Zürich Summer School Lectures

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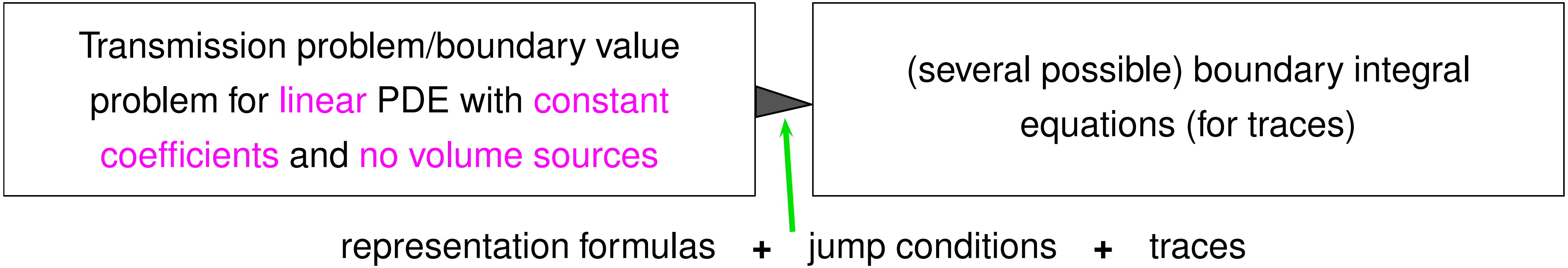
1 Boundary Integral Equations

McLean, W. (2000), *Strongly Elliptic Systems and Boundary Integral Equations*, Cambridge University Press, Cambridge, UK, Chapter 6-9.

Sauter, S. & Schwab, C. (2004), *Randelementmethoden*, BG Teubner, Stuttgart, Chapter 3.

Hackbusch, W. (1995), *Integral equations. Theory and numerical treatment.*, Vol. 120 of *International Series of Numerical Mathematics*, Birkhäuser, Basel, Chapter 7-8.



Transmission problem/boundary value problem for linear PDE with constant coefficients and no volume sources

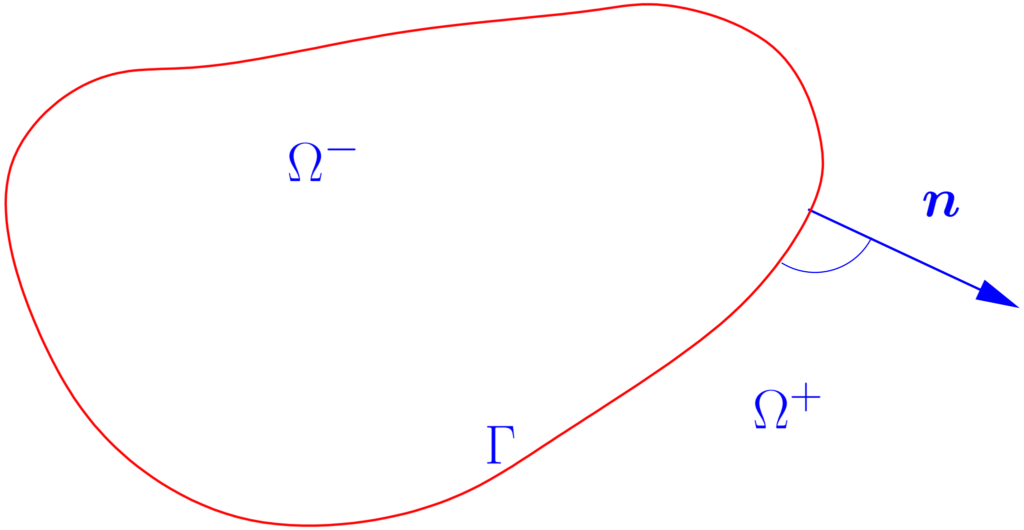
(several possible) boundary integral equations (for traces)

representation formulas + jump conditions + traces

We distinguish
bounded interior domain (scatterer) $\Omega^- \subset \mathbb{R}^d$, $d = 2, 3$ (Simon: Υ)
unbounded exterior domain ("air") $\Omega^+ := \mathbb{R}^d \setminus \bar{\Omega}^-$
($\Omega \hat{=}$ "generic" domain)

We generally assume

Ω^- has **Lipschitz boundary** $\Gamma := \partial\Omega^-$



➤ existence of exterior unit normal vector field $\boldsymbol{n} \in L^\infty(\Gamma)$

Special cases:
- “smooth” C^1-boundary Γ
- piecewise smooth boundary

Example 1 (Simple non-Lipschitz domains).

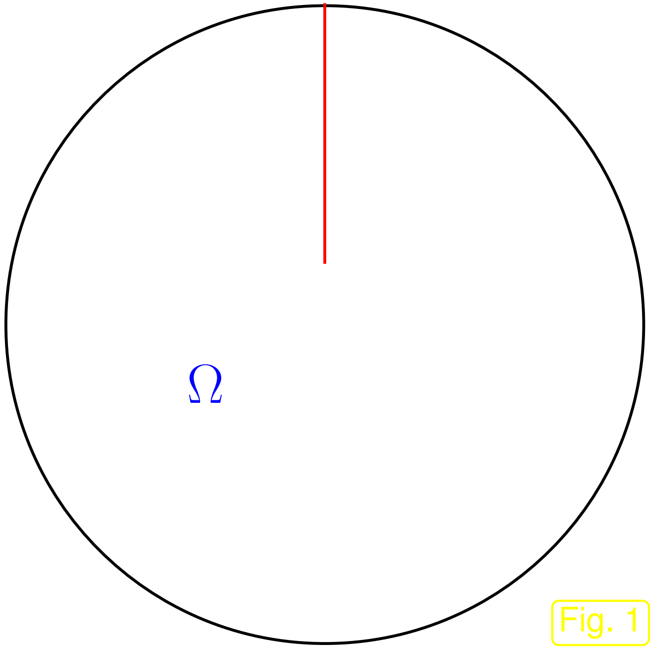


Fig. 1

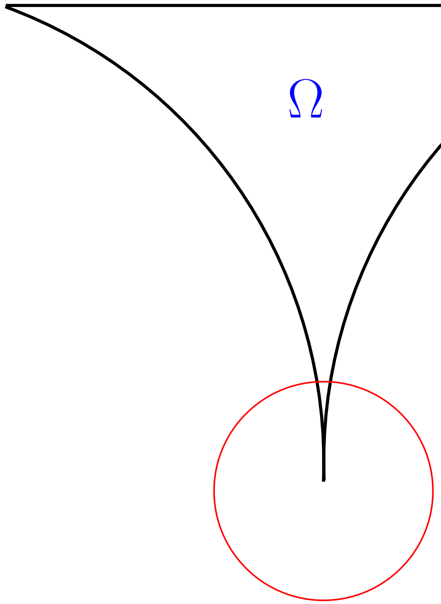


Fig. 2

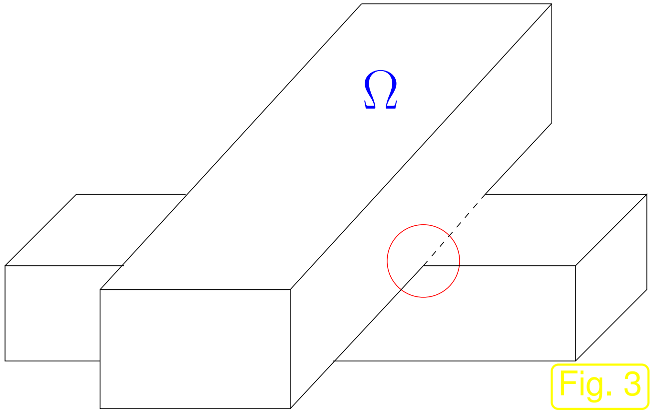


Fig. 3

1.1 Helmholtz equation

Focus on Helmholtz equation: $-\Delta u - \kappa^2 u = 0, \quad \kappa \geq 0$

Definition 1.1.1 (Radiating Helmholtz solution)**.**
A distribution $u \in \mathcal{D}'(\Omega)$ *is a radiating Helmholtz solution, if*

- *it satisfies the Helmholtz equation* $-\Delta u - \kappa^2 u = 0$ *in* Ω*,*
- *(for unbounded* Ω*) it complies with the Sommerfeld radiation conditions*

$$\left|\frac{\partial u}{\partial r}(\boldsymbol{x}) - i\kappa u(\boldsymbol{x})\right| = o(|x|^{(1-d)/2}) \quad \text{uniformly for } |\boldsymbol{x}| \to \infty \ .$$

PDE theory: radiating Helmholtz solutions are analytic inside Ω

1.1.1 Fundamental solutions

fundamental solution $G \in \mathcal{D}'(\mathbb{R}^d)$ = distributional solution in $\mathbb{R}^d$ for point source “δ”:

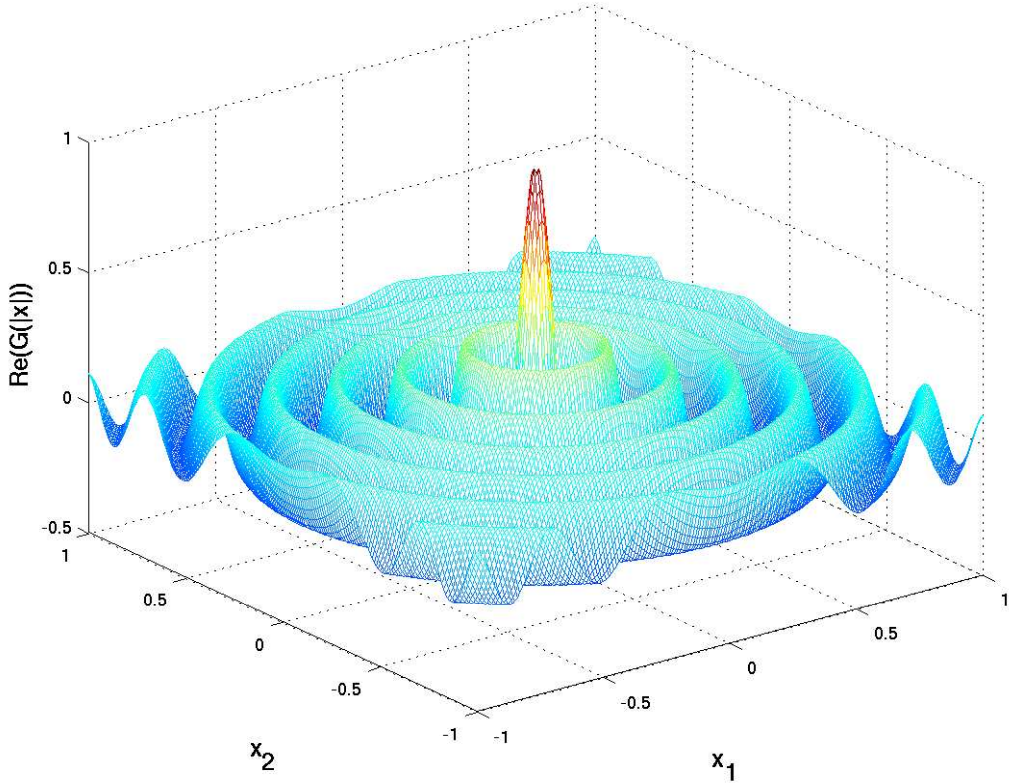
- $-\Delta G - \kappa^2 G = \delta$ in the sense of distributions, $(\delta(\psi) = \psi(0) \quad \forall \psi \in \mathcal{D}(\mathbb{R}^d))$
- u is radiating Helmholtz solution on $\mathbb{R}^d \setminus \{0\}$

Lemma 1.1.2 (Fundamental solution)**.**

$$G(\boldsymbol{x}) = \begin{cases} -\frac{1}{2\pi}\log(\kappa\,|\boldsymbol{x}|) & \textit{for } d = 2,\ \kappa = 0\ , \\ \imath/4 H_0^{(1)}(\kappa\,|\boldsymbol{x}|) & \textit{for } d = 2,\ \kappa > 0\ , \\ \frac{e^{\imath\kappa|\boldsymbol{x}|}}{4\pi|\boldsymbol{x}|} & \textit{for } d = 3\ . \end{cases}$$

▷ Singularity $\begin{array}{l} O(\log|\boldsymbol{x}|),\ d = 2 \\ O(|\boldsymbol{x}|^{-1},\ d = 3 \end{array}$ for $|\boldsymbol{x}| \rightarrow 0$.

G for $d = 2$, $\kappa = 10\pi$ ▷



“Convolution with fundamental solution provides solution operator”:

For $f \in \mathcal{D}(\mathbb{R}^d)$: $\quad u(\boldsymbol{x}) := \int_{\mathbb{R}^d} G(\boldsymbol{x}-\boldsymbol{y}) f(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y}$ solves $-\Delta u - \kappa^2 u = f$
(and complies with Sommerfeld radiation conditions)

▶ Newton potential operator: $\quad (\mathsf{N}_\kappa f)(\boldsymbol{x}) := \int_{\mathbb{R}^d} G(\boldsymbol{x}-\boldsymbol{y}) f(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y}\ .$ (1.1.1)

Lemma 1.1.3 (Newton potential). N_κ *can be extended to an injective operator* $\mathsf{N}_\kappa : H^{-1}_{\mathrm{comp}}(\mathbb{R}^d) \mapsto H^1_{\mathrm{loc}}(\mathbb{R}^d)$.

➤ N_κ is “smoothing operator” of order -2 (inverse of 2nd-order differential operator)

1.1.2 Boundary potentials

Notation: $\gamma_D \mathrel{\hat=}$ “Dirichlet trace”, $\quad (\gamma_D u)(\boldsymbol{x}) = u(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma,\ u \in C^0(\bar{\Omega})$

Recall trace theorem ↔ definition of trace space $H^{\frac{1}{2}}(\Gamma)$:

Theorem 1.1.4 (Trace theorem for $H^1(\Omega)$). → *(McLean 2000, Thm. 3.38)*
For any Lipschitz domain $\gamma_D : C^0(\bar{\Omega}) \mapsto C^0(\Gamma)$ can be extended to a ***continuous*** *and* ***surjective*** *operator $\gamma_1 : H^1_{\mathrm{loc}}(\Omega) \mapsto H^{\frac{1}{2}}(\Gamma)$.*

Recall Green's formula ("integration by parts"):

$$\int_\Omega u\Delta v - v\Delta u \,\mathrm{d}\boldsymbol{x} = \int_\Gamma u\,\mathbf{grad}\,v\cdot\mathbf{n} - v\,\mathbf{grad}\,u\cdot\mathbf{n}\,\mathrm{d}S \quad \forall u,v \in H^1_{\mathsf{loc}}(\Delta;\Omega)\ , \tag{1.1.2}$$

with

$$H^1_{\mathsf{loc}}(\Delta;\Omega) := \{u \in H^1_{\mathrm{loc}}(\Omega)\colon \quad \Delta u \in L^2_{\mathrm{loc}}(\Omega)\}.$$

Notation: $\gamma_N \hat{=}$ "Neumann trace", $(\gamma_N u)(\boldsymbol{x}) = \mathbf{grad}\,u(\boldsymbol{x})\cdot\boldsymbol{n}(\boldsymbol{x})$, $\boldsymbol{x}\in\Gamma$, $u \in C^1(\bar{\Omega})$

(1.1.2) ⇒ $\gamma_N : C^1(\bar{\Omega}) \mapsto C^0(\Gamma)$ can be extended to a **continuous** and **surjective** trace operator
$\gamma_N : H^1_{\mathsf{loc}}(\Delta;\Omega) \mapsto H^{-\frac{1}{2}}(\Gamma)$, $H^{-\frac{1}{2}}(\Gamma) \hat{=}$ dual of $H^{\frac{1}{2}}(\Gamma)$ w.r.t. $L^2(\Gamma)$ pivot space.

Theorem 1.1.5 (Representation formula for Helmholtz solutions)**.**
A radiating Helmholtz solution $u \in H^1_{\mathrm{loc}}(\Omega^- \cup \Omega^+)$ *(→ Def. 1.1.1) on* $\Omega^- \cup \Omega^+$ *has the integral representation (in the sense of distributions)*

$$u(\boldsymbol{x}) = -\boxed{\int_\Gamma G(\boldsymbol{x},\boldsymbol{y})\,[\gamma_N u(\boldsymbol{y})]_\Gamma \,\mathrm{d}S(\boldsymbol{y})} + \boxed{\int_\Gamma \gamma_{N,\boldsymbol{y}} G(\boldsymbol{x},\boldsymbol{y})\,[\gamma_D u(\boldsymbol{y})]_\Gamma \,\mathrm{d}S(\boldsymbol{y})}$$

single layer potential operator Ψ_{SL} double layer potential operator Ψ_{DL}

Notation: jump $[\gamma\cdot]_\Gamma := \gamma^+ \cdot - \gamma^- \cdot$, $\gamma^+ \mathrel{\hat{=}}$ trace from Ω^+, $\gamma^- \mathrel{\hat{=}}$ trace from Ω^-

Cauchy data $(\gamma_D u, \gamma_N u)$ of Helmholtz solution $u \in H^1_{\text{loc}}(\Delta;\Omega)$ $\xrightarrow[\text{formula, Thm. 1.1.5}]{\text{repesentation}}$ pointwise recovery of u in $\Omega^- \cup \Omega^+$

Formal definitions:

single layer potential operator:
$$\Psi_{\mathrm{SL}}(\varphi)(\boldsymbol{x}) := \int_\Gamma G(\boldsymbol{x},\boldsymbol{y})\varphi(\boldsymbol{y})\,\mathrm{d}S(\boldsymbol{y}) \;, \tag{1.1.3}$$

double layer potential operator:
$$\Psi_{\mathrm{DL}}(u)(\boldsymbol{x}) := \int_\Gamma \gamma_{N,\boldsymbol{y}} G(\boldsymbol{x},\boldsymbol{y})u(\boldsymbol{y})\,\mathrm{d}S(\boldsymbol{y}) \;. \tag{1.1.4}$$

Classical formula for $d = 3$: $\Psi_{\mathsf{DL}}(u)(\boldsymbol{x}) = \int_{\Gamma} \frac{e^{\imath|\boldsymbol{x}-\boldsymbol{y}|}(1-\imath\,|\boldsymbol{x}-\boldsymbol{y}|)}{4\pi\,|\boldsymbol{x}-\boldsymbol{y}|} \frac{(\boldsymbol{x}-\boldsymbol{y})\cdot\boldsymbol{n}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|^2} u(\boldsymbol{y})\,\mathrm{d}S(\boldsymbol{y})$.

“Functional analytic” definition: (* tags adjoint w.r.t. pivot space $L^2(\Omega)$, $L^2(\Gamma)$, resp.)

$$\Psi_{\mathsf{SL}} = \mathsf{N}_\kappa^* \circ \gamma_D^* \quad , \quad \Psi_{\mathsf{DL}} = \mathsf{N}_\kappa^* \circ \gamma_N^* \ .$$

▶ $\Psi_{\mathsf{SL}} : H^{-\frac{1}{2}}(\Gamma) \mapsto H^1_{\mathrm{loc}}(\mathbb{R}^d) \cap H^1_{\mathrm{loc}}(\Delta, \Omega^- \cup \Omega^+)$,
$\Psi_{\mathsf{DL}} : H^{\frac{1}{2}}(\Gamma) \mapsto H^1_{\mathrm{loc}}(\Delta, \Omega^- \cup \Omega^+)$ are continuous ! (1.1.5)

Moreover: $\forall\varphi \in H^{-\frac{1}{2}}(\Gamma)$, $\forall u \in H^{\frac{1}{2}}(\Gamma)$ provide $\Psi_{\mathsf{SL}}(\varphi)$, $\Psi_{\mathsf{DL}}(u)$ radiating Helmholtz solutions in $\Omega^- \cup \Omega^+$.

(1.1.6)

▶ trace operators γ_D, γ_N make sense for potentials

Theorem 1.1.6 (Jump relations). $\rightarrow$ *(McLean 2000, Thm. 6.11)*

For all $\varphi \in H^{\frac{1}{2}}(\Gamma)$, $u \in H^{\frac{1}{2}}(\Gamma)$ hold the jump relations:

$$[\gamma_D \Psi_{SL}(\varphi)]_\Gamma = 0 \quad , \quad [\gamma_D \Psi_{DL}(u)]_\Gamma = u \quad \text{in } H^{\frac{1}{2}}(\Gamma) \, ,$$
$$[\gamma_N \Psi_{SL}(\varphi)]_\Gamma = -\varphi \quad , \quad [\gamma_N \Psi_{DL}(u)]_\Gamma = 0 \quad \text{in } H^{-\frac{1}{2}}(\Gamma) \, .$$

1.1.3 Boundary integral operators

Boundary potentials + trace operators ➡ boundary integral operators

Well defined thanks to (1.1.6)

Definition 1.1.7 (Boundary integral operators)**.**

Single layer boundary integral operator: $\mathsf{V}_\kappa := \gamma_D \Psi_{\mathit{SL}} : H^{-\frac{1}{2}}(\Gamma) \mapsto H^{\frac{1}{2}}(\Gamma)$,

Double layer boundary integral operators:

$\mathsf{K}_\kappa := \{\gamma_D \Psi_{\mathit{DL}}\}_\Gamma : H^{\frac{1}{2}}(\Gamma) \mapsto H^{\frac{1}{2}}(\Gamma)$,

$\mathsf{K}'_\kappa := \{\gamma_N \Psi_{\mathit{SL}}\}_\Gamma : H^{-\frac{1}{2}}(\Gamma) \mapsto H^{-\frac{1}{2}}(\Gamma)$,

Hypersingular boundary integral operator: $\mathsf{W}_\kappa := -\gamma_N \Psi_{\mathit{DL}} : H^{\frac{1}{2}}(\Gamma) \mapsto H^{-\frac{1}{2}}(\Gamma)$.

Notation: average $\{\gamma\cdot\}_\Gamma := \frac{1}{2}(\gamma^+ + \gamma^-)$, $\gamma^+ \hat{=}$ trace from Ω^+, $\gamma^- \hat{=}$ trace from Ω^-

Corollary 1.1.8 (Continuity of boundary integral operators in trace norms)**.**

All boundary integral operators of Def. 1.1.7 are continuous

A more refined result:

Theorem 1.1.9 (Continuity of boundary integral operators). → *(McLean 2000, Thm. 7.1)*

The boundary integral operators (→ Def. 1.1.7)

$$\mathsf{V}_\kappa : H^{s-\frac{1}{2}}(\Gamma) \mapsto H^{s+\frac{1}{2}}(\Gamma) \quad , \quad \mathsf{K}_\kappa : H^{s+\frac{1}{2}}(\Gamma) \mapsto H^{s+\frac{1}{2}}(\Gamma) \; ,$$
$$\mathsf{K}'_\kappa : H^{s-\frac{1}{2}}(\Gamma) \mapsto H^{s-\frac{1}{2}}(\Gamma) \quad , \quad \mathsf{W}_\kappa : H^{s+\frac{1}{2}}(\Gamma) \mapsto H^{s-\frac{1}{2}}(\Gamma) \; ,$$

are continuous for any $s \in [-\frac{1}{2}, \frac{1}{2}]$.

Are the operators from Def. 1.1.7 really *boundary integral operators* **?**

(➪ asks for a *boundary integral representation*)

Assumption: Γ is piecewise smooth (boundary of a curvilinear polygon/polyhedron)

- $\forall \varphi \in L^\infty(\Gamma)$: $\mathsf{V}_\kappa \varphi = \int\limits_\Gamma G(\cdot, \boldsymbol{y})\varphi(\boldsymbol{y})\,\mathrm{d}S(\boldsymbol{y})$ in $C^0(\Gamma)$.
- for u p.w. C^1: $\mathsf{K}_\kappa u = \int\limits_\Gamma \gamma_{N,\boldsymbol{y}} G(\cdot, \boldsymbol{y}) u(\boldsymbol{y})\,\mathrm{d}S(\boldsymbol{y})$ a.e. on Γ,

where all integrals are understood as improper surface integrals.

Some *compactness results*:

- For a C^2-boundary: $\mathsf{K}_\kappa, \mathsf{K}'_\kappa : L^2(\Gamma) \mapsto H^1(\Gamma)$ continuous $\rightarrow$ (Hackbusch 1995, Sect. 8.2)
- The following differences of boundary integral operators are compact

$$\mathsf{V}_\kappa - \mathsf{V}_0 : H^{-\frac{1}{2}}(\Gamma) \mapsto H^{\frac{1}{2}}(\Gamma) \quad , \quad \mathsf{K}_\kappa - \mathsf{K}_0 : H^{\frac{1}{2}}(\Gamma) \mapsto H^{\frac{1}{2}}(\Gamma) \; ,$$
$$\mathsf{K}'_\kappa - \mathsf{K}'_0 : H^{-\frac{1}{2}}(\Gamma) \mapsto H^{-\frac{1}{2}}(\Gamma) \quad , \quad \mathsf{W}_\kappa - \mathsf{W}_0 : H^{\frac{1}{2}}(\Gamma) \mapsto H^{-\frac{1}{2}}(\Gamma) \; .$$

▷ $\mathsf{K}^*_\kappa = \mathsf{K}'_\kappa$ ($L^2(\Gamma)$-adjoints) up to compact perturbations

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Boundary integral operators and sesqui-linear forms: by duality of $H^{\frac{1}{2}}(\Gamma)$-$H^{-\frac{1}{2}}(\Gamma)$

$$\mathsf{V}_\kappa : H^{-\frac{1}{2}}(\Gamma) \mapsto H^{\frac{1}{2}}(\Gamma) \quad \triangleright \quad (\varphi,\psi) \mapsto \langle \mathsf{V}_\kappa\varphi,\psi\rangle \in L(H^{-\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Gamma),\mathbb{C}) \; ,$$
$$\mathsf{W}_\kappa : H^{\frac{1}{2}}(\Gamma) \mapsto H^{-\frac{1}{2}}(\Gamma) \quad \triangleright \quad (u,v) \mapsto \langle \mathsf{W}_\kappa u,v\rangle \in L(H^{\frac{1}{2}}(\Gamma) \times H^{\frac{1}{2}}(\Gamma),\mathbb{C}) \; .$$

For p.w. smooth Γ: straightforward from integral representation

$$\langle \mathsf{V}_\kappa\varphi,\psi\rangle = \int_\Gamma \int_\Gamma G(\boldsymbol{x},\boldsymbol{y})\varphi(\boldsymbol{y})\overline{\psi}(\boldsymbol{x})\,\mathrm{d}S(\boldsymbol{y})\mathrm{d}S(\boldsymbol{x}) \quad \forall\varphi,\psi \in L^\infty(\Gamma) \; . \tag{1.1.7}$$

For hypersingular sesqui-linear form: regularization ($\leftarrow$ integration by parts on Γ):

Lemma 1.1.10 (Expression for hypersingular sesqui-linear form). *(McLean 2000, Thm. 9.15)*
For piecewise smooth Γ and $u, v \in W^{1,\infty}(\Gamma)$ and

$$d = 2: \qquad \langle \mathsf{W}_\kappa u, v\rangle = \left\langle \mathsf{V}_\kappa \frac{\partial u}{\partial s}, \frac{\partial v}{\partial s}\right\rangle - \kappa^2 \langle \mathsf{V}_\kappa(u\boldsymbol{n}), v\boldsymbol{n}\rangle \;, \tag{1.1.8}$$

where $\frac{\partial}{\partial s}$ is the derivative along Γ w.r.t. arc length, and

$$d = 3: \qquad \langle \mathsf{W}_\kappa u, v\rangle = \langle \mathsf{V}_\kappa \mathbf{curl}_\Gamma u, \mathbf{curl}_\Gamma v\rangle - \kappa^2 \langle \mathsf{V}_\kappa(u\boldsymbol{n}), v\boldsymbol{n}\rangle \;, \tag{1.1.9}$$

where $\mathbf{curl}_\Gamma$ is the surface rotation (= rotated surface gradient).

Ellipticity of sesqui-linear forms associated with boundary integral operators: → (McLean 2000, Cor. 8.13)

Theorem 1.1.11 (Ellipticity of single layer/hypersingular boundary integral operators)**.**
For $d = 3$ *and* $d = 2$ *in the case of* $\operatorname{diam}\Omega < 1$*:*

$$\exists C = C(\Gamma): \quad \langle \mathsf{V}_0 \varphi, \varphi \rangle \geq C \left\| \varphi \right\|^2_{H^{-\frac{1}{2}}(\Gamma)} \qquad \forall \varphi \in H^{-\frac{1}{2}}(\Gamma) \;,$$

$$\exists C = C(\Gamma): \quad \langle \mathsf{W}_0 v, v \rangle \geq C \left\| v \right\|^2_{H^{\frac{1}{2}}(\Gamma)} \qquad \forall u \in H^{\frac{1}{2}}(\Gamma)/\mathbb{R} \;.$$

► the sesqui-linear forms associated with V_κ, W_κ are $H^{-\frac{1}{2}}(\Gamma)/H^{\frac{1}{2}}(\Gamma)$-coercive **!**

BIG ISSUE: κ-dependence of operator norms/coercivity constants (⟶ Simon's lecture)

1.1.4 Boundary integral equations

Relevant boundary value problems (BVPs) for Helmholtz equation:

- *Exterior Dirichlet problem*:

$$\begin{aligned} -\Delta u - \kappa^2 u &= 0 && \text{in } \Omega^+ \,, \\ \gamma_D u &= g \in H^{\frac{1}{2}}(\Gamma) && \text{on } \Gamma \,, \end{aligned} \quad + \quad \begin{array}{l}\text{Sommerfeld}\\ \text{radiation b.c. at } \infty \,.\end{array} \tag{1.1.10}$$

- *Exterior Neumann problem*:

$$\begin{aligned} -\Delta u - \kappa^2 u &= 0 && \text{in } \Omega^+ \,, \\ \gamma_N u &= \psi \in H^{-\frac{1}{2}}(\Gamma) && \text{on } \Gamma \,, \end{aligned} \quad + \quad \begin{array}{l}\text{Sommerfeld}\\ \text{radiation b.c. at } \infty \,.\end{array} \tag{1.1.11}$$

Extension: mixed BVP $\hat{=}$ Dirichlet/Neumann b.c. on different parts Γ_D/Γ_N of Γ

- *Transmission problem*:

$$\begin{aligned} -\Delta u - \kappa_+^2 u &= 0 && \text{in } \Omega^+ \,, \\ -\Delta u - \kappa_-^2 u &= 0 && \text{in } \Omega^- \,, \\ [\gamma_D u]_\Gamma &= g \in H^{-\frac{1}{2}}(\Gamma) && \text{on } \Gamma \,, \\ [\gamma_N u]_\Gamma &= \psi \in H^{-\frac{1}{2}}(\Gamma) && \text{on } \Gamma \,, \end{aligned} \quad + \quad \begin{array}{l}\text{Sommerfeld}\\ \text{radiation b.c. at } \infty \,.\end{array} \tag{1.1.12}$$

Representation formula + trace operators ➡ boundary integral equations

1.1.4.1 Direct BIE

Given: $u \in H^1_{\mathrm{loc}}(\Delta; \Omega^- \cup \Omega^+)$ = Helmholtz solution in $\Omega^- \cup \Omega^+$

$$\text{Thm. 1.1.5} \quad \Rightarrow \quad \begin{pmatrix} \gamma_D^- u \\ \gamma_N^- u \end{pmatrix} = \underbrace{\begin{pmatrix} \frac{1}{2}\mathsf{Id} - \mathsf{K}_\kappa & \mathsf{V}_\kappa \\ \mathsf{W}_\kappa & \frac{1}{2}\mathsf{Id} + \mathsf{K}'_\kappa \end{pmatrix}}_{\text{interior Calderón projector } \mathsf{P}^-} \begin{pmatrix} \gamma_D^- u \\ \gamma_N^- u \end{pmatrix} \tag{1.1.13}$$

$$\text{Thm. 1.1.5} \quad \Rightarrow \quad \begin{pmatrix} \gamma_D^+ u \\ \gamma_N^+ u \end{pmatrix} = \underbrace{\begin{pmatrix} \frac{1}{2}\mathsf{Id} + \mathsf{K}_\kappa & -\mathsf{V}_\kappa \\ -\mathsf{W}_\kappa & \frac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa \end{pmatrix}}_{\text{exterior Calderón projector } \mathsf{P}^+} \begin{pmatrix} \gamma_D^+ u \\ \gamma_N^+ u \end{pmatrix} \tag{1.1.14}$$

Lemma 1.1.12 (Calderón projectors). *(Sauter & Schwab 2004, Sect. 3.6)*
$\mathsf{P}^-, \mathsf{P}^+ : H^{\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Gamma) \mapsto H^{\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Gamma)$ *are continous* ***projectors*** *with* $\mathsf{P}^- + \mathsf{P}^+ = \mathsf{Id}$.

▷ direct boundary integral equations for exterior Dirichlet problem (1.1.10)

$$\varphi \in H^{-\frac{1}{2}}(\Gamma): \quad -\mathsf{V}_\kappa(\varphi) = (\tfrac{1}{2}\mathsf{Id} - \mathsf{K}_\kappa)g \quad \text{in} \quad H^{\frac{1}{2}}(\Gamma)\,, \tag{1.1.15}$$

$$\varphi \in H^{-\frac{1}{2}}(\Gamma): \quad (\tfrac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa)\varphi = \mathsf{W}_\kappa(g) \quad \text{in} \quad H^{-\frac{1}{2}}(\Gamma)\,. \tag{1.1.16}$$

Unknown: Neumann data $\varphi = \gamma_N^+ u$ (“physical unknowns”)

▷ direct boundary integral equations for exterior Neumann problem (1.1.10)

$$u \in H^{\frac{1}{2}}(\Gamma): \quad (\tfrac{1}{2}\mathsf{Id} + \mathsf{K}_\kappa)u = \mathsf{V}_\kappa(\psi) \quad \text{in } H^{-\frac{1}{2}}(\Gamma)\,, \tag{1.1.17}$$

$$\varphi \in H^{-\frac{1}{2}}(\Gamma): \quad -\mathsf{W}_\kappa(u) = (\tfrac{1}{2}\mathsf{Id} + \mathsf{K}'_\kappa)\psi \quad \text{in } H^{-\frac{1}{2}}(\Gamma)\,. \tag{1.1.18}$$

Unknown: Dirichlet data $u = \gamma_D^+ u$ (“physical unknowns”)

Terminology:	(1.1.15),(1.1.18)	$\hat{=}$	first kind boundary integral equations
	(1.1.16),(1.1.17)	$\hat{=}$	second kind boundary integral equations

Issue: Existence and uniqueness of solutions of direct boundary integral equations

Theorem 1.1.13 (Characterization of Cauchy data). *For* $(u,\varphi) \in H^{\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Gamma)$

$$\big((u,\varphi) \in \mathrm{Im}(\mathsf{P}^-) \Leftrightarrow (u,\varphi) \in \mathrm{Ker}(\mathsf{P}^+)\big) \quad \Longleftrightarrow \quad (u,\varphi) \text{ Cauchy data for Helmholtz sol. in } \Omega^- \;,$$
$$\big((u,\varphi) \in \mathrm{Im}(\mathsf{P}^+) \Leftrightarrow (u,\varphi) \in \mathrm{Ker}(\mathsf{P}^-)\big) \quad \Longleftrightarrow \quad (u,\varphi) \text{ Cauchy data for Helmholtz sol. in } \Omega^+ \;.$$

Known from PDE theory:
→ Simon's lecture

existence & uniqueness of solutions of exterior Neumann/Dirichlet and transmission boundary value problems *for all* $\kappa \geq 0$

BUT direct boundary integral equations have a resonance problem:

Definition 1.1.14 (Interior resonant frequencies).

κ *interior Dirichlet eigenvalue* $:\Leftrightarrow \quad \exists u \in H_0^1(\Omega^-) \setminus \{0\}: \quad -\Delta u = \kappa^2 u \quad$ *in* Ω^- ,

κ *interior Neumann eigenvalue* $:\Leftrightarrow \quad \exists u \in H^1_{loc}(\Delta;\Omega^-) \setminus \{0\}: \quad \begin{cases} -\Delta u = \kappa^2 u & \text{in } \Omega^- , \\ \gamma_N^- u = 0 & \text{on } \Gamma . \end{cases}$

Interior Dirichlet/Neumann eigenvalues are also called interior resonant frequencies.

Note: (both types of) interior resonant frequencies form an discrete sets $\subset \mathbb{R}_0^+$ with no accumulation point

κ interior Dirichlet eigenvalue $\;\Rightarrow\;$ $\exists u \neq 0,\quad -\Delta u - \kappa^2 u = 0 \quad\wedge\quad \gamma_D^- u = 0$

$$\xRightarrow{\text{Thm. 1.1.13}} \quad \mathsf{V}_\kappa(\varphi) = 0 \quad \wedge \quad (\tfrac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa)\varphi = 0 \quad \text{for } \varphi := \gamma_N^- u \neq 0 \; .$$

► $\mathrm{Ker}(\mathsf{V}_\kappa) \neq \{0\}, \quad \mathrm{Ker}(\tfrac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa) \neq \{0\}$ **!**

κ interior Neumann eigenvalue $\;\Rightarrow\;$ $\exists u \neq 0,\quad -\Delta u - \kappa^2 u = 0 \quad\wedge\quad \gamma_N^- u = 0$

$$\xRightarrow{\text{Thm. 1.1.13}} \quad (\tfrac{1}{2}\mathsf{Id} + \mathsf{K}_\kappa)v = 0 \quad \wedge \quad \mathsf{W}_\kappa v = 0 \quad \text{for } v := \gamma_D^- u \neq 0 \; .$$

► $\mathrm{Ker}(\mathsf{W}_\kappa) \neq \{0\}, \quad \mathrm{Ker}(\tfrac{1}{2}\mathsf{Id} + \mathsf{K}_\kappa) \neq \{0\}$ **!**

☹ No uniqueness of solutions of direct BIE for $\kappa =$ interior Dirichlet (1.1.15), (1.1.16) or Neumann (1.1.18), (1.1.17) resonant frequency.

(Nevertheless: solutions exists and, in Ω^+ can be recovered by representation formula)

Theorem 1.1.15 (Existence & uniqueness of solutions of direct BIE)**.**
$\kappa \neq$ *interior* $\begin{matrix}\textit{Dirichlet}\\ \textit{Neumann}\end{matrix}$ *resonant frequency* $\Rightarrow$ $\begin{matrix}(1.1.15), (1.1.16)\\ (1.1.18), (1.1.17)\end{matrix}$ *have unique solutions.*

Remedy for resonance problem: combined field integral equations (CFIE) (Burton & Miller 1971)

Uniqueness of solutions of interior BVP for impedance boundary conditions

➤ Idea: complex linear combination of boundary integral equations of Calderón identities from (1.1.14)

For exterior Helmholtz solution with $\eta > 0$

$$\gamma_D^+ u = (\mathsf{K}_\kappa + \tfrac{1}{2}\mathsf{Id})(\gamma_D^+ u) - \mathsf{V}_\kappa(\gamma_N^+ u)\ , \tag{1.1.19}$$

$$\gamma_N^+ u = -\mathsf{W}_\kappa(\gamma_D^+ u) - (\mathsf{K}'_\kappa - \tfrac{1}{2}\mathsf{Id})(\gamma_N^+ u)\ . \tag{1.1.20}$$

⇓

$$(i\eta(\mathsf{K}_\kappa + \tfrac{1}{2}\mathsf{Id}) - \mathsf{W}_\kappa)(\gamma_D^+ u) - (i\eta\mathsf{V}_\kappa + \tfrac{1}{2}\mathsf{Id} + \mathsf{K}'_\kappa)(\gamma_N^+ u) = 0\ .$$

▷ 2nd-kind integral equation for exterior Dirichlet problem (1.1.10)

$$\varphi \in H^{-\frac{1}{2}}(\Gamma):\quad (i\eta\mathsf{V}_\kappa + \tfrac{1}{2}\mathsf{Id} + \mathsf{K}'_\kappa)(\varphi) = (i\eta(\mathsf{K}_\kappa + \tfrac{1}{2}\mathsf{Id}) - \mathsf{W}_\kappa)(g)\ . \tag{1.1.21}$$

Theorem 1.1.16 (Uniqueness of solutions of CFIE)**.**

$i\eta\mathsf{V}_\kappa + \frac{1}{2}\mathsf{Id} + \mathsf{K}'_\kappa : H^{-\frac{1}{2}}(\Gamma) \mapsto H^{-\frac{1}{2}}(\Gamma)$ *is injective*

Variational formulations of direct BIE (➢ linear variational problems):

❶ No problem for *1st-kind boundary integral equations*: (duality !)

(1.1.15) ⇔ $\varphi \in H^{-\frac{1}{2}}(\Gamma)\colon \quad -\langle \mathsf{V}_\kappa\varphi, \psi\rangle = \left\langle (\tfrac{1}{2}\mathsf{Id} - \mathsf{K}_\kappa)g, \psi \right\rangle \quad \forall\psi \in H^{-\frac{1}{2}}(\Gamma)\,,$ **(1.1.22)**

(1.1.18) ⇔ $u \in H^{\frac{1}{2}}(\Gamma)\colon \quad -\langle \mathsf{W}_\kappa u, v\rangle = \left\langle (\tfrac{1}{2}\mathsf{Id} + \mathsf{K}'_\kappa)\psi, v \right\rangle \quad \forall v \in H^{\frac{1}{2}}(\Gamma)\,.$ **(1.1.23)**

Thm. 1.1.11 ➨ (1.1.22), (1.1.23)coercive variational problems **!**

❶ 2nd-kind boundary integral equations: no duality ➙ no natural variational formulation

➤ variational formulations based on inner products (notation: $(\cdot,\cdot)_X$)

- option: inner products of trace spaces

(1.1.16) ⇔ $\varphi \in H^{-\frac{1}{2}}(\Gamma)\colon \quad \left((\tfrac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa)\varphi, \psi\right)_{H^{-\frac{1}{2}}(\Gamma)} = (\mathsf{W}_\kappa(g), \psi)_{H^{-\frac{1}{2}}(\Gamma)} \quad \forall\psi \in H^{-\frac{1}{2}}(\Gamma)\,,$ **(1.1.24)**

(1.1.17) ⇔ $u \in H^{\frac{1}{2}}(\Gamma)\colon \quad \left((\tfrac{1}{2}\mathsf{Id} + \mathsf{K}_\kappa)u, v\right)_{H^{\frac{1}{2}}(\Gamma)} = (\mathsf{V}_\kappa\psi, v)_{H^{\frac{1}{2}}(\Gamma)} \quad \forall v \in H^{\frac{1}{2}}(\Gamma)\,.$ **(1.1.25)**

Lemma 1.1.17 (Coercivity of operators of 2nd-kind BIE)**.** *(Sauter & Schwab 2004, Sect. 3.8)*

$$(\varphi,\psi) \mapsto \Big((\tfrac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa)\varphi,\psi\Big)_{H^{-\frac{1}{2}}(\Gamma)} \quad \textit{is coercive in} \quad H^{-\frac{1}{2}}(\Gamma)\;,$$

$$(u,v) \mapsto \Big((\tfrac{1}{2}\mathsf{Id} + \mathsf{K}_\kappa)u,v\Big)_{H^{\frac{1}{2}}(\Gamma)} \quad \textit{is coercive in} \quad H^{\frac{1}{2}}(\Gamma)\;.$$

BUT, (1.1.24), (1.1.25) involve **non-local** inner products ➤ not useful for discretization **!**

- option: inner product of $L^2(\Gamma)$

(1.1.16) $\Leftrightarrow$ $\varphi \in L^2(\Gamma)$: $\Big((\tfrac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa)\varphi,\psi\Big)_{L^2(\Gamma)} = (\mathsf{W}_\kappa(g),\psi)_{L^2(\Gamma)} \quad \forall\psi \in L^2(\Gamma)\;,$ (1.1.26)

(1.1.17) $\Leftrightarrow$ $u \in L^2(\Gamma)$: $\Big((\tfrac{1}{2}\mathsf{Id} + \mathsf{K}_\kappa)u,v\Big)_{L^2(\Gamma)} = (\mathsf{V}_\kappa\psi,v)_{L^2(\Gamma)} \quad \forall v \in L^2(\Gamma)\;.$ (1.1.27)

☹ variational formulations not set in *natural trace spaces*

Lemma 1.1.18 (L^2-coercivity of operators of 2nd-kind BIE)**.**
If $d = 2$ *or* $d = 3$ *and* Γ *is* C^2*-smooth, then the sesqui-linear forms of* (1.1.26) *and* (1.1.26) *are coercive.*

Also for CFIE (1.1.21): variational formulation in $L^2(\Gamma)$-framework ➤ same problems.

Remark 2. Theoretical problems with CFIEs do not seem to translate into practical difficulties.

Remark 3 (Regularized CFIE)*.*

"mathematically unsettling": CFIE arising from adding equations set in different trace spaces

▷ lift equations into the same space by use of regularizing operator $\mathsf{M} : H^{-\frac{1}{2}}(\Gamma) \mapsto H^{\frac{1}{2}}(\Gamma)$

▶ regularized CFIE

$$\varphi \in H^{-\frac{1}{2}}(\Gamma){:} \quad (i\eta\mathsf{V}_\kappa + \mathsf{M} \circ (\tfrac{1}{2}\mathsf{Id} + \mathsf{K}'_\kappa))(\varphi) = (i\eta(\mathsf{K}_\kappa + \tfrac{1}{2}\mathsf{Id}) - \mathsf{M} \circ \mathsf{W}_\kappa)(g) \quad \text{in} \;\; H^{\frac{1}{2}}(\Gamma)\;. \tag{1.1.28}$$

Theoretically pleasing, numerically feasible . . . , but really necessary **?**

Buffa, A. & Hiptmair, R. (2005), ‘Regularized combined field integral equations’, *Numer. Math.* **100**(1), 1–19.

1.1.4.2 Transmission BIE

Thm. 1.1.13 $\Rightarrow$ for solution u of transmission problem (1.1.12):

$$\mathsf{P}^{+}_{\kappa^-}\begin{pmatrix}\gamma_D^- u\\ \gamma_N^- u\end{pmatrix} = 0 \quad\wedge\quad \mathsf{P}^{-}_{\kappa^+}\begin{pmatrix}\gamma_D^+ u\\ \gamma_N^+ u\end{pmatrix} = 0\,,$$

+ transmission conditions $\gamma_D^+ u - \gamma_D^- = g$, $\gamma_N^+ u - \gamma_N^- = \psi$:

▶ $$\left(\mathsf{P}^{+}_{\kappa^-} - \mathsf{P}^{-}_{\kappa^+}\right)\begin{pmatrix}\gamma_D^- u\\ \gamma_N^- u\end{pmatrix} = \begin{pmatrix}-\mathsf{K}_{\kappa^-} - \mathsf{K}_{\kappa^+} & \mathsf{V}_{\kappa^-} + \mathsf{V}_{\kappa^+}\\ \mathsf{W}_{\kappa^-} + \mathsf{W}_{\kappa^+} & \mathsf{K}'_{\kappa^-} + \mathsf{K}'_{\kappa^+}\end{pmatrix}\begin{pmatrix}\gamma_D^- u\\ \gamma_N^- u\end{pmatrix} = \mathsf{P}^{-}_{\kappa^+}\begin{pmatrix}g\\ \psi\end{pmatrix}\,. \tag{1.1.29}$$

$\Leftrightarrow$ variational problem: find $u \in H^{\frac{1}{2}}(\Gamma)$, $\varphi \in H^{-\frac{1}{2}}(\Gamma)$

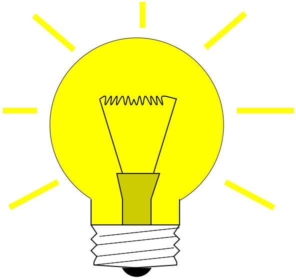
$$\begin{aligned} \langle(\mathsf{W}_{\kappa^-} + \mathsf{W}_{\kappa^+})u, v\rangle \; &+ \; \left\langle(\mathsf{K}'_{\kappa^-} + \mathsf{K}'_{\kappa^+})\varphi, v\right\rangle = \ldots \quad \forall v \in H^{\frac{1}{2}}(\Gamma)\,,\\ -\langle(\mathsf{K}_{\kappa^-} + \mathsf{K}_{\kappa^+})u, \mu\rangle \; &+ \; \langle(\mathsf{V}_{\kappa^-} + \mathsf{V}_{\kappa^+})\varphi, \mu\rangle = \ldots \quad \forall \mu \in H^{-\frac{1}{2}}(\Gamma)\,. \end{aligned} \tag{1.1.30}$$

Theorem 1.1.19 (Existence & uniqueness of solutions of transmission BIE)**.**

For any $\kappa \geq 0$ *and all data* (1.1.30) *has a unique solution.*

1.1.4.3 Indirect BIE

Fact: potentials Ψ_{SL}, Ψ_{DL} provide Helmholtz solutions



Idea: Trial expressions for solutions of BVPs

single layer ansatz: $u = \Psi_{\mathsf{SL}}(\varphi)\ , \quad \varphi \in H^{-\frac{1}{2}}(\Gamma)\ ,$

double layer ansatz: $u = \Psi_{\mathsf{DL}}(u)\ , \quad u \in H^{\frac{1}{2}}(\Gamma)\ .$

▶ (1.1.10) $\Rightarrow$

$$\begin{cases} \gamma_D^+ \Psi_{\mathsf{SL}}(\varphi) = \mathsf{V}_\kappa \varphi = g & \text{in } H^{\frac{1}{2}}(\Gamma)\ , \\ \gamma_D^+ \Psi_{\mathsf{DL}}(u) = (\mathsf{K}_\kappa + \frac{1}{2}\mathsf{Id})u = g & \text{in } H^{\frac{1}{2}}(\Gamma)\ . \end{cases}$$

▶ (1.1.11) $\Rightarrow$ $$\begin{cases} \gamma_N^+ \Psi_{\mathsf{SL}}(\varphi) = (\mathsf{K}'_\kappa - \frac{1}{2}\mathsf{Id})\varphi = \psi & \text{in } H^{-\frac{1}{2}}(\Gamma)\ , \\ \gamma_N^+ \Psi_{\mathsf{DL}}(u) = \mathsf{W}_\kappa(u) = \psi & \text{in } H^{-\frac{1}{2}}(\Gamma)\ . \end{cases}$$

▶ first kind & second kind indirect BIE for unknown densities

☞ analysis and variational formulations as for direct BIEs → Sect. 1.1.4.1

Advantage: economical ↔ no boundary integral operators on the right hand side

Remark 4 (Interpretation of densities in indirect BIE).

φ : jump of Neumann data for solutions of interior/exterior Dirichlet BVPs
u : jump of Drichlet data for solutions of interior/exterior Neumann BVPs

Indirect CFIE: trial expression $u = \imath\eta\Psi_{\mathsf{SL}}(\varphi) + \Psi_{\mathsf{DL}}(\varphi)$

➢ indirect CFIE for exterior Dirichlet problem (1.1.10)

$$\imath\eta\mathsf{V}_\kappa(\varphi) + (\tfrac{1}{2}\mathsf{Id} + \mathsf{K}_\kappa)(\varphi) = g\ . \qquad (1.1.31)$$

☞ uniqueness of solutions & variational formulation in $L^2(\Gamma)$ as above

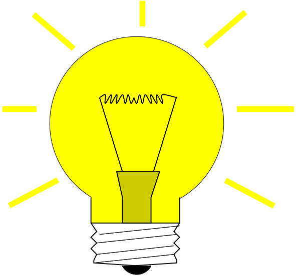
1.1.5 Symmetric Coupling

Boundary value problem, volume source f supported in Ω^-

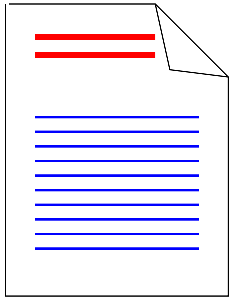
$$-\Delta u - \kappa^2 u = f \quad \text{in } \Omega^- \quad , \quad \text{Sommerfeld radiation b.c. at } \infty \; .$$

Goal: *couple* domain variational formulation in Ω^- (➔ FEM)
boundary integral equation for exterior domain Ω^+ (➔ BEM)
(couple in a variational context)

$$\begin{array}{c} -\Delta u - \kappa^2 u = f \\ \text{in } \Omega^- \end{array} \quad \Leftrightarrow \quad \int_{\Omega^-} \mathbf{grad}\, u \cdot \mathbf{grad}\, v - \kappa^2 uv \,\mathrm{d}\boldsymbol{x} - \int_{\Gamma} \gamma_N u \gamma_D u \,\mathrm{d}S = \int_{\Omega^-} fv \,\mathrm{d}\boldsymbol{x}$$



Idea:
- use transmission condition $[\gamma_D u]_\Gamma = 0$, $[\gamma_{ND} u]_\Gamma = 0$,
- replacement $\gamma_N^+ u = -\mathsf{W}_\kappa(\gamma_D^+ u) - (\mathsf{K}'_\kappa - \frac{1}{2}\mathsf{Id})(\gamma_N^+ u)$, *cf.* (1.1.20),
- extra equation $\gamma_D^+ u = (\mathsf{K}_\kappa + \frac{1}{2}\mathsf{Id})(\gamma_D^+ u) - \mathsf{V}_\kappa(\gamma_N^+ u)$, *cf.* (1.1.19).



Costabel, M. (1987), Symmetric methods for the coupling of finite elements and boundary elements, *in* C. Brebbia, W. Wendland & G. Kuhn, eds, 'Boundary Elements IX', Springer-Verlag, Berlin, pp. 411–420.

▶ coupled variational problem: seek $u \in H^1(\Omega^-)$, $\varphi \in H^{-\frac{1}{2}}(\Gamma)$

$$\begin{aligned}
\int_{\Omega^-} \mathbf{grad}\, u \cdot \mathbf{grad}\, v - \kappa^2 uv \,\mathrm{d}\boldsymbol{x} + \langle \mathsf{W}_\kappa(\gamma_D^- u), \gamma_D^- v\rangle \; - \; \left\langle (\mathsf{K}'_\kappa - \tfrac{1}{2}\mathsf{Id})(\varphi), \gamma_D^- v \right\rangle \; &= \int_{\Omega^-} f v \,\mathrm{d}\boldsymbol{x} \;, \\
\left\langle -(\mathsf{K}_\kappa - \tfrac{1}{2}\mathsf{Id})\gamma_D^- u, \mu \right\rangle \qquad + \qquad \langle \mathsf{V}_\kappa \varphi, \mu\rangle \; &= 0 \;,
\end{aligned}$$

for all $v \in H^1(\Omega^-)$, $\mu \in H^{-\frac{1}{2}}(\Gamma)$

➤ coercive variational problem in natural energy/trace spaces

Note: $\kappa =$ interior Dirichlet resonant frequency $\Rightarrow$ non-uniqueness of solution for φ

➡ “CFIE-type” symmetric coupling necessary **?**

Hiptmair, R. & Meury, P. (2005), Stable FEM-BEM coupling for helmholtz transmission problems, Technical Report 2005-06, SAM, ETH Zürich, Zürich, Switzerland (To appear in SIAM J. Numer. Anal.) `http://www.sam.math.ethz.ch/reports/2005/06`

1.2 Time-harmonic Maxwell’s equations

Topic skipped due to lack of time

1.2.1 Traces

Topic skipped due to lack of time

1.2.2 Representation formula

Topic skipped due to lack of time

1.2.3 Boundary integral operators

Topic skipped due to lack of time

2 Classical Boundary Element Methods

From the perspective of Galerkin discretization:

boundary elements (BEM) $\hat{=}$ finite elements (FEM) for boundary integral equations

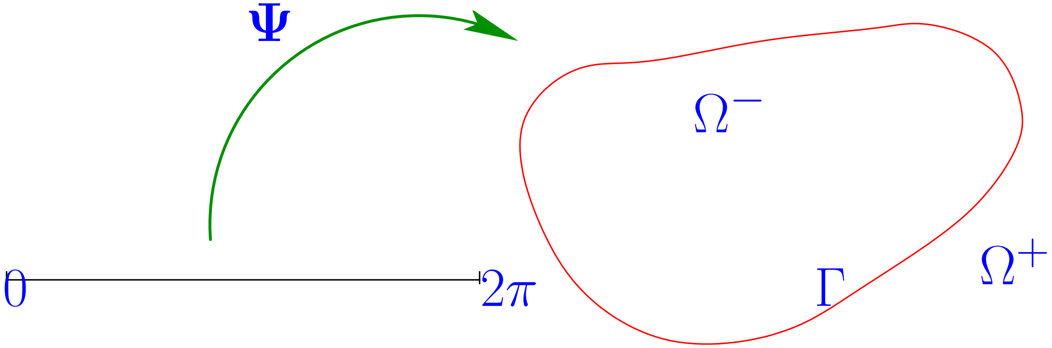
Sauter, S. & Schwab, C. (2004), *Randelementmethoden*, BG Teubner, Stuttgart, Chapter 4.

2.1 Meshes

Assume: $\Gamma =$ boundary of curvilinear polygon ($d = 2$) or Lipschitz polyhedron ($d = 3$) ("CAD geometry")

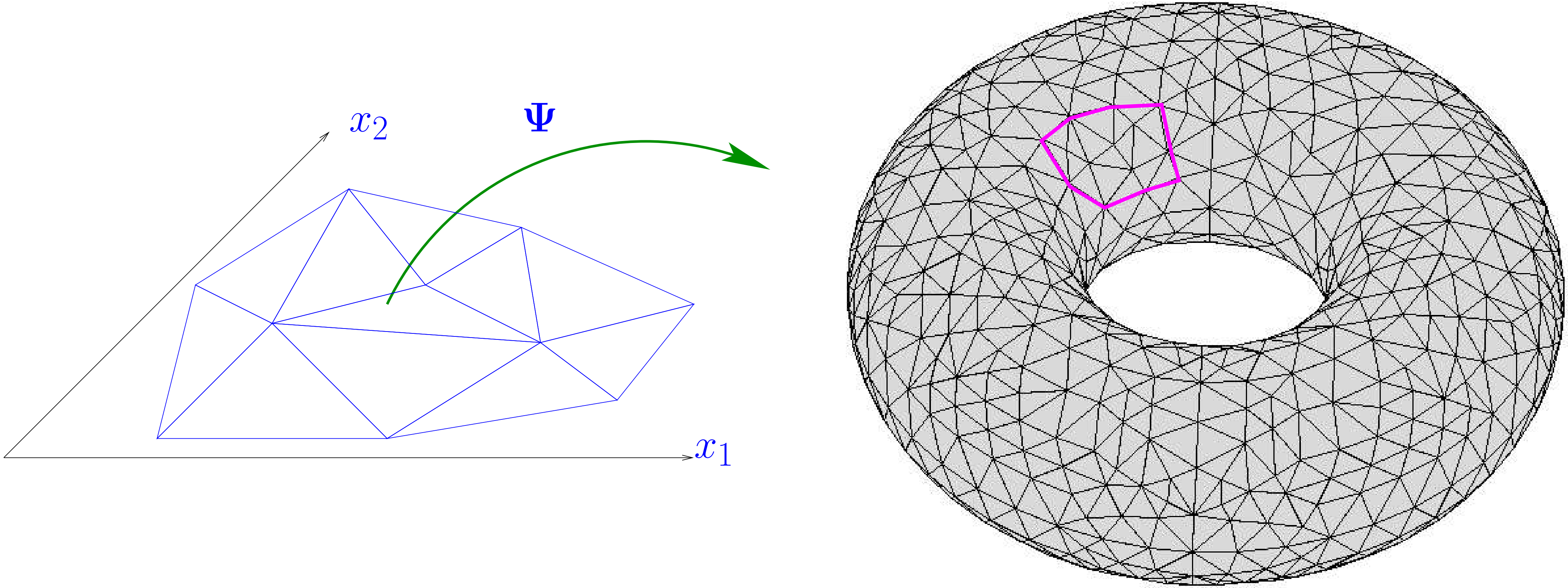
Γ = image of parameter domains $D_i \subset \mathbb{R}^{d-1}$ under (one or several) piecewise smooth charts $\mathbf{\Psi}_i : D_i \mapsto \mathbf{\Psi}(D_i) \subset \Gamma$ (parameterizations)

$d = 2$: $\Gamma = \mathbf{\Psi}([0, 2\pi[)$ ▷



Assume lower and upper bounds (≈ 1) on Gram determinant (limited distortion under $\mathbf{\Psi}_i$)

Definition 2.1.1 (Boundary element mesh)**.**
Parameter domains D_i *equipped with* $\{\mathbf{\Psi}_i\}_i$*-compatible finite element triangulations (triangular/quadrilateral for* $d = 2$*). A (boundary) mesh on* Γ *is their image under the* $\mathbf{\Psi}_i$.



Notions inherited from FEM:

- meshwidth h of a boundary mesh $\mathcal{M}_\Gamma$
- shape-regular families of boundary meshes
- quasi-uniformity of families of boundary meshes

Geometric objects: cells/panels, vertices/nodes, edges of a boundary mesh

Assume: all boundary meshes aligned with corners/edges of Γ

2.2 Standard boundary element spaces

$H^s(D_i)$-conforming finite element spaces on triangulations of parameter domains

▶

$H^s(\Gamma)$-conforming boundary element spaces on $\mathcal{M}_\Gamma$

Note: only holds for $-3/2 < s < 3/2$ in general, for other s smooth Γ required

▷ boundary element spaces $\subset$ trace space $H^{\frac{1}{2}}(\Gamma)$:

Lemma 2.2.1 (Compatibility condition for $H^{\frac{1}{2}}(\Gamma)$)**.**

A p.w. C^1*-function* u *(on closed cells of* $\mathcal{M}_\Gamma$*) belongs to* $H^{\frac{1}{2}}(\Gamma)$ $\iff$ $u \in C^0(\Gamma)$

▼

$H^1(D_i)$-conforming (Lagrangian) finite element spaces $\mathcal{S}_p^0$, $p \in \mathbb{N}$, on triangulations of parameter domains ▶ $H^{\frac{1}{2}}(\Gamma)$-conforming boundary element spaces $\mathcal{S}_p^0(\mathcal{M}_\Gamma)$ on $\mathcal{M}_\Gamma$

polynomial
degree

Mapping under parameterization

▷ boundary element spaces $\subset L^2(\Gamma)/H^{-\frac{1}{2}}(\Gamma)$:

☞ no continuity requirements on boundary element space

piecewise polynomial spaces $\mathcal{S}_p^{-1}$, $p \in \mathbb{N}$, on triangulations of parameter domains ▶ $L^2(\Gamma)$-conforming boundary element spaces $\mathcal{S}_p^{-1}(\mathcal{M}_\Gamma)$ on $\mathcal{M}_\Gamma$

polynomial
degree

Mapping under parameterization

▼

Notions inherited from FEM:
- locally supported nodal basis functions/shape functions
- degrees of freedom ↔ local nodal interpolation operators

Recall: asymptotic best approximation estimates in standard finite element spaces

For
- finite element spaces $X_h = \mathcal{S}_p^0, \mathcal{S}_p^{-1}$ on triangular/quadrilateral mesh of $\Omega \subset \mathbb{R}^{d-1}$,
- $-3/2 < s < 3/2$ in the case $X_h = \mathcal{S}_p^0 \subset C^0(\overline{\Omega})$
  $-1/2 < s < 1/2$ in the case $X_h = \mathcal{S}_p^{-1}$
- $\max\{s, 0\} \leq r \leq p+1$:

$$\exists C = C(s, r, p, \text{shape regularity}): \quad \inf_{v_h \in X_h} \|u - v_h\|_{H^s(\Omega)} \leq C h^{r-s} \|u\|_{H^r(\Omega)} \quad \forall u \in H^r(\Omega)\ . \tag{2.2.1}$$

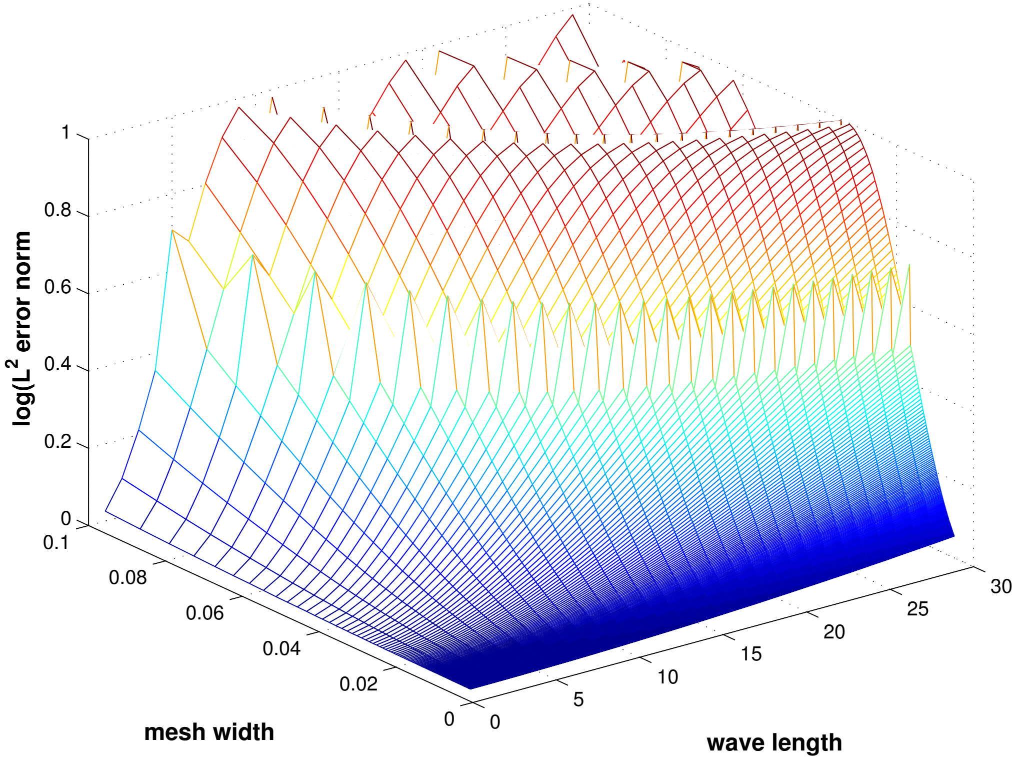
▶ carries over to boundary element spaces derived from $\mathcal{S}_p^0$, $\mathcal{S}_p^{-1}$ (smoothness of Γ may restrict range of valid r)

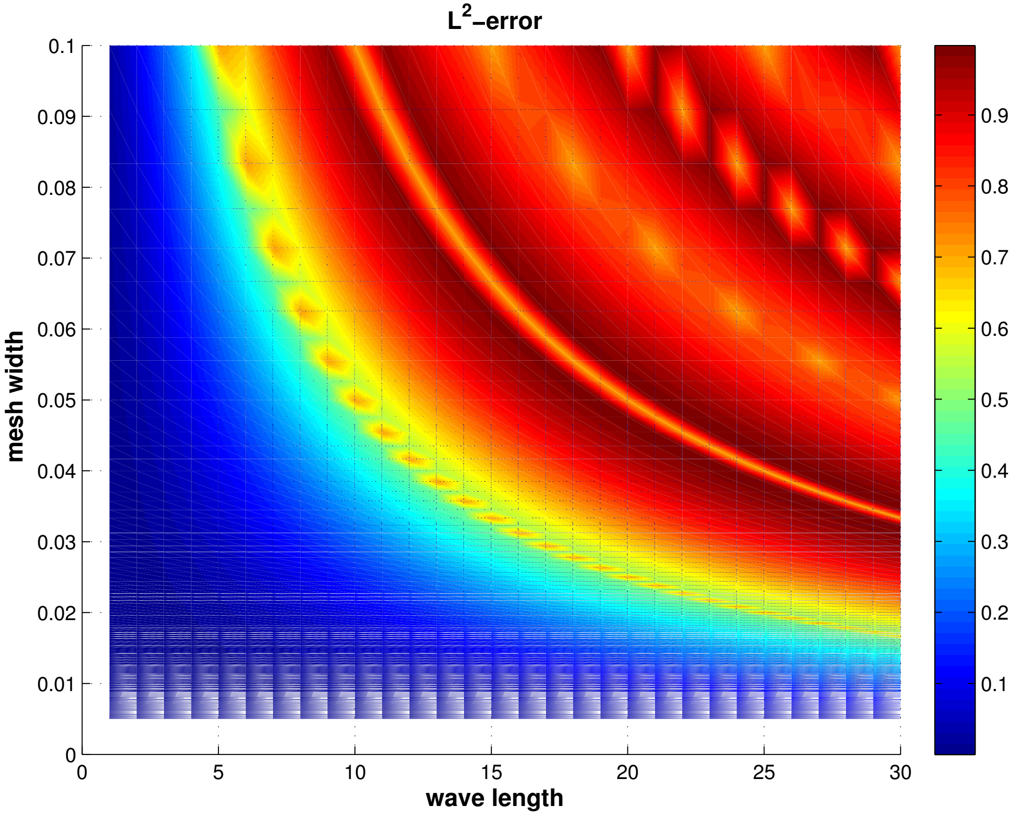
Similar: interpolation error estimates for $\mathcal{S}_p^0(\mathcal{M}_\Gamma)$ (→ edge-by-edge/face-by-face estimates)

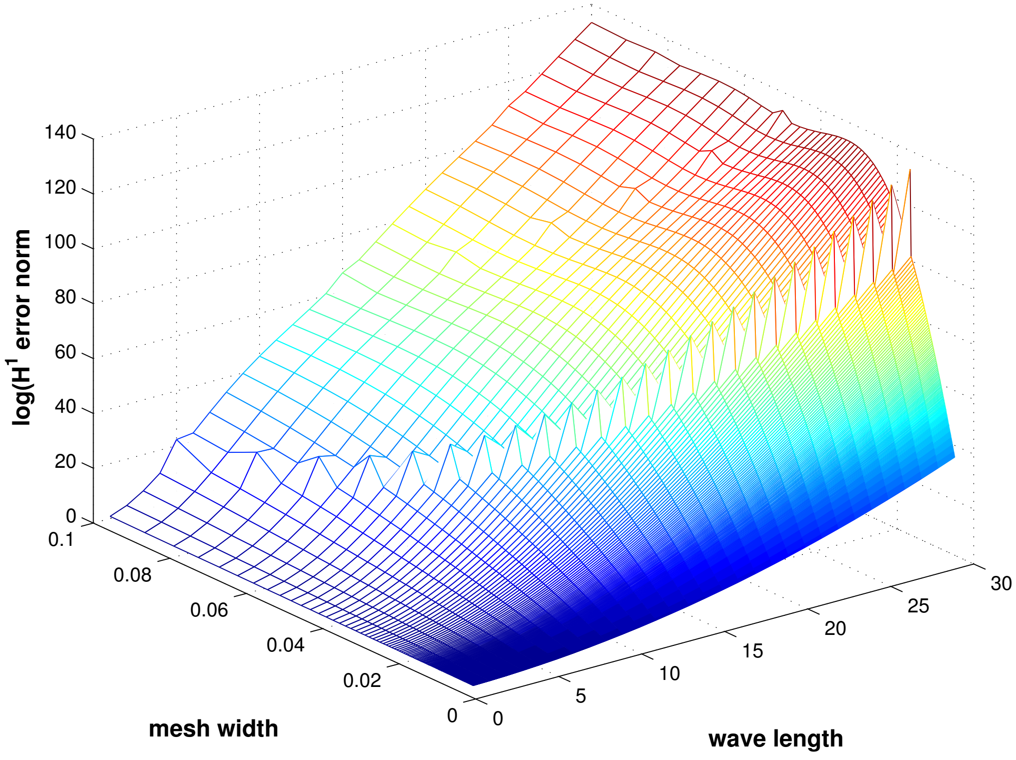
Remark 5. (Almost all) other estimates for finite element spaces (e.g., inverse estimate) have analogues for derived boundary element spaces.

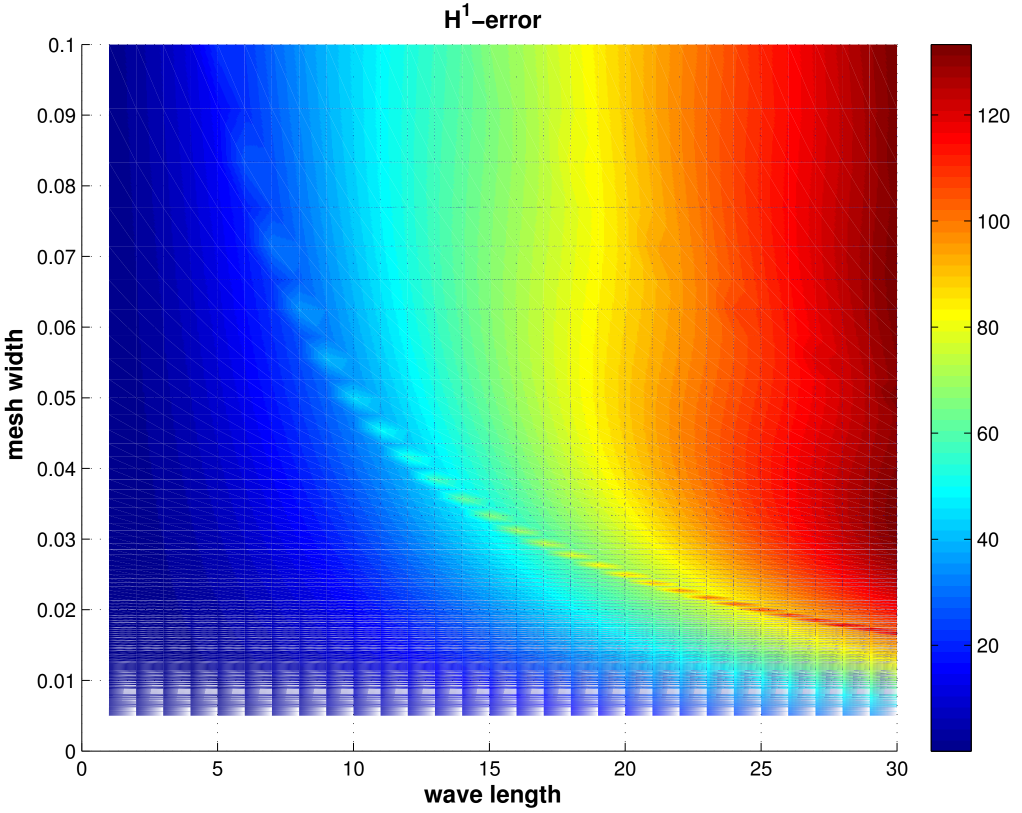
Example 6 (Approximation estimates for oscillatory functions).

Equidistant linear interpolation of $x \mapsto \sin(2\pi k x)$, $k > 0$ on $[0, 1]$.


log(L^2 error norm
1
0.8
0.6
0.4
0.2
0
0.1
0.08
0.06
0.04
0.02
0
mesh width
0
5
10
15
20
25
30
wave length


L^2-error
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
mesh width
0
5
10
15
20
25
30
wave length
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1





➡ minimal resolution required (➞ Nyquist sampling rate) before asymptotic algebraic convergence (2.2.1) sets in.

Meshwidth of $\mathcal{M}_\Gamma$ at least proportional to wavelength $\lambda := \frac{2\pi}{\kappa}$
("Famous" rule: 5-10 points per wavelenght, sampling condition)

2.3 A priori error analysis

Abstract: Linear variational problem posed on Hilbert space V,

$$u \in V\colon \quad \mathsf{a}(u,w) = \langle f,w \rangle_V \quad \forall w \in W \ , \tag{2.3.1}$$

- $\mathsf{a} \in L(V \times W, \mathbb{K})$ continuous sesqui-linear form,
- $f \in W'$ continuous linear form.

Galerkin discretization based on $V_N \subset V$ ➤ Discrete variational problem

$$u_N \in V_N\colon \quad \mathsf{a}(u_N, w_N) = f(w_N) \quad \forall w_N \in W_N \ . \tag{2.3.2}$$

Theorem 2.3.1 (Abstract a priori error estimate for Galerkin discretization)**.**
Let the sesqui-linear form $\mathsf{a} \in L(V \times W, \mathbb{K})$, V, W *Hilbert spaces, give rise to an isomorphism* $\mathsf{A} : V \mapsto W'$. *If the discrete inf-sup conditions*

$$\exists \gamma_N > 0\colon \quad \inf_{v_N \in V_N \setminus \{0\}} \sup_{w_N \in W_N \setminus \{0\}} \frac{|\mathsf{a}(v_N, w_N)|}{\|v_N\|_V \, \|w_N\|_W} \geq \gamma_N \ , \tag{2.3.3}$$

$$\sup_{v_N \in V_N} |\mathsf{a}(v_N, w_N)| > 0 \quad \forall w_N \in W_N \setminus \{0\} \ , \tag{2.3.4}$$

hold, then (2.3.2) *has a unique solution* $u_N \in V_N$ *that satisfies*

$$\|u - u_N\|_V \leq \left(1 + \frac{\|\mathsf{a}\|_{V \times W \mapsto \mathbb{K}}}{\gamma_N}\right) \inf_{v_N \in V_N} \|u - v_N\|_V \ . \tag{2.3.5}$$

Proof. → lecture by M. Melenk ☐

Consider sequence of finite dimensional subspaces $(V_N)_N$, $V_N \subset V$ that is asymptotically dense

$$\forall u \in V\colon \quad \lim_{N \to \infty} \inf_{v_N \in V_N} \|u - v_N\|_V = 0 \ . \tag{2.3.6}$$

Theorem 2.3.2 (Asymptotic convergence estimate for coercive variational problems)**.**
$\mathsf{a} \in L(V \times V, \mathbb{K})$ *coercive and injective* ($a(u,v) = 0\ \forall v \in V \quad \Rightarrow \quad u = 0$)
$\Longrightarrow \quad \exists N_0 \in \mathbb{N}$ *and* $C > 0$*:*

$$\forall N \geq N_0 \colon \quad \forall u \in V \colon \quad \exists_1 u_N \in V_N \colon \quad \begin{array}{c} \mathsf{a}(u_N - u, v_N) = 0 \quad \forall v_N \in V_N \\ \wedge \\ \|u - u_N\|_V \leq C \inf_{v_N \in V_N} \|u - v_N\|_V \ . \end{array}$$

Parlance: Galerkin solution u_N is asymptotically quasi-optimal.

➤ quasi-optimality hinges on minimal resolution of trial space

Observation, *cf.* Ex. 6:

For boundary integral equations related to BVPs for Helmholtz equation
convergence requires “sampling condition” for boundary element space

2.4 Aspects of implementation

2.4.1 Assembly of Galerkin matrix

Entry of single layer Galerkin matrix $\mathbf{A} = \mathbb{C}^{N,N}$, $N =$ dimension of boundary element space with nodal basis $\{b_i\}_{i=1,\dots,N}$,

$$\mathbf{A}_{ij} = \int_\Gamma \int_\Gamma G(\boldsymbol{x},\boldsymbol{y})\, b_i(\boldsymbol{x})\, b_j(\boldsymbol{y})\, \mathrm{S}(\boldsymbol{x})\mathrm{d}S(\boldsymbol{y}) \quad i,j \in \{1,\dots,N\}\,. \tag{2.4.1}$$

▶ to be evaluated: double surface integrals over pairs of panels:

$$\int_{K_1} \int_{K_2} G(\boldsymbol{x},\boldsymbol{y})\, b_i(\boldsymbol{x})\, b_j(\boldsymbol{y})\, \mathrm{S}(\boldsymbol{x})\mathrm{d}S(\boldsymbol{y}) \quad i,j \in \{1,\dots,N\}\,, \quad K_1, k_2 \text{ panels of } \mathcal{M}_\Gamma\,. \tag{2.4.2}$$

kernel $G(\boldsymbol{x},\boldsymbol{y})$ oscillates on scale $\lambda = \frac{2\pi}{\kappa}$, which has to be *resolved by* $\mathcal{M}_\Gamma$, *cf.* Ex. 6.

▶ on the scale of a single panel is **not oscillatory !**

Challenge: kernel $G(\boldsymbol{x}, By)$ has *singularity* for $\boldsymbol{x} = \boldsymbol{y}$

Semi-analytic evaluations

Trick: extract singularity ($\leftrightarrow$ subtract off kernel for $\kappa = 0$), e.g., for $d = 3$

$$G(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{4\pi\,|\boldsymbol{x}-\boldsymbol{y}|} \quad + \quad \frac{e^{\imath\kappa|\boldsymbol{x}-\boldsymbol{y}|} - 1}{4\pi\,|\boldsymbol{x}-\boldsymbol{y}|} \; .$$

(almost) analytic evaluation
➞ faesible for p.w. linear $\mathcal{M}_\Gamma$
(Steinbach 2000)

globally continuous, piecewise C^1 with bounded derivatives
➤ use low order numerical quadrature everywhere

Numerical quadrature

Distinguish two cases in (2.4.2)

❶ K_1, K_2 adjacent ($\overline{K_1} \cap \overline{K_2} \neq 0$) or near
❷ K_1, K_2 well separated

Case ❶: → singularity encountered

- use regularizing transformation (Duffy trick) to obtain smooth integrand
- apply Gaussian quadrature rule to regularized integrals

Case ➨: use low order Gaussion quadrature rules for outer and inner integrals in (2.4.2)

balance: discretization error $\longleftrightarrow$ consistency error due to quadrature (Strang's lemma)
(→ "near field" quadrature order $= O(|\log h|)$)

Detailed recipes:

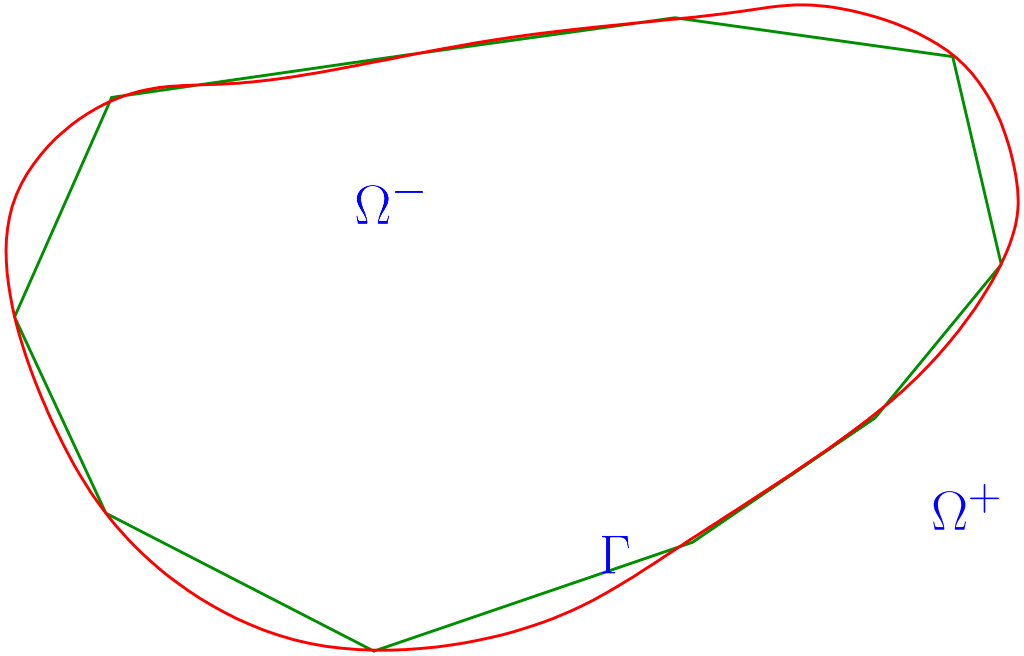
Sauter, S. & Schwab, C. (2004), *Randelementmethoden*, BG Teubner, Stuttgart, Chapter 5.

2.4.2 Boundary approximation

Treat boundary integral equations on curve/surface Γ_h instead of Γ

$\Gamma_h \leftarrow$ "polynomial interpolation" of Γ (isoparametric curve/surface approximation)

Simplest case: piecewise (affine) linear interpolation



balance: discretization error $\longleftrightarrow$ error due to surface approximation (Strang's lemma)

Rule of thumb (p.w. smooth Γ): polynomial degree $p+1$ for surface approximation, if boundary element space derived from p.w. polynomials of degree p

Detailed analysis in forthcoming English edition (chapter 9) of

Sauter, S. & Schwab, C. (2004), *Randelementmethoden*, BG Teubner, Stuttgart.

2.5 Spectral Galerkin methods

Assumptions:

- Γ smooth **&** with *analytic* parameterization $\boldsymbol{\Psi} : [0, 2\pi[\mapsto \Gamma$ ($d = 2$),
  with *analytic* parameterization via the 2-sphere $\boldsymbol{\Psi} : \mathbb{S} \mapsto \Gamma$ ($d = 3$).
  (restrictive assumption on geometry)
- analytic data $\Rightarrow$ analytic Cauchy data of solutions of Helmholtz BVPs

Trial ansd test spaces (for any function space $H^{\frac{1}{2}}(\Gamma)$, $L^2(\Gamma)$, $H^{-\frac{1}{2}}(\Gamma)$):

$d = 2$: use first N (N odd) harmonics

$$V_N := \operatorname{Span}\left\{\boldsymbol{x} \mapsto \exp(\imath k \boldsymbol{\Psi}^{-1}(\boldsymbol{x}))\colon k = -\tfrac{N-1}{2}, \dots, \tfrac{N-1}{2}, \boldsymbol{x} \in \Gamma\right\} .$$

$d = 3$: use first L^2 spherical harmonics up to order L → (Colton & Kress 1998, Sect. 2.3)

$$V_{L^2} := \operatorname{Span}\left\{\boldsymbol{x} \mapsto Y_n^{m-1}(\boldsymbol{\Psi}^{-1}(\boldsymbol{x}))\colon m = -n, \dots, n, m = 1, \dots, L, \boldsymbol{x} \in \Gamma\}\right\} .$$

▶ exponential convergence w.r.t. N ($d = 2$), L ($d = 3$), resp.

BUT minimal resolution requirement entails $N \sim \kappa\,\mathrm{diam}(\Gamma)$ ($d = 2$), $L \sim \kappa\,\mathrm{diam}(\Gamma)$ ($d = 3$).

Important: efficient implementation (using suitable quadrature rules, fast transformations)

Ganesh, M. & Graham, I. (2003), ‘A high-order algorithm for obstacle scattering in three dimensions’, *J. Comp. Phys.* **198**(1), 211–242.

2.6 Boundary elements for electromagnetics

This subject was skipped due to lack of time.

3 Fast Multipole Methods

3.1 Challenge and model problems

Galerkin matrix ↔ boundary integral operator

$$\mathbf{A}_{ij} = \int_\Gamma \int_\Gamma G(\boldsymbol{x},\boldsymbol{y})\, b_i(\boldsymbol{x})\, b_j(\boldsymbol{y})\, \mathrm{S}(\boldsymbol{x})\mathrm{d}S(\boldsymbol{y}) \quad i,j \in \mathcal{I} := \{1,\dots,N\}\ , \tag{3.1.1}$$

- $\Gamma \hat{=}$ compact closed curved ($d = 2$)/surface ($d = 3$), usually the boundary $\Gamma := \partial\Omega^-$,
- $\{b_i\}_{i=1}^N \hat{=}$ (locally supported) basis functions of boundary element space $V_N \subset V$, $\dim V_N = N$ → Sect. 2.2,
- $G(\boldsymbol{x},\boldsymbol{y}) \hat{=}$ non-local kernel function (G9for single layer boundary integral operators)

"Helmholtz kernels": $$G(\boldsymbol{x},\boldsymbol{y}) = \begin{cases} i/4 H_0^{(1)}(\kappa|\boldsymbol{x}-\boldsymbol{y}|) & \text{, for } d=2,\ \kappa \neq 0\ , \\ \frac{\exp(i\kappa|\boldsymbol{x}-\boldsymbol{y}|)}{4\pi|\boldsymbol{x}-\boldsymbol{y}} & \text{, for } d=3\ , \end{cases}$$

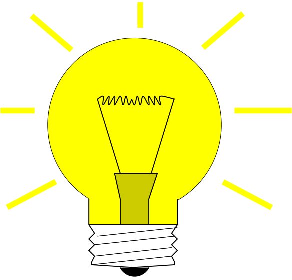
with $\kappa > 0 \hat{=}$ wave number.

▶ $\mathbf{A}$ dense $:\Leftrightarrow$ $\mathrm{nnz}(\mathbf{A}) := \sharp\{(i,j) \in \{1,\dots,N\}^2 \colon \mathbf{A}_{ij} \neq 0\} \approx N^2$

Storage requirements & costs of assembly: $O(N^2)$

Computational cost(matrix × vector): $O(N^2)$

➤ Prohibitively expensive for (realistic) $N \approx 10^4 - 10^6$



Insight: We can merely compute approximate solutions, anyway **!**

Idea: replace $\mathbf{A}$ with approximation $\widetilde{\mathbf{A}} \approx \mathbf{A}$ such that

Storage for $\widetilde{A} =$ $O(N)$ (or slightly worse$^{(*)}$)

Computational cost($\widetilde{\mathbf{A}}$ × vector) $=$ $O(N)$ (or slightly worse$^{(*)}$)

$(*)$: $O(N \log^\gamma N)$ acceptable, with small $\gamma \in \mathbb{N}_0$

Caveats:

- ☞ Watch the constants in the "O" !
- ☞ Also crucial: dependence on wave number κ (for "high frequencies" $\kappa \to \infty$)

Model problem: kernel collocation matrix:

$$\mathbf{A}_{ij} = \begin{cases} G(\boldsymbol{x}_i, \boldsymbol{x}_j) & \text{, if } i \neq j \text{ ,} \\ 0 & \text{else} \end{cases} \quad \in \mathbb{C}^{N,N} \text{ ,} \tag{3.1.2}$$

$\boldsymbol{x}_i$, $i = 1, \ldots, N,$ = collocation points on Γ.

Example 7 (Helmholtz collocation matrix on simple curve).

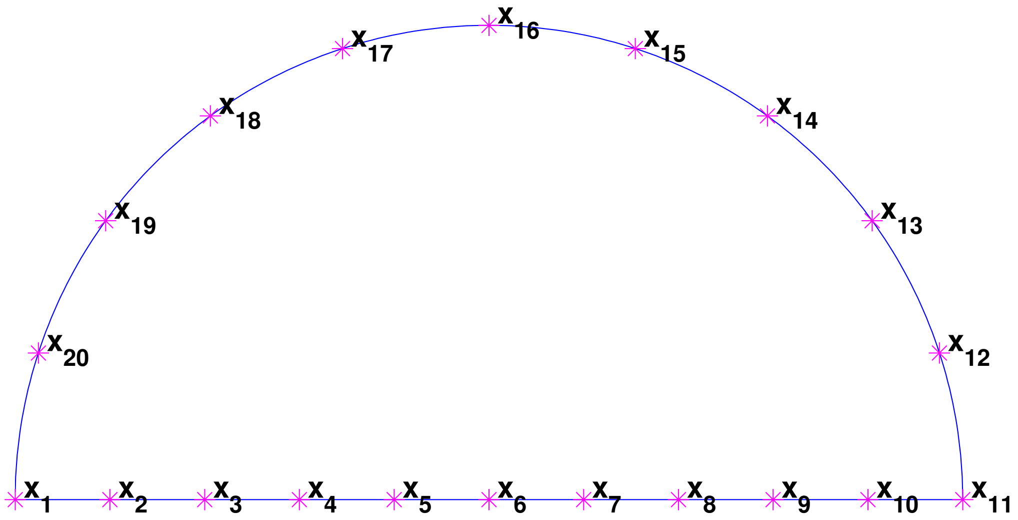
$\Omega \subset \mathbb{R}^2$ half disk (diameter 1), $\Gamma := \partial\Omega$

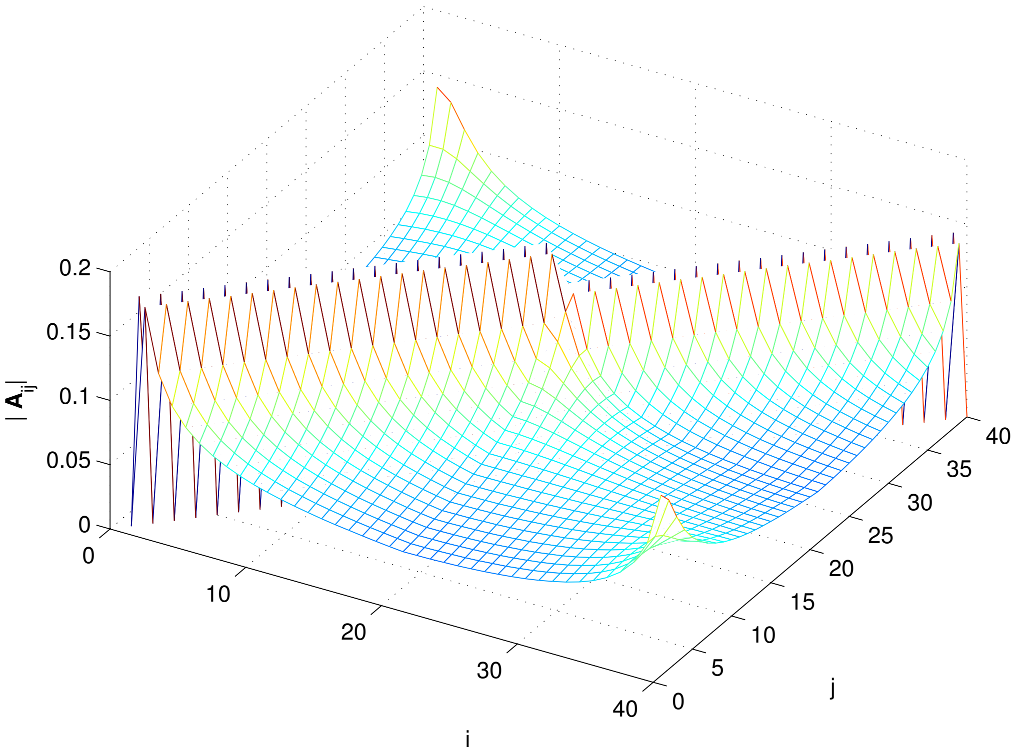
Evenly spaced collocation points $\boldsymbol{x}_i$, $i = 1, \ldots, N$

➤ kernel collocation matrix ($\kappa \neq 0$)

$$\mathbf{A}_{ij} = \begin{cases} i/4 H_0^{(1)}(\kappa |\boldsymbol{x}_i - \boldsymbol{x}_j|) & \text{, if } i \neq j \text{ ,} \\ 0 & \text{, if } i = j \text{ .} \end{cases}$$

▷





◁ modulus of entries of $\mathbf{A}$:

- 40 collocation points
- wave number $\kappa = 8\pi$

Geometric assumptions for the study of N-asymptotics:

Curve/surface Γ not too much “crumpled” (Sauter & Schwab 2004, Ass. 7.3.17)]

$$\exists C > 0\colon \quad \mathrm{vol}(\Gamma \cap B_{r,R}(\boldsymbol{x})) \leq C(R^{d-1} - r^{d-1}) \quad \forall \boldsymbol{x} \in \Gamma, \forall 0 \leq r < R < \infty \;,$$

$B_{r,R}(\boldsymbol{x}) := \{\boldsymbol{y} \in \mathbb{R}^d \colon r < |\boldsymbol{x} - \boldsymbol{y}| < R\}$.

Collocation points "evenly distributed":

the points $\boldsymbol{x}_i$ are vertices of a surface mesh belonging to uniformly shape-regular and quasi-uniform family.

(➭ will be taken for granted in the sequel)

3.2 Abstract approximation error estimates

All "fast" methods employ *approximations of the integral kernel*:

$$\mathbf{A} \quad \longrightarrow \quad \widetilde{\mathbf{A}}_{ij} := \int_\Gamma \int_\Gamma \widetilde{G}(\boldsymbol{x},\boldsymbol{y})\, b_i(\boldsymbol{x}) b_j(\boldsymbol{y})\, \mathrm{d}S(\boldsymbol{y})\mathrm{d}S(\boldsymbol{x}) \; . \tag{3.2.1}$$

➤ (in framework of Galerkin boundary element methods)

Impact of kernal approximation analyzed by means of Strang's lemma

$$\mathsf{a}(u,v) := \int_\Gamma\int_\Gamma G(\boldsymbol{x},\boldsymbol{y})\, v(\boldsymbol{x})u(\boldsymbol{y})\,\mathrm{d}S(\boldsymbol{y})\mathrm{d}S(\boldsymbol{x})\ ,$$
$$\widetilde{\mathsf{a}}(u,v) := \int_\Gamma\int_\Gamma \widetilde{G}(\boldsymbol{x},\boldsymbol{y})\, v(\boldsymbol{x})u(\boldsymbol{y})\,\mathrm{d}S(\boldsymbol{y})\mathrm{d}S(\boldsymbol{x})\ ,$$

V-elliptic and V-continuous.

▶ examine consistency error

$$\|\mathsf{a}-\widetilde{\mathsf{a}}\|_{V\times V\mapsto\mathbb{C}} := \sup_{u_N\in V_N}\sup_{v_N\in V_N}\frac{|\mathsf{a}(u_N,v_N)-\widetilde{\mathsf{a}}(u_N,v_N)|}{\|u_N\|_V\,\|v_N\|_V}\ . \tag{3.2.2}$$

Special case: variational problem in $V = L^2(\Gamma)$: a crude estimate

$$\blacktriangleright\quad \|\mathsf{a}-\widetilde{\mathsf{a}}\|_{L^2(\Gamma)\times L^2(\Gamma)\mapsto\mathbb{C}} \leq \left\|G-\widetilde{G}\right\|_{L^\infty(\Gamma\times\Gamma)}|\Gamma|\ . \tag{3.2.3}$$

To gauge effect of kernel approximation: study $\left\|G-\widetilde{G}\right\|_{L^\infty(\Gamma\times\Gamma)}$!

Remark 8. Impact of kernel approximation on kernel collocation matrix (3.1.2):

$$\left\|\mathbf{A}-\widetilde{\mathbf{A}}\right\| \leq N\cdot\max_{i,j}|G(\boldsymbol{x}_i,\boldsymbol{x}_j)-\widetilde{G}(\boldsymbol{x}_i,\boldsymbol{x}_j)|\ ,\quad \|\cdot\| \mathrel{\hat{=}} \text{Euklidean matrix norm}\ .$$

3.3 Hierarchical clustering for low frequencies

Sauter, S. & Schwab, C. (2004), *Randelementmethoden*, BG Teubner, Stuttgart, Chapter 7.

Study asymptotics: κ fixed & $\left(N \rightarrow \infty \quad \Leftrightarrow \quad h \rightarrow 0 \right)$

Focus: $\kappa \approx 0$ (“Laplacian”) $\longleftrightarrow$ “small objects ↔ large wavelength”

▶ single layer kernel $G(\boldsymbol{x},\boldsymbol{y}) = \begin{cases} -\frac{1}{2\pi}\log(|\boldsymbol{x}-\boldsymbol{y}|) & \text{, for } d=2 \text{ ,} \\ \frac{1}{4\pi}\frac{1}{|\boldsymbol{x}-\boldsymbol{y}|} & \text{, for } d=3 \text{ ,} \end{cases}$ $\boldsymbol{x} \neq \boldsymbol{y}$.

Notation: $Q_0 \subset \mathbb{R}^d \mathrel{\hat{=}}$ bounding box for Γ ($\Gamma \subset Q_0$, $Q_0 = \prod_{i=1}^{d} [\alpha_i, \beta_i]$)

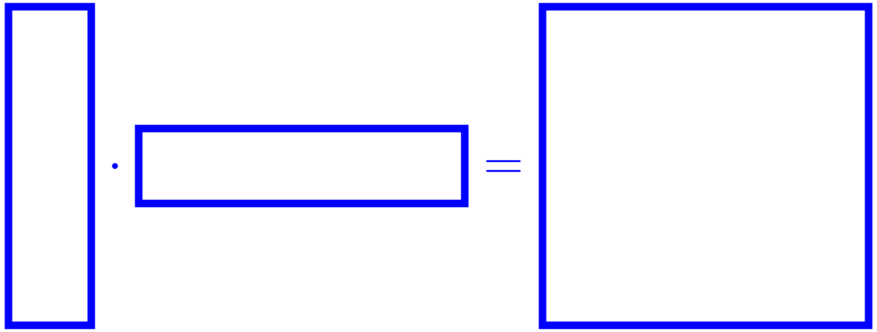
3.3.1 Idea: separable kernel approximation

What if . . . kernel $G(\boldsymbol{x},\boldsymbol{y})$ was separable: $G(\boldsymbol{x},\boldsymbol{y}) = g(\boldsymbol{x})\overline{h(\boldsymbol{y})}$ **?**

($g, h : Q_0 \mapsto \mathbb{C}$ continuous)

▶ $$\mathbf{A} = (g(\boldsymbol{x}_i))_{i=1}^{N} \cdot ((h(\boldsymbol{x}_j))_{j=1}^{N})^H \in \mathbb{C}^{N,N} \;,$$

vectors $\in \mathbb{C}^N$!



(3.3.1)

➡ Storage required for $\mathbf{A}$: $2N$ `complex` numbers

Cost($\mathbf{A}$ × vector) $= 2N$ multiplications $+$ $2N-2$ additions

If kernel $G(\boldsymbol{x},\boldsymbol{y})$ = linear combination of separable functions:

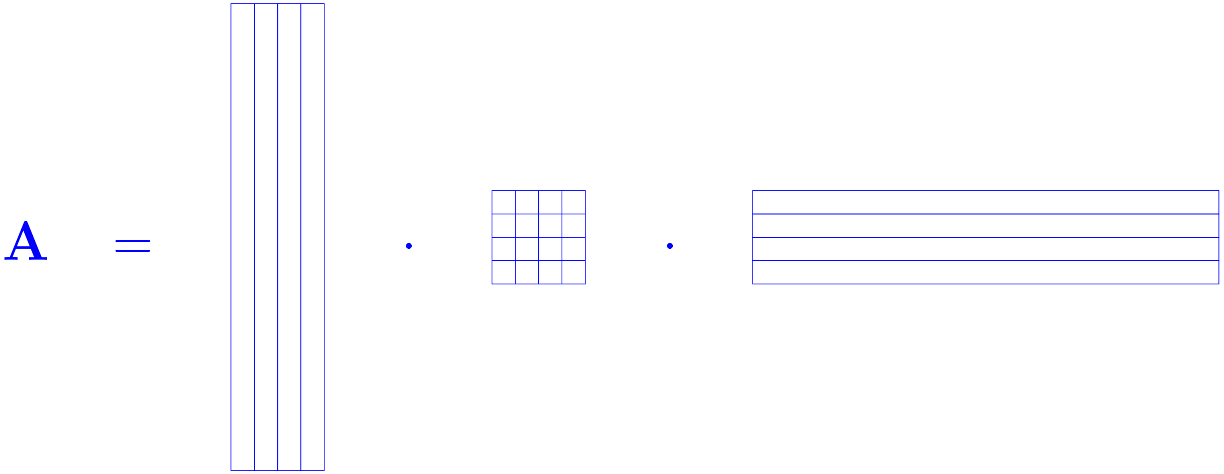
$$G(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^{P}\sum_{j=1}^{P} \gamma_{ij} g_i(\boldsymbol{x})\overline{h}_j(\boldsymbol{y}) \;, \quad (g_i, h_j : Q_0 \mapsto \mathbb{C} \text{ continuous}, \gamma_{ij} \in \mathbb{C}\,). \qquad (3.3.2)$$

▶ $$\mathbf{A} = \mathbf{U}\cdot\mathbf{C}\cdot\mathbf{V}^H \;,$$

$$\mathbf{U} := \big(g_j(\boldsymbol{x}_i)\big)_{\substack{i=1,\dots,N\\ j=1,\dots,P}} \in \mathbb{C}^{N,P} \;,$$

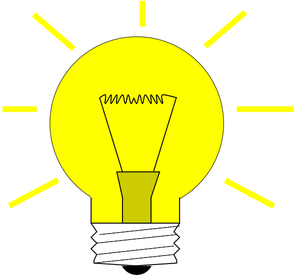
$$\mathbf{C} := \big(\gamma_{ij}\big)_{i,j=1,\dots,P}$$ (coupling matrix) , (3.3.3)

$$\mathbf{V} := \big(h_j(\boldsymbol{x}_i)\big)_{\substack{i=1,\dots,N\\ j=1,\dots,P}} \in \mathbb{C}^{N,P} \;.$$



Note: $P < N$ ➢ $\operatorname{rank}(\mathbf{A}) \leq P$: $P \ll N$ ➙ $\mathbf{A} =$ “low rank matrix”.

➡ Storage required for $\mathbf{A}$: $2PN + P^2$ `complex` numbers
Cost($\mathbf{A} \times$ vector) $= 2NP + P^2$ multiplications $+$ $2(N-1)P - (P-1)^2$ additions



Idea: (semi-)separable kernel approximation

$$G(\boldsymbol{x}, \boldsymbol{y}) \approx \sum_{i=1}^{P} \sum_{j=1}^{P} \gamma_{ij} g_i(\boldsymbol{x}) \overline{h}_j(\boldsymbol{y}) \ , \tag{3.3.4}$$

$g_i, h_j : Q_0 \mapsto \mathbb{C}$ continuous, $\gamma_{ij} \in \mathbb{C}$.

Example 9 (Global separable approximation of kernel collocation matrix).

Definition 3.3.1 (Singular value decomposition). → *(Golub & Van Loan 1989)*
$\mathbf{A} = \mathbf{U}\,\mathrm{diag}(\sigma_1,\dots,\sigma_N)\mathbf{V}^H$ *is the singular value decomposition of* $\mathbf{A} \in \mathbb{C}^{N,N}$, *if* $\mathbf{U},\mathbf{V} \in \mathbb{C}^{N,N}$ *are* unitary *matrices and* $\sigma_i \geq 0$. *The* σ_i *are the singular values of* $\mathbf{A}$.

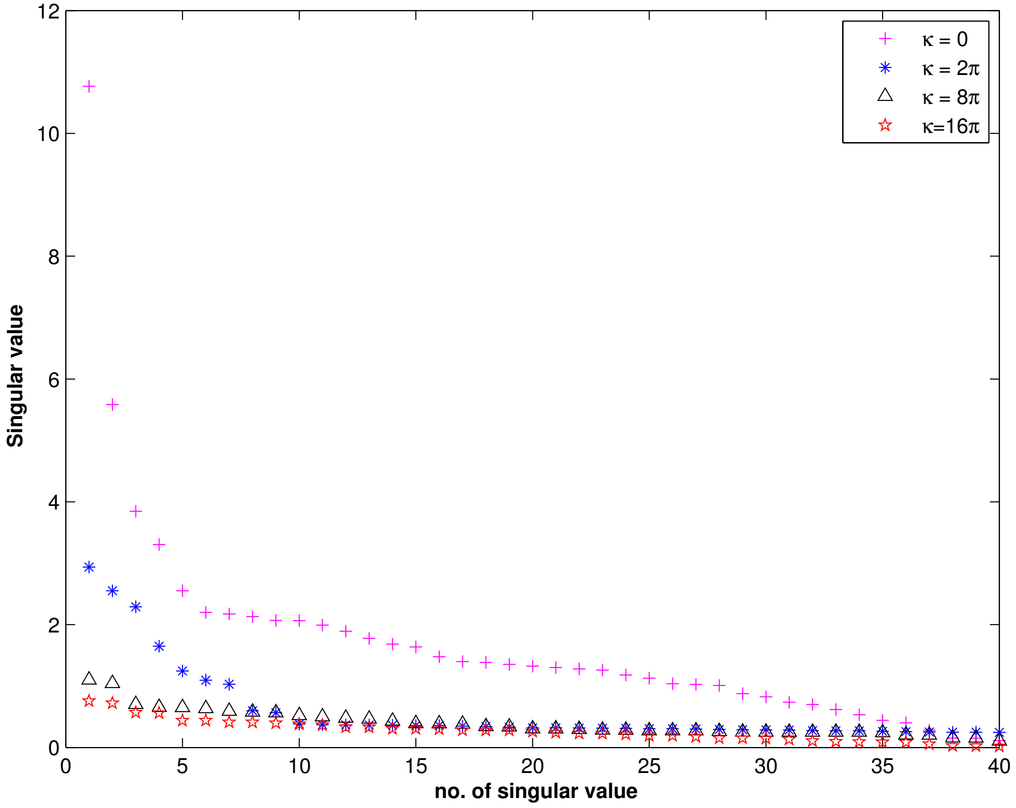
Convention: singular values sorted $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_N \geq 0$

Singular values ↔ approximability of $\mathbf{A}$ by low rank matrices:

Theorem 3.3.2 (Low rank best approximation).

$$\mathbf{A} \in \mathbb{C}^{N,N}: \quad \inf\{\|\mathbf{A}-\mathbf{F}\| : \mathrm{rank}(\mathbf{F}) \leq k\} = \sigma_{k+1}\ , \quad k = 1,\dots,N-1\ ,$$

where $\|\cdot\|$ = *Euklidean matrix norm or Frobenius norm.*



Setting of Ex. 7:

(40 collocation points)

◁ Singular values of Helmholtz kernel collocation matrix for different wavenumbers κ

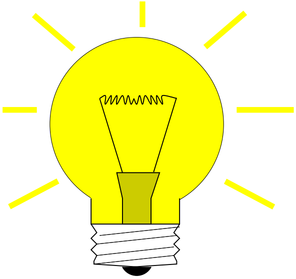
➠ Slow decay of singular values

Poor approximability of $\mathbf{A}$ in terms of low rank matrices.

Singularity of kernel for $\boldsymbol{x} = \boldsymbol{y}$ ⟷↯ separable and smooth approximation

How to avoid the singularities **?**

Idea: local separable approximation



Use tensor product tiling: $Q_0 \times Q_0 = \bigcup_k Q_k^x \times Q_k^y, \quad Q_k^x, Q_k^y \subset \mathbb{R}^d$

$$▶ \quad G(\boldsymbol{x},\boldsymbol{y}) \approx \sum_{i=1}^{P}\sum_{j=1}^{P} \gamma_{ij}^k g_i^k(\boldsymbol{x})\overline{h}_j^k(\boldsymbol{y}) \quad \boxed{\text{for} \quad \boldsymbol{x} \in Q_k^x, \boldsymbol{y} \in Q_k^y},$$

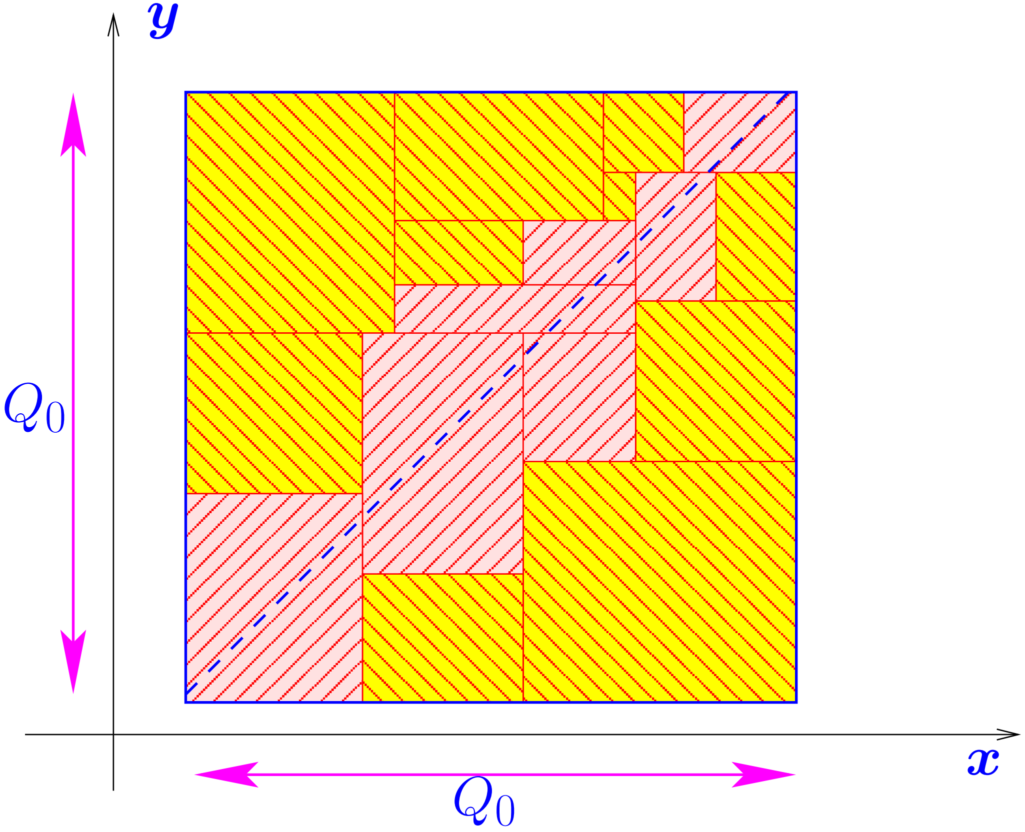
with (local) expansion functions $g_i^k, h_j^k : Q_0 \mapsto \mathbb{C}$ continuous, $\gamma_{ij}^k \in \mathbb{C}$.

“avoiding the singularity”

$\updownarrow$

$Q_k^x \cap Q_k^x = \emptyset$

Parlance: $Q_k^x \times Q_k^y$ called a block



Remark 10 (Separable approximation of other kernels).

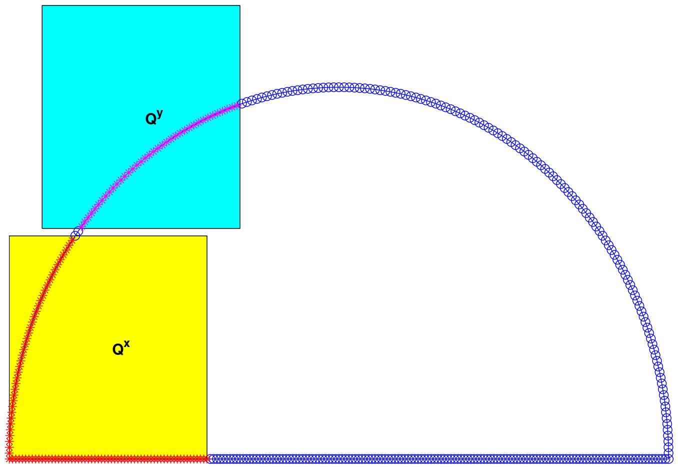
If $\widehat{G}(\boldsymbol{x},\boldsymbol{y}) = \partial_{\boldsymbol{y}} G(\boldsymbol{x},\boldsymbol{y})$, $\partial_{\boldsymbol{y}} \hat{=}$ differential operator acting on $\boldsymbol{y}$, e.g. double layer kernel,

$$\widehat{G}(\boldsymbol{x},\boldsymbol{y}) \approx \sum_{i=1}^{P}\sum_{j=1}^{P} \gamma_{ij}^{k} g_i^k(\boldsymbol{x})(\partial_{\boldsymbol{y}} h_j^k)(\boldsymbol{y}) \quad \text{for} \quad \boldsymbol{x} \in Q_k^x,\ \boldsymbol{y} \in Q_k^y\ .$$

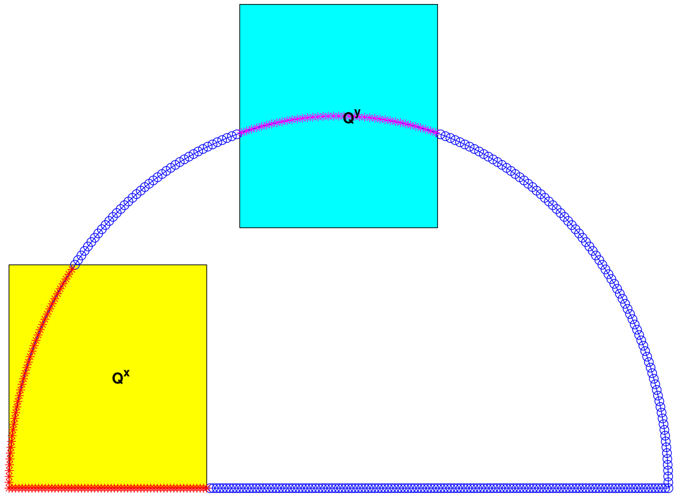
Example 11 (“Off diagonal” separable approximation).

Setting of Ex. 7, 400 collocation points, *Laplacian case* $\kappa = 0$

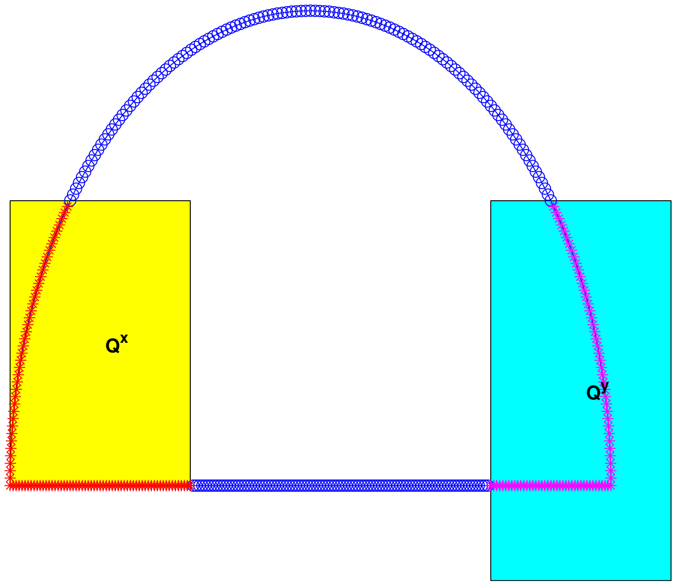
Monitored: singular values of sub-blocks of Helmholtz kernel collocation matrix (corresponding to rectangles Q^x, Q^y)



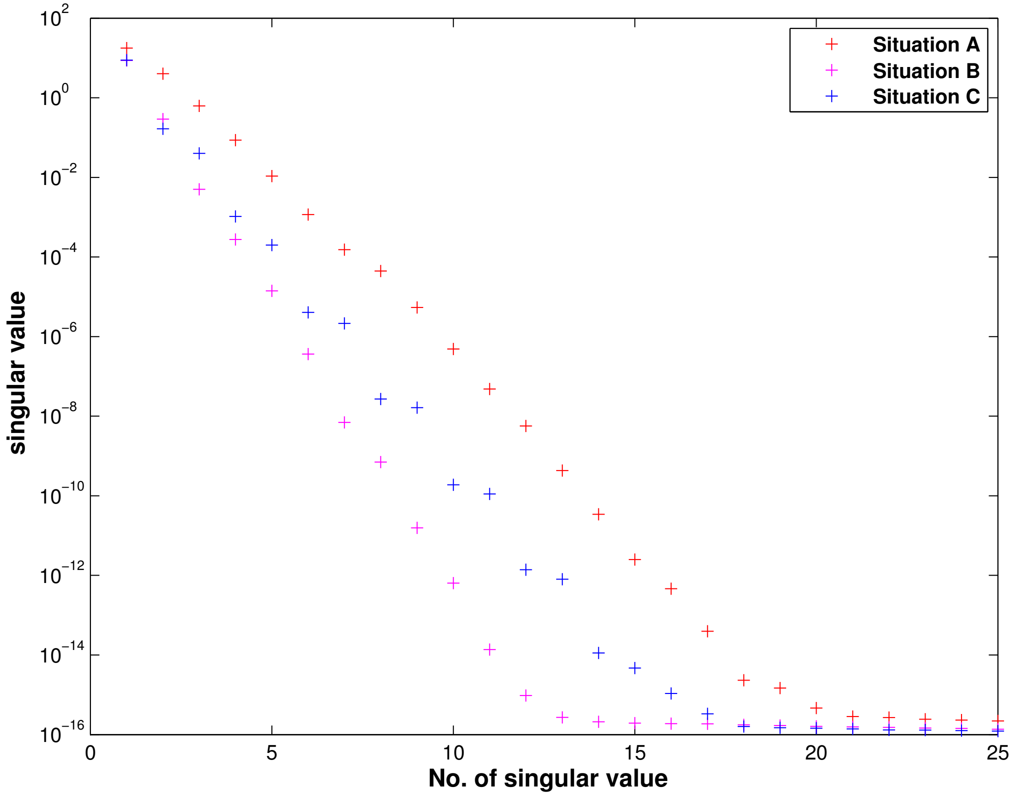
Situation A



Situation B

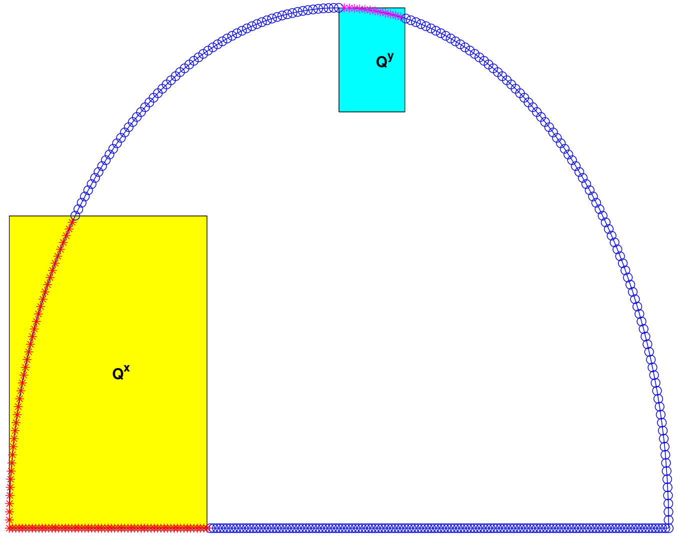


Situation C

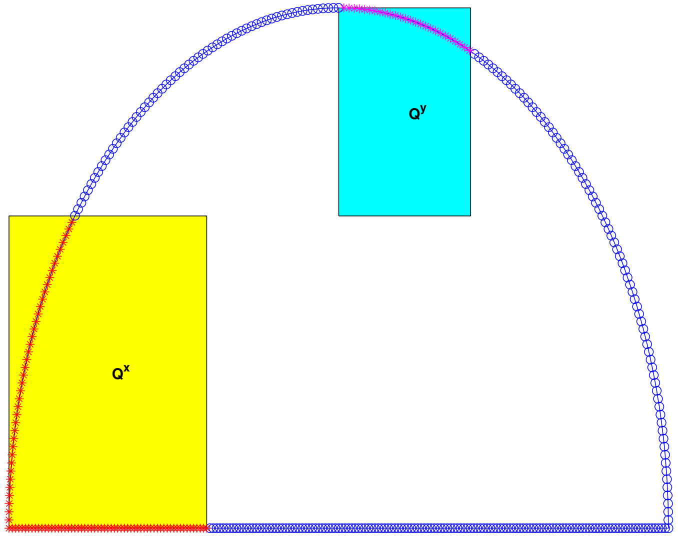


◁ Observation:

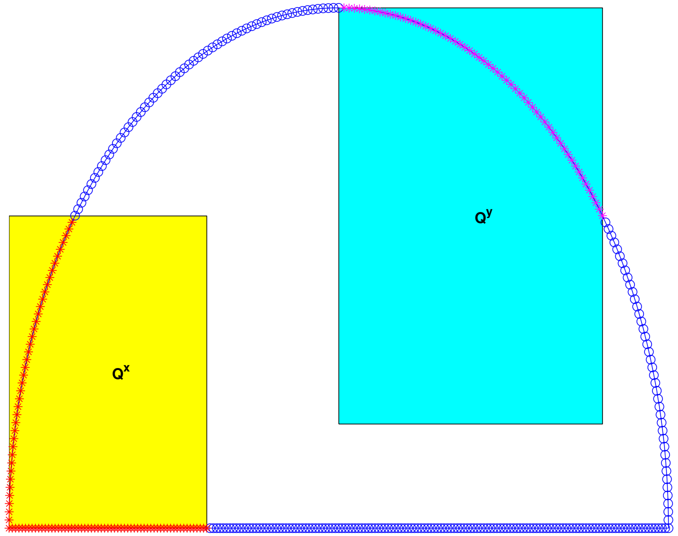
- exponential decay of singular values
- better separation of boxes
  - ➢ faster rate of decay of singular values



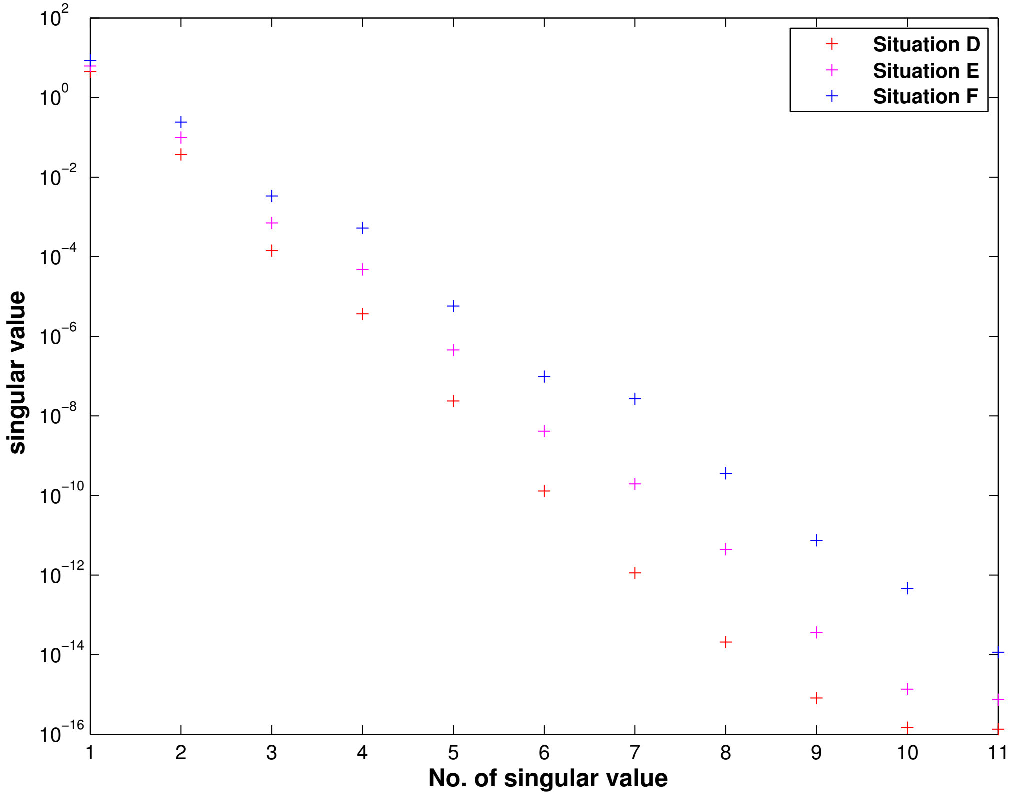
Situation D



Situation E



Situation F



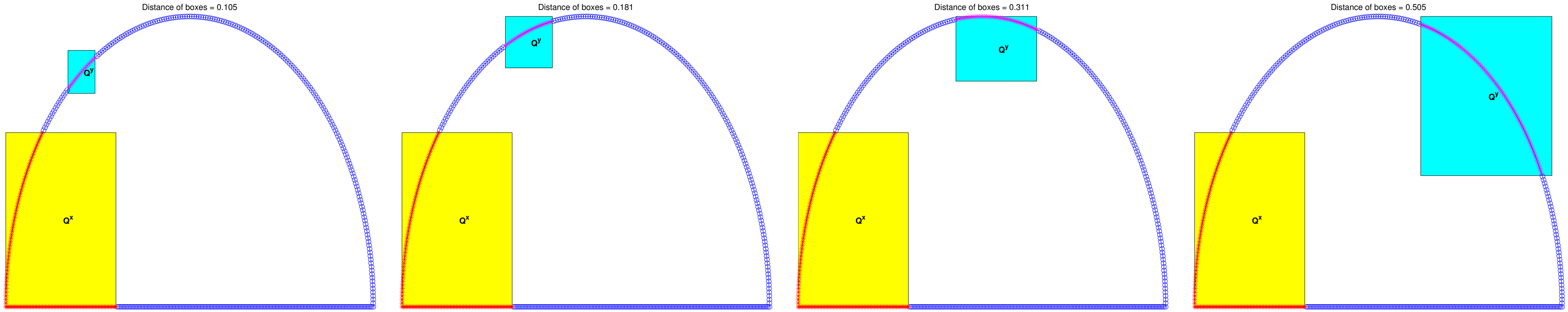
$\lhd$ Observation:

- In the case of constant distance: faster exponential decay of singular values for smaller boxes

Example 12 (Low rank approximation and admissibility condition).

Setting of Ex. 7, 400 collocation points, *Laplacian case* $\kappa = 0$

Ex. 11 ➪ try to balance distance of boxes $\longleftrightarrow$ size of boxes

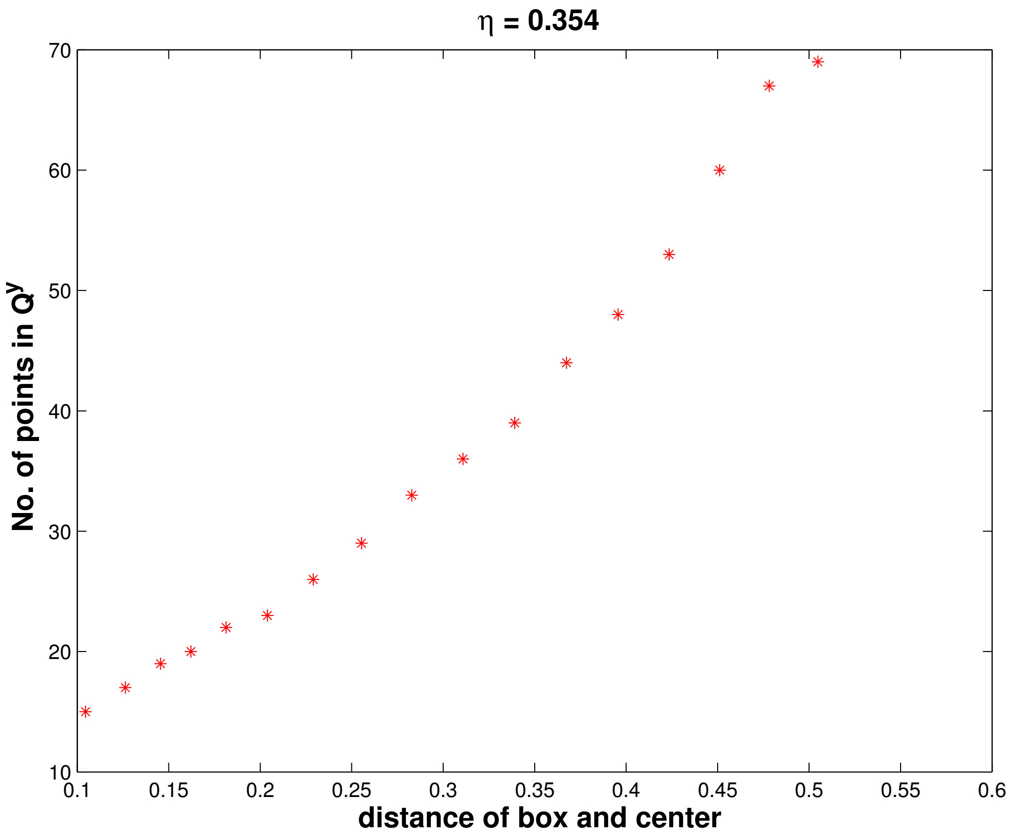


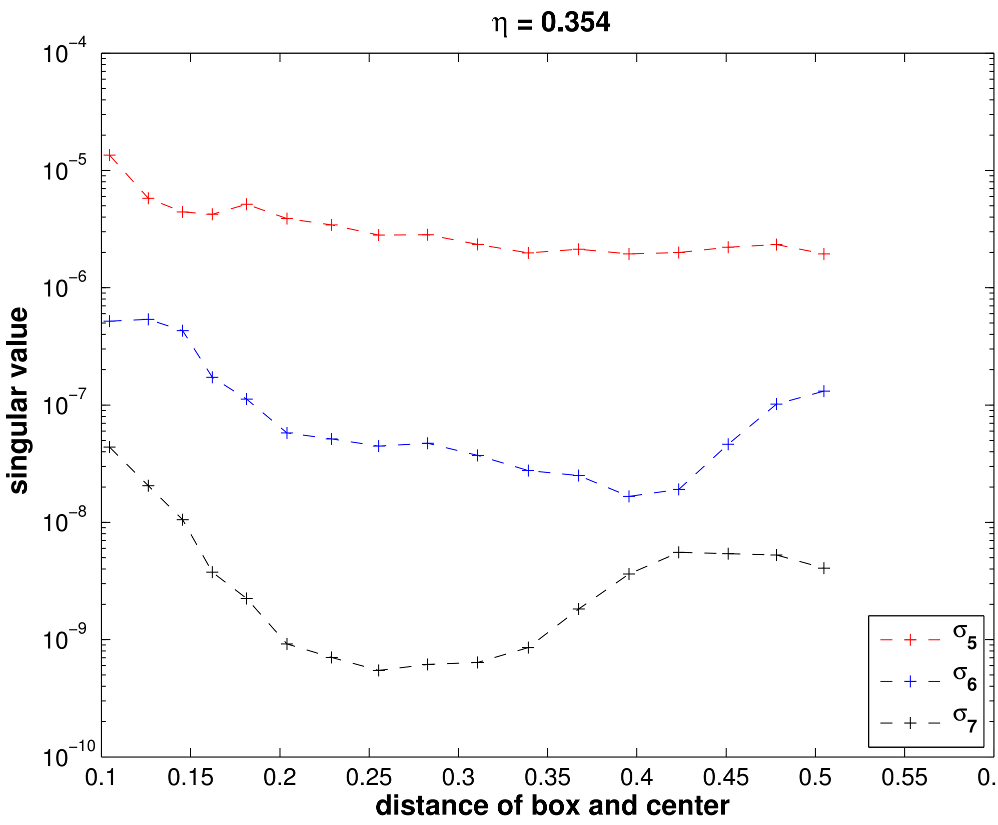
Monitored: σ_i, $i=5,6,7$ for $Q^x=[0,0.3]\times[0,0.3]$, $\eta=\frac{1}{4}\sqrt{2}$,

$$Q^y = \{\boldsymbol{x}\in\mathbb{R}^2\colon\ \|\boldsymbol{x}-\boldsymbol{c}\|_\infty \leq \eta\,\mathrm{dist}(\boldsymbol{c};Q^x)\}\ ,$$

$$\boldsymbol{c}\in\left\{\begin{pmatrix}\frac{1}{2}+\frac{1}{2}\cos(\varphi)\\ \frac{1}{2}\sin(\varphi)\end{pmatrix}\colon \varphi\in\{0.3\pi,0.325\pi,\dots,0.7\pi\}\right\}\ .$$

➤ fixed ratio of (size of Q^y) : (distance of Q^x, Q^y).





Definition 3.3.3 (Admissibilty of blocks)**.**

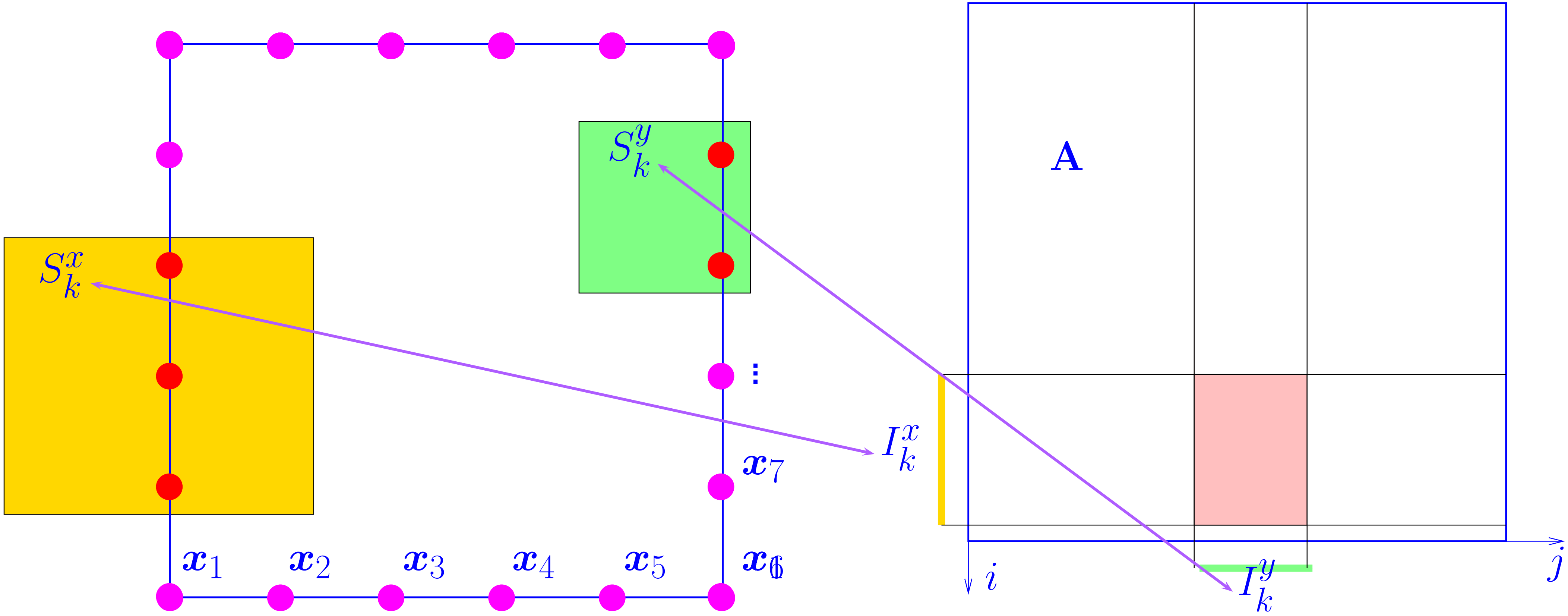
A tensor product domain $Q^x \times Q^y$, $Q^x, Q^y \subset Q_0$ *is called* *η-admissible*, $\eta > 0$, *if*

$$\eta \, \mathrm{dist}(Q^x; Q^y) \geq \max\{\mathrm{diam}\, Q^x, \mathrm{diam}\, Q^y\} \; .$$

Ex. 12 ☞ “uniform” accuracy of rank-k-approximation on admissible blocks

Another perspective: tiling induces *block partitioning* of matrix $\mathbf{A}$:

Visualization (for kernel collocation matrix):



Q_k^x and Q_k^y

Index sets $S_k^x := \{i \colon \boldsymbol{x}_i \in Q_k^x\}$,
$S_k^y := \{i \colon \boldsymbol{x}_i \in Q_k^y\}$.

tensor product tiling
$\{Q_k^{\boldsymbol{x}} \times Q_k^{\boldsymbol{y}}\}_k$ of $Q_0 \times Q_0$ ⇒ block partitioning $\{S_k^x \times S_k^y\}_k$ of $\mathcal{I} \times \mathcal{I}$
($\mathcal{I} := \{1, \ldots, N\} \mathrel{\hat{=}}$ index set)

Parlance: tensor product subset of $\mathcal{I} \times \mathcal{I} \hat{=}$ block cluster

block cluster partitioning $\{S_k^x \times S_k^y\}_k$ of $\mathcal{I} \times \mathcal{I}$ $\Rightarrow$ tensor product tiling $\{Q_k^{\boldsymbol{x}} \times Q_k^{\boldsymbol{y}}\}_k$ of neighborhood of $\Gamma \times \Gamma$ by means of bounding boxes

$$S_k^z \quad \longrightarrow \quad Q_k^z = \mathrm{Box}(S_k^z) := \prod_{j=1}^{d} [\min\{(\boldsymbol{x}_i)_j \colon i \in S_k^z\}, \max\{(\boldsymbol{x}_i)_j \colon i \in S_k^z\}] \;, \quad z = x, y \;.$$

➤ Extension of Def. 3.3.3

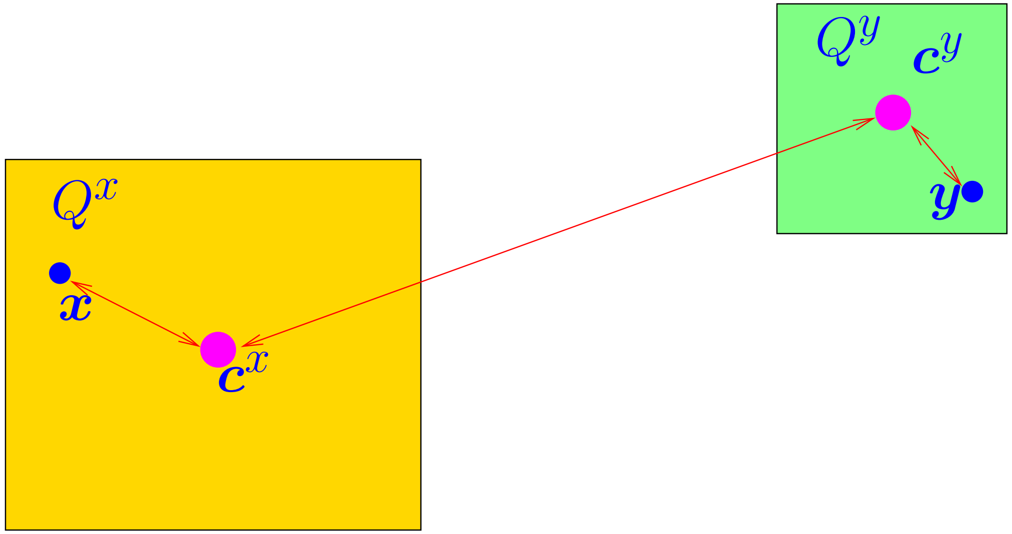
block cluster $I^x \times I^y$, $I^x, I^y \subset I$, admissible, if tensor product of bounding boxes admissible

3.3.2 Separable polynomial approximation

For $\kappa = 0$: kernel function $G(\boldsymbol{x}, \boldsymbol{y})$ asymptotically smooth: for all multi-indices $\boldsymbol{\alpha} \in \mathbb{N}_0^d$, $|\boldsymbol{\alpha}| > 0$

$$\exists C = C(|\boldsymbol{\alpha}|) > 0 \colon \quad |D^{\boldsymbol{\alpha}} G(\boldsymbol{x}, \boldsymbol{y})| \leq C |\boldsymbol{x} - \boldsymbol{y}|^{2-d-|\alpha|} \quad \forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d, \boldsymbol{x} \neq \boldsymbol{y} \;. \tag{3.3.5}$$

Multi-dimensional Taylor expansion



$$\begin{aligned} G(\boldsymbol{x},\boldsymbol{y}) =& G(|\boldsymbol{x}-\boldsymbol{c}^x+\boldsymbol{c}^x-\boldsymbol{c}^y+\boldsymbol{c}^y-\boldsymbol{y}|) \\ &= \sum_{j=0}^{P} \frac{1}{j!} f^{(j)}(0)(\underbrace{\boldsymbol{d},\dots,\boldsymbol{d}}_{j \text{ times}}) \\ &\quad + \frac{1}{(P+1)!} f^{(P+1)}(\delta)(\boldsymbol{d},\dots,\boldsymbol{d}) \;, \end{aligned}$$

$f(t)=G(|\boldsymbol{c}^x-\boldsymbol{c}^y+t(\underbrace{\boldsymbol{x}-\boldsymbol{c}^x+\boldsymbol{c}^y-\boldsymbol{y})}_{=:\boldsymbol{d}}|)$, some $0 \leq \delta \leq 1$.

Note: $f^{(j)}(0)(\underbrace{\boldsymbol{d},\dots,\boldsymbol{d}}_{j \text{ times}}) = g(\boldsymbol{x})h(\boldsymbol{y})$, $g,h =$ multivariate polynomials of (separate) degree $\leq j$ in components of $\boldsymbol{x}$, $\boldsymbol{y}$, resp.

Asymptotic smoothness (3.3.5)
&
Admissibility condition, Def. 3.3.3

▶ Exponential decay (w.r.t. expansion order P) of remainder of Taylor expansion of $G(\boldsymbol{x},\boldsymbol{y})$ *on admissible block*.

Crucial: exponential $L^\infty(Q^x \times Q^y)$ convergence of local separable kernel approximation w.r.t. P

Hackbusch, W. & Nowak, Z. (1989), ‘On the fast matrix multiplication in the boundary element method by panel clustering’, *Numer. Math.* **54**, 463–491.

Alternative to Taylor expansion: *tensor product polynomial interpolation*

Börm, S. & Grasedyck, L. (2004), ‘Low-rank approximation of integral operators by interpolation’, *Computing* **72**(3-4), 325–332.

Sect. 7.1.3 of Sauter, S. & Schwab, C. (2004), *Randelementmethoden*, BG Teubner, Stuttgart.

❶ Pick block $Q^x \times Q^y$, where $Q^x, Q^y \subset \mathbb{R}^d$, $Q^x \cap Q^y = \emptyset$ are “bricks”

$$\exists \alpha_i < \beta_i\colon \quad Q^z = \prod_{i=1}^{d} [\alpha_i, \beta_i] \subset \mathbb{R}^d \;, \quad z = \boldsymbol{x}, \boldsymbol{y} \;. \tag{3.3.6}$$

❷ Given polynomial degree $p \in \mathbb{N}$, choose interpolation nodes

$$\alpha_i \le \xi_1^i < \xi_1^i < \cdots < \xi_p^i \le \beta_i \;,$$

(α_i, β_i from (3.3.6)) ➢ $(\xi_l^1, \xi_m^2)^T$, $1 \le l, m \le p$ ➤ interpolation nodes in Q^z ($d = 2$).

❸ $\mathcal{P}_{p-1}(\mathbb{R})$:= (univariate) polynomials of degree $< p$, L_l^i := l-th Lagrange polynomial, $l = 1, \ldots, p$, for nodes $\{\xi_j^i\}_{j=1}^p$:

$$L_l^i \in \mathcal{P}_{p-1}\colon \quad L_l^i(\xi_j) = \delta_{lj} \quad \text{(Kronecker symbol)}\ , \quad i, j = 1, \ldots, p\ . \tag{3.3.7}$$

separable approximation for $d = 2$ on block $Q^x \times Q^y$: $\quad (P = p^4)$

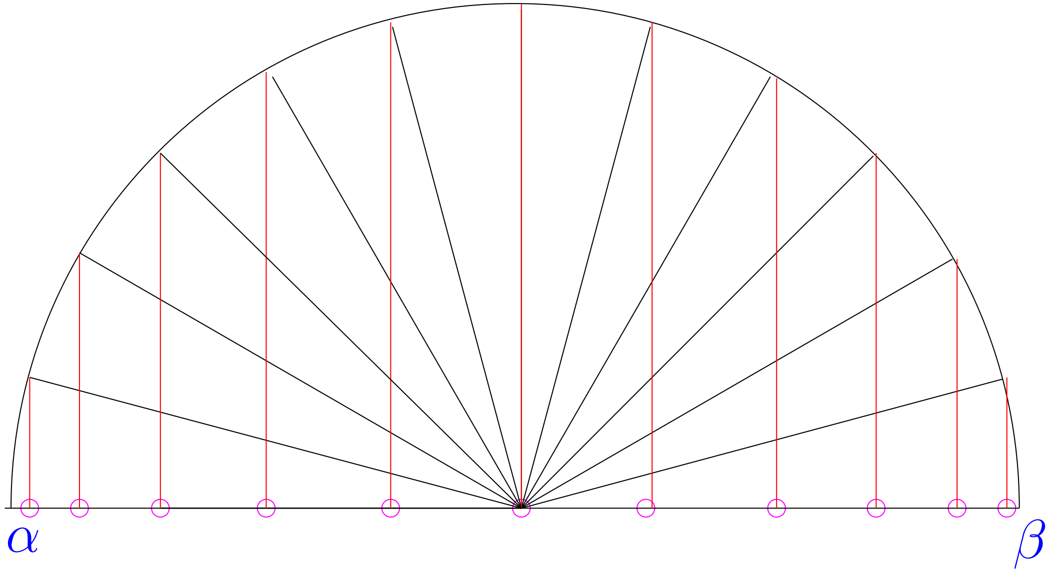
$$\widetilde{G}(\boldsymbol{x}, \boldsymbol{y}) = \sum_{l=1}^{p} \sum_{j=1}^{p} \sum_{m=1}^{p} \sum_{n=1}^{p} \underbrace{G(\xi_l^{1,x} \xi_j^{2,x}, \xi_m^{1,y} \xi_n^{2,y})}_{\gamma_{(lj),(mn)}} \underbrace{L_l^{1,x}(x_1) L_j^{2,x}(x_2)}_{g_{lj}(\boldsymbol{x})} \underbrace{L_m^{1,y}(y_1) L_n^{2,y}(y_2)}_{h_{mn}(\boldsymbol{y})}\ . \tag{3.3.8}$$

for tensor product polynomial interpolation: expansion functions $g_i(\boldsymbol{x})/h_i(\boldsymbol{y})$ on block $Q^x \times Q^y$ **only** depend on Q^x/Q^y, resp. **!**

Recall:
special choice of interpolation nodes on $[\alpha_i, \beta_i]$
(for stability reasons):

Chebychev nodes:

$$\xi_l^i = \alpha_i + \frac{\beta_i - \alpha_i}{2}\left(\cos\left(\frac{2l-1}{2p}\pi\right) + 1\right) \quad (3.3.9)$$
$$l = 1, \ldots, p \; .$$



Remark 13 (Separable approximation by harmonic polynomials).

Rokhlin, V. (1985), ‘Rapid solution of integral equations of classical potential theory’, *J. Comp. Phys.* **60**(2), 187–207.

Idea: for $\kappa = 0$ ➤ $\boldsymbol{x} \mapsto G(\boldsymbol{x}, \boldsymbol{y})$ and $\boldsymbol{y} \mapsto G(\boldsymbol{x}, \boldsymbol{y})$ are *harmonic*

▶ Choose *harmonic* expansion functions $g(\boldsymbol{x})$, $h(\boldsymbol{y})$ **!**

For $\kappa = 0$, $d = 2$ with indentification $\mathbb{R}^2 \cong \mathbb{C}$ ($\boldsymbol{x} \leftrightarrow x \in \mathbb{C}$, $\boldsymbol{y} \leftrightarrow y \in \mathbb{C}$):

$$\log(|\boldsymbol{x} - \boldsymbol{y}|) = \mathrm{Re}(\log(x - y)) = \mathrm{Re}\left\{ \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l} \left(\frac{y}{x}\right)^l \right\} , \quad \text{for } |y| < |x| .$$

▶ for $\boldsymbol{x} \in Q^x$, $\boldsymbol{y} \in Q^y$, $Q^x \times Q^y$ admissible block (→ Def. 3.3.3)

$$\begin{aligned} G(\boldsymbol{x}, \boldsymbol{y}) &= \log|\boldsymbol{c}_y - \boldsymbol{c}_x - (\boldsymbol{c}_x - \boldsymbol{x} + \boldsymbol{y} - \boldsymbol{c}_y)| = \mathrm{Re}\left\{ \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l} \left(\frac{c_x - x + y - c_y}{c_y - c_x} \right)^l \right\} \\ &= \mathrm{Re}\left\{ \sum_{l=1}^{\infty} (-1)^{l-1} \frac{1}{c_y - c_x} \sum_{k=0}^{l} \binom{l}{k} (c_x - x)^k (y - c_y)^{l-k} \right\} . \end{aligned}$$

Approximation by truncation of the series:

$$G(\boldsymbol{x}, \boldsymbol{y}) \approx \mathrm{Re}\left\{ \sum_{l=1}^{P} \frac{(-1)^{l-1}}{l} \frac{1}{c_y - c_x} \sum_{k=0}^{l} \binom{l}{k} \underbrace{(c_x - x)^k}_{\leftrightarrow\, g_{kl}(\boldsymbol{x})} \underbrace{(y - c_y)^{l-k}}_{\leftrightarrow\, h_{kl}(\boldsymbol{x})} \right\} . \tag{3.3.10}$$

☛ more economical than tensor product interpolation (fewer expansion functions)

Note: expansion functions $g_{kl}(\boldsymbol{x})/h_{kl}(\boldsymbol{y})$ only depend on Q^x/Q^y (as in the case of tensor product polynomial interpolation)

Local error estimates

Focus: case of Laplacian $\kappa = 0$,
local separable kernel approximation through tensor product Chebychev interpolation, see (3.3.9)

Asymptotic smoothness (3.3.5)
&
Admissibility condition, Def. 3.3.3

►

Uniform local exponential convergence (w.r.t. expansion order P) of tensor product Chebychev interpolants on *admissible block*.

Theorem 3.3.4 (Kernel approximation error estimate for tensor product Chebychev interpolation). → *(Sauter & Schwab 2004, Thm. 7.3.12)*
There are $\eta_0 > 0$, $C_0, C_1 > 0$ *such that*

$$\left\| G - \widetilde{G} \right\|_{L^\infty(Q^x \times Q^y)} \leq C_0 \left(\frac{C_1 \eta}{2 + C_1 \eta} \right)^P \frac{1}{\operatorname{dist}(Q^x; Q^y)} ,$$

with $\widetilde{G}$ *obtained by tensor product Chebychev interpolation* (3.3.8).

Goal: (asymptotically) kernel approximation error $\approx$ discretization error

$= O(h^q) = O(N^{-dq})$, $q \in \mathbb{N}$, for q-th order scheme

► choose $\boxed{P = O(\log N)}$, if Galerkin discretization converges algebraically

3.3.3 Clustering

Goal: find block partitioning $\boldsymbol{\mathcal{B}} := \{S_k^x \times S_k^y\}_k$ of $\mathcal{I} \times \mathcal{I}$ such that

- $\sharp\left((\mathcal{I} \times \mathcal{I}) \setminus \{S_k^x \times S_k^y \colon S_k^x \times S_k^y \in \boldsymbol{\mathcal{B}} \text{ admissible}\}\right) = O(N)$

- ∃ "small" collection

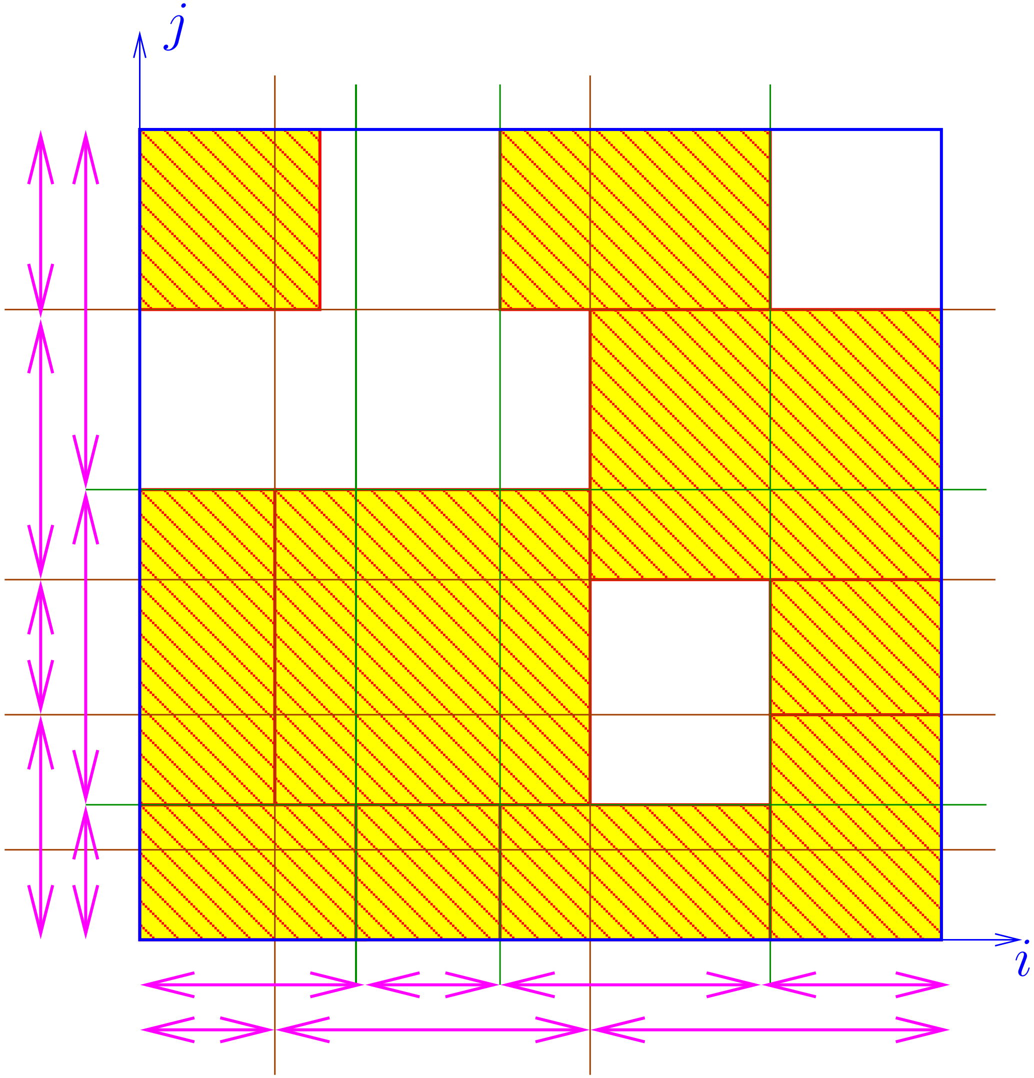
$$\mathcal{T} := \{S_1,\dots,S_K\} \subset 2^{\mathcal{I}}$$

such that

$\bigcup S_k = \mathcal{I}$, $\sharp\mathcal{C} \ll \sharp\boldsymbol{\mathcal{B}}$, and $\boldsymbol{\mathcal{B}} \subset \mathcal{T}\times\mathcal{T}$

(only "a few" possibilities for components of block clusters)

block partitioning of matrix $\mathbf{A}$ ▷



▶ related: $\mathcal{H}$-matrices

Börm, S., Grasedyk, L. & Hackbusch, W. (2003), Hierarchical matrices, Lecture note 21/2003, Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany. `http://www.mis.mpg.de/preprints/ln/lecturenote-2103.pdf`.

Terminology: sets $S_k \subset \mathcal{I}$ are called clusters

Definition 3.3.5 (Near field and far field)**.**
Given block (cluster) partitioning $\boldsymbol{\mathcal{B}} := \{S_k^x \times S_k^y\}_k$ *of* $\mathcal{I} \times \mathcal{I}$

Far field: $\boldsymbol{\mathcal{B}}_{\mathrm{far}} := \{S_k^x \times S_k^y \in \boldsymbol{\mathcal{B}}\colon S_k^x \times S_k^y \text{ admissible}\} \subset \boldsymbol{\mathcal{B}}$,

Near field: $\boldsymbol{\mathcal{B}}_{\mathrm{near}} := \boldsymbol{\mathcal{B}} \setminus \boldsymbol{\mathcal{B}}_{\mathrm{far}}$.

Summary: local separable kernel approximation on far field blocks

---

How to construct the clusters **?** ☞ Tree techniques

Definition 3.3.6 (Cluster tree). → *(Sauter & Schwab 2004, Def. 7.1.4)*

The cluster tree $\mathcal{T}$ is a tree (→ graph theory) such that

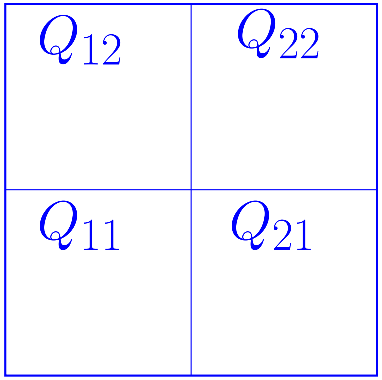
1. *the nodes are clusters (subsets of $\mathcal{I}$),*
2. *the root $\mathrm{root}(\mathcal{T})$ is $\mathcal{I}$,*
3. *the set of leaves is $\mathrm{leaves}(\mathcal{T}) = \{\{i\} \colon i \in \mathcal{I}\}$,*
4. *the set of sons $\mathrm{sons}(S)$ of $S \in \mathcal{T}$ is $\Sigma(S) := \{S' \in \mathcal{T} \colon S' \subset S\}$.*

$$S \in \mathcal{T}\colon \quad \mathrm{level}(S) := \begin{cases} 0 & \text{, if } S = \mathrm{root}(\mathcal{T}) \ , \\ \mathrm{level}(S') + 1 & \text{, if } S \in \mathrm{sons}(S'), S' \in \mathcal{T} \ . \end{cases} \quad ➤ \quad \mathcal{T}_l := \{S \in \mathcal{T}\colon \ \mathrm{level}(S) = l\} \ .$$

Note: $\displaystyle\sum_{S \in \mathcal{T}_l} \sharp S \leq N$

Algorithm: Quadtree/Octree based generation of cluster tree (shown for $d = 2$)

```
function  $\mathcal{T}$  =  gentree($Q$,$\{\boldsymbol{x}_1,\dots,\boldsymbol{x}_N\}$)
% $Q = [\alpha_1,\beta_1]\times[\alpha_2,\beta_2]\subset\mathbb{R}^2 \hat{=}$ box
% $\{\boldsymbol{x}_1,\dots,\boldsymbol{x}_N\} \hat{=}$ collocation points
    $\mathcal{T} := \{i\colon \boldsymbol{x}_i \in Q\}$;
    if  $\mathcal{T}=\emptyset$  return;
    $d_j := \beta_j - \alpha_j, \quad j = 1,2$;
    $Q_{lm} := [\alpha_1 + \frac{1}{2}(l-1)d_1, \beta_1 + \frac{1}{2}ld_1] \times [\alpha_2 + \frac{1}{2}(m-1)d_2, \beta_2 + \frac{1}{2}md_2], \quad l,m \in \{1,2\}$;
    $\mathcal{T} := \mathcal{T} \cup \bigcup_{l,m=1}^{2}$ gentree($Q_{lm}, \{\boldsymbol{x}_1,\dots,\boldsymbol{x}_N\}$);
end
```



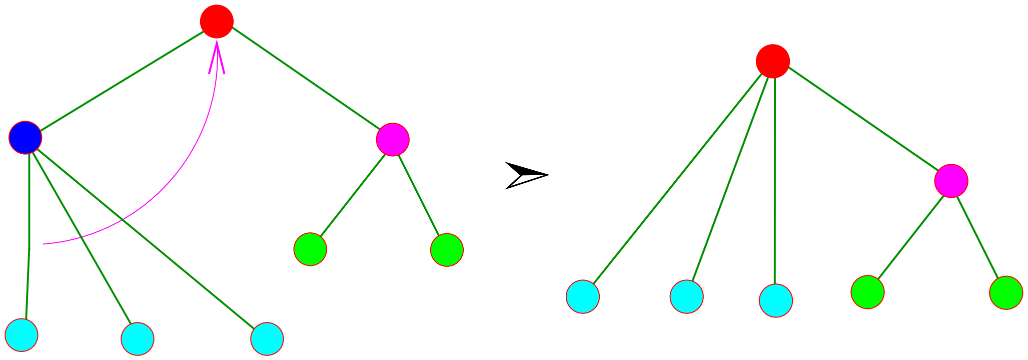
☞ invoke `gentree(`Q_0,$\{\boldsymbol{x}_1,\dots,\boldsymbol{x}_N\}$`)` ➤ cluster tree $\mathcal{T}$

Remark 14 (Minimal number of sons).

Postprocessing of $\mathcal{T}$: balancing

Ensure:

$$\forall S \in \mathcal{T} \setminus \mathrm{leaves}(\mathcal{T}): \quad \sharp\,\mathrm{sons}(S) \geq 4\ .$$



Under the geometric assumptions of Sect. 3.1: (Sauter & Schwab 2004, Sect. 7.4.1)

☞ computational effort (smart implementation !): $O(N \log N)$ comparisons

☞ number of clusters $\sharp\mathcal{T} = O(N)$

(Constants depend on Γ, η, and $\boldsymbol{x}_i$ ↔ shape-regularity of underlying mesh)

► costs(generation of cluster tree): $= O(N \log N)$ (comparisons)

How to construct near field and far field (⟶ Def. 3.3.5) **?** ☞ Tree techniques

Algorithm: (based on given cluster tree $\mathcal{T}$ → Def. 3.3.6)

```
function [$\mathcal{B}_{\text{near}}, \mathcal{B}_{\text{far}}$] = divide($(S,S')$,$\mathcal{B}_{\text{near}}$, $\mathcal{B}_{\text{far}}$)
% $(S,S')$ $\hat{=}$ pair of clusters
% $\mathcal{B}_{\text{near}}$ $\hat{=}$ variable storing near field
% $\mathcal{B}_{\text{far}}$ $\hat{=}$ variable storing far field
    if ( $(S,S')$ admissible ) then $\mathcal{B}_{\text{far}} := \mathcal{B}_{\text{far}} \cup \{(S,S')\}$; end
    elseif $(S,S') \in \text{leaves}(\mathcal{T}) \times \text{leaves}(\mathcal{T})$ then $\mathcal{B}_{\text{near}} := \mathcal{B}_{\text{near}} \cup \{(S,S')\}$; end
    else
        if $S \in \text{leaves}(\mathcal{T})$ then $\mathcal{S}^x := \{S\}$; else $\mathcal{S}^x := \text{sons}(S)$; end
        if $S' \in \text{leaves}(\mathcal{T})$ then $\mathcal{S}^y := \{S'\}$; else $\mathcal{S}^y := \text{sons}(S')$; end
        for all $(s,s') \in \mathcal{S}^x \times \mathcal{S}^y$ do divide($(s,s')$,$\mathcal{B}_{\text{near}}$,$\mathcal{B}_{\text{far}}$); end
    end
end
```

➽ Computational effort $= O(N)$ (checking admissibility)

Analysis: under the geometric assumptions of Sect. 3.1 and

assume: $\forall (S,R) \in \mathcal{B} := \mathcal{B}_{\text{near}} \cup \mathcal{B}_{\text{far}}$: $\text{level}(S) = \text{level}(R)$. (3.3.11)

$\exists$ constants $C = C(\Gamma, \eta,$distribution of collocation points$) > 0$ such that

- $\sharp\boldsymbol{\mathcal{B}}_{\mathrm{near}} \leq CN$ (only $O(N)$ pairs of collocation points in near field)
- $\sharp\boldsymbol{\mathcal{B}}_{\mathrm{far}} \leq CN$ (separable approximation on only $O(N)$ blocks)
- $O(1)$ occurrences of each cluster $\in \mathcal{T}$ in the far field:

$$\forall S \in \mathcal{T}\colon \quad \sharp\{S' \in \mathcal{T}\colon (S, S') \in \boldsymbol{\mathcal{B}}_{\mathrm{far}}\} \leq C \; . \tag{3.3.12}$$

3.3.4 Matrix×vector algorithm

Given:
- cluster tree $\mathcal{T} \subset 2^{\mathcal{I}}$ → Def. 3.3.6
- $\forall S \in \mathcal{T}$: expansion functions $g_i^S(\boldsymbol{x})$, $h_i^S(\boldsymbol{y})$, $i = 1, \dots, P_S$, $P_S \in \mathbb{N}$
  (for single layer kernels usually $g_i^S = h_i^S$ ↔ symmetry)

- kernel approximation

$$\widetilde{G}(\boldsymbol{x}_i,\boldsymbol{y}_j)=\begin{cases}0 & \text{, if } i=j\ ,\\ G(\boldsymbol{x}_i,\boldsymbol{x}_j) & \text{, if } \{i\}\times\{j\}\in\boldsymbol{\mathcal{B}}_{\mathrm{near}}\ ,\\ \sum\limits_{k=1}^{P_S}\sum\limits_{l=1}^{P_R}\gamma_{kl}^{S,R}g_k^S(\boldsymbol{x}_i)h_l^R(\boldsymbol{x}_j) & \text{, if } i\in S,\ j\in R\text{:}\quad (S,R)\in\boldsymbol{\mathcal{B}}_{\mathrm{far}}\ .\end{cases}\tag{3.3.13}$$

$\Rightarrow$ approximate kernel collocation matrix $\widetilde{\mathbf{A}}=\left(\widetilde{G}(\boldsymbol{x}_i,\boldsymbol{x}_j)\right)_{i,j=1}^{N}$

Algorithm: evaluation of $\vec{\varphi}=\widetilde{\mathbf{A}}\vec{\xi}$

$$\varphi_i=\sum_{j=1}^{N}\widetilde{G}(\boldsymbol{x}_i,\boldsymbol{y}_j)\xi_j=\boxed{\sum_{j=\boldsymbol{\mathcal{B}}_{\mathrm{near}}(i)}\widetilde{\mathbf{A}}_{ij}\xi_j}+\boxed{\sum_{\substack{S\in\mathcal{T}\\ i\in S}}\ \sum_{\substack{R\in\mathcal{T}\\ (S,R)\in\boldsymbol{\mathcal{B}}_{\mathrm{far}}}}\ \sum_{j\in R}\widetilde{\mathbf{A}}_{ij}\xi_j}\ ,\quad i=1,\ldots,N\ ,$$

near field contributions

far field contributions

where $\boldsymbol{\mathcal{B}}_{\mathrm{near}}(i):=\{j\in\mathcal{I}\text{: }\{i\}\times\{j\}\in\boldsymbol{\mathcal{B}}_{\mathrm{near}}\}$

With $(\mathbf{A}_{\text{near}})_{ij} := \begin{cases} G(\boldsymbol{x}_i, \boldsymbol{x}_j) & \text{, if } \{i\} \times \{j\} \in \boldsymbol{\mathcal{B}}_{\text{near}} \quad \wedge \quad i \neq j \;, \\ 0 & \text{, else.} \end{cases}$

$$\begin{aligned} \varphi_i &= (\mathbf{A}_{\text{near}}\vec{\xi})_i + \sum_{\substack{S\in\mathcal{T} \\ i\in S}} \sum_{\substack{R\in\mathcal{T} \\ (S,R)\in\boldsymbol{\mathcal{B}}_{\text{far}}}} \sum_{j\in R} \sum_{k=1}^{P_S} \sum_{l=1}^{P_R} \gamma_{kl}^{S,R} g_k^S(\boldsymbol{x}_i) \overline{h}_l^R(\boldsymbol{x}_j)\, \xi_j \\ &= (\mathbf{A}_{\text{near}}\vec{\xi})_i + \sum_{\substack{S\in\mathcal{T} \\ i\in S}} \sum_{\substack{R\in\mathcal{T} \\ (S,R)\in\boldsymbol{\mathcal{B}}_{\text{far}}}} \left(\mathbf{U}_S \mathbf{C}_{S,R} \mathbf{V}_R^H \vec{\xi}_{|R} \right)_i \;, \end{aligned}$$

where

$$\mathbf{U}_S := \left(g_k^S(\boldsymbol{x}_i) \right)_{\substack{i\in S \\ l=1,\dots,P^S}} \in \mathbb{C}^{\sharp S, P_S} \;, \tag{3.3.14}$$

$$\mathbf{V}_R := \left(h_l^R(\boldsymbol{y}_j) \right)_{\substack{j\in R \\ l=1,\dots,P^R}} \in \mathbb{C}^{\sharp R, P_R} \;, \tag{3.3.15}$$

$$\mathbf{C}_{S,R} := \left(\gamma_{kl}^{S,R} \right)_{\substack{k=1,\dots,P_S \\ l=1,\dots,P_R}} \in \mathbb{C}^{P_S, P_R} \;. \tag{3.3.16}$$

Note: symmetric local expansion $g_k^S = h_k^S \quad \forall S \in \mathcal{T}$ ➤ $\mathbf{U}_S = \mathbf{V}_S \quad \forall S \in \mathcal{T}$

Steps of the algorithm:

❶ ("setup"): Computation of $\boldsymbol{\mathcal{B}}_{\text{near}}, \boldsymbol{\mathcal{B}}_{\text{far}}$: costs $= O(N \log N)$

Assembly of $\mathbf{U}_S$, $\mathbf{V}_R$: costs $\overset{(*)}{=} O(PN \log N)$

Assembly of $\mathbf{C}_{S,R}$, $(S,R) \in \boldsymbol{\mathcal{B}}_{\text{far}}$: costs $\overset{(*)}{=} O(P^2 N)$

$(*)$ if $P^R \leq P$ for all clusters R ($\leftrightarrow$ uniform expansion order)

❷: $\forall R \in \mathcal{T} \setminus \text{leaves}(\mathcal{T})$: compute $\vec{\mu}_R := \mathbf{V}_R^H \vec{\xi}_{|R}$ ➔ costs $\lesssim \sharp R \cdot P^R$

➤ total costs $\lesssim \sum_{R \in \mathcal{T}} \sharp R \cdot P^R \overset{(*)}{\lesssim} P \cdot N \log N$,

❸: $\forall R, S \in \boldsymbol{\mathcal{B}}_{\text{far}}$: compute $\vec{\nu}_S := \mathbf{C}_{S,R} \vec{\mu}_R$ ➔ costs $\lesssim P_S P_R$

➤ total costs $\lesssim \sum_{(S,R) \in \boldsymbol{\mathcal{B}}_{\text{far}}} P_S P_R \overset{(*)}{\lesssim} N P^2$,

❹: $\forall S \in \mathcal{T} \setminus \text{leaves}(\mathcal{T})$: compute $\vec{\varphi}_{|S} \leftarrow \vec{\varphi}_{|S} + \mathbf{U}_S \vec{\nu}_S$ ➔ costs $\lesssim \sharp S \cdot P^S$

➤ total costs $\lesssim \sum_{S \in \mathcal{T}} \sharp S \cdot P^S \overset{(*)}{\lesssim} P \cdot N \log N$,

Special case: kernel approximation by tensor product Chebychev interpolation with polynomials of degree $O(\log N)$

▶ $\boxed{\text{total computational costs} = O(N \log^{2d} N)}$

Remark 15 (Variable order interpolation).

Polynomial kernel approximation: we can "afford" low polynomial degrees on high levels:

$$\forall S \in \mathcal{T}: \quad p_S \sim \mathrm{depth}(\mathcal{T}) - \mathrm{level}(S)\ .$$

Sauter, S. (2000), 'Variable order panel clustering', *Computing* **64**, 223–261.

Krzebeck, N. & Sauter, S. (2003), 'Fast cluster techniques for BEM', *Engineering Analysis with Boundary Elements* **27**, 455–467.

3.3.5 Interpolation techniques

Consider: kernel approximation by polynomials of uniform degree $\leq p$, symmetric expansion

➤ $$\forall S \in \mathcal{T}: \quad g_k^S \in \mathcal{P}_p(\mathbb{R}^d),\ k = 1, \dots, P$$

► $$\forall S \in \mathcal{T}\colon\quad \forall_{\substack{s \in \mathrm{sons}(S)\\ s \notin \mathrm{leaves}(\mathcal{T})}}\colon\quad \exists \tau_{kl}^{S,s},\ 1 \leq k,l \leq P\colon\quad g_k^S = \sum_{l=1}^{P} \tau_{kl}^{S,s} g_l^s \quad \forall k = 1,\dots,P\ .$$

$\tau_{kl}^{S,s} \mathrel{\hat{=}}$ shift coefficients

If $s \in \mathrm{sons}(S) \cap \mathrm{leaves}(\mathcal{T})$:
$$\tau_{kl}^{S,s} = \begin{cases} g_k^S(\boldsymbol{x}_i) & \text{, if } l = 1\ , \\ 0 & \text{else.} \end{cases}$$

➤ interlevel transfer matrix: $\mathbf{T}^{S,s} := \left(\tau_{kl}^{S,s}\right)_{k,l=1,\dots,P} \in \mathbb{C}^{P,P}$, $s \in \mathrm{sons}(S)$

► "upward" (from leaves to root) computation of $\vec{\mu}_R$, $R \in \mathcal{T} \setminus \mathrm{leaves}(\mathcal{T})$, in step ❷ of algorithm:

$$(\vec{\mu}_S)_k = \sum_{j\in S} g_k^S(\boldsymbol{x}_j)\xi_j = \sum_{s\in\mathrm{sons}(S)} \sum_{j\in s} g_k^S(\boldsymbol{x}_j)\xi_j = \sum_{s\in\mathrm{sons}(S)} \sum_{j\in s} \sum_{l=1}^{P} \tau_{kl}^{S,s} g_l^s(\boldsymbol{x}_j)\xi_j$$
$$= \sum_{s\in\mathrm{sons}(S)} \sum_{l=1}^{P} \tau_{kl}^{S,s} (\vec{\mu}_s)_l = \sum_{s\in\mathrm{sons}(S)} \left(\mathbf{T}^{S,s}\vec{\mu}_s\right)_k\ .$$

```
function $\vec{\mu}$ = setmu(cluster $S$)
    if $S \in \text{leaves}(\mathcal{T})$ then $\vec{\mu}_S := (\xi_i, 0, \dots, 0)^T$, $S = \{i\}$; end
    else
        $\vec{\mu}_S = 0$;
        foreach $s \in \text{sons}(S)$ do $\vec{\mu}_S := \vec{\mu}_S + \mathbf{T}^{S,s}\cdot$setmu($s$);
    end
end
```

(If) Transfer matrices have special structure (e.g., Kronecker products !)

➡ Recursive (multilevel) computation of $\vec{\mu}_S$ more efficient than direct computation **!**

Related: $\mathcal{H}^2$-matrices

Hackbusch, W. & Börm, S. (2002), '$\mathcal{H}^2$-matrix approximation of integral operators by interpolation', *Appl. Numer. Math.* **43**(1-2), 129–143.

Remark 16 (Approximate transfers).

In the case of variable order interpolation: no nesting $g_k^S \in \mathrm{span}\{g_l^s : l = 1, \dots, P_s\}$ not guaranteed for $s \in \mathrm{sons}(S)$ **!**

Idea: approximation $$g^S_{k\,|\,\mathrm{Box}(s)} \approx \sum_{l=1}^{P_s} \tau^{S,s}_{kl} g^s_l$$

(will introduce new source of error !)

(Krzebeck & Sauter 2003): $O(N)$-effort for (sufficiently accurate !) matrix×vector operations for discrete boundary integral operators (for Laplacian, $\kappa = 0$)

3.4 Hierarchical clustering for high frequencies

Sect. 2.2: necessary for accuracy of standard Galerkin BEM solution for (high frequency) scattering problems:

surface mesh resolves waves: $$N = \begin{cases} O(\kappa) & \text{for } d = 2\,, \\ O(\kappa^2) & \text{for } d = 3\,. \end{cases} \quad \Leftrightarrow \quad \kappa = \begin{cases} O(N) & \text{for } d = 2\,, \\ O(N^{1/2}) & \text{for } d = 3\,. \end{cases}$$

☞ the "curse of high wave numbers" (➙ lectures by S. Chendler-Wilde)

➤ Asymptotics: minimal resolution $\kappa = O(N^{1/d})$ for $N \to \infty$

Focus: Efficient matrix×vector operation for kernel collocation matrix (3.1.2) and $\kappa = O(N^{1/d-1})$ ➙ Sect. 3.1

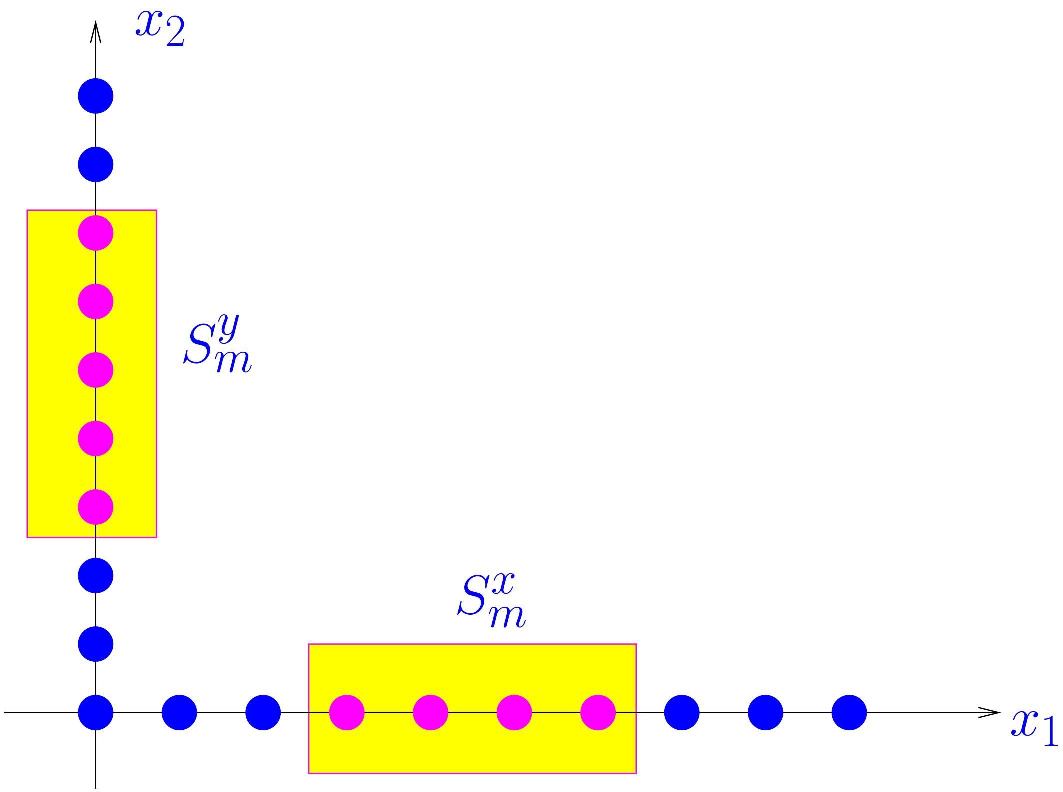
("nice" geometry of Γ, uniform distribution of collocation points $\boldsymbol{x}_i$ may be assumed)

3.4.1 Failure of low rank approximation

At the heart of p-*uniform* exponentially convergent polynomial kernel approximation on *admissible blocks*: asymptotic smoothness (3.3.5) !

BUT . . . $G(\boldsymbol{x},\boldsymbol{y})$ **not** asymptotically smooth for $\kappa > 0$!

Example 17 (Required block ranks for admissible clusters).



Collocation points

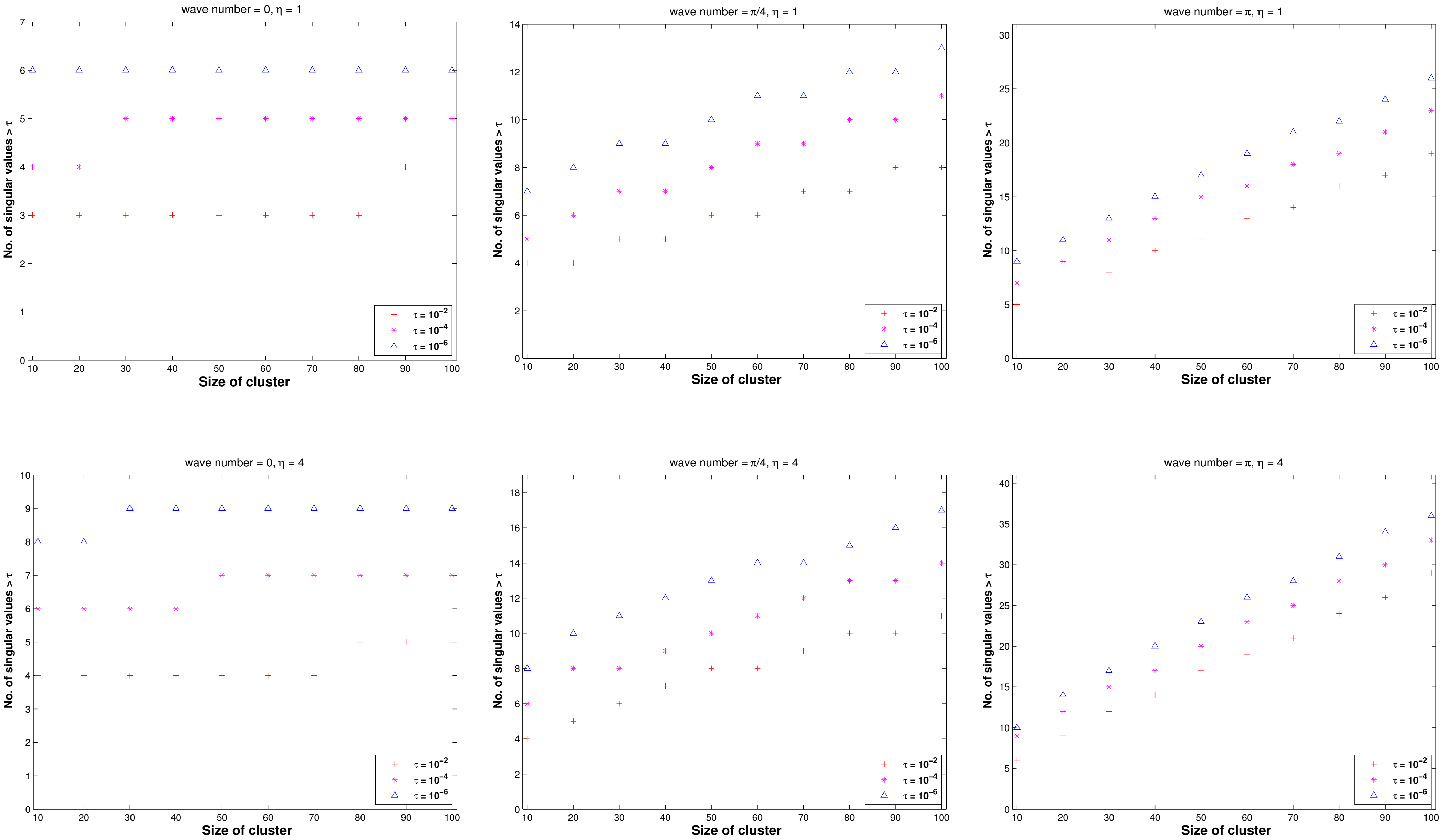
$$\{\boldsymbol{x}_i^1, \boldsymbol{x}_i^2\}\ ,\quad i \in \mathbb{N}_0\ ,$$
$$\boldsymbol{x}_i^1 = (ih, 0)^T\ ,\quad \boldsymbol{x}_i^2 = (0, ih)^T\ ;.$$

Clusters ($m \leftrightarrow$ size of cluster, $\eta > 0$):

$$S_m^x := \{\boldsymbol{x}_{l(m)}^1, \dots, \boldsymbol{x}_{r(m)}^1\}\ ,$$
$$S_m^y := \{\boldsymbol{x}_{l(m)}^2, \dots, \boldsymbol{x}_{r(m)}^2\}\ ,$$
$$l(m) = \frac{m}{\sqrt{2}\eta}\ ,\quad r(m) = m + l(m)\ .$$

➢ η-admissible clusters (⟶ Def. 3.3.3)

Monitored: minimal rank of low rank approximation $\widetilde{\mathbf{B}}$ of sub-block $\mathbf{B}$ ($\leftrightarrow$ (S_m^x, S_m^y)) of Helmholtz kernel collocation matrix for $\left\|\widetilde{\mathbf{B}} - \mathbf{B}\right\| \leq \tau$, $\tau > 0$



$\kappa h \approx 1$ ▷ required rank increases linearly with $\mathrm{diam}(\mathrm{Box}(S_m^x))$ **!**

wavelength ≈ meshwidth ▶ Constant rank low-rank approximation
on admissible clusters impossible

How to salvage the clustering based kernel approximation **?**

Obtain efficient algorithm despite large $P_S = P_S(\mathrm{diam}\,\mathrm{Box}(S))$ by

- reduced costs for coupling matrix $\mathbf{C}\times$vector:
  ➞ achieve: $\mathbf{C}$ diagonal, Toeplitz, circulant, etc.
- inexpensive computation of $\vec{\mu}_R$ by efficient interpolation → Sect. 3.3.5

3.4.2 Cylindrical wave approximation

Fcous: $d = 2$, $\Gamma =$ curve, $G(\boldsymbol{x}, \boldsymbol{y}) = i/4 H_0^{(1)}(\kappa|\boldsymbol{x} - \boldsymbol{y}|)$

✍: (polar coordinates) $\boldsymbol{x} \in \mathbb{R}^2 \setminus \{0\}$: $(|\boldsymbol{x}|, \varphi_{\boldsymbol{x}}) \in \mathbb{R}^+ \times [0, 2\pi[$, $x_1 = |\boldsymbol{x}| \cos \varphi_{\boldsymbol{x}}, x_2 = |\boldsymbol{x}| \sin \varphi_{\boldsymbol{x}}$

Theorem 3.4.1 (Graf's addition theorem). → *(Abramowitz & Stegun 1970, (9.1.79))*

For $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^2$, $|\boldsymbol{y}| < |\boldsymbol{x}|$, *we have the convergent series expansion*

$$H_n^{(1)}(|\boldsymbol{x}-\boldsymbol{y}|) = \sum_{m=-\infty}^{\infty} H_{m+n}^{(1)}(|\boldsymbol{x}|) J_m(|\boldsymbol{y}|) \exp(\imath m(\varphi_{\boldsymbol{x}} - \varphi_{\boldsymbol{y}})) e^{-\imath n(\varphi_{\boldsymbol{x}-\boldsymbol{y}} - \varphi_{\boldsymbol{x}})} , \qquad (3.4.1)$$

and for all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^2$

$$J_n(|\boldsymbol{x}-\boldsymbol{y}|) e^{\pm \imath n \varphi_{[\boldsymbol{x}-\boldsymbol{y}]}} = \sum_{m=-\infty}^{\infty} J_{n+m}(|\boldsymbol{x}|) J_m(|\boldsymbol{y}|) e^{\pm \imath m(\varphi_{\boldsymbol{x}} - \varphi_{\boldsymbol{y}})} , \qquad (3.4.2)$$

where $H_n^{(1)} \hat{=}$ *Hankel functions,* $J_n \hat{=}$ *Bessel functions of the first kind.*

Interpretation of (3.4.1) for $n = 0$ (= single layer kernel): ▷

source in $\boldsymbol{x}$

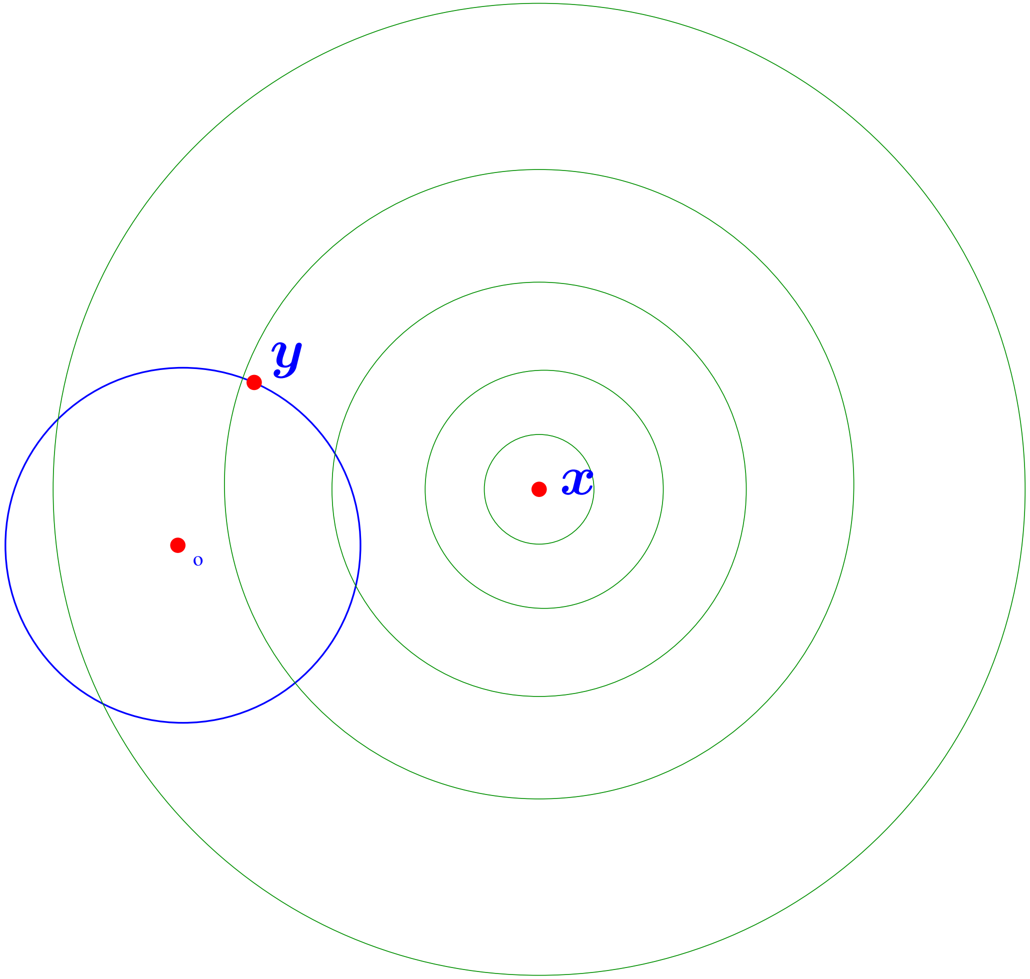
↓

cylindrical wave (—)

↓

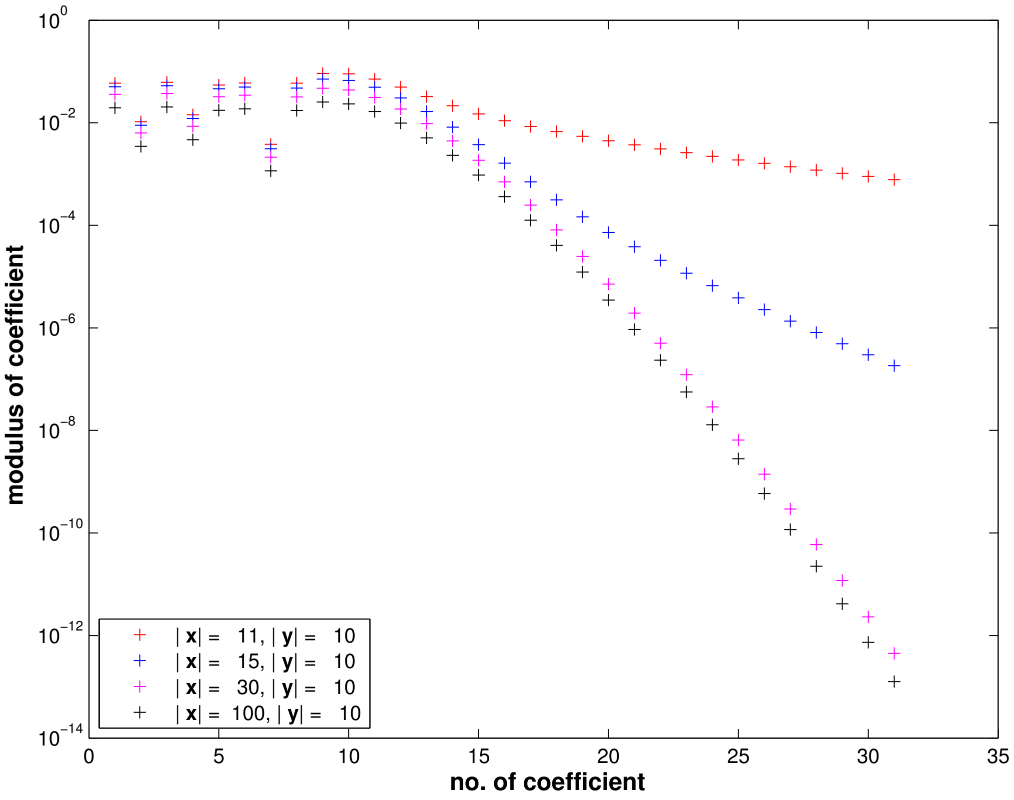
sum of (incoming) cylindrical waves (w.r.t. origin)

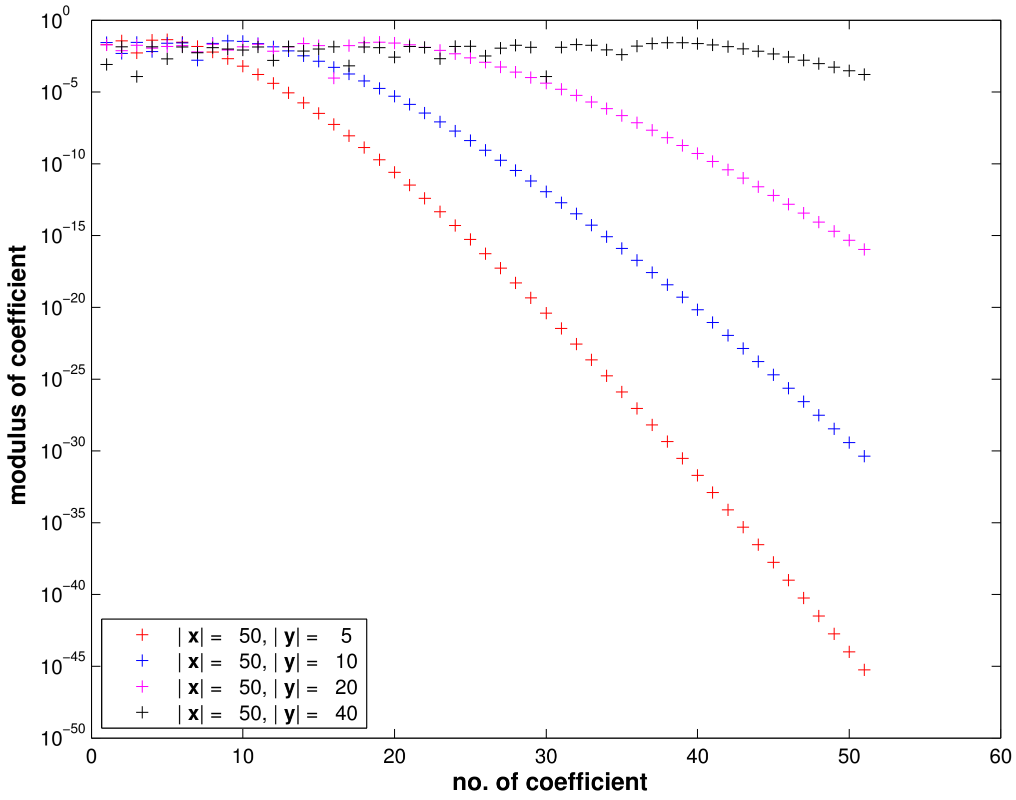
(3.4.1) = shift theorem



Example 18 (Spectral content of far field).

Modulus of terms in (3.4.1) for different $|\boldsymbol{x}|$, $|\boldsymbol{y}|$:



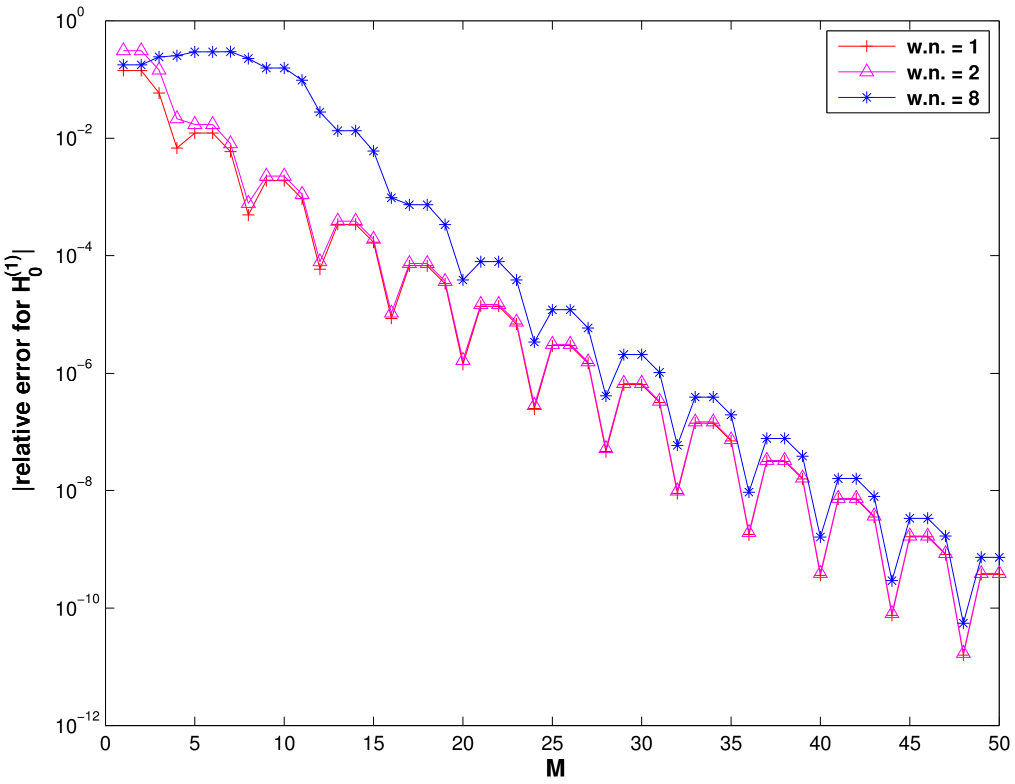


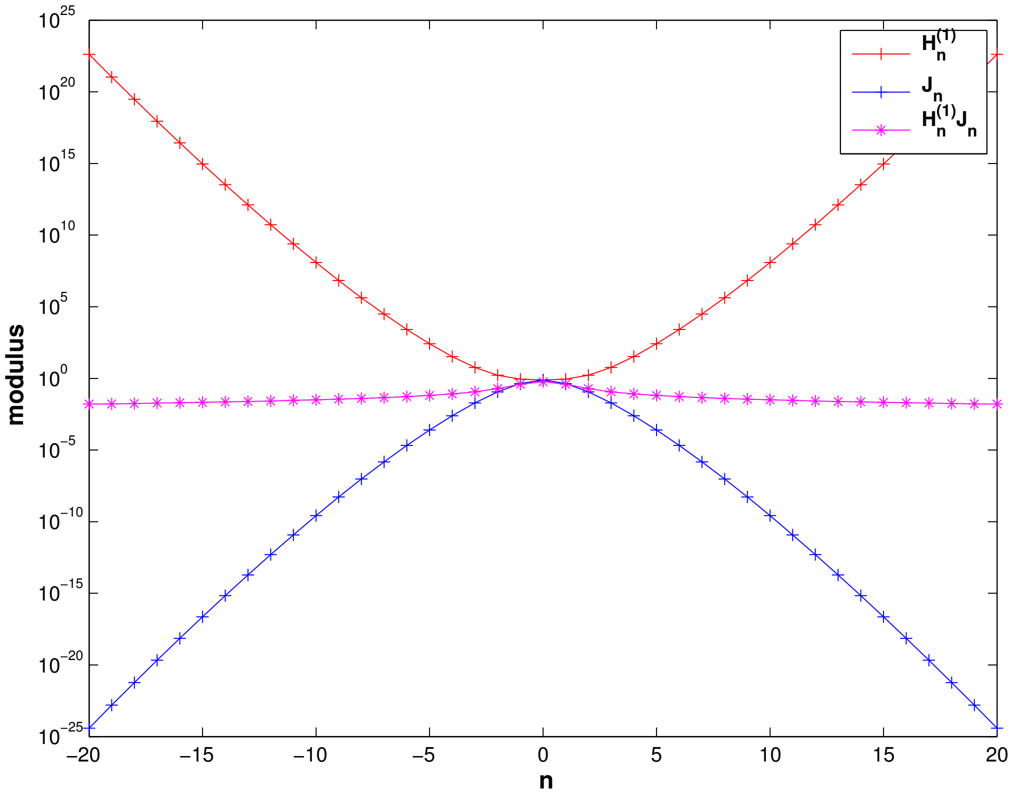
$$|\boldsymbol{y}| \left\{\begin{matrix}\text{large}\\ \text{small}\end{matrix}\right\} \blacktriangleright \left\{\begin{matrix}\text{large}\\ \text{small}\end{matrix}\right\}$$ "practical bandwidth" of wave near 0

$$\boldsymbol{x} \left\{\begin{matrix}\text{far}\\ \text{near}\end{matrix}\right\} \blacktriangleright \left\{\begin{matrix}\text{small}\\ \text{large}\end{matrix}\right\}$$ "practical bandwidth" of wave near 0

Example 19 (Convergence of (3.4.1)).

Study of convergence of series (3.4.1) for $\boldsymbol{x} = \binom{2}{0}$, $\boldsymbol{y} = \binom{1}{1}$:





➤ Observed: ("precarious") exponential convergence

Thm. 3.4.1 ➤ (infinite) "separable" expansion of $G(\boldsymbol{x},\boldsymbol{y})$ on admissible (→ Def. 3.3.3) block $Q^x \times Q^y$:

Geometric situation ($d = 2$)

$\boldsymbol{c}^x/\boldsymbol{c}^y$ = "centers" of Q^x/Q^y:

$$\begin{aligned} G(\boldsymbol{x},\boldsymbol{y}) = G(|\boldsymbol{x}-\boldsymbol{y}|) &= \\ G(|\boldsymbol{x}-\boldsymbol{c}^x+\boldsymbol{c}^x-\boldsymbol{c}^y+\boldsymbol{c}^y-\boldsymbol{y}|) &= \\ G(|(\boldsymbol{c}^x-\boldsymbol{c}^y)+(\boldsymbol{x}-\boldsymbol{c}^x+\boldsymbol{c}^y-\boldsymbol{y})|) &. \end{aligned}$$

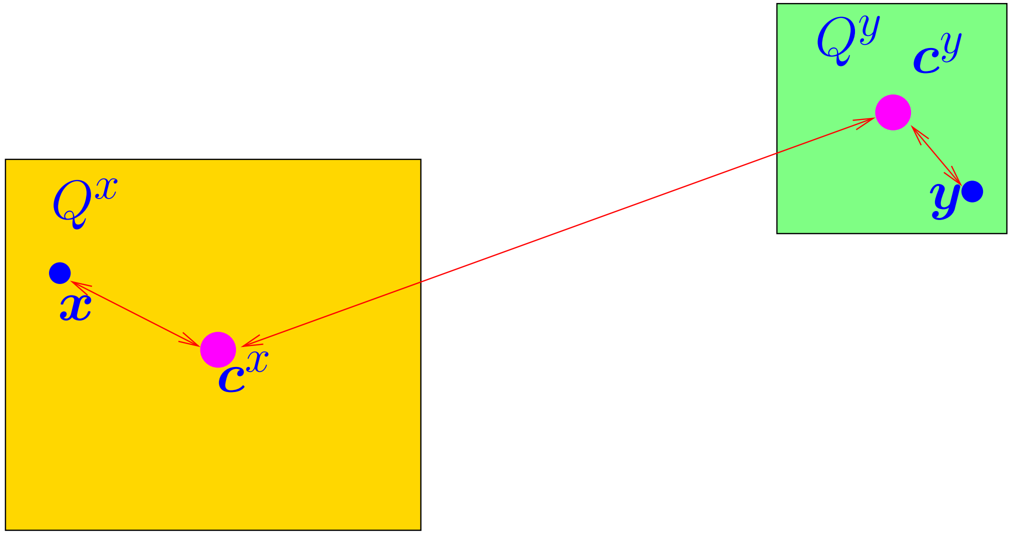


Fig. 4

Q^x, Q^y η-admissible, $\eta > 0$ sufficiently large

$$\Rightarrow \quad |\boldsymbol{c}^x-\boldsymbol{c}^y| > |\boldsymbol{x}-\boldsymbol{c}^x+\boldsymbol{c}^y-\boldsymbol{y}|$$

Pick $\boldsymbol{x} \in Q^x$, $\boldsymbol{y} \in Q^y$ $\quad$ ($\boldsymbol{d} := \kappa(\boldsymbol{c}^x-\boldsymbol{c}^y)$, $\boldsymbol{q} := -\kappa(\boldsymbol{x}-\boldsymbol{c}^x+\boldsymbol{c}^y-\boldsymbol{y})$) ➢ $\kappa(\boldsymbol{x}-\boldsymbol{y}) = \boldsymbol{d}-\boldsymbol{q}$)

Combined translation formulas of Thm. 3.4.1 (double series expansion):

$$H_0^{(1)}(\kappa\,|\boldsymbol{x}-\boldsymbol{y}|) = H_0^{(1)}(|\boldsymbol{d}-\boldsymbol{q}|) = \sum_{m=-\infty}^{\infty} H_m^{(1)}(|\boldsymbol{d}|)J_m(|\boldsymbol{q}|)e^{\imath m(\varphi_{\boldsymbol{d}}-\varphi_{\boldsymbol{q}})}$$

$$= \sum_{m=-\infty}^{\infty} H_m^{(1)}(|\boldsymbol{d}|)e^{\imath m\varphi_{\boldsymbol{d}}} \sum_{l=-\infty}^{\infty} J_{m+l}(\kappa\,|\boldsymbol{y}-\boldsymbol{c}^y|)e^{-\imath(m+l)\varphi_{[\boldsymbol{y}-\boldsymbol{c}^y]}} J_l(\kappa\,|\boldsymbol{x}-\boldsymbol{c}^x|)e^{\imath l\varphi_{[\boldsymbol{x}-\boldsymbol{c}^x]}}$$

$$= \sum_{l=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} J_l(\kappa\,|\boldsymbol{x}-\boldsymbol{c}^x|)e^{\imath l\varphi_{[\boldsymbol{x}-\boldsymbol{c}^x]}} H_{m-l}^{(1)}(|\boldsymbol{d}|)e^{\imath(m-l)\varphi_{\boldsymbol{d}}} J_m(\kappa\,|\boldsymbol{y}-\boldsymbol{c}^y|)e^{-\imath m\varphi_{[\boldsymbol{y}-\boldsymbol{c}^y]}}\,. \qquad (3.4.3)$$

Next: Truncation of series ↔ kernel approximation ▶ separable approximation

$$G(\boldsymbol{x},\boldsymbol{y}) \approx \frac{\imath}{4}\sum_{l=-M}^{M}\sum_{m=-M}^{M} \underbrace{J_l(\kappa\,|\boldsymbol{x}-\boldsymbol{c}^x|)e^{\imath l\varphi_{[\boldsymbol{x}-\boldsymbol{c}^x]}}}_{\leftrightarrow\, g_l(\boldsymbol{x})} \underbrace{H_{m-l}^{(1)}(|\boldsymbol{d}|)e^{\imath(m-l)\varphi_{\boldsymbol{d}}}}_{\leftrightarrow\, \gamma_{lm}} \underbrace{J_m(\kappa\,|\boldsymbol{y}-\boldsymbol{c}^y|)e^{-\imath m\varphi_{[\boldsymbol{y}-\boldsymbol{c}^y]}}}_{\leftrightarrow\, \overline{g}_m(\boldsymbol{y})}\,, \qquad (3.4.4)$$

with “suitable” $M \in \mathbb{N}$ ▷ expansion order $P = (2M+1)^2$.

Note: Coupling matrix $\mathbf{C} := (\gamma_{lm})$ is Toeplitz matrix $^{(*)}$

$(*)$: cost(matrix×vector) = $O(n\log n)$ for $n \times n$ Toeplitz matrix **!**

How to choose M (depending on block cluster) **?**

☹ Drawback of cylindrical wave expansion:

Efficient interpolation not available !

3.4.3 Plane wave approximation

An alternative separable expansion on admissible (⟶ Def. 3.3.3) block $Q^x \times Q^y$:

Derivation in 2D

☛ Geometric situation/notations as in Fig. 4

Pick $\boldsymbol{x} \in Q^x$, $\boldsymbol{y} \in Q^y$ $(\boldsymbol{d} := \kappa(\boldsymbol{c}^x - \boldsymbol{c}^y)$, $\boldsymbol{q} := -\kappa(\boldsymbol{x} - \boldsymbol{c}^x + \boldsymbol{c}^y - \boldsymbol{y}))$ ➢ $\kappa(\boldsymbol{x} - \boldsymbol{y}) = \boldsymbol{d} - \boldsymbol{q})$

$$\text{(3.4.1)} \quad \Rightarrow \quad H_0^{(1)}(\kappa\,|\boldsymbol{x} - \boldsymbol{y}|) = H_0^{(1)}(|\boldsymbol{d} - \boldsymbol{q}|) = \sum_{m=-\infty}^{\infty} H_m^{(1)}(|\boldsymbol{d}|) J_m(|\boldsymbol{q}|) e^{\imath m(\varphi_{\boldsymbol{d}} - \varphi_{\boldsymbol{q}})} \,. \qquad (3.4.5)$$

+ Bessel function values as Fourier coefficients (Abramowitz & Stegun 1970, (9.1.79))

$$J_m(x) = \frac{1}{2\pi\imath^m}\int_0^{2\pi} e^{\imath x\cos t} e^{-\imath m t}\,\mathrm{d}t\ . \tag{3.4.6}$$

➤ $$J_m(|\boldsymbol{q}|)e^{-\imath m\varphi_{\boldsymbol{q}}} = \frac{1}{2\pi\imath^m}\int\limits_0^{2\pi} e^{\imath|\boldsymbol{q}|\cos(t-\varphi_{\boldsymbol{q}})} e^{-\imath m t}\,\mathrm{d}t = \frac{1}{2\pi\imath^m}\int\limits_0^{2\pi} e^{\imath\boldsymbol{q}\cdot\widehat{\boldsymbol{s}}(t)} e^{-\imath m t}\,\mathrm{d}t\ , \tag{3.4.7}$$

with $\widehat{\boldsymbol{s}}(t) = \begin{pmatrix}\cos t\\ \sin t\end{pmatrix}$, $\boldsymbol{q}\cdot\widehat{\boldsymbol{s}} \hat{=}$ Euklidean scalar product of vectors in $\mathbb{R}^2$.

Use $\boldsymbol{q} = -\kappa(\boldsymbol{x} - \boldsymbol{c}^x + \boldsymbol{c}^y - \boldsymbol{y}))$ ▷ “integrand separates”:

$$J_m(|\boldsymbol{q}|)e^{-\imath m\varphi_{\boldsymbol{q}}} = \frac{1}{2\pi\imath^m}\int\limits_0^{2\pi} e^{-\imath\kappa(\boldsymbol{x}-\boldsymbol{c}^x)\cdot\widehat{\boldsymbol{s}}(t)}\cdot e^{\imath\kappa(\boldsymbol{y}-\boldsymbol{c}^y)\cdot\widehat{\boldsymbol{s}}(t)}\cdot e^{-\imath m t}\,\mathrm{d}t\ .$$

$$H_0^{(1)}(\kappa\,|\boldsymbol{x}-\boldsymbol{y}|) = \sum_{m=-\infty}^{\infty} \frac{1}{2\pi\imath^m}\int\limits_0^{2\pi} \underbrace{H_m^{(1)}(\kappa\,|\boldsymbol{c}^x-\boldsymbol{c}^y|)e^{\imath m\varphi[\boldsymbol{c}^x-\boldsymbol{c}^y]}}_{\leftrightarrow\ \gamma_{mt}} \underbrace{e^{\imath\kappa(\boldsymbol{c}^x-\boldsymbol{x})\cdot\widehat{\boldsymbol{s}}(t)}}_{\leftrightarrow\ g_{m,t}(\boldsymbol{x})}\cdot\underbrace{e^{\imath\kappa(\boldsymbol{y}-\boldsymbol{c}^y)\cdot\widehat{\boldsymbol{s}}(t)}}_{\leftrightarrow\ h_{m,t}(\boldsymbol{y})}\cdot e^{-\imath mt}\mathrm{d}t\;. \tag{3.4.8}$$

⚠ integration and summation may not be exchanged ! → Ex. 19

“Discretizing” (3.4.8): two steps of approximation

❶ Truncation of Hankel function series (3.4.5): with $M \in \mathbb{N}$

$$H_0^{(1)}(\kappa\,|\boldsymbol{x}-\boldsymbol{y}|) \approx \sum_{m=-M}^{M} \frac{1}{2\pi\imath^m}\int\limits_0^{2\pi} H_m^{(1)}(\kappa\,|\boldsymbol{c}^x-\boldsymbol{c}^y|)e^{\imath m\varphi[\boldsymbol{c}^x-\boldsymbol{c}^y]}\cdot e^{\imath\kappa(\boldsymbol{c}^x-\boldsymbol{x})\cdot\widehat{\boldsymbol{s}}(t)}\cdot e^{\imath\kappa(\boldsymbol{y}-\boldsymbol{c}^y)\cdot\widehat{\boldsymbol{s}}(t)}\cdot e^{-\imath mt}\mathrm{d}t\;.$$

❷ Numerical quadrature: trapezoidal rule $\displaystyle \frac{1}{2\pi}\int_0^{2\pi} f(t)\,\mathrm{d}t \approx \frac{1}{L}\sum_{l=0}^{L-1} f(\tfrac{2\pi}{L}l)$

“Magic” of trapezoidal rule: $\boxed{\text{Exact integration of trigonometric polynomials of degree } \leq L\textbf{!}}$

$$H_0^{(1)}(\kappa\,|\boldsymbol{x}-\boldsymbol{y}|) \approx \sum_{l=0}^{L-1} \underbrace{\sum_{m=-M}^{M} \frac{1}{L\imath^m} H_m^{(1)}(\kappa\,|\boldsymbol{c}^x-\boldsymbol{c}^y|) e^{\imath m\varphi[\boldsymbol{c}^x-\boldsymbol{c}^y]} \cdot e^{-\imath m\frac{2\pi l}{L}}}_{\leftrightarrow\,\gamma_l} \cdot$$

$$\underbrace{e^{\imath\kappa(\boldsymbol{c}^x-\boldsymbol{x})\cdot\widehat{\boldsymbol{s}}(\frac{2\pi l}{L})}}_{\leftrightarrow\,g_l(\boldsymbol{x})} \cdot \underbrace{e^{\imath\kappa(\boldsymbol{y}-\boldsymbol{c}^y)\cdot\widehat{\boldsymbol{s}}(\frac{2\pi l}{L})}}_{\leftrightarrow\,h_l(\boldsymbol{y})} \,,$$

$$\Updownarrow$$

$$H_0^{(1)}(\kappa\,|\boldsymbol{x}-\boldsymbol{y}|) \approx \sum_{l=0}^{L-1} \underbrace{e^{\imath\kappa(\boldsymbol{c}^x-\boldsymbol{c}^y)\cdot\widehat{\boldsymbol{s}}(\frac{2\pi l}{L})} \cdot \sum_{m=-M}^{M} \frac{1}{L\imath^m} H_m^{(1)}(\kappa\,|\boldsymbol{c}^x-\boldsymbol{c}^y|) e^{\imath m\varphi[\boldsymbol{c}^x-\boldsymbol{c}^y]} \cdot e^{-\imath m\frac{2\pi l}{L}}}_{\leftrightarrow\,\gamma_l} \cdot$$

$$\underbrace{e^{-\imath\kappa\boldsymbol{x}\cdot\widehat{\boldsymbol{s}}(\frac{2\pi l}{L})}}_{\leftrightarrow\,g_l(\boldsymbol{x})} \cdot \underbrace{e^{\imath\kappa\boldsymbol{y}\cdot\widehat{\boldsymbol{s}}(\frac{2\pi l}{L})}}_{\leftrightarrow\,\overline{g}_l(\boldsymbol{y})} \,. \tag{3.4.9}$$

☞ local separable kernel approximation with $P = L$ and plane wave expansion functions

$$g_l(\boldsymbol{x}) = e^{-\imath\kappa\boldsymbol{x}\cdot\widehat{\boldsymbol{s}}(\frac{2\pi l}{L})}\ , \quad l = 0,\dots,L-1\ .$$

plane wave, wavelength $\lambda := \frac{2\pi}{\kappa}$, direction $\widehat{\boldsymbol{s}}(\frac{2\pi l}{L})$

Again (→ Sect. 3.3.2): expansion functions intrinsic to block/cluster **!**

(3.4.9) $\hat{=}$ general separable kernel approximation (3.3.4) with **diagonal** coupling matrix $\mathbf{C} = (\gamma_{ij})$

Derivation in 3D

Rahola, J. (1996), ‘Diagonal form of the translation operators in the fast multipole algorithm for scattering problems’, *BIT* **36**(2), 333–358.

Darve, E. (2000*a*), ‘The fast multipole method i: Error analysis and asymptotic complexity’, *SIAM J. Numer. Anal.* **38**(1), 98–128.

Tool: another addition theorem (translation formula) for special functions

Theorem 3.4.2 (Gegenbauer's addition theorem). *(Abramowitz & Stegun 1970, (10.1.45) & (10.1.46))*
For $\boldsymbol{x}, \boldsymbol{q} \in \mathbb{R}^3$, $|\boldsymbol{x}| > |\boldsymbol{q}|$, *we have the convergent series expansion*

$$\frac{e^{\imath|\boldsymbol{d}+\boldsymbol{q}|}}{|\boldsymbol{d}+\boldsymbol{q}|} = \imath \sum_{m=0}^{\infty} (2m+1)(-1)^m h_m^{(1)}(|\boldsymbol{d}|) j_m(|\boldsymbol{q}|) P_m(\widehat{\boldsymbol{d}} \cdot \widehat{\boldsymbol{q}}) \;, \tag{3.4.10}$$

$h_m^{(1)} \mathrel{\hat{=}}$ *spherical Hankel functions of the first kind,* $j_m \mathrel{\hat{=}}$ *spherical Bessel functions,* $P_l \mathrel{\hat{=}}$ *Legendre polynomials,* $\widehat{\boldsymbol{x}} := \boldsymbol{x}/|\boldsymbol{x}|$.

+ spherical integral representation formula, *cf.* (3.4.7)

$$j_m(|\boldsymbol{q}|) P_m(\widehat{\boldsymbol{d}} \cdot \widehat{\boldsymbol{q}}) = \frac{1}{4\pi\imath^m} \int_{\mathbb{S}} e^{\imath \boldsymbol{q}\cdot\widehat{\boldsymbol{s}}(\boldsymbol{\omega})} P_m(\widehat{\boldsymbol{d}} \cdot \widehat{\boldsymbol{s}}(\boldsymbol{\omega}))\, \mathrm{d}S(\boldsymbol{\omega}) \;, \tag{3.4.11}$$

where $\mathbb{S} \mathrel{\hat{=}}$ unit sphere in $\mathbb{R}^3$, $\widehat{\boldsymbol{s}}(\omega) \mathrel{\hat{=}}$ unit vector in direction $\boldsymbol{\omega}$.

► as before apply (3.4.10) **&** (3.4.11) to $\boldsymbol{d} := \kappa(\boldsymbol{c}^x - \boldsymbol{c}^y)$, $\boldsymbol{q} := \kappa(\boldsymbol{x} - \boldsymbol{c}^x + \boldsymbol{c}^y - \boldsymbol{y})$) ➢ $\kappa(\boldsymbol{x} - \boldsymbol{y}) = \boldsymbol{d} - \boldsymbol{q}$) for $\boldsymbol{x} \in Q^x$, $\boldsymbol{y} \in Q^y$, $Q^x \times Q^y$ = admissible block.

▼

$$\frac{e^{\imath|\boldsymbol{d}+\boldsymbol{q}|}}{|\boldsymbol{d}+\boldsymbol{q}|} = \imath\sum_{m=0}^{\infty}(2m+1)(-1)^m h_m^{(1)}(|\boldsymbol{d}|)\frac{1}{4\pi\imath^m}\int_{\mathbb{S}} e^{\imath\boldsymbol{q}\cdot\widehat{\boldsymbol{s}}(\boldsymbol{\omega})} P_m(\widehat{\boldsymbol{d}}\cdot\widehat{\boldsymbol{s}}(\boldsymbol{\omega}))\,\mathrm{d}S(\boldsymbol{\omega})$$

$$= \imath\sum_{m=0}^{\infty}\int_{\mathbb{S}} \underbrace{e^{\imath\kappa(\boldsymbol{x}-\boldsymbol{c}^x)\cdot\widehat{\boldsymbol{s}}(\boldsymbol{\omega})}}_{\leftrightarrow\, g_{\boldsymbol{\omega}}(\boldsymbol{x})}\cdot(2m+1)(-1)^m h_m^{(1)}(|\boldsymbol{d}|)\frac{1}{4\pi\imath^m}\cdot\underbrace{e^{-\imath\kappa(\boldsymbol{y}-\boldsymbol{c}^y)\cdot\widehat{\boldsymbol{s}}(\boldsymbol{\omega})}}_{\leftrightarrow\, \overline{g}_{\boldsymbol{\omega}}(\boldsymbol{y})}\,\mathrm{d}S(\boldsymbol{\omega})\,.$$

As before: “discretization” **=** truncation of series **&** numerical quadrature

$$\frac{e^{\imath|\boldsymbol{d}+\boldsymbol{q}|}}{|\boldsymbol{d}+\boldsymbol{q}|} \approx \imath\sum_{l=1}^{L}\underbrace{e^{\imath\kappa\boldsymbol{x}\cdot\widehat{\boldsymbol{s}}(\boldsymbol{\omega}_l)}}_{\leftrightarrow\, g_l(\boldsymbol{x})}\cdot\underbrace{\rho_l e^{\imath\kappa(\boldsymbol{c}^y-\boldsymbol{c}^x)}\sum_{m=0}^{M}(2m+1)(-1)^m h_m^{(1)}(|\boldsymbol{d}|)\frac{1}{4\pi\imath^m}}_{\leftrightarrow\, \gamma_l}\cdot\underbrace{e^{-\imath\kappa\boldsymbol{y})\cdot\widehat{\boldsymbol{s}}(\boldsymbol{\omega}_l)}}_{\leftrightarrow\, \overline{g}_l(\boldsymbol{y})}\ ,$$

where $\{(\rho_l,\boldsymbol{\omega}_l)\}_{l=1,\dots,L} \mathrel{\hat{=}}$ quadrature weights/nodes for 2-sphere $\mathbb{S}$, *cf.* (3.4.9).

Recall:

$$\begin{tikzcd}
\text{2D} \arrow[d, leftrightarrow] & & \text{3D} \arrow[d, leftrightarrow] \\
\text{Fourier harmonics } t \mapsto e^{\imath nt},\ t\in[0,2\pi[\arrow[rr, leftrightarrow] & & \text{spherical harmonics } Y_n^m(\boldsymbol{\omega}),\ \boldsymbol{\omega}\in\mathbb{S}
\end{tikzcd}$$

➤ choose quadrature rule that is exact for spherical harmonics up to a certain order n (Requires $O(n^2)$ quadrature points)

McLaren, A. (1963), ‘Optimal numerical integration on a sphere’, *Math. Comp.* **17**(84), 361–383.

Remark 20 (Drawbacks of plane wave expansion).

- approximation of Bessel function term in (3.4.1), (3.4.10), whose rapid decay is crucial for convergence, *cf.* Ex. 19

  → numerical instability for large M

- for small κ: plane waves become (almost) linearly dependent

  → numerical instability for small κ

▶ Potential remedy: inhomogeneous plane wave expansions

Darve, E. & Havé, P. (2004), ‘A fast multipole method for maxwell equations stable at all frequencies’, *Phil. Trans. R. Soc. London A* **362**(1816), 603–628.

3.4.4 Kernel approximation error estimates

☞ combined analysis of truncation error and quadrature error

Error estimates in two dimensions

Amini, S. & Profit, A. (1999), ‘Analysis of a diagonal form of the fast multipole algorithm for scattering theory’, *BIT* **39**, 585–602.

Labreuche, C. (1998), ‘A convergence theorem for the fast multipole method for two-dimensional scattering problems’, *Math. Comp.* **67**(222), 553–591.

Error in kernel approximation ($\boldsymbol{x} \in Q^x$, $\boldsymbol{y} \in Q^y$, $Q^x \times Q^y$ admissible block, see Fig. 4):

$$G(\boldsymbol{x},\boldsymbol{y}) = \sum_{m=-\infty}^{\infty} \frac{\imath/4}{2\pi\imath^m}\int\limits_0^{2\pi} H_m^{(1)}(|\boldsymbol{d}|)e^{\imath m\varphi_{\boldsymbol{d}}} e^{\imath\kappa(\boldsymbol{c}^x-\boldsymbol{x})\cdot\widehat{\boldsymbol{s}}(t)} e^{\imath\kappa(\boldsymbol{y}-\boldsymbol{c}^y)\cdot\widehat{\boldsymbol{s}}(t)} e^{-\imath m t}\,\mathrm{d}t\,,$$

$$\updownarrow$$

$$\widetilde{G}(\boldsymbol{x},\boldsymbol{y}) = \sum_{m=-M}^{M}\sum_{l=0}^{L-1} \frac{\imath/4}{L\imath^m} H_m^{(1)}(|\boldsymbol{d}|)e^{\imath m\varphi_{\boldsymbol{d}}+\imath\boldsymbol{d}\cdot\widehat{\boldsymbol{s}}(\frac{2\pi l}{L})} e^{-\imath\kappa\boldsymbol{x}\cdot\widehat{\boldsymbol{s}}(\frac{2\pi l}{L})} e^{\imath\kappa\boldsymbol{y}\cdot\widehat{\boldsymbol{s}}(\frac{2\pi l}{L})} e^{-\imath m\frac{2\pi l}{L}}\,.$$

❶ Separating quadrature error from truncation error

$$\delta G(\boldsymbol{x},\boldsymbol{y}) = \tfrac{\imath}{4}\sum_{\substack{m=-\infty\\|m|>M}}^{\infty} H_m^{(1)}(|\boldsymbol{d}|)J_m(|\boldsymbol{q}|)e^{\imath m(\varphi_{\boldsymbol{d}}-\varphi_{\boldsymbol{q}})} +$$

$$\tfrac{\imath}{4}\sum_{m=-M}^{M} H_m^{(1)}(|\boldsymbol{d}|)e^{\imath m\varphi_{\boldsymbol{d}}}\left(J_m(|\boldsymbol{q}|) - \widetilde{J}_m(|\boldsymbol{q}|)\right)e^{\imath m\varphi_{\boldsymbol{q}}} ,$$

with quadrature approximation

$$\widetilde{J}_m(|\boldsymbol{q}|)e^{-\imath m\varphi_{\boldsymbol{q}}} := \frac{1}{\imath^m L}\sum_{l=0}^{L-1} e^{\imath\boldsymbol{q}\cdot\widehat{\boldsymbol{s}}(\frac{2\pi}{L}l)}\cdot e^{-\imath m\frac{2\pi}{L}l} .$$

Tool: Jacobi-Anger expansion: → (Abramowitz & Stegun 1970, (9.1.41))

$$e^{\imath x\cos\psi} = \sum_{k=-\infty}^{\infty} \imath^k J_k(x)e^{\imath k\psi} , \quad x\in\mathbb{R},\ \psi\in[0,2\pi[. \tag{3.4.12}$$

►
$$\widetilde{J}_m(|\boldsymbol{q}|)e^{-\imath m\varphi_{\boldsymbol{q}}} = \frac{1}{\imath^m L}\sum_{l=0}^{L-1}\sum_{k=-\infty}^{\infty}\imath^k J_k(|\boldsymbol{q}|)e^{\imath k(\frac{2\pi}{L}l-\varphi_{\boldsymbol{q}})}e^{-\imath m\frac{2\pi}{L}l}$$

$$= \sum_{k=-\infty}^{\infty}\imath^{k-m}J_k(|\boldsymbol{q}|)e^{-\imath k\varphi_{\boldsymbol{q}}}\cdot \underbrace{\frac{1}{L}\sum_{l=0}^{L-1}e^{\imath(k-m)\frac{2\pi}{L}l}}_{=\begin{cases}1 & \text{, if } k-m\equiv 0 \mod L\,,\\ 0 & \text{, else.}\end{cases}}$$

▼

$$\sum_{m=-M}^{M} H_m^{(1)}(|\boldsymbol{d}|)e^{\imath m\varphi_{\boldsymbol{d}}}\left(J_m(|\boldsymbol{q}|)-\widetilde{J}_m(|\boldsymbol{q}|)\right)e^{\imath m\varphi_{\boldsymbol{q}}} =$$

$$\sum_{\substack{k=-\infty\\ k\neq 0}}^{\infty}\sum_{m=-M}^{M}\imath^{kL}J_{kL+m}(|\boldsymbol{q}|)e^{-\imath(kL+m)\varphi_{\boldsymbol{q}}}H_m^{(1)}(|\boldsymbol{d}|)e^{\imath m\varphi_{\boldsymbol{d}}}\,.$$

Heuristics: L such that quadrature error terms only contain Bessel functions have have also been discarded when truncating the series

➡ $\boxed{L = 2M+1}$

$$\boxed{\delta G(\boldsymbol{x},\boldsymbol{y}) = \frac{\imath}{4}\sum_{\substack{m=-\infty\\|m|>M}}^{\infty} J_m(|\boldsymbol{q}|)e^{-\imath\varphi_{\boldsymbol{q}}}\left(H_m^{(1)}(|\boldsymbol{d}|)e^{\imath m\varphi_{\boldsymbol{d}}} + \imath^{m-r}H_r^{(1)}(|\boldsymbol{d}|)e^{\imath r\varphi_{\boldsymbol{d}}}\right)}\;, \tag{3.4.13}$$

where $r \in \{-M,\dots,M\}$, $r \equiv m \mod L$.

Lemma 3.4.3 (Behavior of Hankel and Bessel functions). → *(Amini & Profit 2000, Lemma 2)*

- *For fixed* $m > 0$*:* $x \mapsto \left|H_m^{(1)}(x)\right|$ *strictly decreasing*
- $x \mapsto J_m(x)$, $m \in \mathbb{N}$, *is positive and increasing in* $x \in [0, m]$.
- *For fixed* $x > 0$*:* $m \mapsto |H_m^{(1)}|$ *is strictly increasing.*

▶ Require $L > \frac{1}{2}\kappa \max\{\operatorname{diam} Q^x, \operatorname{diam} Q^y\}$

$$\blacktriangleright \quad |\delta G(\boldsymbol{x},\boldsymbol{y})| \leq \frac{1}{4}\sum_{\substack{m=-\infty\\|m|>M}}^{\infty} |J_m(2\kappa \max\{\operatorname{diam} Q^x, \operatorname{diam} Q^y\})| \cdot \Big(|H_m^{(1)}(\kappa \operatorname{dist}(Q^x;Q^y))| + |H_M^{(1)}(\kappa \operatorname{dist}(Q^x;Q^y))| \Big)$$

$$\leq \frac{1}{2}\sum_{\substack{m=-\infty\\|m|>M}}^{\infty} |J_m(2\kappa \max\{\operatorname{diam} Q^x, \operatorname{diam} Q^y\})| \cdot |H_m^{(1)}(\eta^{-1}\kappa \max\{\operatorname{diam} Q^x, \operatorname{diam} Q^y\})| \;,$$

in the case of an η-admissible block $Q^x \times Q^y$.

➢ $\eta < 1$: $|\delta G(\boldsymbol{x},\boldsymbol{y})| <$ remainder term for series (3.4.1) **!**

➢ if $L > \frac{1}{2}\kappa \max\{\operatorname{diam} Q^x, \operatorname{diam} Q^y\}$, exponential convergence w.r.t. L on η-admissible blocks, *cf.* Ex. 19.

Rigorous estimate from (Labreuche 1998, Thm. 2): uniform exponential convergence $|\delta G(\boldsymbol{x},\boldsymbol{y})| \to 0$ w.r.t L on $Q^x \times Q^y$, for $L \geq C\kappa$ (for some $C > 0$), $\eta > 0$ sufficiently large.

Error estimates in three dimensions

Quentin, C. & Collino, F. (2005), 'Error estimates in the fast multipole method for scattering problems. ii. truncation of the Gegenbauer series', *ESAIM, Math. Model. Numer. Anal.* **39**(1), 183–221.

Koc, S., Song, J.-M. & Chew, W. (1999), 'Error analysis for the numerical evaluation of the diagonal forms of the scalar spherical addition theorem', *SIAM J. Numer. Anal.* **36**(3), 906–921.

Darve, E. (2000*a*), 'The fast multipole method I: Error analysis and asymptotic complexity', *SIAM J. Numer. Anal.* **38**(1), 98–128.

Bound for number M of terms in Gegenbauer expansion (3.4.10) for η-admissible block ($\eta < 1$) and (relative !) error threshold $\epsilon > 0$ →(Quentin & Collino 2005):

$$M \simeq \kappa d + (\tfrac{1}{2})^{5/3} W^{2/3} \left(\left(\frac{1+\eta}{1-\eta} \right)^{3/2} \frac{\kappa d}{4\epsilon^6} \right) \sqrt[3]{d\kappa} - \frac{1}{2} \; ,$$

where
- $W \hat{=}$ Lambert function: $W(\xi)e^{W(\xi)} = \xi$, $\xi > 0$, $W(\xi) \asymp \log(\frac{\xi}{\log \xi})$ for $\xi \to \infty$
- $d = \max\{\operatorname{diam} Q^x, \operatorname{diam} Q^y\}$ $\hat{=}$ size of block

Choice of quadrature rule on $\mathbb{S}$: integrate spherical harmonics up to order $2M$ exactly → (Darve 2000*a*).

3.4.5 Plane wave FMM: Algorithm

Implementation in 2D

☛ Multilevel clustering algorithm (→ Sects. 3.3.4, 3.3.5) based on (3.4.9)

Recall: for cluster $S \in \mathcal{T}$ ▷ truncation parameter $L_S = O(\kappa \cdot \mathrm{diam}(\mathrm{Box}(S)))$!
(variable expansion length)

Main issue: efficient evaluation of (necessarily inexact) transfers
($\hat{=}$ fast products with transfer matricces $\mathbf{T}^{S,s}$)

$s \in \mathrm{sons}(S) \quad \Rightarrow \quad \mathrm{diam}(\mathrm{Box}(s)) < \mathrm{diam}(\mathrm{Box}(S))$ (usually $\mathrm{diam}(\mathrm{Box}(s)) \approx \frac{1}{2}\mathrm{diam}(\mathrm{Box}(S))$)
$L_s < L_S$ (smaller expansion system on smaller clusters)

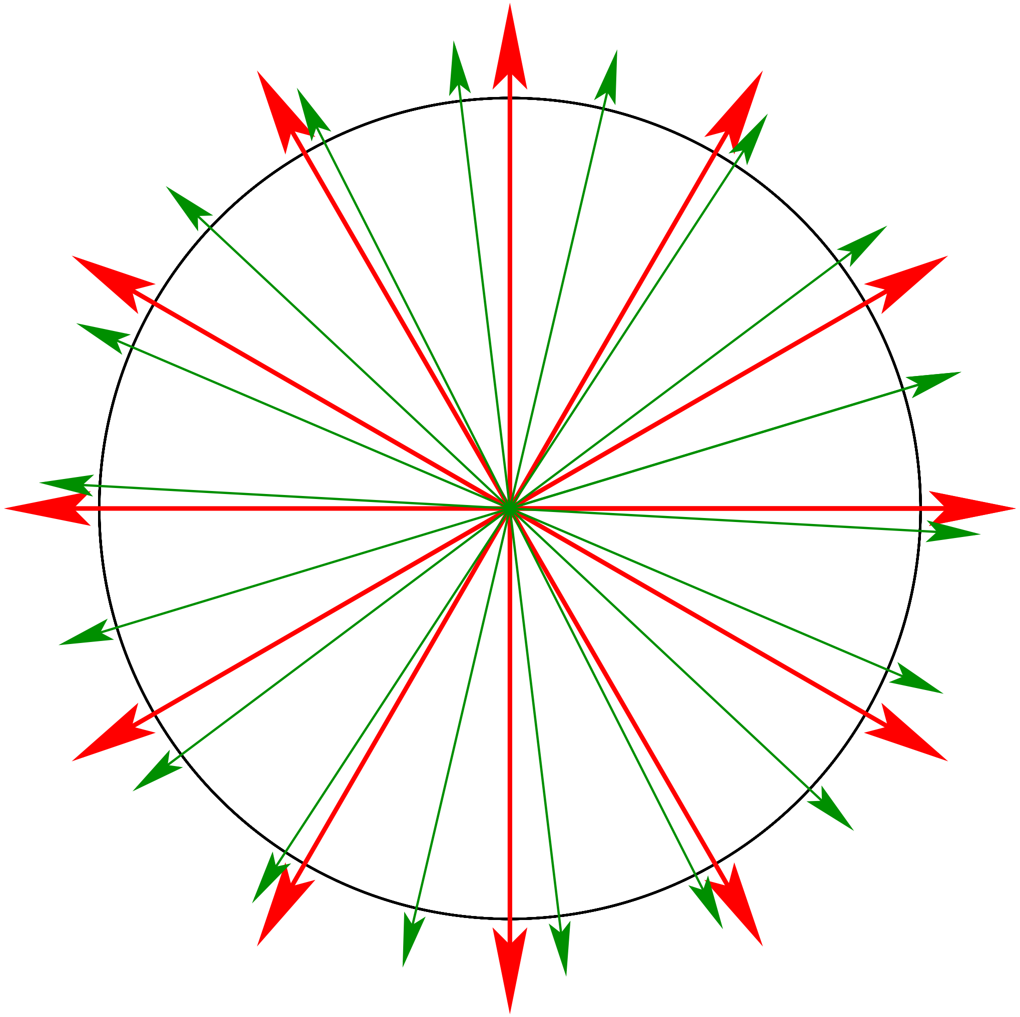
Task: Given: $S \in \mathcal{T}$, $s \in \mathrm{sons}(S)$ with centers (of bounding boxes) $\boldsymbol{c}$ and $\boldsymbol{b}$, w.l.o.g. $\boldsymbol{b} = 0$.
Expansion lengths on S/s: L,l, resp.: $L > l$

Find $\mathbf{T}^{S,s} = (\tau^{S,s}_{kj})_{\substack{k=1,\dots,L\\ j=1,\dots,l}}$ such that

$$\sum_{j=1}^{l} \tau^{S,s}_{kj} e^{\imath\kappa \boldsymbol{x}\cdot\widehat{\boldsymbol{s}}(\frac{2\pi}{l}j)} \approx e^{\imath\kappa(\boldsymbol{x}-\boldsymbol{c})\cdot\widehat{\boldsymbol{s}}(\frac{2\pi}{L}k)}\ , \quad k=1,\dots,L\ .$$

expansion functions on s expansion functions on S

How to approximate a plane wave in a set of plane waves with other directions **?**



Idea: use Jacobi-Anger expansion (3.4.12)

plane wave (father)

$\downarrow$

cylindrical wave

$\downarrow$

(truncation)

$\downarrow$

plane wave (son)

$$\sum_{k=1}^{L}\alpha_k e^{\imath\kappa(\boldsymbol{x}-\boldsymbol{c})\cdot\widehat{s}(\frac{2\pi}{L}k)} = \sum_{k=1}^{L}\big(\underbrace{\alpha_k e^{-\imath\boldsymbol{c}\cdot\widehat{s}(\frac{2\pi}{L}k)}}_{=:\alpha'_k}\big)e^{\imath\kappa\boldsymbol{x}\cdot\widehat{s}(\frac{2\pi}{L}k)}$$

$$= \sum_{m=-\infty}^{\infty}\Big(\sum_{k=1}^{L}\alpha'_k e^{-\imath m\frac{2\pi}{L}k}\Big)J_m(\kappa\,|\boldsymbol{x}|)e^{\imath m\varphi_{\boldsymbol{x}}}$$

$$\approx \sum_{m=-\infty}^{\infty}\Big(\sum_{k=1}^{l}\beta_j e^{-\imath m\frac{2\pi}{l}j}\Big)J_m(\kappa\,|\boldsymbol{x}|)e^{\imath m\varphi_{\boldsymbol{x}}} = \sum_{j=1}^{l}\beta_j e^{\imath\kappa\boldsymbol{x}\cdot\widehat{s}(\frac{2\pi}{l}k)}\ ,$$

Desired: $$\sum_{k=1}^{L}\alpha'_k e^{-\imath m\frac{2\pi}{L}k} \approx \sum_{k=1}^{l}\beta_j e^{-\imath m\frac{2\pi}{l}j}\quad \forall m\in\mathbb{Z}\ . \qquad (3.4.14)$$

In (3.4.14): demand equality for $m = 0,\dots,l-1$: $\boxed{\vec{\beta}\text{ from }\vec{\alpha'}\text{ by 2 FFTs}}$

➤ Costs for transfers S ↔ four sons $= O(L\log L))$

Total costs for transfers:

assume $L_S = C2^{\text{level}_{\max} - \text{level}(S)} \approx \sharp S$ & “nice” geometry, point distribution

$$\text{Costs} \lesssim \sum_{S \in \mathcal{T} \setminus \text{leaves}(\mathcal{T})} L_S \log L_S \lesssim \sum_{S \in \mathcal{T} \setminus \text{leaves}(\mathcal{T})} \sharp S(\text{level}_{\max} - \text{level}(S))$$

$$\lesssim \log N \sum_{S \in \mathcal{T} \setminus \text{leaves}(\mathcal{T})} \sharp S = O(N \log^2 N) \; .$$

▶ Computational costs of plane wave FMM $= O(N \log^2 N)$

Implementation in 3D

Darve, E. (2000*b*), ‘The fast multipole method: Numerical implementation’, *J. Comp. Phys.* **160**(1), 195–240.

4 Preconditioning Techniques

4.1 The rationale

➜ Matrix compression by Fast Multipole Methods (Ch. 3) ➢ no matrix available **!**

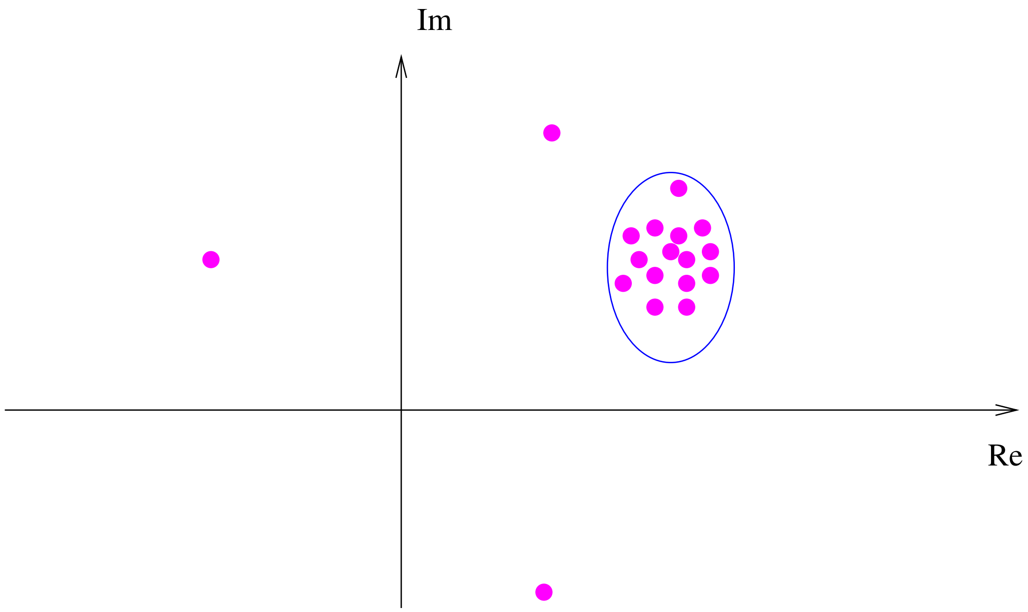
- ▷ cannot use direct solvers (also ruled out for $N \gg 1$)
- ▷ only matrix×vector at one's disposal

► iterative solution techniques for discrete boundary integral equations (usually: Krylov method)

➜ Speed of convergence of iterative solvers for $\mathbf{A}\vec{\xi} = \vec{\varphi}$ "linked to"

- Euklidean norms of $\mathbf{A}$, $\mathbf{A}^{-1}$
- distribution of eigenvalues of $\mathbf{A}^{(*)}$

“Simple theory” only for Hermitian matrices (↔ CG, MINRES), convergence theory available for GMRES (without restart).



$(*)$ desirable distribution of eigenvalues:

bulk of the spectrum clustered around $z \neq 0$

Bad: bulk of spectrum clustered around 0 or ∞

A preconditioner $\mathbf{B}$ for $\mathbf{A}$ is a “matrix” (↔ linear operator in $\mathbb{R}^N$),

- so that Krylov subspace solvers applied to $\mathbf{BA}$ converge much faster than for $\mathbf{A}$ (“approximate inverse”)
- for which costs($\mathbf{B}\times$vector) $\approx$ costs($\mathbf{A}\times$ vector)

Do we need preconditioners for discrete BIE **?**

Consider: shape-regular, quasi-uniform family of meshes of Γ, Sect. 2.1, meshwidth h, standard boundary element space (→ Sect. 2.2) with $L^2(\Gamma)$-stable nodal basis

❶ First-kind integral equations (1.1.15), (1.1.18) (assume: no resonance problem)

$$\varphi \in H^{-\frac{1}{2}}(\Gamma): \quad -\mathsf{V}_\kappa(\varphi) = (\tfrac{1}{2}\mathsf{Id} - \mathsf{K}_\kappa)g \quad \text{in } H^{\frac{1}{2}}(\Gamma) \;,$$
$$\varphi \in H^{-\frac{1}{2}}(\Gamma): \quad -\mathsf{W}_\kappa(u) = (\tfrac{1}{2}\mathsf{Id} + \mathsf{K}'_\kappa)\psi \quad \text{in } H^{-\frac{1}{2}}(\Gamma) \;.$$

BEM Galerkin matrices: $\mathbf{A}_V \longleftrightarrow \langle \mathsf{V}_\kappa\varphi, \psi\rangle$, $\mathbf{A}_W \longleftrightarrow \langle \mathsf{W}_\kappa u, v\rangle$

⇒ **sharp** estimates

$$h \lesssim \frac{|\vec{\varphi}^H \mathbf{A}_V \vec{\psi}|}{|\vec{\varphi}||\vec{\psi}|} \lesssim 1 \quad , \quad 1 \lesssim \frac{|\vec{\mu}^H \mathbf{A}_W \vec{\nu}|}{|\vec{\mu}||\vec{\nu}|} \lesssim h \quad \forall \vec{\varphi}, \vec{\psi}, \ldots \in \mathbb{C}^N \;, \tag{4.1.1}$$

asymptotically for fixed κ, $h \to 0$, constants depend on κ.

(Possible) clustering of eigenvalues at 0, ∞

❷ Second-kind integral equations (1.1.16), (1.1.17)

$$\varphi \in H^{-\frac{1}{2}}(\Gamma): \quad (\tfrac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa)\varphi = \mathsf{W}_\kappa(g) \quad \text{in } H^{-\frac{1}{2}}(\Gamma) \;,$$
$$u \in H^{\frac{1}{2}}(\Gamma): \quad (\tfrac{1}{2}\mathsf{Id} + \mathsf{K}_\kappa)u = \mathsf{V}_\kappa(\psi) \quad \text{in } H^{\frac{1}{2}}(\Gamma) \;.$$

BEM Galerkin matrices: $\mathbf{A}_K \longleftrightarrow \left((\frac{1}{2}\mathsf{Id} + \mathsf{K}_\kappa)u, v\right)_{L^2(\Gamma)}$, $\mathbf{A}_{K'} \longleftrightarrow \left((\frac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa)\varphi, \psi\right)_{L^2(\Gamma)}$

Assume: uniform discrete inf-sup condition w.r.t. $L^2(\Gamma)$-norm

▶ $$1 \lesssim \frac{|\vec{\varphi}^H \mathbf{A}_K \vec{\psi}|}{|\vec{\varphi}||\vec{\psi}|} \lesssim 1 \quad , \quad 1 \lesssim \frac{|\vec{\mu}^H \mathbf{A}_{K'} \vec{\nu}|}{|\vec{\mu}||\vec{\nu}|} \lesssim 1 \quad \forall \vec{\varphi}, \vec{\psi}, \ldots \in \mathbb{C}^N \; , \tag{4.1.2}$$

Spectrum uniformly bounded away from 0, ∞

❷ Second-kind integral equations ↔ sesqui-linear form

$$(u, v) \mapsto ((\mathsf{Id} + \mathsf{K})u, v)_{L^2(\Gamma)} \; , \quad u, v \in L^2(\Gamma) \; ,$$

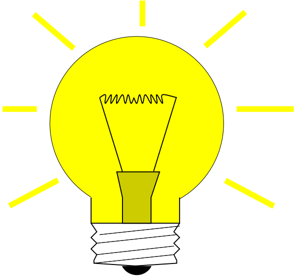
with $\mathsf{K} : L^2(\Gamma) \mapsto L^2(\Gamma)$ compact

▶ Spectrum of Galerkin matrix clustered around 1

▼

Preconditioning required for 1st-kind discrete BIE on fine meshes

4.2 Operator preconditioning



Idea: Operator of “opposite order” provide good approximate inverses

(typical “Elliptic”, “low frequency” reasoning)

4.2.1 Abstract framework

- V, W refl. Banach spaces, $\mathsf{A} \in L(V, V')$, $\mathsf{B} \in L(W, W')$ isomorphisms.
- Finite dimensional trial/test spaces $V_h \subset V$, $W_h \subset W$ such that

  ❶ $\mathsf{A}_h := \mathsf{A}_{|V_h} : V_h \mapsto V_h'$, $\mathsf{B}_h := \mathsf{B}_{|W_h} : W_h \mapsto W_h'$ (h-uniformly) stable

  ❷ $\dim V_h = \dim W_h$
- Stable discrete duality pairing: sesqui-linear form $d \in L(V \times W, \mathbb{C})$

$$\exists c_D > 0: \quad \sup_{v_h \in V_h} \frac{|d(v_h, w_h)|}{\|v_h\|_V} \geq c_D \, \|w_h\|_W \quad \forall w_h \in W_h \ .$$

Theorem 4.2.1 (Operator preconditioning)**.**

Spectral condition number satisfies:

$$\kappa(\mathbf{D}^{-1}\mathbf{B}\mathbf{D}^{-T}\mathbf{A}) \leq \|\mathsf{A}_h\|\,\|\mathsf{A}_h^{-1}\|\;\|\mathsf{B}_h\|\,\|\mathsf{B}_h^{-1}\|\frac{\|d\|^2}{c_D^2}$$

Galerkin matrices

S. CHRISTIANSEN AND J.-C. NÉDÉLEC, *Des préconditionneurs pour la résolution numérique des équations intégrales de frontiére de l'acoustique*, C.R. Acad. Sci. Paris, Ser. I Math, 330 (2000), pp. 617–622.

4.2.2 Boundary element application

- First-kind integral equations (1.1.22) (assume: no resonance problem)

$$\text{(1.1.15)} \quad \Leftrightarrow \quad \varphi \in H^{-\frac{1}{2}}(\Gamma)\colon \quad \langle \mathsf{V}_\kappa\varphi,\psi\rangle = -\left\langle (\tfrac{1}{2}\mathsf{Id} - \mathsf{K}_\kappa)g,\psi\right\rangle \quad \forall\psi \in H^{-\frac{1}{2}}(\Gamma)\ . \qquad (1.1.22)$$

- Galerkin discretization by means of $\mathcal{M}_\Gamma$-p.w. constant boundary element functions $\longrightarrow V_h$

(1.1.22) ↔ single layer BI-Op. $\mathsf{V}_\kappa : H^{-\frac{1}{2}}(\Gamma) \mapsto H^{\frac{1}{2}}(\Gamma)$

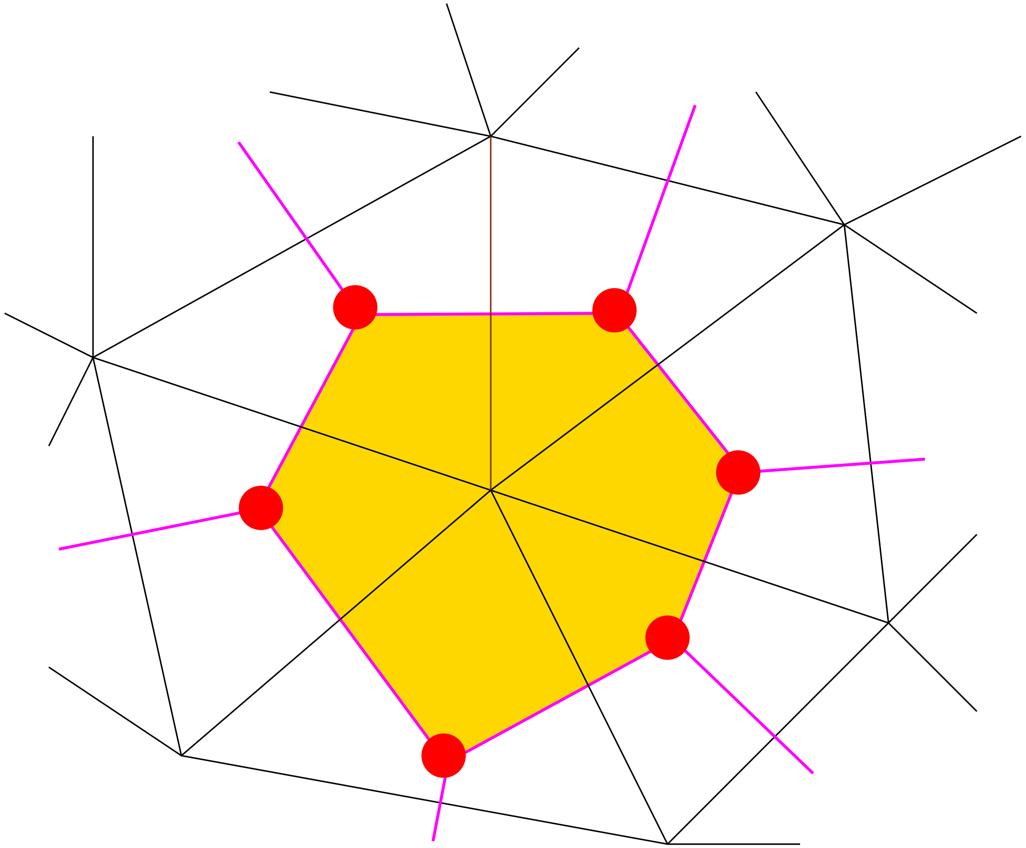
Thm. 4.2.1: natural candidates

$$\boxed{W = H^{\frac{1}{2}}(\Gamma), \quad \mathsf{B} = \mathsf{W}_\kappa}$$

Duality pairing between $V = H^{-\frac{1}{2}}(\Gamma)$ and $W = H^{\frac{1}{2}}(\Gamma)$:

$$d(u,v) := \int_\Gamma u\bar{v}\,\mathrm{d}S$$ ► trivially stable

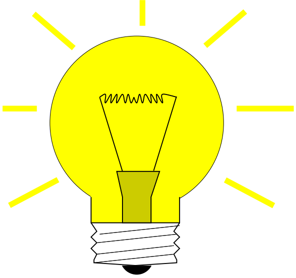
$V_h \not\subset W$ ➢ $W_h = V_h$ not an option: What is W_h **?**



$d = 3$:

mesh $\mathcal{M}$	$\leftrightarrow$	dual mesh $\widetilde{\mathcal{M}}$
nodes	$\leftrightarrow$	cells
edges	$\leftrightarrow$	edges
cells	$\leftrightarrow$	nodes

(Incidence matrices of $\widetilde{\mathcal{M}}$ = transposed incidence matrices of $\mathcal{M}$)

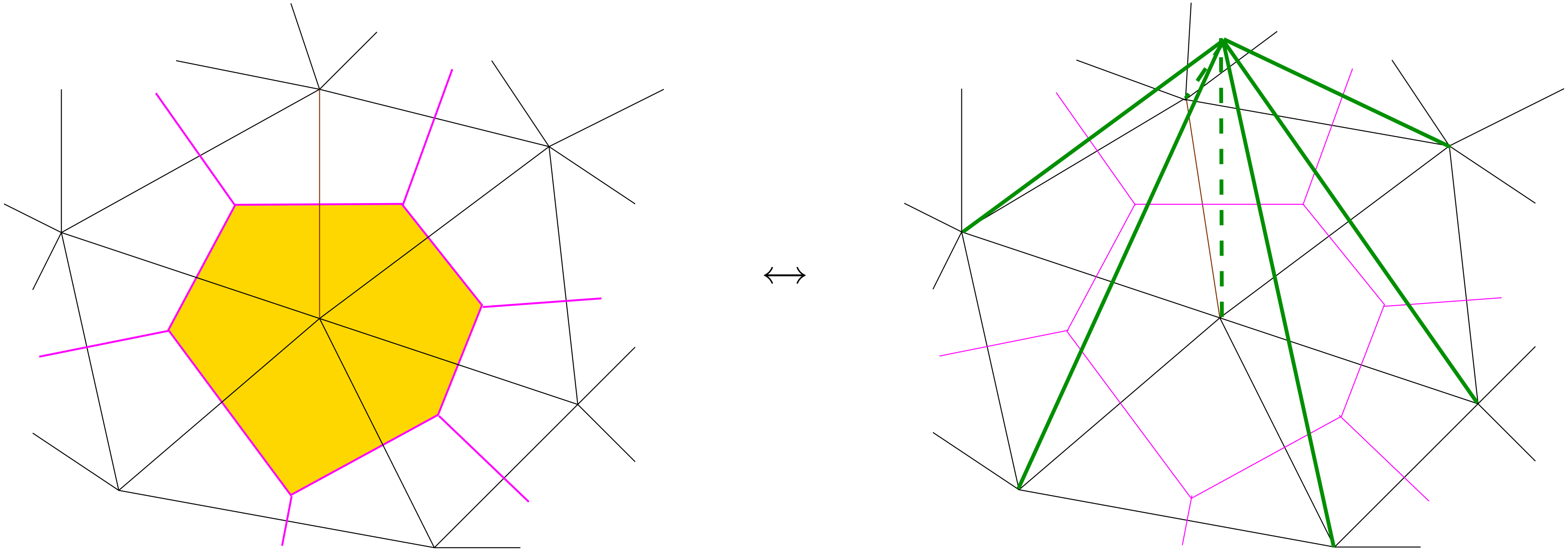


Idea:

$V_h \leftrightarrow$ cells of $\mathcal{M}$ $\Leftrightarrow$ $W_h \leftrightarrow$ vertices of $\widetilde{\mathcal{M}}$

For $V = H^{-\frac{1}{2}}(\Gamma)$:

$$\begin{tikzcd}
V_h \arrow[r, leftrightarrow] \arrow[d, leftrightarrow] & W_h \arrow[d, leftrightarrow] \\
\text{p.w. constant on cells of } \mathcal{M} \arrow[r, leftrightarrow] & \text{“p.w. linear” } \textbf{\&} \ C^0 \text{ on } \widetilde{\mathcal{M}}
\end{tikzcd}$$



h-uniform stability of discrete duality paiting $(u,v) \mapsto \int uv \, \mathrm{d}S$ on $V_h \times W_h$

O. Steinbach, *On a generalized L_2 projection and some related stability estimates in Sobolev spaces*, Numer. Math., 90 (2002), pp. 775–786.

Remark 21 (Operator preconditioning based on Calderon projectors).

By derivation: operator preconditioning controls spectrum for $h \to 0$

Can it be more powerful ?

By projector property of Calderón projectors (→ Sect. 1.1.4.1): $\mathsf{P}^{\pm}\mathsf{P}^{\pm} = \mathsf{P}^{\pm}$:

$$\begin{aligned} \mathsf{K}_\kappa \mathsf{V}_\kappa &= \mathsf{V}_\kappa \mathsf{K}'_\kappa \quad , \quad & \mathsf{W}_\kappa \mathsf{K}_\kappa &= \mathsf{K}'_\kappa \mathsf{W}_\kappa \ , \\ \mathsf{V}_\kappa \mathsf{W}_\kappa &= \tfrac{1}{4}\mathsf{Id} - \mathsf{K}_\kappa^2 \quad , \quad & \mathsf{W}_\kappa \mathsf{V}_\kappa &= \tfrac{1}{4}\mathsf{Id} - \mathsf{K}'^2_\kappa \ . \end{aligned}$$

Γ smooth ➤ K_κ, K'_κ compact ➤ operator preconditioning achieves clustering of spectrum **?**

Issue: impact of κ on quality of operator preconditioning ?

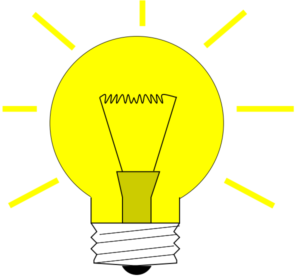
4.3 Asymptotic preconditioning

Neumann-to-Dirichlet operator $\mathsf{S} : H^{-\frac{1}{2}}(\Gamma) \mapsto H^{\frac{1}{2}}(\Gamma)$ for exterior Helmholtz BVP:

$$\mathsf{S}\varphi := \gamma_D u, \quad \text{where } u \text{ solves} \quad \begin{aligned} -\Delta u - \kappa^2 u &= 0 \ \text{ in } \Omega^+ \ , \\ \gamma_N^+ u &= \varphi \ \text{ on } \Gamma \end{aligned} \qquad +r.c.$$

$$(1.1.14) \quad \Rightarrow \quad -\mathsf{W}_\kappa \circ \mathsf{S} + (\tfrac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa) = \mathsf{Id}\ . \tag{4.3.1}$$

BVP: exterior Neumann problem for Helmholtz equation (1.1.11)



Idea: exploit (4.3.1) in context of *indirect BIE* → Sect. 1.1.4.3

trial expression: $u = \Psi_{\mathsf{SL}}(\varphi) + \Psi_{\mathsf{DL}}(\widetilde{\mathsf{S}}\varphi)$,

where $\widetilde{\mathsf{S}} \approx \mathsf{S}$.

➤ BIE: $(-\mathsf{W}_\kappa \circ \widetilde{\mathsf{S}} + (\tfrac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa))\varphi = \psi$

(4.3.1) ▶ if $\widetilde{\mathsf{S}} \approx \mathsf{S} \quad \Rightarrow \quad -\mathsf{W}_\kappa \circ \widetilde{\mathsf{S}} + (\tfrac{1}{2}\mathsf{Id} - \mathsf{K}'_\kappa) \approx \mathsf{Id}$

How to find suitable $\widetilde{\mathsf{S}}$ **?**

For large frequencies: (plane wave scattering) use Kirchhoff approximation (half-space approximation (local approximation of S)

Antoine, X. & Darbas, M. (2005), ‘Alternative integral equations for the iterative solution of acoustic scattering problems’, *Quaterly Journal of Mechanics and Applied Mathematics* **58**(1), 107–128.

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