IDEFIX Group Seminar

# Computing singular and near-singular integrals in high-order boundary elements

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1. Integral equations

2. Weakly singular integrals

3. Numerical experiments

4. Strongly singular integrals

# Integral equations – Direct & inverse problems

## Direct & inverse scattering problems

- An incident wave $u^i$ is scattered by an obstacle, total field $u = u^i + u^s$
  - Direct problem = scatterer known → determine the scattered field
  - Inverse problem = scattered field known → determine the scatterer

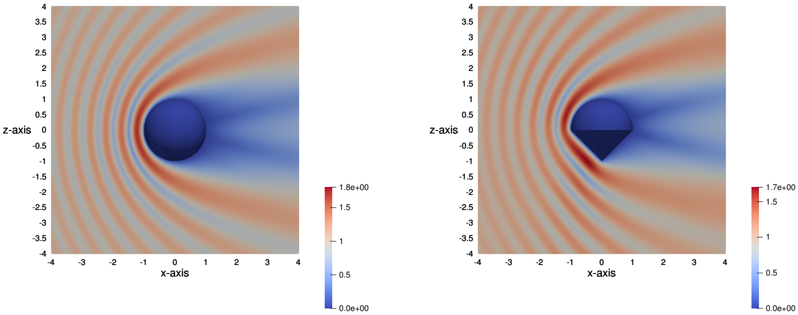


Figure: *Acoustic scattering of a plane wave by a sphere and a cone-sphere in 3D.*

# Integral equations – Direct & inverse problems

## Direct & inverse scattering problems

- An incident wave $u^i$ is scattered by an obstacle, total field $u = u^i + u^s$
  - Direct problem = scatterer known $\rightarrow$ determine the scattered field
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## Applications

- EDF applications
  - Defect and crack detection in materials
  - Dike inspection
  - Eddy-current imaging in pipes
  - Steam generator monitoring
- Military applications
  - Radar and sonar technology
  - Underwater mine detection
- Other applications
  - Medical imaging

# Integral equations – Layer potentials

## Background

- Time-harmonic acoustic waves solutions to 3D Helmholtz $\Delta u + k^2 u = 0$
- May be rewritten as a 2D integral equation on the scatterer's boundary
- Applies to Maxwell's eqns. (electromagnetic waves) and elasticity (elastic waves)

## Single-layer potential

- The radiating solution to $\Delta u + k^2 u = 0$ in $\mathbb{R}^3 \setminus \overline{\Omega}$ with $u = u_D$ on $\Gamma = \partial\Omega$, for some bounded $\Omega$ whose complement is connected, can be obtained via

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

- $G$ is the Green's function of the Helmholtz equation in 3D,

$$G(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{4\pi} \frac{e^{ik|\boldsymbol{x}-\boldsymbol{y}|}}{|\boldsymbol{x}-\boldsymbol{y}|}$$

- Once the equation is solved for $\varphi$, unique if $k^2$ is not an e-value of $-\Delta$ in $\Omega$, the solution $u$ may be represented by the LHS for all $\boldsymbol{x} \in \mathbb{R}^3 \setminus \Omega$

# Integral equations – Layer potentials

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- May be rewritten as a 2D integral equation on the scatterer's boundary
- Applies to Maxwell's eqns. (electromagnetic waves) and elasticity (elastic waves)

## Double-layer potential

- The radiating solution to $\Delta u + k^2 u = 0$ in $\mathbb{R}^3 \setminus \overline{\Omega}$ with $u = u_D$ on $\Gamma = \partial\Omega$, for some bounded $\Omega$ whose complement is connected, can be obtained via

$$\int_\Gamma \frac{\partial G(\boldsymbol{x}, \boldsymbol{y})\varphi(\boldsymbol{y})}{\partial \boldsymbol{n}(\boldsymbol{y})} d\Gamma(\boldsymbol{y}) + \frac{\varphi(\boldsymbol{x})}{2} = u_D(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma$$

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# Integral equations – Numerical methods

**Integral equation**

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

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

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

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

- High-order but restricted in terms of geometry

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

- Based on a variational formulation of the integral equation

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

- Flexible with respect to geometry but often low-order

# Integral equations – Challenges

**Integral equation**

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

**Numerical challenges**

- The resulting linear system $Ax = b$ is dense
  - For large wavenumbers $k$, iterative methods are required ($N \uparrow k$)
  - High-order schemes may be helpful in enlarging the interval of feasible $k$
- These yield singular/near-singular integrals for which standard methods fail
  - Singular $\rightarrow$ intrinsic to the integral equation formulation
  - Near-singular $\rightarrow$ nearby objects (*e.g.*, thin layers), resonant cavities

**Goals**

1. High-order method for enlarging the interval of feasible wavenumbers $k$
2. Robust with respect to geometry, *e.g.*, handles corners & nearby objects

# Weakly singular integrals – Setup

**Boundary element methods**

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

**Singular integrals**

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

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

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

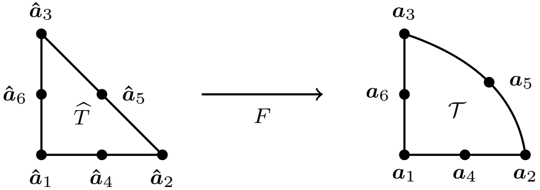


Figure: *A quadratic element $\mathcal{T}$ and its mapping $F$.*

# Weakly singular integrals – Cancel & subtract

## A simple example

- Consider the following integral that is singular at the origin

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

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

- Change of variables such that the Jacobian cancels the singularity

$$I = \int_0^1 \int_0^{2\pi} \frac{\varphi(\rho\cos\theta, \rho\sin\theta)}{\rho} \rho d\rho d\theta = \int_0^1 \int_0^{2\pi} \varphi(\rho\cos\theta, \rho\sin\theta) d\rho d\theta$$

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

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

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

# Weakly singular integrals – Continuation

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

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

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

## A more complicated example

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

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

- Continuation approach still works and yields

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

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

# Weakly singular integrals – Method

**Problem**

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

**Method**

- Step 1 – Mapping back to the reference element

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

- 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

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

- Steps 4 & 5 – Integrating $T_{-1}$ with continuation & transplanted quadrature

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

# Weakly singular integrals – Step 1

Goal ▶ Mapping back $I(\boldsymbol{x}_0) = \int_{\mathcal{T}} \frac{\varphi(F^{-1}(\boldsymbol{x}))}{|\boldsymbol{x}-\boldsymbol{x}_0|} dS(\boldsymbol{x}) = \int_{\widehat{T}} \frac{\varphi(\hat{\boldsymbol{x}})|J_1(\hat{\boldsymbol{x}})\times J_2(\hat{\boldsymbol{x}})|}{|F(\hat{\boldsymbol{x}})-\boldsymbol{x}_0|} dS(\hat{\boldsymbol{x}})$

## Map and Jacobian matrix

- A quadratic triangle $\mathcal{T} \subset \mathbb{R}^3$ is defined by six points $\boldsymbol{a}_j \in \mathbb{R}^3$ and the map $F : \widehat{T} \to \mathcal{T}$

$$F(\hat{\boldsymbol{x}}) = \sum_{j=1}^{6} \varphi_j(\hat{\boldsymbol{x}})\boldsymbol{a}_j \in \mathbb{R}^3$$

- The $3 \times 2$ Jacobian matrix $J$ is then defined by

$$J(\hat{\boldsymbol{x}}) = \left( J_1(\hat{\boldsymbol{x}}) \;\middle|\; J_2(\hat{\boldsymbol{x}}) \right) = \left( F_{\hat{x}_1}(\hat{\boldsymbol{x}}) \;\middle|\; F_{\hat{x}_2}(\hat{\boldsymbol{x}}) \right) \in \mathbb{R}^{3\times 2}$$

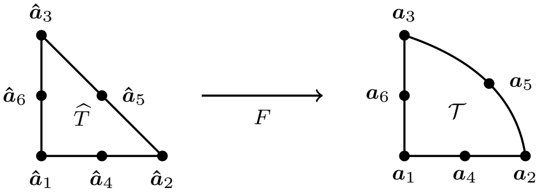


Figure: *A quadratic element $\mathcal{T}$ and its mapping $F$.*

# Weakly singular integrals – Step 2

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

**Cost function**

- Given $\mathcal{T}$ and a point $\boldsymbol{x}_0$, find $\hat{\boldsymbol{x}}_0$ such that $F(\hat{\boldsymbol{x}}_0)$ is the closest point to $\boldsymbol{x}_0$ on $\mathcal{T}$
- Minimize $E(\hat{\boldsymbol{x}}) = |F(\hat{\boldsymbol{x}}) - \boldsymbol{x}_0|^2$, the output $\hat{\boldsymbol{x}}_0$ is such that

$$\boldsymbol{x}_0 = F(\hat{\boldsymbol{x}}_0) - h\boldsymbol{e}_h, \quad h = |F(\hat{\boldsymbol{x}}_0) - \boldsymbol{x}_0|, \quad \boldsymbol{e}_h = \frac{F(\hat{\boldsymbol{x}}_0) - \boldsymbol{x}_0}{h}$$

- We make the assumption that $h \ll \rho$ (diameter of $\mathcal{T}$)

**Numerical optimization**

- Compute closest point on the surface with Newton's method

$$\hat{\boldsymbol{x}}_0^{\text{new}} = \hat{\boldsymbol{x}}_0 + \alpha p(\hat{\boldsymbol{x}}_0), \quad p(\hat{\boldsymbol{x}}_0) = -H(\hat{\boldsymbol{x}}_0)^{-1}\nabla E(\hat{\boldsymbol{x}}_0)$$

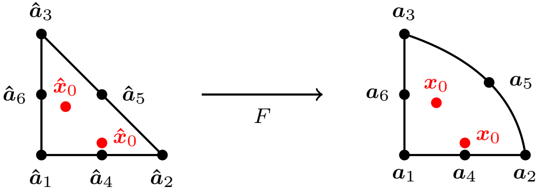


Figure: *Nearest singularity is computed with optimization.*

# Weakly singular integrals – Step 3

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

## First-order Taylor series

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

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

- Since $|J(\hat{\boldsymbol{x}}_0)(\hat{\boldsymbol{x}} - \hat{\boldsymbol{x}}_0)|^2 \sim \rho^2\delta\hat{x}^2$ and $h\mathcal{O}(\delta\hat{x}^2) \sim h\rho\delta\hat{x}^2$, the latter may be neglected
- From the expansion of $R^2$, we obtain that of $\psi R^{-1}$

$$\frac{\psi(\hat{\boldsymbol{x}})}{|F(\hat{\boldsymbol{x}}) - \boldsymbol{x}_0|} \approx \frac{\psi(\hat{\boldsymbol{x}}_0)}{\sqrt{|J(\hat{\boldsymbol{x}}_0)(\hat{\boldsymbol{x}} - \hat{\boldsymbol{x}}_0)|^2 + h^2}}$$

## Higher-order expansions

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

$$T_0(\hat{\boldsymbol{x}}, h) = \frac{\psi_0'}{\left[|J(\hat{\boldsymbol{x}}_0)\delta\hat{\boldsymbol{x}}|^2 + h^2\right]^{\frac{1}{2}}} - \frac{h\psi_0}{2}\sum_{j=1}^{3} a_j \frac{\delta\hat{x}_1^{3-j}\delta\hat{x}_2^{j-1}}{\left[|J(\hat{\boldsymbol{x}}_0)\delta\hat{\boldsymbol{x}}|^2 + h^2\right]^{\frac{3}{2}}} - \dots$$

# Weakly singular integrals – Step 3

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

## First-order Taylor series

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

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# Weakly singular integrals – Step 4

Goal ▶ Transform $\int T_{-1}$ with the continuation approach

**Continuation approach**

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

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

- When the origin is far from an edge (close to), integrand is analytic (but near-singular)

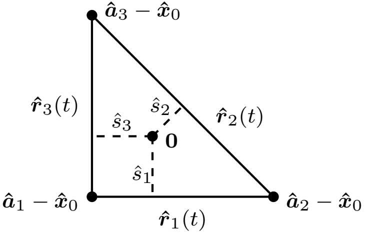



Figure: *The integrals are computed along the edges of $\widehat{T} - \hat{\boldsymbol{x}}_0$.*

# Weakly singular integrals – Step 5

Goal ▶ Compute $\int T_{-1}$ with 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 $g_\epsilon$ such that $g_\epsilon(\pm 1) = \pm 1$, *e.g.*, $g_\epsilon(z) = \epsilon \sinh\left[\operatorname{arcsinh}\left(\frac{1}{\epsilon}\right) z\right]$

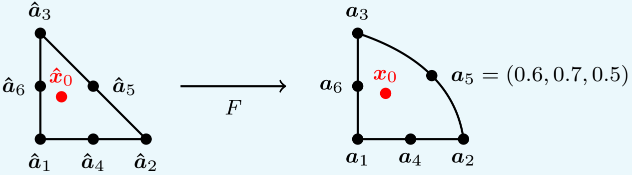
$$I(\epsilon) = \int_{-1}^{1} g_\epsilon'(t) f_\epsilon(g_\epsilon(t))dt \approx \sum_{k=1}^{n} w_k g_\epsilon'(t_k) f_\epsilon(g_\epsilon(t_k))$$

- Integrates $f_\epsilon$ 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 $\ell$

# Numerical experiments – 2D near-singular integral

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

Setup



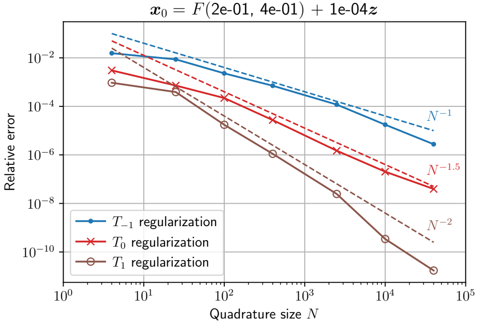
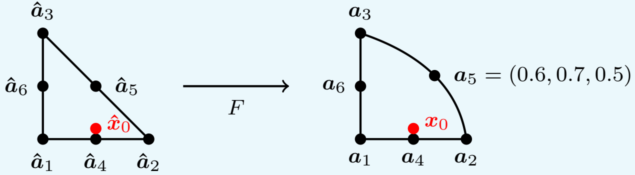




Figure: *Error versus quadrature size.*

# Numerical experiments – 2D singular integral

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

Setup



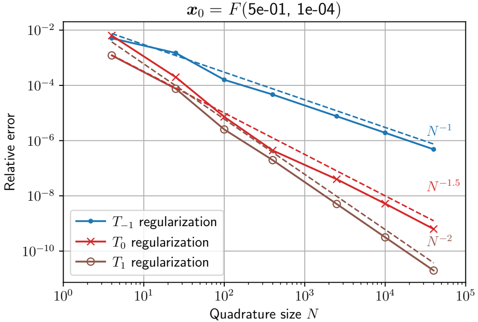




Figure: *Error versus quadrature size.*

# Numerical experiments – 2D singular integral

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

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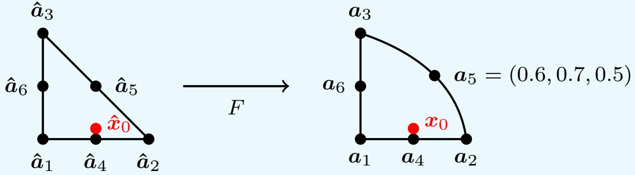


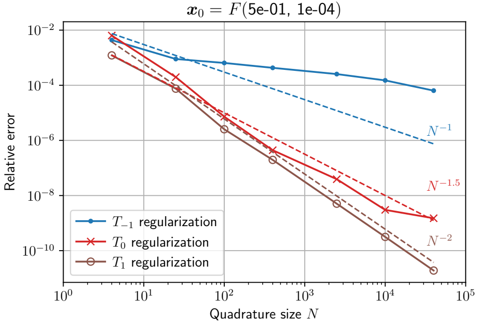


Figure: *Error versus quadrature size.*

# Numerical experiments – 4D singular integral

**Goal** ▶ Computing $\int_{\mathcal{T}} \int_{\mathcal{T}} \frac{dS(\boldsymbol{y})dS(\boldsymbol{x})}{|\boldsymbol{x}-\boldsymbol{y}|}$

**Method**

- We map the $\boldsymbol{y}$-integral back to $\widehat{T}$ and discretize it with $N$-point Gauss quadrature

$$I = \int_{\mathcal{T}} \int_{\widehat{T}} \frac{\psi(\hat{\boldsymbol{y}})}{|\boldsymbol{x} - F(\hat{\boldsymbol{y}})|} dS(\hat{\boldsymbol{y}}) dS(\boldsymbol{x}) \approx I_N = \sum_{n=1}^{N} w_n \psi(\hat{\boldsymbol{y}}_n) \int_{\mathcal{T}} \frac{dS(\boldsymbol{x})}{|\boldsymbol{x} - F(\hat{\boldsymbol{y}}_n)|}$$

- There remain $N$ integrals, which we compute with $T_{-1}$ regularization using $N$ points

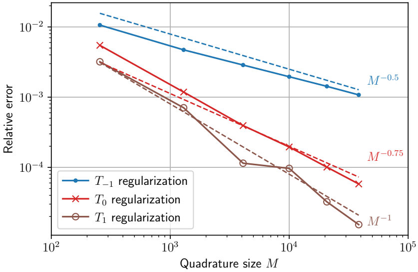


Figure: *Error versus quadrature size ($M = N^2$ is the total number of points).*

# Numerical experiments – Helmholtz (setup)

Goal ► Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

**Method**

- Single-layer potential formulation yields the computation of integrals of the form

$$I = \frac{1}{4\pi}\int_{\mathcal{T}_\ell}\int_{\mathcal{T}_{\ell'}} \frac{e^{ik|\boldsymbol{x}-\boldsymbol{y}|}}{|\boldsymbol{x}-\boldsymbol{y}|}\varphi_{j'}(F_{\ell'}^{-1}(\boldsymbol{y}))dS(\boldsymbol{y})\varphi_j(F_\ell^{-1}(\boldsymbol{x}))dS(\boldsymbol{x})$$

- We map the $\boldsymbol{y}$-integral back to $\widehat{T}$ and discretize it with $N$-point Gauss quadrature

$$I \approx I_N = \frac{1}{4\pi}\sum_{n=1}^{N} w_n \psi_{j'}(\hat{\boldsymbol{y}}_n)\int_{\mathcal{T}_\ell} \frac{e^{ik|\boldsymbol{x}-F_{\ell'}(\hat{\boldsymbol{y}}_n)|}}{|\boldsymbol{x}-F_{\ell'}(\hat{\boldsymbol{y}}_n)|}\varphi_j(F_\ell^{-1}(\boldsymbol{x}))dS(\boldsymbol{x})$$

- We are left with the computations of $N$ integrals of the form

$$\int_{\mathcal{T}_\ell} \frac{e^{ik|\boldsymbol{x}-\boldsymbol{x}_n|}-1}{|\boldsymbol{x}-\boldsymbol{x}_n|}\varphi_j(F_\ell^{-1}(\boldsymbol{x}))dS(\boldsymbol{x}) + \int_{\mathcal{T}_\ell} \frac{\varphi_j(F_\ell^{-1}(\boldsymbol{x}))}{|\boldsymbol{x}-\boldsymbol{x}_n|}dS(\boldsymbol{x}).$$

- First integral discretized with $N$-point Gauss quadrature—convergence $\mathcal{O}(N^{-1.5})$
- Second one discretized with $T_{-1}$ regularization—convergence $\mathcal{O}(N^{-1})$

# Numerical experiments – Helmholtz (unit sphere)

Goal ▶ Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

**Far-field error**

- Find solution $u^s$ such that $u = u^i + u^s = 0$ on $\Gamma$ for $u^i(r,\theta) = e^{ikr\cos\theta}$
- Single-layer potential formulation of the integral equation $\mathcal{S}_h \varphi_h^s = -u_h^i$
- Solve for $\varphi_h^s$, then evaluate $u_h^s$ at "infinity" $\longrightarrow u_h^\infty$ (far-field)

$$|u^\infty(\boldsymbol{x}) - u_h^\infty(\boldsymbol{x})| \leq c\left(h^{2(p+1)+1}\|\varphi^s\|_{H^{p+1}(\Gamma)} + h^{2q}\|\varphi^s\|_{L_2(\Gamma)}\right)$$

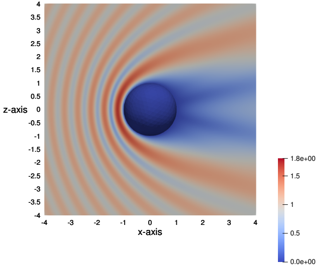


Figure: *Acoustic scattering of a plane wave by a sphere in 3D.*

# Numerical experiments – Helmholtz (unit sphere)

Goal ▶ Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

**Far-field error**

- Find solution $u^s$ such that $u = u^i + u^s = 0$ on $\Gamma$ for $u^i(r,\theta) = e^{ikr\cos\theta}$
- Single-layer potential formulation of the integral equation $\mathcal{S}_h \varphi_h^s = -u_h^i$
- Solve for $\varphi_h^s$, then evaluate $u_h^s$ at "infinity" $\longrightarrow u_h^\infty$ (far-field)

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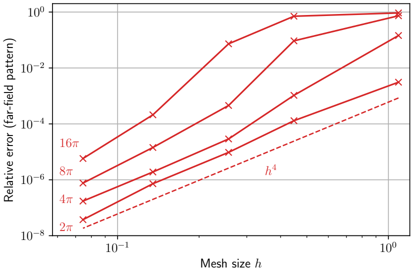


Figure: *Error in far-field versus mesh size $h$ ($p = q = 2$).*

# Numerical experiments – Helmholtz (unit sphere)

Goal ► Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

**Far-field error**

- Find solution $u^s$ such that $u = u^i + u^s = 0$ on $\Gamma$ for $u^i(r,\theta) = e^{ikr\cos\theta}$
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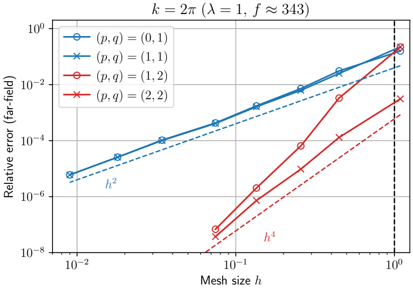


Figure: *Error in far-field versus mesh size $h$.*

# Numerical experiments – Helmholtz (unit sphere)

Goal ▶ Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

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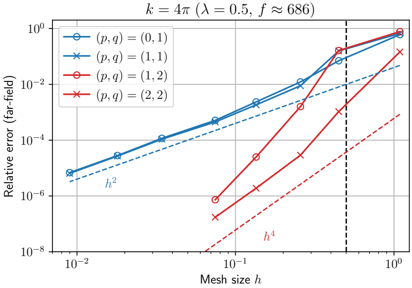


Figure: *Error in far-field versus mesh size $h$.*

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Goal ▶ Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

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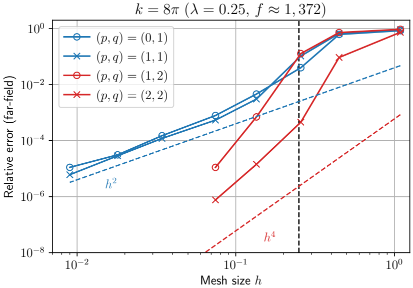


Figure: *Error in far-field versus mesh size $h$.*

# Numerical experiments – Helmholtz (unit sphere)

Goal ▶ Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

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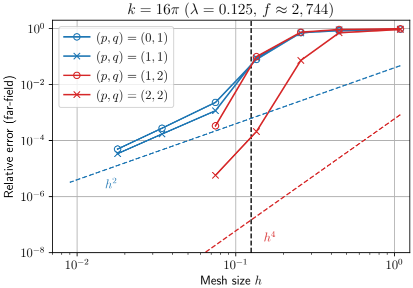


Figure: *Error in far-field versus mesh size $h$.*

# Numerical experiments – Helmholtz (unit sphere)

Goal ▶ Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

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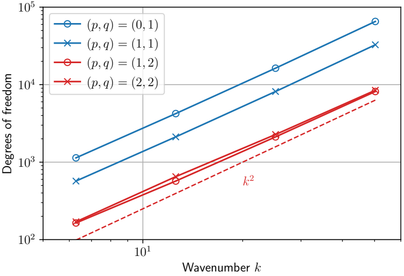


Figure: *DoFs versus wavenunber $k$ for target error $\epsilon \approx 10^{-3}$: Goal #1 achieved.*

# Numerical experiments – Helmholtz (cone-sphere)

Goal ▶ Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

**Far-field error**

- Find solution $u^s$ such that $u = u^i + u^s = 0$ on $\Gamma$ for $u^i(r,\theta) = e^{ikr\cos\theta}$
- Single-layer potential formulation of the integral equation $\mathcal{S}_h \varphi_h = -u_h^i$
- Solve for $\varphi_h^s$, then evaluate $u_h^s$ at "infinity" $\longrightarrow u_h^\infty$ (far-field)

$$|u^\infty(\boldsymbol{x}) - u_h^\infty(\boldsymbol{x})| \le c\left(h^{p+2}\|\varphi^s\|_{H^{p+1}(\Gamma)} + h^{q+1}\|\varphi^s\|_{L_2(\Gamma)}\right)$$

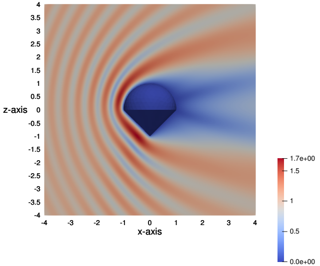


Figure: *Acoustic scattering of a plane wave by a cone-sphere in 3D.*

# Numerical experiments – Helmholtz (cone-sphere)

Goal ▶ Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

**Far-field error**

- Find solution $u^s$ such that $u = u^i + u^s = 0$ on $\Gamma$ for $u^i(r,\theta) = e^{ikr\cos\theta}$
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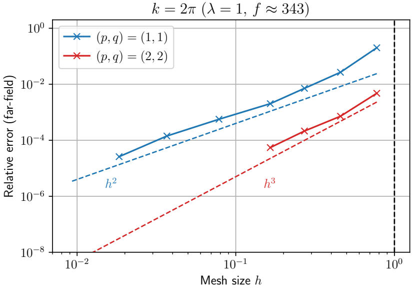


Figure: *Error in far-field versus mesh size $h$.*

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Goal ▶ Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

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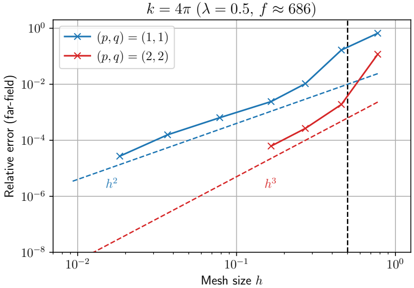


Figure: *Error in far-field versus mesh size $h$.*

# Numerical experiments – Helmholtz (cone-sphere)

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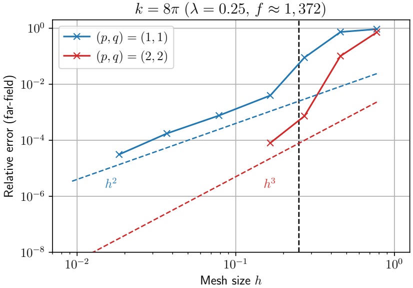


Figure: *Error in far-field versus mesh size $h$.*

# Numerical experiments – Helmholtz (cone-sphere)

Goal ▶ Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

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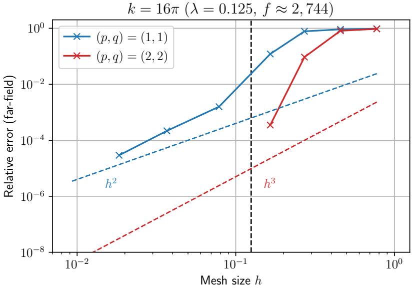


Figure: *Error in far-field versus mesh size $h$.*

# Numerical experiments – Helmholtz (cone-sphere)

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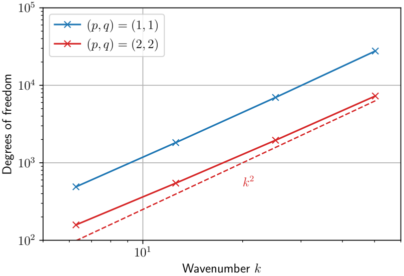


Figure: *DoFs versus wavenunber $k$ for target error $\epsilon \approx 10^{-3}$: Goal #1 achieved.*

# Numerical experiments – Helmholtz (cone-sphere)

Goal ▶ Solving 3D Helmholtz $\Delta u + k^2 u = 0$ (exterior Dirichlet problem)

**Far-field error**

- Find solution $u^s$ such that $u = u^i + u^s = 0$ on $\Gamma$ for $u^i(r,\theta) = e^{ikr\cos\theta}$
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$$|u^\infty(\boldsymbol{x}) - u_h^\infty(\boldsymbol{x})| \leq c \left( h^{p+2} \|\varphi^s\|_{H^{p+1}(\Gamma)} + h^{q+1} \|\varphi^s\|_{L_2(\Gamma)} \right)$$

Table: *Computer time to build the single-layer $\mathcal{S}$ and its $LU$ factors, and memory.*

| $k$ | Build ($\mathcal{S}$) | Memory ($\mathcal{S}$) | Build ($LU$) | Memory ($L$) |
|---|---|---|---|---|
| $2\pi$ | 1.45e+1 | 872.37 MB | 4.52e+1 | 301.17 MB |
| $4\pi$ | 1.72e+1 | 999.79 MB | 7.38e+1 | 375.09 MB |
| $8\pi$ | 2.20e+2 | 1235.0 MB | 1.87e+2 | 572.26 MB |
| $2\pi$ | 1.40e+1 | 179.88 MB | 7.89e+0 | 68.007 MB |
| $4\pi$ | 1.55e+1 | 208.40 MB | 1.38e+1 | 85.899 MB |
| $8\pi$ | 1.83e+1 | 260.30 MB | 3.64e+1 | 132.35 MB |

# Numerical experiments – Helmholtz (half-spheres)

Goal ▶ Solving 3D Helmholtz $\Delta u_\delta + k^2 u_\delta = 0$ (exterior Dirichlet problem)

**Far-field error**

- Find solution $u_\delta^s$ such that $u_\delta = u^i + u_\delta^s = 0$ on $\Gamma$ for $u^i(r,\theta) = e^{ikr\cos\theta}$
- Single-layer potential formulation of the integral equation $\mathcal{S}_\delta \varphi_\delta^s = -u^i$
- Solve for $\varphi_\delta^s$ with $h \ll 1$, then evaluate $u_\delta^s$ at "infinity" $\longrightarrow u_\delta^\infty$ (far-field)

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

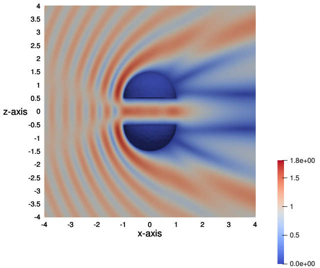


Figure: *Acoustic scattering of a plane wave by half-spheres in 3D* ($\delta = 0.5$).

# Numerical experiments – Helmholtz (half-spheres)

Goal ▶ Solving 3D Helmholtz $\Delta u_\delta + k^2 u_\delta = 0$ (exterior Dirichlet problem)

**Far-field error**

- Find solution $u_\delta^s$ such that $u_\delta = u^i + u_\delta^s = 0$ on $\Gamma$ for $u^i(r,\theta) = e^{ikr\cos\theta}$
- Single-layer potential formulation of the integral equation $\mathcal{S}_\delta \varphi_\delta^s = -u^i$
- Solve for $\varphi_\delta^s$ with $h \ll 1$, then evaluate $u_\delta^s$ at "infinity" $\longrightarrow u_\delta^\infty$ (far-field)

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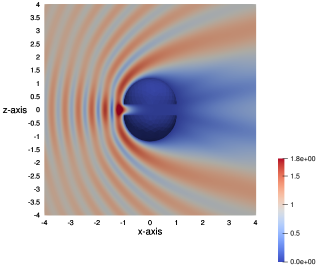


Figure: *Acoustic scattering of a plane wave by half-spheres in 3D* $(\delta = 0.2)$.

# Numerical experiments – Helmholtz (half-spheres)

Goal ▶ Solving 3D Helmholtz $\Delta u_\delta + k^2 u_\delta = 0$ (exterior Dirichlet problem)

**Far-field error**

- Find solution $u_\delta^s$ such that $u_\delta = u^i + u_\delta^s = 0$ on $\Gamma$ for $u^i(r,\theta) = e^{ikr\cos\theta}$
- Single-layer potential formulation of the integral equation $\mathcal{S}_\delta \varphi_\delta^s = -u^i$
- Solve for $\varphi_\delta^s$ with $h \ll 1$, then evaluate $u_\delta^s$ at "infinity" $\longrightarrow u_\delta^\infty$ (far-field)

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

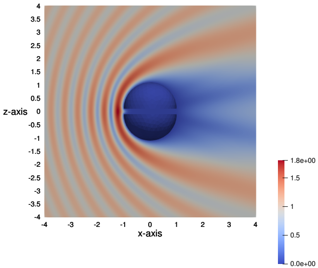


Figure: *Acoustic scattering of a plane wave by half-spheres in 3D* $(\delta = 0.1)$.

# Numerical experiments – Helmholtz (half-spheres)

Goal ▶ Solving 3D Helmholtz $\Delta u_\delta + k^2 u_\delta = 0$ (exterior Dirichlet problem)

**Far-field error**

- Find solution $u_\delta^s$ such that $u_\delta = u^i + u_\delta^s = 0$ on $\Gamma$ for $u^i(r, \theta) = e^{ikr\cos\theta}$
- Single-layer potential formulation of the integral equation $\mathcal{S}_\delta \varphi_\delta^s = -u^i$
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$$|u^\infty(\boldsymbol{x}) - u_\delta^\infty(\boldsymbol{x})| \leq c\delta^\ell$$

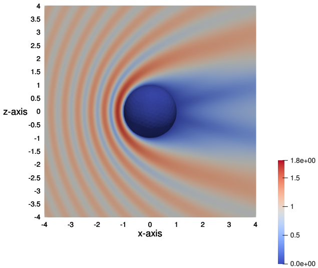


Figure: *Acoustic scattering of a plane wave by half-spheres in 3D* $(\delta = 0)$.

# Numerical experiments – Helmholtz (half-spheres)

Goal ▶ Solving 3D Helmholtz $\Delta u_\delta + k^2 u_\delta = 0$ (exterior Dirichlet problem)

**Far-field error**

- Find solution $u_\delta^s$ such that $u_\delta = u^i + u_\delta^s = 0$ on $\Gamma$ for $u^i(r,\theta) = e^{ikr\cos\theta}$
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$$|u^\infty(\boldsymbol{x}) - u_\delta^\infty(\boldsymbol{x})| \le c\delta^\ell$$

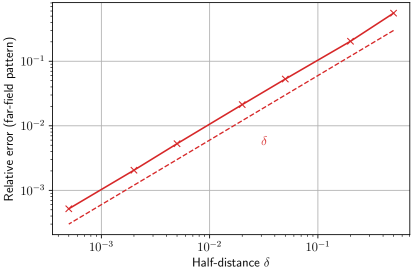



Figure: *Convergence of the far-field of the half-spheres as $\delta \to 0$: Goal #2 achieved.*

# Numerical experiments – Software

## Singular integrals

- Implemented in Python, available on GitHub (≈ 2000 ++)
- Shorter code for simple examples, available in 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++, available as part of `castor` (≈ 3,000 ++)
- 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

# Strongly singular integrals – Setup & Method

## Setup

- The double-layer potential involves the gradient

$$\nabla_{\boldsymbol{y}} G = \frac{1}{4\pi}\frac{(\boldsymbol{x}-\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|^3} + \frac{k^2}{8\pi}\frac{(\boldsymbol{x}-\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|} + \frac{S(|\boldsymbol{x}-\boldsymbol{y}|)}{4\pi}(\boldsymbol{x}-\boldsymbol{y})$$

- Therefore, we have to compute strongly singular integrals of the form of

$$\mathcal{J}(\boldsymbol{x}_0) = \int_{\widehat{T}} \frac{(F(\hat{\boldsymbol{x}}) - F(\hat{\boldsymbol{x}}_0) - h\boldsymbol{n}_0/|\boldsymbol{n}_0|)\cdot \boldsymbol{n}(F(\hat{\boldsymbol{x}}))}{|F(\hat{\boldsymbol{x}}) - \boldsymbol{x}_0|^3}\varphi(\hat{\boldsymbol{x}})dS(\hat{\boldsymbol{x}})$$

## Method

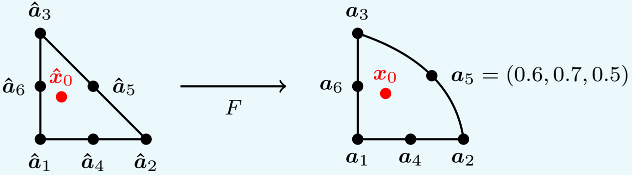
- If $h = 0$, then the integrand $\mathcal{O}(\delta\hat{x}^{-1})$
  - No regularization gives $\mathcal{O}(N^{-0.5})$, $T_{-1}$ regularization yields $\mathcal{O}(N^{-1})$
- If $h \neq 0$, then the integrand is $\mathcal{O}(\delta\hat{x}^{-2})$
  - Need $T_{-2}$ regularization to get $\mathcal{O}(N^{-0.5})$, $T_{-1}$ regularization yields $\mathcal{O}(N^{-1})$
- Steps 1–5 as before, some subtleties when regularizing, *e.g.*,

$$T_{-2}(\hat{\boldsymbol{x}}, h) = \frac{-h}{[|\hat{\boldsymbol{x}} - \hat{\boldsymbol{x}}_0|^2 + h^2]^{\frac{3}{2}}}$$

# Strongly singular integrals – Experiments

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

**Setup**



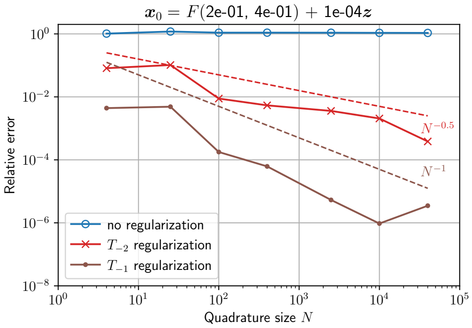
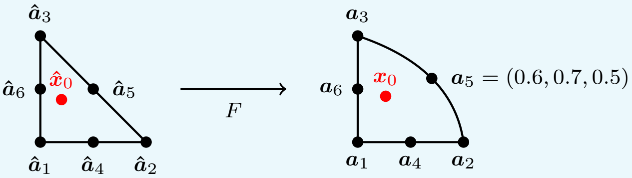




Figure: *Error versus quadrature size.*

# Strongly singular integrals – Experiments

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

Setup



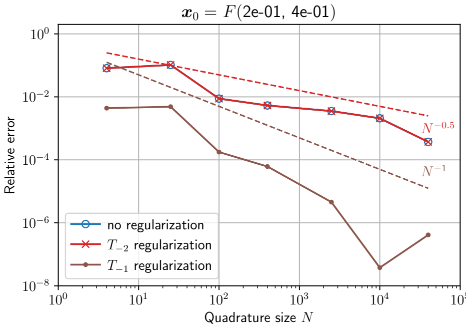




Figure: *Error versus quadrature size.*

# Future work

Goal ▶ High-order methods for scattering by 3D geometric objects

**Outine**

- Strongly singular integrals in high-order elements (*ongoing*)
- Inverse scattering problems in uncertain environments (*ongoing*)
- Hierarchical solvers for high-order elements (*short-term*)
- Study of 3D resonators (*short-term*)
- More sophisticated models (*long-term*)
  - Multi-trace boundary formulations
  - Forward and inverse Maxwell's equations and elasticity problems

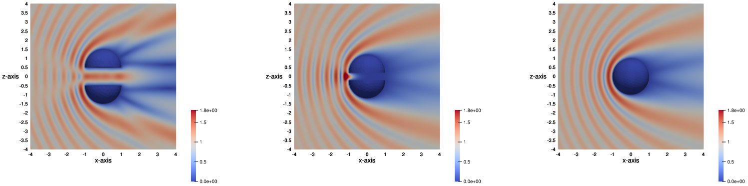



Figure: *Acoustic scattering of a plane wave by half-spheres in 3D.*