence of the far-field u_δ to the far-field u corresponding to $\delta = 0$ as $\delta \to 0$

$$|u(\boldsymbol{x}) - u_\delta(\boldsymbol{x})| \leq c\delta^\ell$$



Numerical experiments (4/4)

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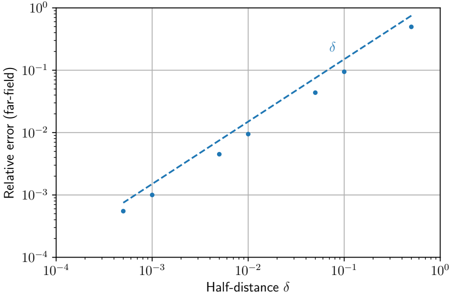

Software

Singular integrals

- Implemented in Python, soon available on GitHub (≈ 900 ++)
- Shorter code for simple examples, available in upcoming paper (≈ 60 ++)

```
# Step 1 - Mapping back:
a, b, c = 0.6, 0.7, 0.5
Fx = lambda x: x[0] + 2*(2*a-1)*x[0]*x[1]
Fy = lambda x: x[1] + 2*(2*b-1)*x[0]*x[1]
Fz = lambda x: 4*c*x[0]*x[1]
F = lambda x: np.array([Fx(x), Fy(x), Fz(x)])                          # map
J1 = lambda x: np.array([1 + 2*(2*a-1)*x[1], 2*(2*b-1)*x[1], 4*c*x[1]])  # Jacobian (1st col)
J2 = lambda x: np.array([2*(2*a-1)*x[0], 1 + 2*(2*b-1)*x[0], 4*c*x[0]])  # Jacobian (2nd col)
x0 = F([0.5, 1e-4]) + 1e-4*np.array([0, 0, 1])                         # singularity

# Step 2 - Locating the singularity:
e = lambda x: F(x) - x0
E = lambda x: np.linalg.norm(e(x))**2                                  # cost function
dE = lambda x: 2*np.array([e(x) @ J1(x), e(x) @ J2(x)])                # gradient
x0h = minimize(E, np.zeros(2), method='BFGS', jac=dE, tol=1e-12).x     # minimization
h = np.linalg.norm(F(x0h) - x0)
```

Singular integrals + boundary elements

- Implemented in C++, soon available as part of `castor` (≈ 2,000 ++)
- Gmsh for quadrilateral elements—more generally, any `ply` or `vtk` files
- Hierarchical matrices for compression
- Parallel computations—Intel Xeon Gold (3.00 GHz, 36 cores) with 512 GB of RAM

Summary

Method

- Novel method for computing weakly singular/near-singular integrals
- Based on singularity subtraction and the continuation approach
- Transplanted Gauss quadrature circumvents near-singular issues

Future

- Applicable to quadrilateral elements with some tweaks
- Extension to strongly and hyper singular integrals, *e.g.*,

$$\frac{\partial}{\partial n(\boldsymbol{x})} \int_\Gamma \frac{\partial G(\boldsymbol{x}, \boldsymbol{y})}{\partial n(\boldsymbol{y})} q(\boldsymbol{y}) d\Gamma(\boldsymbol{y}) = u_N(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma$$

  for the 3D Neumann problem $\Delta u + k^2 u = 0$ in $\mathbb{R}^3 \setminus \overline{\Omega}$ with $\partial u / \partial n = u_N$ on Γ
- Maxwell's equations, elasticity problems, etc.