

An introduction to high-order boundary integral equation methods

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Why learn boundary integral equations?

In some applications boundary integral equation are

- Faster
- More accurate

than volume discretization schemes.

Useful in both academic and industrial context:

- Airbus
- Shell
- Naval group
- ...

Can be combined with volume methods such as FEM or finite volume to exploit the best of both worlds (FEM+BEM coupling)

Why learn high-order BIE methods?

- For smooth solutions, high-order tends to be faster than refining the mesh, specially in applications requiring high accuracy.
- Increasing the order does not incur in extra fill-in for BIE methods
- Accurate computation of matrix entries can improve conditioning
- Most importantly: **complementary** to other techniques such as adaptive mesh refinement

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- 2 Discretization techniques
- 3 Singular quadratures
- 4 Nyström method: an example

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Notation and problem formulation

Example of B.V.P. problem

$$\Delta u = 0$$

$$r \in \Omega,$$

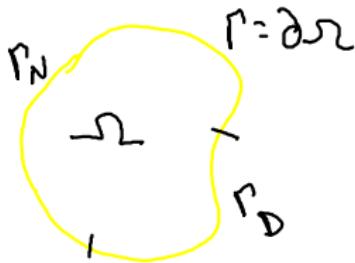
$$u = f$$

$$x \in \Gamma_D,$$

$$\partial_n u = g$$

$$x \in \Gamma_N.$$

- $\Omega \subset \mathbb{R}^d$: open and bounded domain with boundary $\Gamma = \partial\Omega$
- $u : \Omega \rightarrow \mathbb{R}$ is the solution
- f, g are the boundary datum



Reciprocity relation

Let u, v be sufficiently regular. Then by **divergence theorem**:

Reciprocity for Laplace

$$\begin{aligned}\int_{\Omega} (v \Delta u - u \Delta v) \, d\Omega &= \int_{\Omega} \nabla \cdot (u \nabla v - v \nabla u) \, d\Omega \\ &= \int_{\Gamma} \left(\underbrace{u}_{\gamma_0 u} \underbrace{\nabla v \cdot n}_{\gamma_1 v} - \underbrace{v}_{\gamma_0 v} \underbrace{\nabla u \cdot n}_{\gamma_1 u} \right) \, d\Gamma\end{aligned}$$

- γ_0 is the Dirichlet trace operator
- γ_1 is the Neumann trace operator
- Formally viewed as



$$(\gamma_0 u)(x) = \lim_{\varepsilon \rightarrow 0^+} u(x - \varepsilon n)$$

$$(\gamma_1 u)(x) = \lim_{\varepsilon \rightarrow 0^+} \nabla u(x - \varepsilon n) \cdot n(x)$$

Boundary integral representation: idea

Reciprocity for Laplace

$$\int_{\Omega} (v \Delta u - u \Delta v) \, d\Omega = \int_{\Gamma} (\underbrace{u}_{\gamma_0 u} \underbrace{\nabla v \cdot n}_{\gamma_1 v} - \underbrace{v}_{\gamma_0 v} \underbrace{\nabla u \cdot n}_{\gamma_1 u}) \, d\Gamma$$

- Let u be a solution of $\Delta u = 0$
- For a fixed \mathbf{x} , let $v(\mathbf{y}) = G(\mathbf{x}, \mathbf{y})$, with $\Delta G = -\delta(\mathbf{x} - \mathbf{y})$.
- If $\mathbf{x} \notin \overline{\Omega}$,

$$0 = \int_{\Gamma} (\gamma_0 u(\mathbf{y}))(\gamma_1 G(\mathbf{x}, \mathbf{y})) - (\gamma_0 G(\mathbf{x}, \mathbf{y}))(\gamma_1 u(\mathbf{y})) \, d\Gamma(\mathbf{y})$$

- If $\mathbf{x} \in \Omega$
 - Consider a punctured domain $\Omega_{\varepsilon}(\mathbf{x}) = \Omega \setminus B_{\varepsilon}(\mathbf{x})$
 - Apply the reciprocity identity on $\Omega_{\varepsilon}(\mathbf{x})$
 - Let $\varepsilon \rightarrow 0$ and compute contributions from $\partial\Omega_{\varepsilon}(\mathbf{x})$



⇒ Boundary integral representation.

Boundary integral representation

Leads to the following **fundamental relation**

Greens representation formula

$$\mathcal{S}[\gamma_1 u](\mathbf{x}) - \mathcal{D}[\gamma_0 u](\mathbf{x}) = \begin{cases} u(\mathbf{x}) & \mathbf{x} \in \Omega \\ 0 & \mathbf{x} \notin \bar{\Omega} \end{cases}$$

where:

Definition (Single and double-layer potentials)

$$\mathcal{S}[\sigma](\mathbf{x}) := \int_{\Gamma} G(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) \, d\Gamma(\mathbf{y})$$

$$\mathcal{D}[\sigma](\mathbf{x}) := \int_{\Gamma} (\nabla_{\mathbf{y}} G(\mathbf{x}, \mathbf{y}) \cdot \mathbf{n}(\mathbf{y})) \sigma(\mathbf{y}) \, d\Gamma(\mathbf{y})$$

⚠ Valid for $\mathbf{x} \notin \Gamma$!

Boundary integral representation

Greens (interior) representation formula

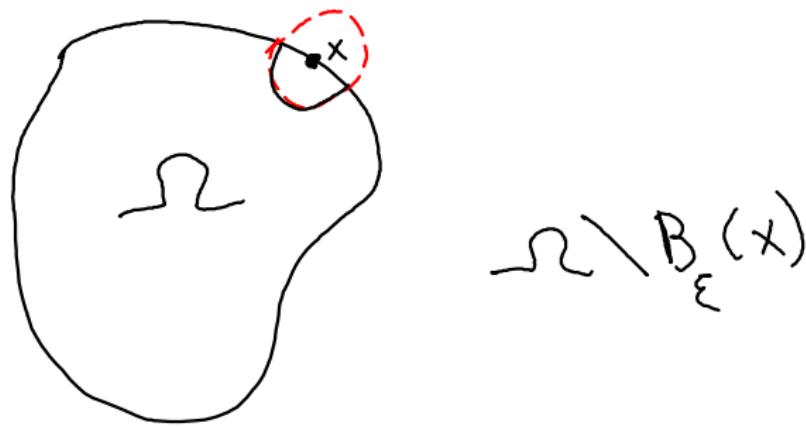
$$\mathcal{S}[\gamma_1 u](\mathbf{x}) - \mathcal{D}[\gamma_0 u](\mathbf{x}) = \begin{cases} u(\mathbf{x}) & \mathbf{x} \in \Omega \\ 0 & \mathbf{x} \notin \bar{\Omega} \end{cases}$$

Important remarks:

- This is a representation, **not an equation**
- The traces $\gamma_0 u$ and $\gamma_1 u$ fully determine the solution
- Typically one trace is given as B.C., and you find the other
- A fundamental solution $G(\mathbf{x}, \mathbf{y})$ must be known
- The kernels in \mathcal{S} and \mathcal{D} are analytic for $\mathbf{x} \notin \Gamma$
- As $\Omega \ni \mathbf{x} \rightarrow \mathbf{y} \in \Gamma$ kernels blow up since $G(\mathbf{x}, \mathbf{x})$ is singular

⇒ next step: obtain an equation from the representation

Boundary integral equations: sketch



Boundary integral equation

“Applying” the trace operators to the representation formula:

Greens' identities

$$\frac{1}{2}(\gamma_0 u)(x) = S[\gamma_1 u](x) - D[\gamma_0 u](x) \quad x \in \Gamma$$

$$\frac{1}{2}(\gamma_1 u)(x) = D'[\gamma_1 u](x) - T[\gamma_0 u](x) \quad x \in \Gamma$$

Definition (Boundary integral operators)

$$S[\sigma](x) := \int_{\Gamma} G(x, y) \sigma(y) d\Gamma(y), \quad (\text{Single-layer})$$

$$D[\sigma](x) := \text{p.v.} \int_{\Gamma} (\gamma_{1,y} G(x, y)) \sigma(y) d\Gamma(y), \quad (\text{Double-layer})$$

$$D'[\sigma](x) := \text{p.v.} \int_{\Gamma} (\gamma_{1,x} G(x, y)) \sigma(y) d\Gamma(y), \quad (\text{Adjoint double-layer})$$

$$T[\sigma](x) := \text{f.p.} \int_{\Gamma} \gamma_{1,x} (\gamma_{1,y} G(x, y)) \sigma(y) d\Gamma(y) \quad (\text{Hypersingular})$$

Boundary integral operators

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- The **fast** and **accurate** approximation of S, D, D', T are fundamental components of BIE methods
- **fast** \approx acceleration techniques (FMM, H-Matrices, ...)
- **accurate** \approx singular integration

⚠ We will return to the meaning of p.v. and f.p. later. For the moment keep in mind that these are not classical integrals!

Generalization: some examples

Many other PDEs which are amenable to BIE formulation:

$$\mathcal{L}u = \begin{cases} -\Delta u & (\text{Laplace}), \\ -\Delta u - (\omega/c)^2 u & (\text{Helmholtz}), \\ -\mu\Delta u - (\mu + \lambda)\nabla(\nabla \cdot u) & (\text{elastostatic}), \\ -\mu\Delta u - (\mu + \lambda)\nabla(\nabla \cdot u) - \omega^2\rho u & (\text{elastodynamic}), \end{cases}$$

The definition of the traces has to be modified:

$$(\gamma_1 u)(\mathbf{x}) = \begin{cases} \lim_{\varepsilon \rightarrow 0^+} \nabla u(\mathbf{x} - \varepsilon \mathbf{n}(\mathbf{x})) \cdot \mathbf{n}(\mathbf{x}) & (\text{Laplace/Helmholtz}) \\ \lim_{\varepsilon \rightarrow 0^+} \{ \lambda (\nabla \cdot u(\mathbf{x} - \varepsilon \mathbf{n}(\mathbf{x}))) \mathbf{n}(\mathbf{x}) + 2\mu \nabla u(\mathbf{x} - \varepsilon \mathbf{n}(\mathbf{x})) \cdot \mathbf{n}(\mathbf{x}) \\ + \mu \mathbf{n}(\mathbf{x}) \times (\nabla \times u(\mathbf{x} - \varepsilon \mathbf{n}(\mathbf{x}))) \} & (\text{Elastostatics/elastodynamics}). \end{cases}$$

William McLean and William Charles Hector McLean. *Strongly elliptic systems and boundary integral equations*. Cambridge university press, 2000

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Outline of a BIE solution process

- ① Choose a boundary integral representation
- ② Discretize the required boundary integral operators
- ③ Solve the resulting linear system
- ④ Compute the quantity of interest using the representation

The three classes of methods

Consider the following integral equation on Γ :

$$\frac{1}{2} u(\mathbf{x}) + \int_{\Gamma} K(\mathbf{x}, \mathbf{y}) u(\mathbf{y}) \, d\Gamma(\mathbf{y}) = f(\mathbf{x}),$$

- $K(\mathbf{x}, \mathbf{y})$ is a known kernel (think $K(\mathbf{x}, \mathbf{y}) = G(\mathbf{x}, \mathbf{y})$)
- f is known

There are essentially three classes of BIE methods:

- Collocation method
- Galerkin method
- Nyström method

Collocation method

Continuous problem

$$u(x) + \int_{\Gamma} K(x, y) u(y) d\Gamma(y) = f(x)$$

4

Discrete problem

$$(I + A)c = f$$

- ① Expand $u(x) \approx \sum_{j=1}^N c_j v_j(x)$ where v_n are appropriate basis functions
- ② Replace into equation and enforce equality on N collocation points x_i :

$$\sum_j c_j \underbrace{v_j(x_i)}_{I_{ij}} + \sum_j c_j \underbrace{\int_{\Gamma} K(x_i, y) v_j(y) d\Gamma(y)}_{A_{ij}} = f(x_i).$$

- ③ Solve linear system for c_j

Note that if v_j are nodal basis functions, I is the identity matrix.

Continous problem

$$u(x) + \int_{\Gamma} K(x, y) u(y) d\Gamma(y) = f(x)$$

Discrete problem

$$(I + A) c = f$$

- ① Expand $u(x) \approx \sum_{j=1}^N c_j v_j(x)$ where v_j are trial functions.
- ② Multiply equation by test functions v_i , integrate, and reinforce equality:

$$\sum_j c_j \underbrace{\int_{\Gamma} v_i(x) v_j(x) d\Gamma(x)}_{I_{ij}} + \sum_j c_j \underbrace{\int_{\Gamma} \int_{\Gamma} v_i(x) K(x, y) v_j(y) d\Gamma(y) d\Gamma(x)}_{A_{ij}} = \int_{\Gamma} v_i(x) f(x) d\Gamma(x).$$

- ③ Solve linear system for c_j

Note the double integrals in A_{ij} .

Nyström method

Continous problem

$$u(\mathbf{x}) + \int_{\Gamma} K(\mathbf{x}, \mathbf{y}) u(\mathbf{y}) d\Gamma(\mathbf{y}) = f(\mathbf{x})$$

Discrete problem

$$(\mathbf{I} + \mathbf{A}) \mathbf{c} = \mathbf{f}$$

- ① Use a quadrature $\mathcal{Q} = \{\mathbf{x}_i, w_i\}_{i=1}^N$ to approximate the integral:

$$\int_{\Gamma} K(\mathbf{x}, \mathbf{y}) u(\mathbf{y}) dy \approx \sum_{j=1}^N K(\mathbf{x}, \mathbf{x}_j) \underbrace{u(\mathbf{x}_j)}_{c_j} w_j$$

- ② Replace this approximation into the equation, and impose equality on \mathbf{x}_i :

$$c_i + \sum c_j \underbrace{K(\mathbf{x}_i, \mathbf{x}_j) w_j}_{\mathbf{A}_{ij}} = f(\mathbf{x}_i)$$

- ③ Solve for c_j

- ④ Use **Nystrom interpolant**: $u(\mathbf{x}) \approx f(\mathbf{x}) - \sum_{j=1}^N K(\mathbf{x}, \mathbf{x}_j) w_j$

The three methods

$$A[\sigma](\mathbf{x}) := \int_{\Gamma} K(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) \, d\Gamma(\mathbf{y}) \approx \dots$$

Collocation: \mathbf{x}_i collocation points, v_j basis functions

$$A_{ij} = \int_{\Gamma} K(\mathbf{x}_i, \mathbf{y}) v_j(\mathbf{y}) \, d\Gamma(\mathbf{y}),$$

Galerkin: v_j test/trial functions

$$A_{ij} = \int_{\Gamma} \int_{\Gamma} v_i(\mathbf{x}) K(\mathbf{x}, \mathbf{y}) v_j(\mathbf{y}) \, d\Gamma(\mathbf{y}) d\Gamma(\mathbf{x})$$

Nystrom: $\mathcal{Q} = \{\mathbf{x}_i, w_i\}$ surface quadrature

$$A_{ij} = K(\mathbf{x}_i, \mathbf{x}_j) w_j$$

We need to talk about quadratures...

The three methods

Important remarks:

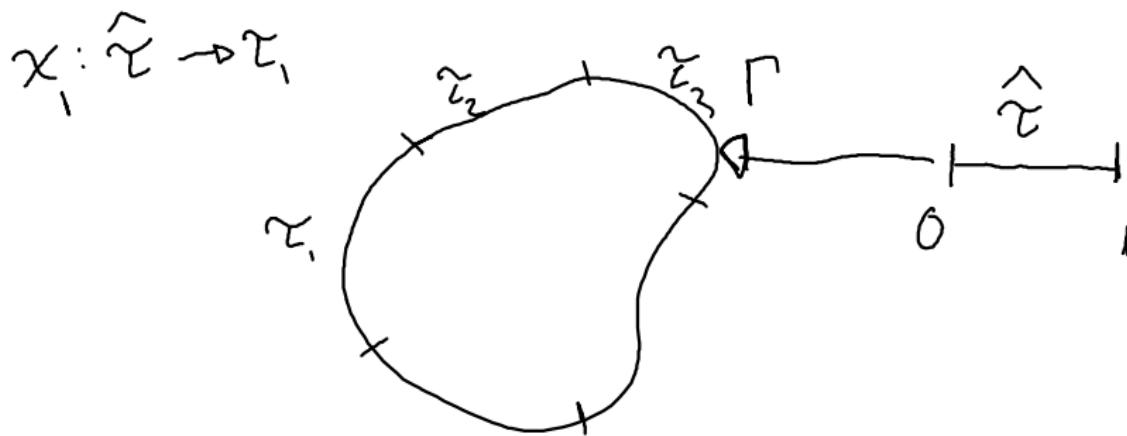
- All methods have advantages and disadvantages
- Some techniques we will see apply to all three methods, some require modifications
- Choice of method depends on available code, geometry representation, desired accuracy, ...

Focus on Nyström methods

Geometry representation

Let $\Gamma \subset \mathbb{R}^d$ be our curve/surface. We will suppose:

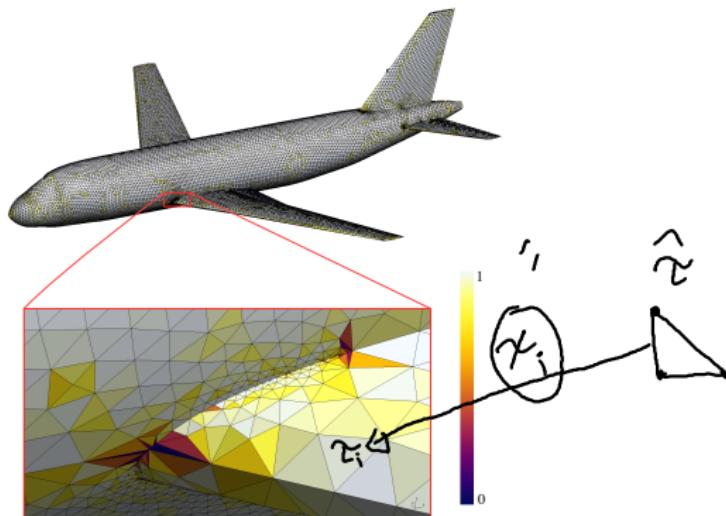
- ① We have an open covering by τ_m elements: $\Gamma = \bigcup_{m=1}^M \overline{\tau_m}$
- ② The elements are non-overlapping: $\tau_i \cap \tau_j = \emptyset$ if $i \neq j$
- ③ A bijective map χ_m from a reference element $\hat{\tau} \subset \mathbb{R}^{d-1}$ to $\tau \subset \mathbb{R}^d$ is given



Geometry representation

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⚠ For realistic problems this is non-trivial step.

Passing through the reference element

The decomposition of Γ means:

$$\int_{\Gamma} K(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) d\Gamma(\mathbf{y}) = \sum_m \int_{\tau_m} \underbrace{K(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y})}_{x \text{ near } \gamma_m} d\Gamma(\mathbf{y})$$
$$= \sum_m \int_{\hat{\tau}} K(\mathbf{x}, \chi_m \circ \hat{\mathbf{y}}) \sigma(\chi_m \circ \hat{\mathbf{y}}) \mu_m(\hat{\mathbf{y}}) d\hat{\mathbf{y}}$$

- $\mu_m = \sqrt{\det(J^\top J)}$ is a metric, where J is the jacobian of μ_m .
- For a fixed $\mathbf{x} \in \tau_n$, $\mathbf{x} = \chi_n(\hat{\mathbf{x}})$, difficulties arise for elements “near” τ_n
- With some bookkeeping, suffices to consider integrals in reference domain

$$\int_{\hat{\tau}} \underbrace{K(\chi_n \circ \hat{\mathbf{x}}, \chi_m \circ \hat{\mathbf{y}}) \mu_m(\hat{\mathbf{y}})}_{\hat{K}_{m,n}(\hat{\mathbf{x}}, \hat{\mathbf{y}})} \underbrace{\sigma(\chi_m \circ \hat{\mathbf{y}})}_{\hat{\sigma}_m(\hat{\mathbf{y}})} d\hat{\mathbf{y}}$$

⚠ We will often use a *hat* to denote variables in parameter space

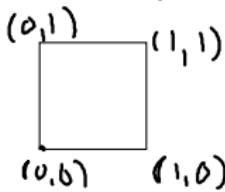
Reference domains

Three reference domains $\hat{\tau}$ will be considered:

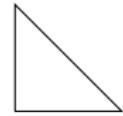
Reference line



Reference square



Reference triangle



For each, will develop quadrature rules for integrating functions which are singular (or nearly-singular) on $\hat{\tau}$.

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Quadratures

- A quadrature is just a set of nodes and weights used to approximate an integral: $\mathcal{Q}_N = \{\hat{x}_i, w_i\}_{i=1}^N$

$$Q[f] := \int_{\hat{\tau}} f(\hat{x}) d\hat{x} \approx \mathcal{Q}_N[f] := \sum_{i=1}^N f(\hat{x}_i) w_i$$

- Depending on domain $\hat{\tau}$, several choices are available
- Error can be studied as $N \rightarrow \infty$, or as $|\hat{\tau}| \rightarrow 0$
- Most quadratures are designed to accurately integrate regular functions
- In 1D, two very important rules: Gauss-Legendre and Trapezoidal

Regular quadratures: Gauss-Legendre

Theorem (Gauss-Legendre quadrature)

Let P_N be the Legendre polynomial of degree n normalized so that

$P_n(1) = 1$. Let x_i be the i -th root of P_n , and $w_i = \frac{2}{(1-x_i^2)P'_n(x_i)^2}$. Then

$$\int_{-1}^1 x^k dx = \sum_{i=1}^n x_i^k w_i \quad \forall \quad 0 \leq k \leq 2N - 1.$$

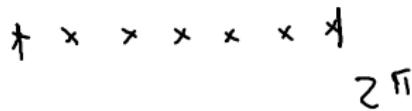
$$\int_{-1}^1 P_i(x) P_j(x) dx = \delta_{ij}$$

Regular quadratures: trapezoidal

Theorem (Trapezoidal quadrature)

Let $g : \mathbb{R} \rightarrow \mathbb{R}$ be analytic and 2π -periodic. Then $\exists s > 0, M > 0$ s.t.

$$\left| \int_0^{2\pi} g(x) dx - \frac{1}{2n} \sum_{j=0}^{2n-1} g(j\pi/n) \right| \leq M (\coth ns - 1) = \mathcal{O}(e^{-2ns})$$



Weakly singular kernels

For the first part, focus on weakly-singular operators:

$$A[\sigma](x) = \int_{\Gamma} K(x, y) \sigma(y) \, d\Gamma(y)$$

Definition (Weakly-singular kernel)

A kernel K is said to be weakly singular if K is defined and continuous for all x and $y \neq x$ in $\Gamma \subset \mathbb{R}^d$, and there exists constants $\alpha \in (0, 2]$ and $M > 0$ such that for all $x, y \in \Gamma$, $y \neq x$, we have

$$|K(x, y)| \leq M|x - y|^{\alpha-d+1}$$

- $d = 2 \rightarrow K(x, y) \sim \log(|x - y|)$ is weakly-singular
- $d = 3 \rightarrow K(x, y) \sim 1/|x - y|$ is weakly-singular
- $G(x, y)$ is always weakly-singular

⚠ Lead to integrable singularities and compact operators on $C(\Gamma)$

David Colton and Rainer Kress. *Integral equation methods in scattering theory*.
SIAM, 2013, Section 1.1

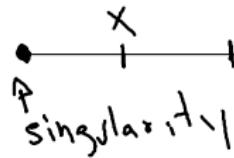
Weakly-singular operators

Change-of-variable quadratures

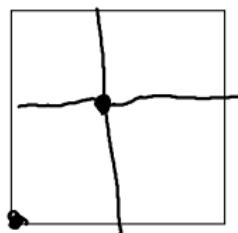
$$\int_{\hat{\tau}} K(\hat{x}, \hat{y}) \hat{\sigma}(\hat{y}) d\hat{y}, \quad \hat{x} \in \hat{\tau}$$

- K is weakly-singular
- $\hat{\tau}$ is one of the following:

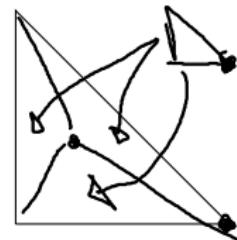
Reference line



Reference square



Reference triangle



- Base case: singularity \hat{x} is always at a vertex (draw)

Weakly-singular operators

One-dimensional case

$$\int_{\hat{\tau}} K(\hat{x}, \hat{y}) \hat{\sigma}(\hat{y}) d\hat{y}, \quad \hat{x} \in \hat{\tau}$$

- K is weakly-singular
- $\hat{\tau}$ is a reference line



Develop quadrature rules for this type of integrals:

$$\int_0^1 g(s) ds, \quad g \sim \log |s| \quad \text{as } s \rightarrow 0$$

Weakly-singular operators in two dimensions

Change-of-variable quadratures

$$\int_0^1 g(s) \, ds, \quad g \sim \log |s| \quad \text{as } s \rightarrow 0$$

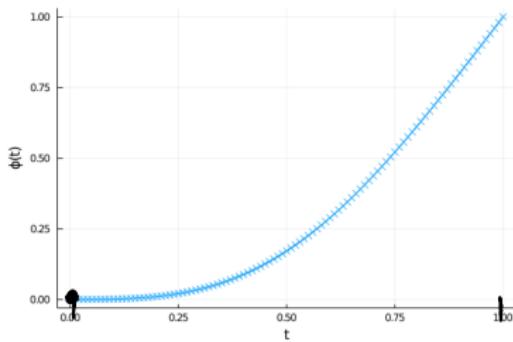
- Let $\phi(t)$ be

$$\phi \sim t^{P+1}$$

- Bijective
- Monotonically increasing
- Infinitely differentiable.
- $\phi^{(n)}(0) = 0, n = 1, \dots, P$

- Then letting $s = \phi(t)$ we obtain

$$\int_0^1 g(s) \, ds = \int_0^1 g(\phi(t))\phi'(t) \, dt$$



Proposition (Regularity of integrand)

The integrand $\tilde{g}(t) := g(\phi(t))\phi'(t)$ is $P - 1$ times continuously differentiable.

$$\log 1+t^1 t^P$$

Weakly-singular operators in two dimensions

Change-of-variable quadratures

Theorem (Convergence of Gauss-Legendre quadrature)

If $f \in C^{P-1}$ for some $k > 2$, the error of the n -point Gauss-Legendre quadrature decays as $\mathcal{O}(n^{-P-1})$

- Convergence is polynomial, controlled by the regularity
- Combining this with previous result, we obtain

$$\left| \int_{-1}^1 g(\phi(t))\phi'(t) dt - \sum_{n=1}^N g(\phi(t_i))\phi'(t_i)w_i \right| = \mathcal{O}\left(\frac{1}{N^{P+1}}\right)$$

where t_i, w_i are the Gauss-Legendre nodes and weights.

- \Rightarrow the modified quadrature $\mathcal{Q} = \{\phi(t_i), w_i\phi'(t_i)\}$ converges to high-order

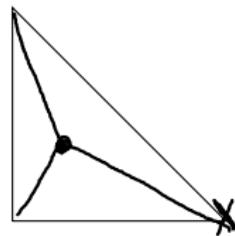
Shuhuang Xiang and Folkmar Bornemann. "On the convergence rates of Gauss and Clenshaw–Curtis quadrature for functions of limited regularity". In: *SIAM Journal on Numerical Analysis* 50.5 (2012), pp. 2581–2587

Weakly-singular operators

Reference triangle

$$\int_{\hat{\tau}} K(\hat{x}, \hat{y}) \hat{\sigma}(\hat{y}) \, d\hat{y}, \quad \hat{x} \in \hat{\tau}$$

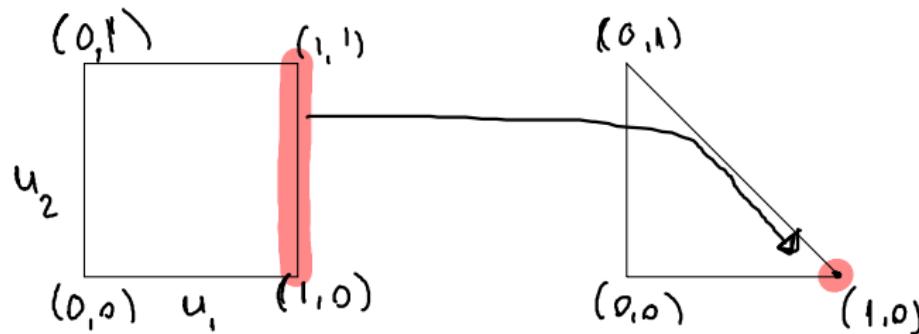
- K is weakly-singular
- $\hat{\tau}$ is a reference triangle



Weakly-singular operators

Duffy change of variables

- $\phi(\mathbf{u}) = (u_1, (1 - u_1)u_2)$. Maps $\square \rightarrow \triangle$:



- Jacobian is

$$\begin{bmatrix} 1 & -u_2 \\ 0 & 1-u_1 \end{bmatrix}$$

- Singular at $(1,0)$ edge of triangle

Weakly-singular operators

Duffy quadrature

- Let $f(\hat{\mathbf{x}}) = \frac{g(\hat{\mathbf{x}})}{\|\hat{\mathbf{x}} - (1,0)\|}$, $g(\mathbf{x}) \in C^\infty$
- Change variables : $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2) = \phi(\mathbf{u}) = (u_1, (1-u_1)u_2)$

$$\int_0^1 \int_0^{1-\hat{x}_1} \frac{g(\hat{\mathbf{x}})}{\sqrt{(\hat{x}_1 - 1)^2 + \hat{x}_2^2}} d\hat{x}_2 d\hat{x}_1$$
$$= \int_0^1 \int_0^1 \frac{g(\phi(\mathbf{u}))}{|u_1 - 1| \sqrt{1 + u_2^2}} |u_1 - 1| du_1 du_2$$

- Apply regular quadrature over unit square

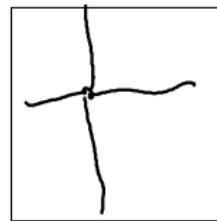


Weakly-singular operators

Change-of-variable quadratures

$$\int_{\hat{\tau}} K(\hat{\mathbf{x}}, \hat{\mathbf{y}}) \hat{\sigma}(\hat{\mathbf{y}}) d\hat{\mathbf{y}}, \quad \hat{\mathbf{x}} \in \hat{\tau}$$

- K is weakly-singular
- $\hat{\tau}$ is a reference square



- Option 1: split into rectangles + tensorize one-dimensional C.O.V.
- Option 2: split into triangles + Duffy C.O.V

Weakly-singular operators: recap

Saw how to compute integrals of the form

$$\int_{\hat{\tau}} K(\hat{\mathbf{x}}, \hat{\mathbf{y}}) \hat{\sigma}(\hat{\mathbf{y}}) d\hat{\mathbf{y}}, \quad \hat{\mathbf{x}} \in \hat{\tau}$$

where

- K is weakly-singular
- $\hat{\tau}$ is a reference segment, square, or triangle

by

- ➊ Splitting τ into base cases with singularity at endpoint/vertex
- ➋ Performing a degenerate change of variables ϕ
- ➌ Applying a regular quadrature on the transformed integral
- ➍ Mapping weights and nodes back to $\hat{\tau}$ if needed

Weakly-singular operators: recap

Many other methods for weakly-singular kernels not based on change-of-variables:

- Fourier decomposition + trapezoidal rule
- Quadrature-by-expansion (QBX)
- Density-interpolation
- Analytic integration for low order
- ...

Change-of-variable quadratures are generic and easy to understand

Singular integrals: principal value

- Weakly-singular operators are “just” improper integrals:

$$\int_{-1}^1 \frac{\log |t-s| f(s)}{\sqrt{\epsilon}} ds = \lim_{\epsilon \rightarrow 0} \int_{-1}^{-\delta_1(\epsilon)} \log |t-s| f(s) ds + \lim_{\epsilon \rightarrow 0} \int_{\delta_2(\epsilon)}^1 \log |t-s| f(s) ds$$

where $\delta_1, \delta_2 > 0$, $\delta_1, \delta_2 = o(1)$ as $\epsilon \rightarrow 0$.

- Singular integrals do not have a similar meaning:

$$t \in (-1, 1) \quad \int_{-1}^1 \frac{1}{t-s} f(s) ds \stackrel{?}{=} \lim_{\epsilon \rightarrow 0} \int_{-1}^{-\delta_1(\epsilon)} \frac{1}{t-s} f(s) ds + \lim_{\epsilon \rightarrow 0} \int_{\delta_2(\epsilon)}^1 \frac{1}{t-s} f(s) ds$$

⚠ The limits depends on *how* δ_1, δ_2 go to zero.

Singular integrals: principal value

- The Cauchy principal value is the limit when a ball is removed:

$$\text{p.v.} \int_{-1}^1 \frac{1}{t-s} f(s) \, ds := \lim_{\varepsilon \rightarrow 0} \int_{(-1,1) \setminus B_\varepsilon(t)} \frac{1}{t-s} f(s) \, ds$$

Example (Principal value)

$$\begin{aligned} \text{p.v.} \int_{-1}^1 \frac{1}{t-s} \, ds &= \lim_{\varepsilon \rightarrow 0} \int_{-1}^{t-\varepsilon} \frac{1}{t-s} \, ds + \lim_{\varepsilon \rightarrow 0} \int_{t+\varepsilon}^1 \frac{1}{t-s} \, ds \\ &= \log \varepsilon - \log(1+t) - \log \varepsilon + \log(1-t) \\ &\Rightarrow = \log \left(\frac{1-t}{1+t} \right) \end{aligned}$$

⚠ This corresponds closely to the limiting process behind the derivation of our boundary integral operators.

Singular integrals: principal value

Example (Principal value)

Let $f \in C^{0,\alpha}$ for some $\alpha > 0$. Then

$$\begin{aligned} \text{p.v.} \int_{-1}^1 \frac{1}{t-s} f(s) \, ds &= \int_{-1}^1 \underbrace{\frac{f(s) - f(t)}{t-s}}_{t-s} \, ds + f(t) \underbrace{\text{p.v.} \int_{-1}^1 \frac{1}{t-s} \, ds}_{\log\left(\frac{1-t}{1+t}\right)} \\ &= \underbrace{\int_{-1}^1 \frac{f(s) - f(t)}{t-s} \, ds}_{\text{p.v.}} + f(t) \log\left(\frac{1-t}{1+t}\right) \end{aligned}$$

- For a curve $\Gamma \subset \mathbb{R}^d$, define similarly

$$\text{p.v.} \int_{\Gamma} K(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) \, d\Gamma(\mathbf{y}) := \lim_{\varepsilon \rightarrow 0} \int_{\Gamma \setminus B_{\varepsilon}(\mathbf{t})} K(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) \, d\Gamma(\mathbf{y}) \, ds$$

⚠ Some assumptions are required on K for this definition to make sense¹.

¹Stefan A Sauter and Christoph Schwab. *Boundary element methods*. Springer, 2010, pp. 183–287, Section 5.1.2.

Singular integrals: finite part

- Can we make sense of even stronger singularities? Try similar idea:

$$\begin{aligned} \int_{-1}^1 \frac{1}{(t-s)^2} ds &\stackrel{?}{=} \lim_{\varepsilon \rightarrow 0} \int_{-1}^{t-\varepsilon} \frac{1}{(t-s)^2} ds + \lim_{\varepsilon \rightarrow 0} \int_{t+\varepsilon}^1 \frac{1}{(t-s)^2} ds \\ &= \frac{1}{t-s} \Big|_{-1}^{t-\varepsilon} + \frac{1}{t-s} \Big|_{t+\varepsilon}^1 \\ &= \underbrace{\left(\frac{2}{\varepsilon}\right)}_{\text{finite part}} + \underbrace{\frac{1}{1+t} - \frac{1}{1-t}}_{\text{finite part}} \end{aligned}$$

- Keep the finite part, and notice that

$$\frac{1}{1+t} - \frac{1}{1-t} = \frac{d}{dt} \log \frac{1+t}{1-t} = \underbrace{\frac{d}{dt} \text{p.v.} \int_{-1}^1 \frac{1}{s-t} ds}_{\text{finite part}}$$

Singular integrals: finite part

- Suggests defining

$$\text{f.p.} \int_{-1}^1 \frac{f(s)}{(s-t)^2} ds = \frac{d}{dt} \left\{ \text{p.v.} \int_{-1}^1 \frac{f(s)}{s-t} ds \right\}$$

- Alternatively, for $f \in C^{1,\alpha}$, $\alpha > 0$,

$$\begin{aligned} \text{f.p.} \int_{-1}^1 \frac{f(s)}{(s-t)^2} ds &= \int_{-1}^1 \frac{f(s) - f(t) - (s-t)f'(t)}{(s-t)^2} ds \\ &\quad + f(t)\text{f.p.} \int_{-1}^1 \frac{1}{(s-t)^2} ds \\ &\quad - f'(t)\text{p.v.} \int_{-1}^1 \frac{1}{s-t} ds \end{aligned}$$

⚠ Definition for a surface is more involved, but the idea is similar...

Singular integrals in BIE

- Cauchy principal value and Hadamard finite part integrals are an important component of BIE methods
- Change-of-variable quadratures cannot be directly applied
- Analytic manipulations are often performed to reduce the problem to a weakly-singular integral (e.g. integration by parts, subtracting an exact solution)
- In what follows we will discuss one possible regularization technique

Regularized formulation

$$\log r \rightarrow \frac{1}{r} \rightarrow \frac{1}{\gamma^2}$$

Definition (Boundary integral operators)

$$S[\sigma](\mathbf{x}) := \int_{\Gamma} G(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) d\Gamma(\mathbf{y}), \quad (\text{Single-layer})$$

$$D[\sigma](\mathbf{x}) := \text{p.v.} \int_{\Gamma} (\gamma_{1,y} G(\mathbf{x}, \mathbf{y})) \sigma(\mathbf{y}) d\Gamma(\mathbf{y}), \quad (\text{Double-layer})$$

$$D'[\sigma](\mathbf{x}) := \text{p.v.} \int_{\Gamma} (\gamma_{1,x} G(\mathbf{x}, \mathbf{y})) \sigma(\mathbf{y}) d\Gamma(\mathbf{y}), \quad (\text{Adjoint double-layer})$$

$$T[\sigma](\mathbf{x}) := \text{f.p.} \int_{\Gamma} \gamma_{1,x} (\gamma_{1,y} G(\mathbf{x}, \mathbf{y})) \sigma(\mathbf{y}) d\Gamma(\mathbf{y}) \quad (\text{Hypersingular})$$

derivative

- For Laplace/Helmholtz and sufficiently regular Γ (e.g. C^2), the double and adjoint double-layer kernels are weakly-singular
- We will focus on a regularization technique for the hypersingular based on Greens identities²

²Marc Bonnet. *Boundary integral equation methods for solids and fluids*. John Wiley, 1995.

Regularized formulation

Hypersingular operator for Laplace

- Suppose we wish to compute:

$$\rightarrow \left| T[\sigma](\mathbf{x}) := \text{f.p.} \int_{\Gamma} \gamma_{1,\mathbf{x}} (\gamma_{1,\mathbf{y}} G(\mathbf{x}, \mathbf{y})) \sigma(\mathbf{y}) d\Gamma(\mathbf{y}) \right|$$

- Fix $\mathbf{x} \in \Gamma$. In order to “regularize” this formulation, consider:

$$T[\sigma](\mathbf{x}) = \overbrace{\text{f.p.} \int_{\Gamma} \gamma_{1,\mathbf{x}} (\gamma_{1,\mathbf{y}} G(\mathbf{x}, \mathbf{y})) \{\sigma(\mathbf{y}) - \underline{\sigma(\mathbf{x})}\} d\Gamma(\mathbf{y})}^{} \\ + \underbrace{\sigma(\mathbf{x}) \text{f.p.} \int_{\Gamma} \gamma_{1,\mathbf{x}} (\gamma_{1,\mathbf{y}} G(\mathbf{x}, \mathbf{y})) d\Gamma(\mathbf{y})}_{}$$

⚠ Very similar to how one may define f.p. for one-dimensional integrals

Regularized formulation

Hypersingular operator for Laplace

$$\rightarrow \begin{cases} T[\sigma](\mathbf{x}) = \text{f.p.} \int_{\Gamma} \gamma_{1,\mathbf{x}} (\gamma_{1,\mathbf{y}} G(\mathbf{x}, \mathbf{y})) \{\underline{\sigma(\mathbf{y}) - \sigma(\mathbf{x})}\} d\Gamma(\mathbf{y}) \\ + \sigma(\mathbf{x}) \int_{\Gamma} \gamma_{1,\mathbf{x}} (\gamma_{1,\mathbf{y}} G(\mathbf{x}, \mathbf{y})) \underline{d\Gamma(\mathbf{y})} \end{cases}$$

- The first term has been regularized because of $\underline{\sigma(\mathbf{y}) - \sigma(\mathbf{x})}$.
- The second term can be simplified using Greens identity

Greens' identities

$$\frac{1}{2}(\gamma_0 u)(\mathbf{x}) = S[\gamma_1 u](\mathbf{x}) - D[\gamma_0 u](\mathbf{x}) \quad \gamma_1 \underline{=} ?$$
$$\frac{1}{2}(\gamma_1 u)(\mathbf{x}) = D'[\gamma_1 u](\mathbf{x}) - T[\gamma_0 u](\mathbf{x}) \quad = 0$$

- Since $u = 1$ is an interior solution of Laplace, it follows that $\underline{T[1]} = 0$

Regularized formulation

Hypersingular operator for Laplace

$$T[\sigma](\mathbf{x}) = \text{p.v.} \int_{\Gamma} \gamma_{1,\mathbf{x}}(\gamma_{1,\mathbf{y}} G(\mathbf{x}, \mathbf{y})) \underbrace{\{\sigma(\mathbf{y}) - \sigma(\mathbf{x})\}}_{f \cdot p} d\Gamma(\mathbf{y})$$

- Still a principal value integral
- Idea: interpolate σ to higher-order

$$T[\sigma](\mathbf{x}) = \underbrace{T[\sigma - \Psi](\mathbf{x})}_{\text{interp.}} + \underbrace{T[\Psi](\mathbf{x})}_{\text{Greens id}}$$

- For this to work, need:
 - ① $\sigma - \Psi = \mathcal{O}(|\mathbf{x} - \mathbf{y}|^2)$ as $\Gamma \ni \mathbf{y} \rightarrow \mathbf{x} \in \Gamma$
 - ② $T[\Psi]$ should be regular or easy to compute
- We will take $\Psi(\mathbf{y}; \mathbf{x}) = \sigma(\mathbf{x}) + \mathbf{c}(\mathbf{x}) \cdot \mathbf{y}$

Regularized formulation

Hypersingular operator for Laplace

- Since Ψ is harmonic:

$$T[\gamma_0 \Psi](\mathbf{x}) = D'[\gamma_1 \Psi](\mathbf{x}) - \frac{1}{2}(\gamma_1 \Psi)(\mathbf{x})$$

where

$$\gamma_1 \Psi(\mathbf{y}; \mathbf{x}) = \mathbf{c}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{y})$$

- Impose $\mathbf{c}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = 0$; i.e. $\mathbf{c}(\mathbf{x}) = c_1 t_1(\mathbf{x}) + c_2 t_2(\mathbf{x})$ where t_1, t_2 are vectors tangent to Γ at \mathbf{x} .
- Impose that $\sigma(\mathbf{y}) - \Psi(\mathbf{y}; \mathbf{x})$ vanish to second-order along Γ . That is, c_1, c_2 match surface derivatives of $\sigma(\mathbf{x})$. Similar to a Taylor series, but on a surface.

Regularized formulation

Hypersingular operator for Laplace

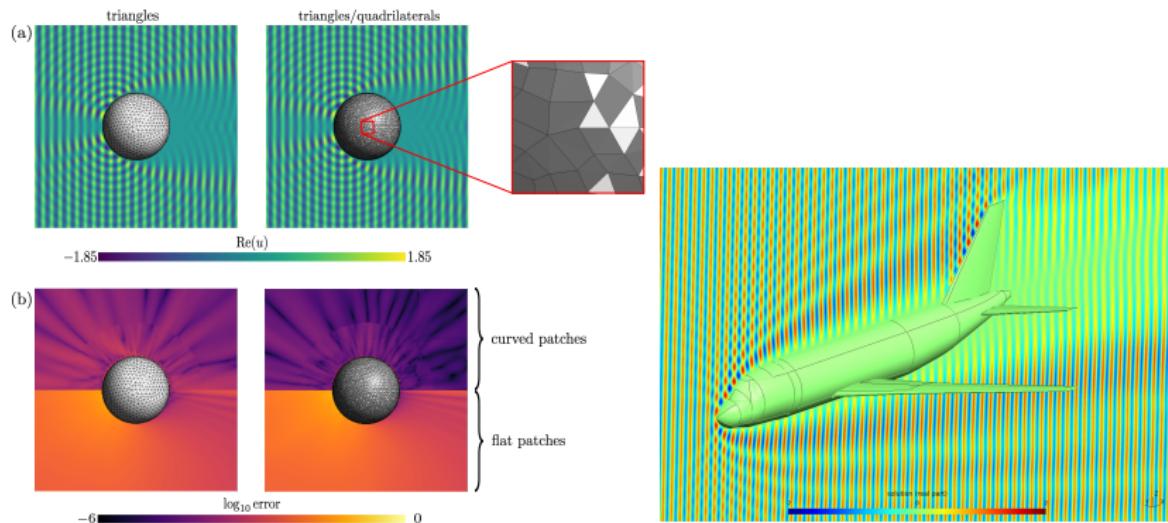
$$\begin{aligned} T[\sigma](\mathbf{x}) &= \underbrace{T[\sigma - \Psi](\mathbf{x})}_{\text{weakly-singular}} + \underbrace{T[\Psi](\mathbf{x})}_{\text{Greens}} \\ &= T[\sigma - \Psi](\mathbf{x}) + \underbrace{D'[\gamma_1 \Psi](\mathbf{x})}_{\text{weakly-singular}} - \frac{1}{2} \gamma_1 \Psi(\mathbf{x}) \end{aligned}$$

- Problem reduced to weakly-singular operators. Previous techniques apply.
- With minor modifications, can be applied to other PDEs
- Can be made dimension and kernel independent
- Also useful to regularize p.v. value integrals in elasticity

Regularized formulation

Hypersingular operator for Laplace

- Ideas can be generalized to arbitrarily high-order becoming an alternative to the aforementioned singular integration techniques³.



³Luiz M Faria, Carlos Pérez-Arcibia, and Marc Bonnet. “General-purpose kernel regularization of boundary integral equations via density interpolation”. In: *Computer methods in Applied mechanics and Engineering* (In press).

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- 1 A brief review
- 2 Discretization techniques
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- 4 Nyström method: an example

Putting it all together

Unwinding the stack

Problem

$$\begin{aligned}\Delta u = 0, \quad & \mathbf{x} \in \Omega, \\ \gamma_0 u = f, \quad & \mathbf{x} \in \Gamma\end{aligned}$$



Formulation

$$u(\mathbf{x}) = S[\sigma](\mathbf{x}), \quad \mathbf{x} \in \Omega$$

Equation

$$S[\sigma](\mathbf{x}) = f(\mathbf{x}), \quad \mathbf{x} \in \Gamma$$

- $\Gamma = \bigcup_{m=1}^M \tau_m$, where $\underline{\chi}_m : \hat{\Gamma} \rightarrow \tau_m$ is given
- Goal: assemble a high-order approximation of S

Putting it all together

$$\mathcal{S}[\sigma](\mathbf{x}) = f(\mathbf{x}), \quad \mathbf{x} \in \Gamma$$

- ① For each τ_m , construct a quadrature $\underline{\mathcal{Q}_m} = \{\underline{\mathbf{x}_{m,q}}, \underline{w_{m,q}}\}_{q=1}^P$
- ② Construct a glob2loc map: $i \rightarrow (m, q)$ and loc2glob map $(m, q) \rightarrow i$, where $1 \leq i \leq N = MP$ are the global indices
- ③ For $1 \leq i, j \leq N$, set $\underline{\mathbf{S}_{ij}^{(0)} = G(\mathbf{x}_i, \mathbf{x}_j)w_i}$ (dense)
- ④ Build $\mathbf{S}^{(1)}$ to correct the large errors on $\mathbf{S}^{(0)}$ for entries (i, j) for which $\underline{\mathbf{x}_i, \mathbf{x}_j}$ are close (sparse)

$$\mathbf{S} = \mathbf{S}^{(0)} + \mathbf{S}^{(1)} \quad \int_{\Gamma} G(\mathbf{x}_i, \mathbf{y}) \underline{v_j(\mathbf{y})}$$

↓ ↓

. . .

Correction matrix

- $m \rightarrow \mathcal{I}_m$ gives list of all indices i s.t. x_i is near τ_m

Algorithm 1: Correction matrix

Initialize $S^{(1)}$ to an $N \times N$ matrix of zeros

for $m = 1$ to M do loop over el,

 for $i \in \mathcal{I}_m$ do loop over near points

$w \leftarrow \text{singularWeights}(x_i, \tau_m)$ (vector of P elements)

 for $p = 1$ to P do

$j \leftarrow \text{loc2glob}(m, p)$

$S^{(1)}[i, j] = w[p] - S^0[i, j]$

 end

 end

end

return $S^{(1)}$

$$\sum_{\tau_m} k(x_i, y) \dots d\tau_m(y)$$

e.g. $x_i \in \tau_m$

Singular weights

Algorithm 2: singularWeights(\mathbf{x}_i, τ_m)

```
{ $\hat{\mathbf{x}}_p$ }p=1P ← quadrature nodes on reference element  $\hat{\tau}$ 
 $p^* \leftarrow \arg \min_{1 \leq p \leq P} |\chi_m(\hat{\mathbf{x}}_p) - \mathbf{x}_i|$ 
 $\ell_j(\hat{\mathbf{x}}) \leftarrow$  Lagrange interpolating polynomial;  $\underbrace{\ell_j(\hat{\mathbf{x}}_p)}_{\ell_j(\hat{\mathbf{x}}_p) = \delta_{jp}} = \delta_{jp}$ 
for  $p = 1$  to  $P$  do
     $w_j \leftarrow$  singularIntegration( $\underbrace{G(\mathbf{x}_i, \chi_m \circ \hat{\mathbf{y}}) \mu_m(\hat{\mathbf{y}}) \ell_j(\hat{\mathbf{y}})}_{\text{integrand}}, \hat{\tau}, \hat{\mathbf{x}}_{p^*})$ 
end
return { $w_j$ }j=1P
```

$$\int_{\hat{\tau}} g(\hat{\mathbf{x}}) d\hat{\mathbf{x}}$$

- $\mu_m = \sqrt{\det(J_m^\top J_m)}$ is the surface element, χ_m the parametrization
- The function singularIntegration is exactly what we worked on!

Singular weights

- For a fixed τ_m and $i \in \mathcal{I}_m$, the singular weights w_j are such that

$$\int_{\tau_m} G(\mathbf{x}_i, \mathbf{y}) \sigma(\mathbf{y}) \, d\Gamma(\mathbf{y}) \approx \sum_{p=1}^P \sigma(\mathbf{x}_{m,p}) w_p$$

- even when \mathbf{x}_i is close to (or on) the element τ_m
- Replace columns $\{\text{loc2glob}(\mathfrak{m}, p)\}_{p=1}^P$ on the i -th row
- Final approximation: $S^{(0)} + S^{(1)}$

Conclusions

What we covered:

- Reviewed some BIE methods
- Learned about singular integrals
- And how to discretize them using singular quadratures
- Putting the pieces together yields a high-order Nyström method

And important things we ignored:

- How to choose a good boundary integral formulation
- Effect of mesh quality
- Conditioning and iterative solvers
- Adaptive refinement strategies
- How to make things fast