OBERWOLFACH, 26–30 SEPTEMBER 2022

SCA & NA FOR WAVE SCATTERING PROBLEMS

Non-polynomial methods for the Helmholtz equation

Andrea Moiola

`https://euler.unipv.it/moiola/`

UNIVERSITÀ DI PAVIA
Department of Mathematics
“Felice Casorati"

Polynomials or not?

Goal:
Numerical approximation of BVPs for the Helmholtz eq. $\Delta u + \kappa^2 u = 0$.

Classical FEM & BEM use piecewise-polynomial approximants.

Why polynomials?

- Easy & cheap to evaluate, manipulate, differentiate, integrate. . .
- Approximation properties:
  - Can approximate all functions
  - Complete theory, convergence rates, only depend on smoothness

Why not polynomials?

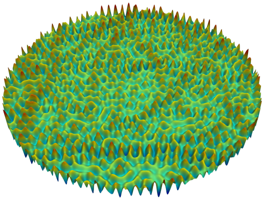
- Can we do better?
  Classical methods at large frequencies are not very satisfactory
- Not adapted to Helmholtz: polynomials are general-purpose tool
- Main goal: more accuracy for fewer DOFs

Everything can/might be extended to
time-harmonic electromagnetic and elastic waves.

Outline

- FEM-type methods: (discretise PDE in Ω)
  - Trefftz methods
  - Meshless methods, method of fundamental solutions (MFS)
  - Partition of unity (PUM)
  - Trefftz discontinuous Galerkin (TDG/UWVF)
  - Quasi-Trefftz
- Approximation properties
- Instability and possible remedy
- BEM-type methods: (discretise BIE on $\partial\Omega$)
  Hybrid-numerical asymptotics BEM (HNA BEM)
  (talk by F. Ecevit)

See also talk by T. Chaumont-Frelet
on approximation by
"Gaussian coherent states".



Part I

FEM-type methods

Trefftz methods

HIPTMAIR, M., PERUGIA 2016, *A survey of Trefftz methods for the Helmholtz eq.*

A **Trefftz** method is a finite-element-type scheme where all discrete functions are solutions of the PDE to be approximated in each element of a mesh.

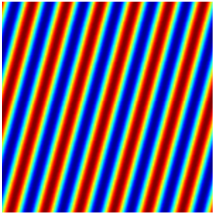
Named after Erich Trefftz's 1926 paper.

E.g.: piecewise harmonic polynomials for Laplace equation $\Delta u = 0$.

Main point: expect more accuracy for fewer DOFs.

Homogeneous Helmholtz eq. does not admit polynomial solutions: Trefftz methods for Helmholtz are non-polynomial.

Trefftz bases



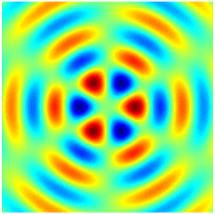
Typical basis: (propagative) plane waves (PPWs):

$$\mathbf{x} \mapsto \mathrm{e}^{\mathrm{i}\kappa\mathbf{d}\cdot\mathbf{x}} \qquad \mathbf{d} \in \mathbb{R}^n \quad \mathbf{d}\cdot\mathbf{d} = 1$$

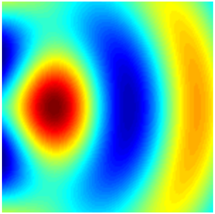
PPWs are just complex exponentials:
as easy & cheap to manipulate, evaluate, differentiate, integrate. . . as polynomials

→ Usually preferred to other choices of Trefftz bases, e.g.:

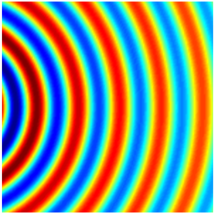
circular waves
$J_\ell(\kappa r)\mathrm{e}^{\mathrm{i}\ell\theta}, \ell \in \mathbb{Z}$



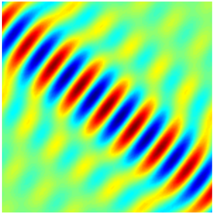
corner waves
$J_\xi(\kappa r)\mathrm{e}^{\mathrm{i}\xi\theta}, \xi \notin \mathbb{Z}$



fundamental sol.
$\Phi_\kappa(\mathbf{x}, \mathbf{y}_j)$

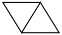


wavebands
$\int_{\varphi_1}^{\varphi_2} \mathrm{e}^{\mathrm{i}\kappa\mathbf{x}\cdot\binom{\cos\varphi}{\sin\varphi}}\,\mathrm{d}\varphi$



Meshless methods and MFS

Trefftz basis functions cannot be "glued" across mesh elements.



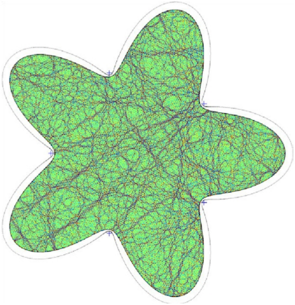
▶ **Solution #1**: meshless methods.

Herrera, Zieliński, Zienkiewicz. . . since 1970s.
Includes "Fokas transform method".

Prominent example:
Method of fundamental solutions (MFS)

Solution u approximated by

$$u_{MFS}(\mathbf{x}) = \sum_{j=1}^{N} a_j H_0^{(1)}(\kappa|\mathbf{x} - \mathbf{y}_j|)$$



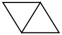
(BARNETT, BETCKE 2008)

Nodes $\mathbf{y}_j$ on a curve exterior to domain.
Coefficients a_j computed by minimising error vs boundary conditions.

+ Simple, highly accurate, bounded or unbounded domains
– Delicate choice of nodes $\mathbf{y}_j$, little analysis, mostly 2D, instability.

Related: "Lightning method" for polygons (GOPAL, TREFETHEN 2019).

Partition of unity method

Trefftz basis functions cannot be "glued" across mesh elements. 

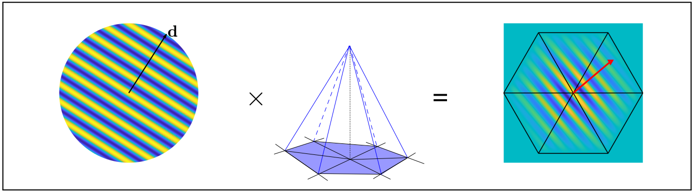
▶ **Solution #2**: Partition of unity method (PUM/PUFEM)

(Melenk, Babuška, 1995–97)

Multiply
- Trefftz basis $\{e^{i\kappa \mathbf{d}_m \cdot \mathbf{x}}\}_{m=1,\dots,M}$
- partition of unity $\{\varphi_j\}_{j=1,\dots,J} \subset H^1(\Omega)$

→ $M \cdot J$ DOFs non Trefftz

Simple choice of PU: piecewise-linear or bilinear finite elements

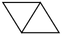


$V_{PUM} = \mathrm{span}\{e^{i\kappa \mathbf{d}_m \cdot \mathbf{x}} \varphi_j(\mathbf{x})\} \subset H^1(\Omega)$: can use classical variational form.:

e.g. $$\int_\Omega (\nabla u \cdot \nabla \overline{v} - \kappa^2 u \overline{v}) + i\kappa \int_{\partial\Omega} u \overline{v} = \int_{\partial\Omega} g v \qquad \forall v \in V_{PUM} \subset H^1(\Omega)$$

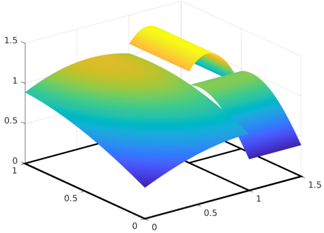
Trefftz DG methods

Trefftz basis functions cannot be “glued” across mesh elements.



▶ **Solution #3**:
Allow discrete functions to be discontinous across mesh face: discontinuous Galerkin (DG) method.

Variational formulation weakly enforces continuity and boundary conditions.

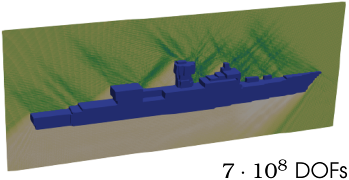


Examples: UWVF, TDG/PWDG, DEM, VTCR, WBM, LS, FLAME, . . .

NGSolve code by P. Stocker: `https://paulst.github.io/NGSTrefftz`

A concrete Trefftz methods depends on 2 choices:

- DG formulation
- discrete space



$7 \cdot 10^8$ DOFs
TDG simulation by M. Sirdey

TDG: sketch of the derivation

Consider Helmholtz equation with impedance (Robin) b.c.:

$$\begin{aligned} -\Delta u - \kappa^2 u &= 0 && \text{in } \Omega \subset \mathbb{R}^n \text{ bdd., Lip., } n = 2, 3 \\ \nabla u \cdot \mathbf{n} + \mathrm{i}\kappa u &= g && \in L^2(\partial\Omega); \end{aligned}$$

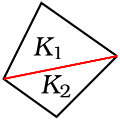
① Partition Ω with a mesh $\mathcal{T}_h$, choose discrete Trefftz space $V_p(\mathcal{T}_h)$

② Multiply with test v, integrate by parts twice on element $K \in \mathcal{T}_h$ ("ultraweak" formulation): $\forall v_p \in V_p(\mathcal{T}_h)$

$$\int_K u_p \underbrace{\overline{(-\Delta v_p - \kappa^2 v_p)}}_{=0} \mathrm{d}V + \int_{\partial K} (-\partial_{\mathbf{n}} u_p \, \overline{v_p} + u_p \, \overline{\partial_{\mathbf{n}} v_p}) \, \mathrm{d}S = 0$$

③ Replace traces on ∂K with "numerical fluxes" to weakly enforce inter-element continuity and BCs:

$$\begin{aligned} u_p &\to \{\!\{u_p\}\!\} - \frac{\beta}{\mathrm{i}\kappa} [\![\nabla_h u_p]\!]_N \\ \nabla u_p &\to \{\!\{\nabla_h u_p\}\!\} - \alpha \mathrm{i}\kappa [\![u_p]\!]_N \end{aligned} \qquad \alpha, \beta > 0$$



$\{\!\{\cdot\}\!\}$ = averages, $[\![\cdot]\!]_N$ = normal jumps on the interfaces

TDG quasi-optimality

Summing over K we get variational formulation:

$$\text{find } u_p \in V_p(\mathcal{T}_h) \quad \text{s.t.} \quad \mathcal{A}_h(u_p, v_p) = \mathcal{F}(v_p) \quad \forall v_p \in V_p(\mathcal{T}_h)$$

$$V_p(\mathcal{T}_h) \subset T(\mathcal{T}_h) := \Big\{ v \in L^2(\Omega) : \; -\Delta v - \kappa^2 v = 0 \text{ in each } K \in \mathcal{T}_h \Big\}$$

$$\left.\begin{array}{l} \quad \forall\, v, w \in T(\mathcal{T}_h) : \\ \mathrm{Im}\, \mathcal{A}_h(v,v) = |||v|||^2_{\mathcal{F}_h} \\ |\mathcal{A}_h(w,v)| \le 2\, |||w|||_{\mathcal{F}_h^+} |||v|||_{\mathcal{F}_h} \end{array}\right\}$$

⇒ Well-posedness & quasi-optimality:

$$|||u - u_p|||_{\mathcal{F}_h} \le 3 \inf_{v_p \in V_p(\mathcal{T}_h)} |||u - v_p|||_{\mathcal{F}_h^+}$$

Holds for all discrete Trefftz spaces $V_p(\mathcal{T}_h) \subset T(\mathcal{T}_h)$

$$|||v|||^2_{\mathcal{F}_h} := \frac{1}{\kappa} \left\| \sqrt{\beta} [\![\nabla_h v]\!]_N \right\|^2_{\mathcal{F}_h^I} + \kappa \left\| \sqrt{\alpha} [\![v]\!]_N \right\|^2_{\mathcal{F}_h^I} + \frac{1}{\kappa} \left\| \sqrt{\delta} \partial_{\mathbf{n}} v \right\|^2_{\partial\Omega} + \kappa \left\| \sqrt{1-\delta}\, v \right\|^2_{\partial\Omega}$$

$$|||v|||^2_{\mathcal{F}_h^+} := |||v|||^2_{\mathcal{F}_h} + \kappa \left\| \beta^{-1/2} \{\!\{ v \}\!\} \right\|^2_{\mathcal{F}_h^I} + \frac{1}{\kappa} \left\| \alpha^{-1/2} \{\!\{ \nabla_h v \}\!\} \right\|^2_{\mathcal{F}_h^I} + \kappa \left\| \delta^{-1/2} v \right\|^2_{\partial\Omega}$$

Duality technique of (MONK, WANG 1999) allows to control L^2 norm of the error: $\quad \|u - u_p\|_{L^2(\Omega)} \le C(\kappa) |||u - u_p|||_{\mathcal{F}_h}$

Part II

Approximation in Trefftz spaces

Best approximation estimates

The analysis of any plane wave Trefftz method requires best approximation estimates:

$$-\Delta u - \kappa^2 u = 0 \qquad \text{in } D \in \mathcal{T}_h, \qquad u \in H^{k+1}(D),$$

$$\mathrm{diam}(D) = h, \qquad p \in \mathbb{N}, \qquad \mathbf{d}_1, \dots, \mathbf{d}_p \in \mathbb{S}^{N-1},$$

$$\inf_{\vec{\alpha} \in \mathbb{C}^p} \left\| u - \sum_{\ell=1}^{p} \alpha_\ell e^{i\kappa\, \mathbf{d}_\ell \cdot \mathbf{x}} \right\|_{H^j(D)} \le C\, \epsilon(h,p)\ \|u\|_{H^{k+1}(D)}$$

Want to study convergence rate: $\epsilon(h,p) \xrightarrow[p\to\infty]{h\to 0} 0$

2 techniques:

- Show that $\forall u \in T(\mathcal{T}_h),\ \exists u_p \in V_p(K)$ with the same Taylor polynomial at a given $\mathbf{x}_K$ (CESSENAT, DESPRÉS 1998)
- Vekua theory (MELENK 1995, M., HIPTMAIR, PERUGIA 2011)

Approximation by plane waves: Vekua theory

Analytical tool from (VEKUA 1942, 1967)

Allows to reduce
approximation of Helmholtz solution by plane and circular waves
↓
approximation of harmonic functions by harmonic polynomials
(MELENK 1995, MOIOLA 2011)

$$\begin{tikzcd}
-\Delta u - \kappa^2 u = 0 \arrow[r, "V^{-1}"] & -\Delta V^{-1}[u] = 0 \arrow[d, "\text{harmonic approx.}"'] \\
\text{Circular waves} \arrow[d, "(\text{Jacobi–Anger})^{-1}"] & \text{Harmonic polyn.} \arrow[l, "V"'] \\
\text{Plane waves} &
\end{tikzcd}$$

Vekua operators

$D \subset \mathbb{R}^n$ star-shaped wrt. $\mathbf{0}$.

Define two continuous functions:

$$M_1(\mathbf{x}, t) = -\frac{\kappa|\mathbf{x}|}{2} \frac{\sqrt{t}^{n-2}}{\sqrt{1-t}} J_1\left(\omega|\mathbf{x}|\sqrt{1-t}\right)$$

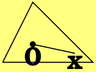
$$M_2(\mathbf{x}, t) = -\frac{i\kappa|\mathbf{x}|}{2} \frac{\sqrt{t}^{n-3}}{\sqrt{1-t}} J_1\left(i\omega|\mathbf{x}|\sqrt{t(1-t)}\right)$$

$M_1, M_2 : D \times [0,1] \to \mathbb{R}$

$J_1 =$ Bessel f.

$$V[\phi](\mathbf{x}) := \phi(\mathbf{x}) + \int_0^1 M_1(\mathbf{x}, t)\phi(t\mathbf{x})\,\mathrm{d}t$$

$$V_2[\phi](\mathbf{x}) := \phi(\mathbf{x}) + \int_0^1 M_2(\mathbf{x}, t)\phi(t\mathbf{x})\,\mathrm{d}t$$



$\mathbf{x} \in D$

$V : C^0(D) \to C^0(D)$ is linear operator such that:

- $V_2 = V^{-1}$
- $\Delta\phi = 0 \quad \Longleftrightarrow \quad \left(-\Delta - \kappa^2\right) V[\phi] = 0$
- $P =$ harmonic polynomial $\Longleftrightarrow$ $V[P] =$ circular/spherical wave
- V, V^{-1} continuous in Sobolev norms, explicit in κ $\left(H^j(D), W^{j,\infty}(D)\right)$

Approximation by circular/spherical waves

Approximation of u by

$$\operatorname{span}\left\{J_\ell(\kappa|\mathbf{x}|)\ \mathrm{e}^{\mathrm{i}\ell\theta}\right\}_{|\ell|\le L} \qquad \text{2D}$$

$$\operatorname{span}\left\{j_\ell(\kappa|\mathbf{x}|)\ Y_\ell^m\left(\tfrac{\mathbf{x}}{|\mathbf{x}|}\right)\right\}_{0\le\ell\le L,|m|\le\ell} \qquad \text{3D}$$

$$\begin{aligned}
\inf_{P\in\left\{\substack{\text{harmonic}\\ \text{polynomials}\\ \text{of degree } \le L}\right\}} \Big\| \underbrace{u - V[P]}_{=V[V^{-1}[u]-P]} \Big\|_{j,\kappa,D} &\le C \inf_{P} \left\|V^{-1}[u] - P\right\|_{j,\kappa,D} && \text{contin. of } V, \\
&\le C\, \epsilon(h,L)\ \left\|V^{-1}[u]\right\|_{k+1,\kappa,D} && \text{harmonic approx. results,} \\
&\le C\, \epsilon(h,L)\ \|u\|_{k+1,\kappa,D} && \text{contin. of } V^{-1}.
\end{aligned}$$

$\Rightarrow$ Orders of convergence for Helmholtz-by-CWs are the same as harmonic functions-by-harmonic polynomials: $L \ge k$

$$\epsilon(h,L) \sim L^{\lambda(k+1-j)} h^{k+1-j}$$

The constant C depends explicitly on κh: $C = C\cdot(1+\kappa h)^{j+6}\mathrm{e}^{\frac{3}{4}\kappa h}$

Approximation of circular waves by plane waves

Link between plane waves and circular/spherical waves:
Jacobi–Anger expansion

2*D* $$e^{iz\cos\theta} = \sum_{\ell\in\mathbb{Z}} i^\ell J_\ell(z)\, e^{i\ell\theta} \qquad z\in\mathbb{C},\ \theta\in\mathbb{R}$$

3*D* $$\underbrace{e^{ir\boldsymbol{\xi}\cdot\boldsymbol{\eta}}}_{\text{plane wave}} = 4\pi\sum_{\ell\geq 0}\sum_{m=-\ell}^{\ell} i^\ell\ \underbrace{j_\ell(r)\ Y_{\ell,m}(\boldsymbol{\xi})}_{\text{spherical w.}}\overline{Y_{\ell,m}(\boldsymbol{\eta})} \qquad \boldsymbol{\xi},\ \boldsymbol{\eta}\in\mathbb{S}^2,\ r\geq 0$$

We need the other way round:

circular wave ≈ linear combination of plane waves

- truncation of J–A expansion
- careful choice of directions (in 3D)
- solution of a linear system
- residual estimates

→ explicit error bound

Final approximation by plane waves

$\forall u \in H^{k+1}(D), \qquad -\Delta u - \kappa^2 u = 0, \qquad D \subset \mathbb{R}^n, \qquad n \in \{2, 3\},$

$$\inf_{\vec{\alpha} \in \mathbb{C}^p} \left\| u - \sum_{\ell=1}^{p} \alpha_\ell \mathrm{e}^{\mathrm{i}\kappa\, \mathbf{x} \cdot \mathbf{d}_\ell} \right\|_{H^j(D)} \leq C(\kappa h)\; h^{k+1-j} p^{-\frac{\lambda(k+1-j)}{n-1}}\; \|u\|_{H^{k+1}(D)}$$

$h = \mathrm{diam}(D), \qquad p =$ PPW space dimension, $\qquad D =$ mesh element

Better rates than polynomials!

If u extends outside D: exponential convergence.

Smooth-coefficient PDEs: quasi-Trefftz methods

All this is for constant-coefficients Helmholtz eq.: $\Delta u + \kappa^2 u = 0$.
What about $\mathcal{L}u = \nabla \cdot \big(a(\mathbf{x})\nabla u\big) + \kappa^2 n(\mathbf{x})u = 0$?

We don't know exact solutions → no Trefftz method possible.

Quasi-Trefftz idea: (IMBERT-GÉRARD 2014–. . .)
use discrete functions that are approximate PDE solutions, $\mathcal{L}u_h \approx 0$.

More precisely,
degree-q Taylor polynomial (centred at a given $\mathbf{x}_K$) of $\mathcal{L}v_h$ is 0:

$T^{q+1}_{\mathbf{x}_K}[\mathcal{L}u_h] = 0 \quad \Rightarrow$ Small residual: $\mathcal{L}v_h(\mathbf{x}) = \mathcal{O}(|\mathbf{x}-\mathbf{x}_K|^{q+1}), \quad \mathbf{x} \in K$

Can construct quasi-Trefftz spaces

- with polynomials, or
- with generalised plane waves: $\mathrm{e}^{\mathrm{i}\kappa P(\mathbf{x})}$

Basis construction and h-approximation properties are available

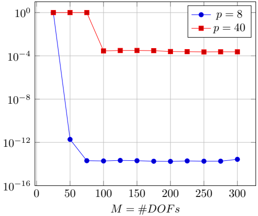
PPW instability

Plane-wave-based Trefftz-DG methods

- have great approximation properties
- are quasi-optimal (→ convergence is guaranteed)
- are simple (exponential basis)

So why isn't everybody using plane waves?

The issue is "instability".
Increasing # of PPWs,
at some point convergence stagnates.



Discrete space contains
an accurate approximation,
but linear system cannot find it.

Numerical phenomenon: due to computer arithmetic+cancellation.

PPW instability already observed in all PPW-based Trefftz methods.
Usually described and treated as ill-conditioning issue.

Part III

PPW instability and evanescent PWs

E. Parolin, D. Huybrechs, A. Moiola arXiv:2202.05658
Stable approximation of Helmholtz solutions by evanescent plane waves Julia code on:
`https://github.com/EmileParolin/evanescent-plane-wave-approx`

Adcock–Huybrechs theory

BEN ADCOCK, DAAN HUYBRECHS, SiRev 2019 & JFAA 2020,
"Frames and numerical approximation I & II"

Goal: Approximate some $v \in V$ with linear combination of $\{\phi_m\} \subset V$.

Result: If there exists $\sum_{m=1}^{M} a_m \phi_m$ with

- good approximation of v,
- small coefficients a_m,

then the approximation of v in computer arithmetic is stable,
if one uses oversampling and SVD regularization.

Denoting $P^{\epsilon}_{\{\phi_m\}}$ the truncated SVD projection with truncation ϵ,

$$\left\| v - P^{\epsilon}_{\{\phi_m\}} v \right\|_V \leq \inf_{\mathbf{a} \in \mathbb{C}^M} \left(\left\| v - \sum_{m=1}^{M} a_m \phi_m \right\|_V + \sqrt{\epsilon} \, \|\mathbf{a}\|_{\mathbb{C}^M} \right)$$

(Improvement: $\sqrt{\epsilon} \to \epsilon$ using oversampling.)

Stability does not depend on (LS, Galerkin,. . .) matrix conditioning.

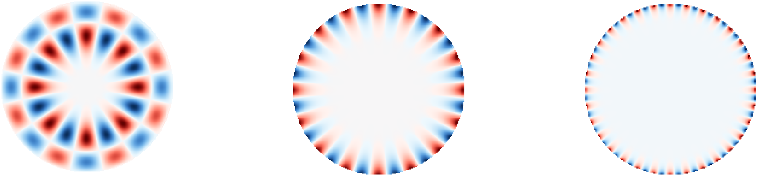
Fourier–Bessel basis on the disc

Let us focus on the unit disc $B_1 \subset \mathbb{R}^2$.

Separable solutions in polar coordinates:

$$\boxed{b_p(r,\theta) := \beta_p J_p(\kappa r) \mathrm{e}^{\mathrm{i}p\theta}} \qquad \forall p \in \mathbb{Z}, \quad (r,\theta) \in B_1$$

$\beta_p =$ normalization, e.g. in $H^1(B_1)$ norm. $\beta_p \sim \kappa \big(\frac{2|p|}{\mathrm{e}\kappa}\big)^{|p|}$ as $p \to \infty$.



$p = 8 = \kappa/2$
Propagative mode

$p = 16 = \kappa$

$p = 32 = 2\kappa$
Evanescent mode

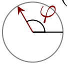
$\{b_p\}_{p \in \mathbb{Z}}$ is orthonormal basis of $\mathcal{B} := \{u \in H^1(B_1) : -\Delta u - \kappa^2 u = 0\}$

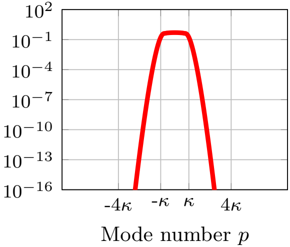
Stable PPW approximation is impossible

The Jacobi–Anger expansion relates PPWs and circular waves b_p:

$$\mathrm{PW}_{\varphi}(\mathbf{x}) := \mathrm{e}^{\mathrm{i}\kappa \mathbf{d}\cdot\mathbf{x}} = \sum_{p\in\mathbb{Z}} \left(\mathrm{i}^p \mathrm{e}^{-\mathrm{i}p\varphi} {\beta_p}^{-1}\right) b_p(r,\theta)$$

$\mathbf{d} = (\cos\varphi, \sin\varphi)$





Modulus of Fourier coefficient
$|\mathrm{i}^p \mathrm{e}^{-\mathrm{i}p\varphi} \beta_p^{-1}| = |\beta_p^{-1}| \sim |p|^{-|p|}$ indep. of φ.

Approximation of $u = \sum_p \widehat{u}_p b_p \in \mathcal{B}$
requires exponentially large coefficients.

$u \in H^s(B_1), s \geq 1 \iff |\widehat{u}_p| \sim o(|p|^{-s+\frac{1}{2}})$
but $|\beta_p^{-1}| \sim |p|^{-|p|}$ is much smaller!

$$\begin{array}{c} \forall p \in \mathbb{Z} \\ \forall M \in \mathbb{N} \\ \forall \boldsymbol{\mu} \in \mathbb{C}^M \\ \forall \eta \in (0,1) \end{array} \qquad \left\| b_p - \sum_{m=1}^{M} \mu_m \mathrm{PW}_{\frac{2\pi m}{M}} \right\|_{\mathcal{B}} \leq \eta \quad \Longrightarrow \quad \|\boldsymbol{\mu}\|_{\ell^1(\mathbb{C}^M)} \geq (1-\eta)\, \underbrace{|\beta_p|}_{\sim |p|^{|p|}}$$

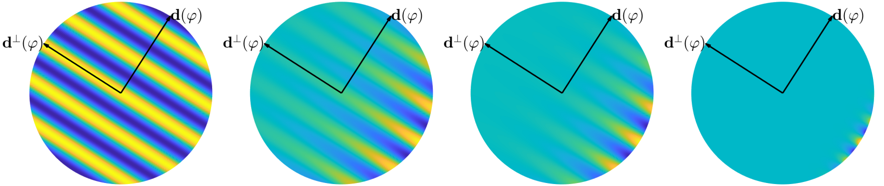
Evanescent plane waves

Idea: use PPWs & evanescent plane waves (EPW)

$$e^{i\kappa \mathbf{d}\cdot\mathbf{x}} \qquad \mathbf{d}\in\mathbb{C}^2 \quad \mathbf{d}\cdot\mathbf{d}=1$$

Complex $\mathbf{d}$!

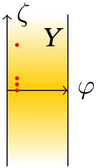
Again: exponential Helmholtz solutions.



$\zeta = 0$ $\zeta = 0.1$ $\zeta = 0.2$ $\zeta = 1$ $\kappa = 16$

Parametrised by φ = direction, ζ = "evanescence".

Parametric cylinder: $\mathbf{y} := (\varphi, \zeta) \in Y := [0, 2\pi) \times \mathbb{R}$.



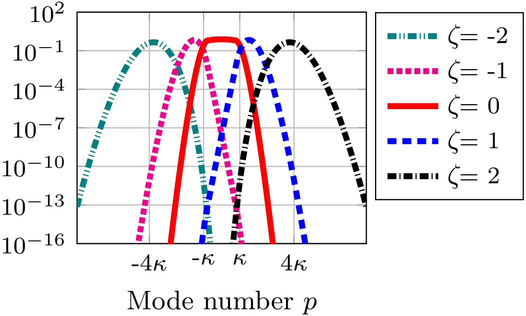
$$\mathbf{d}(\mathbf{y}) := \big(\cos(\varphi + i\zeta), \sin(\varphi + i\zeta)\big) \in \mathbb{C}^2$$

EPW modal analysis

Jacobi–Anger expansion holds also for EPWs:

$$\mathrm{EW}_{\mathbf{y}}(\mathbf{x}) = \mathrm{e}^{\mathrm{i}\kappa \mathbf{d}(\mathbf{y})\cdot\mathbf{x}} = \sum_{p\in\mathbb{Z}} \left(\mathrm{i}^p \mathrm{e}^{-\mathrm{i}p\varphi} {\color{red}\mathrm{e}^{p\zeta}} \beta_p^{-1}\right) b_p(\mathbf{x}).$$

Absolute values of Fourier coefficients $|\mathrm{i}^p \mathrm{e}^{-\mathrm{i}p\varphi} \mathrm{e}^{p\zeta} \beta_p^{-1}|$, $\kappa = 16$:



Looks promising!

We can hope to approximate large-p Fourier modes with EPWs & small coefficients v_m:

$$b_p(\mathbf{x}) \approx \sum_{m=1}^{M} v_m \mathrm{EW}_{\mathbf{y}_m}(\mathbf{x})$$

Helmholtz solutions are EPW superpositions

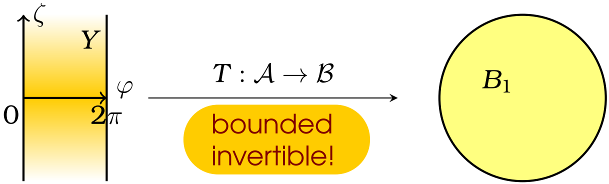
We want to represent $u \in \mathcal{B}$ as continuous superposition of EPWs:

$$u(\mathbf{x}) = \int_Y \mathrm{EW}_{\mathbf{y}}(\mathbf{x})\ v(\mathbf{y})\ w^2(\mathbf{y})\,\mathrm{d}\mathbf{y} =: (Tv)(\mathbf{x}) \qquad \mathbf{x} \in B_1$$

with density $v \in L^2(Y; w^2)$ and weight $w^2 = \mathrm{e}^{-2\kappa \sinh|\zeta| + \frac{1}{2}|\zeta|}$

Parametric space

Physical space



bounded invertible!

Herglotz density

$v \in \mathcal{A} = \overline{\mathrm{span}\{a_p\}} \subset L^2(Y; w^2)$

Helmholtz solution

$u \in \mathcal{B} = \overline{\mathrm{span}\{b_p\}} \subset H^1(B_1)$

Every Helmholtz solution is (continuous) linear combination of EPWs with small coefficients: $\|v\|_{\mathcal{A}} \leq \tau_-^{-1} \|u\|_{\mathcal{B}}$

How to sample $\mathcal{A}$? How to choose $\{\mathbf{y}_m\}_m \in Y$?

Idea from (COHEN, MIGLIORATI 2017).

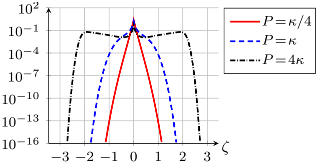
Fix $P \in \mathbb{N}$, set $\mathcal{A}_P := \operatorname{span}\{a_p\}_{|p|\leq P} \subset \mathcal{A}$.

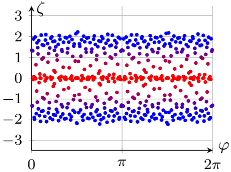
Define probability density

$$\boxed{\rho(\mathbf{y}) := \frac{w^2}{2P+1} \sum_{|p|\leq P} |a_p(\mathbf{y})|^2 \qquad \text{on } Y}$$

ρ^{-1} = "Christoffel function"

Generate $M \in \mathbb{N}$ nodes $\{\mathbf{y}_m\}_{m=1,\dots,M} \subset Y$ distributed according to ρ:





$p = 4\kappa$

We expect that any $u \in \operatorname{span}\{b_p\}_{|p|\leq P}$ can be approximated by EPWs with parameters $\{\mathbf{y}_m\}$ with small coefficients.

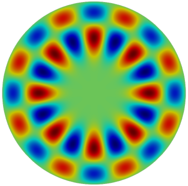
→ Stable approx. in computer arithmetic using SVD & oversampling.

The M-dimensional EPW space depends on truncation parameter P: the space is tuned to approximate the Fourier modes b_p with $|p| \leq P$.

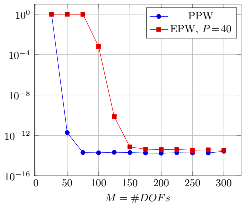
Approximation of b_p by PPWs and by EPWs

$\kappa = 16, \qquad \epsilon = 10^{-14}, \qquad S = \max\{2M, 2|p|\}$

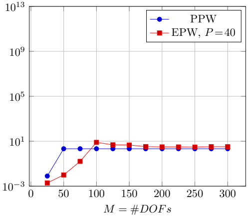
$p = 8$

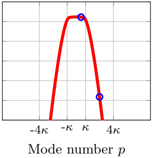


b_p, $p = 8$, residual $\|A\boldsymbol{\xi}_\epsilon - \mathbf{c}\|/\|\mathbf{c}\|$

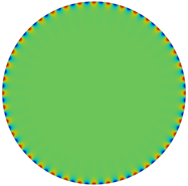


b_p, $p = 8$, coefficient norm $\|\boldsymbol{\xi}_\epsilon\|$

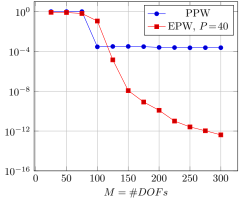




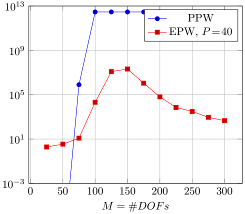
$p = 40$

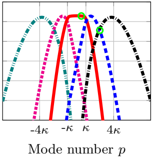


b_p, $p = 40$, residual $\|A\boldsymbol{\xi}_\epsilon - \mathbf{c}\|/\|\mathbf{c}\|$



b_p, $p = 40$, coefficient norm $\|\boldsymbol{\xi}_\epsilon\|$



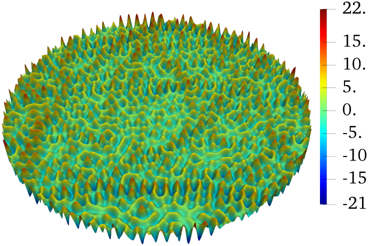


Ill-conditioning does not spoil EPW accuracy

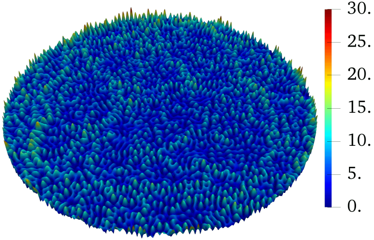
Approximation of general Helmholtz solution

$$u = \sum_{|p|\le P} \hat{u}_p b_p, \quad \hat{u}_p \sim (\max\{1, |p| - \kappa\})^{-1/2}, \quad \kappa = 100, \quad P = 2\kappa, \quad M = 802$$

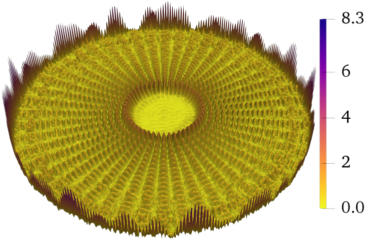
$\Re\{u\}$



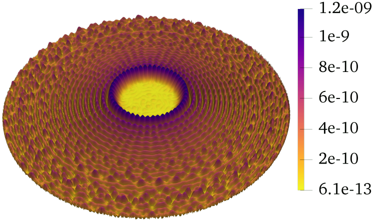
$|u|$



$|u - PPW|$



$|u - EPW|$

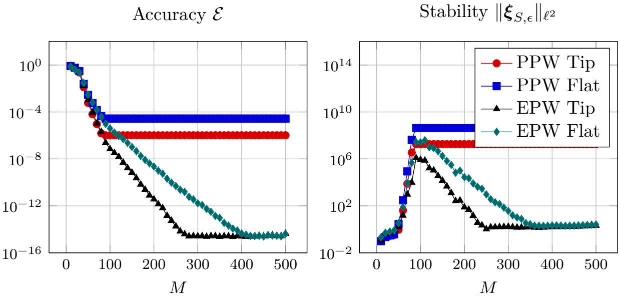


$\|u - PPW\|_{L^\infty} \gtrsim 7 \cdot 10^9 \, \|u - EPW\|_{L^\infty}$

DOFs/wavelength $= \lambda\sqrt{M/|B_1|} \approx 1$

Convex polygon, same discrete space

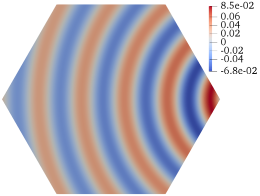
$\kappa = 16, \qquad M = 200, \qquad u =$ fundamental solution at distance 0.25



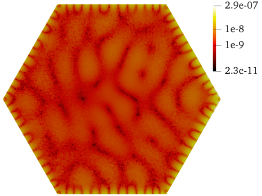
Accuracy $\mathcal{E}$

Stability $\|\boldsymbol{\xi}_{S,\epsilon}\|_{\ell^2}$

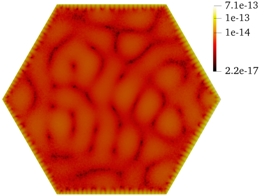
$\Re\{u\}$



$|u - PPW|$



$|u - EPW|$



Part IV

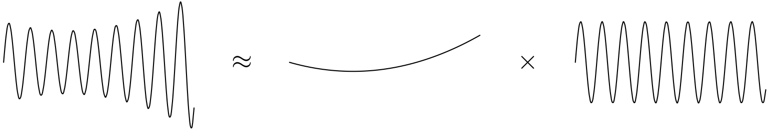
BEM-type methods: HNA

Hybrid numerical-asymptotic approach

- FEM/BEM approximates u by a piecewise polynomial on a mesh.
- GO/GTD approximates u by a sum of WKB solutions (corresponding to incident, reflected, diffracted waves):

$$u(\mathbf{x}) \sim \sum_{j=1}^{J} v_j(\mathbf{x}) \mathrm{e}^{\mathrm{i}\kappa\phi_j(\mathbf{x})}, \qquad \kappa \to \infty.$$

  Phases ϕ_j and amplitudes v_j found by ray tracing, solving ODEs along rays, and asymptotic matching.

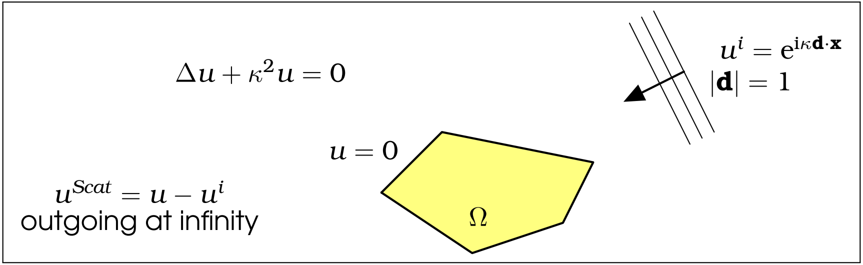


- HNA methods use a FEM/BEM approximation space incorporating oscillatory basis functions, with GO/GTD phases and numerically computed piecewise-polynomial amplitudes.

Goal: Controllable accuracy and $O(1)$ computational cost as $\kappa \to \infty$.

Sound-soft convex polygonal scatterer

HNA survey: (Chandler-Wilde, Graham, Langdon, Spence 2012)
This setting: (Chandler-Wilde, Langdon 2007)



Green's representation theorem: $\Phi(\mathbf{x},\mathbf{y}) := \frac{\mathrm{i}}{4} H_0^{(1)}(\kappa|\mathbf{x}-\mathbf{y}|)$

$$u(\mathbf{x}) = u^i(\mathbf{x}) - \int_\Gamma \Phi(\mathbf{x},\mathbf{y}) \partial_{\mathbf{n}} u(\mathbf{y})\, \mathrm{d}s(\mathbf{y}), \qquad \mathbf{x} \in \mathbb{R}^2 \setminus \overline{\Omega}$$

Taking traces gives a boundary integral equation for $\partial_{\mathbf{n}} u(\mathbf{y})$, e.g.

$$\int_\Gamma \Phi(\mathbf{x},\mathbf{y}) \partial_{\mathbf{n}} u(\mathbf{y})\, \mathrm{d}s(\mathbf{y}) = u^i(\mathbf{x}), \quad \mathbf{x} \in \partial\Omega.$$

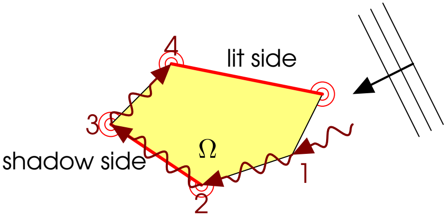
Incident, reflected and diffracted waves

According to geometric theory of diffraction (GTD), for $\kappa \to \infty$

on a "lit" side $$\partial_{\mathbf{n}} u \sim \underbrace{2\frac{\partial u^i}{\partial n}}_{\text{incident + reflected}} + \underbrace{Ae^{i\kappa s} + Be^{-i\kappa s}}_{\text{diffracted}}$$

on a "shadow" side $$\partial_{\mathbf{n}} u \sim \underbrace{Ae^{i\kappa s} + Be^{-i\kappa s}}_{\text{diffracted}}$$

where s is the arclength along the boundary.



Higher-order multiply-diffracted waves have the same phases $e^{\pm i\kappa s}$, but amplitudes A, B are harder to compute.

Hybrid numerical-asymptotic BEM

On each side Γ_j, HNA BEM uses the ansatz

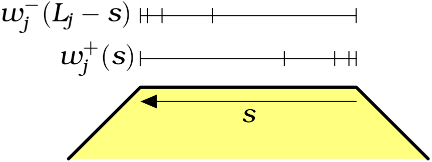
$$\partial_{\mathbf{n}} u(\mathbf{x}(s)) = \underbrace{\begin{bmatrix} 2\partial_{\mathbf{n}} u^i \\ 0 \end{bmatrix}}_{\text{GO}} + \underbrace{v_j^+(s)\mathrm{e}^{\mathrm{i}\kappa s} + v_j^-(L_j - s)\mathrm{e}^{-\mathrm{i}\kappa s}}_{\text{GTD}} \qquad \mathbf{x} \in \Gamma_j$$

$$\approx \begin{bmatrix} 2\partial_{\mathbf{n}} u^i \\ 0 \end{bmatrix} + w_j^+(s)\mathrm{e}^{\mathrm{i}\kappa s} + w_j^-(L_j - s)\mathrm{e}^{-\mathrm{i}\kappa s} = \psi_{HNA}(s)$$

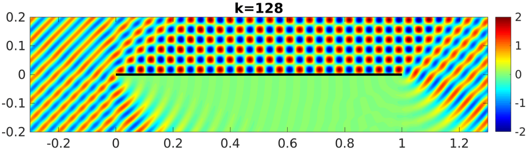
where $w_j^\pm$ are piecewise-polynomials.

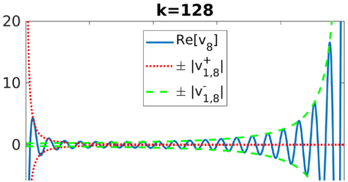
$v_j^\pm(s)$ are analytic in $\Re\{s\} > 0$, slowly oscillating, singular only at $s = 0$:

→ approximated by piecewise-polynomials $w_j^\pm$
on two overlapping geometric meshes, graded towards the corners:



Convergence of *hp*-HNA BEM





(Gibbs, Hewett, Huybrechs, Parolin 2020)

"hp" approximation strategy: increase polynomial degree p simultaneously with the number of layers n in the mesh ($n = cp$)

Hewett, Langdon, Melenk 2013

$$\|\partial_{\mathbf{n}} u - \psi_{HNA}\|_{L^2(\Gamma)} \quad + \quad \frac{\|u - u_{HNA}\|_{L^\infty(D)}}{\|u\|_{L^\infty(D)}} \leq C\kappa^{5/2}\mathrm{e}^{-\tau p}.$$

$\#DOFs = \mathcal{O}(n(p+1)) \sim \log^2 \kappa$ is enough to maintain any given accuracy for $\kappa \to \infty$

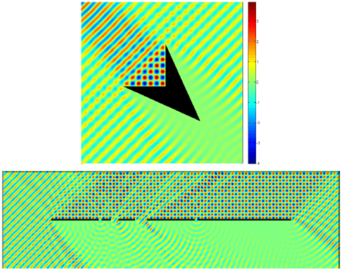
In practice, the method is κ-independent!

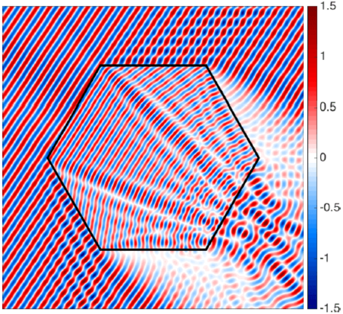
Analysis assumes the use of the "star-combined formulation"

Problems treated with HNA or related methods

- Smooth scatterers
  (ECEVIT, GRAHAM. . .)
- Flat screens in 2D and 3D
- Some non-convex polygons
- Multiple obstacles
- Transmission problems
- Curvilinear polygons
- . . .

Non-polynomial PUM-type BEM: extended isogeometric BEM (XIBEM)
(PEAKE, TREVELYAN, COATES 2013)





Summary

- FEM-type methods:
  - Trefftz methods
  - Meshless methods, method of fundamental solutions (MFS)
  - Partition of unity (PUM)
  - Trefftz discontinuous Galerkin (TDG/UWVF)
  - Quasi-Trefftz
- Approximation properties of plane/circular/spherical waves
- Instability and possible remedy, evanescent plane waves
- BEM-type methods: HNA

Thank you!

Not discussed:

- Choice of PW directions: a priori & a posteriori adaptivity
- Other Trefftz formulations, UWVF framework
- Virtual elements (VEM): PUM and Trefftz versions (PERUGIA. . .)

Part V

Extras

TDG: derivation — I

1. Consider Helmholtz equation with impedance (Robin) b.c.:

$$\begin{aligned} -\Delta u - \kappa^2 u = 0 &\qquad \text{in } \Omega \subset \mathbb{R}^n \text{ bdd., Lip., } n = 2,3 \\ \nabla u \cdot \mathbf{n} + \mathrm{i}\kappa u = g &\qquad \in L^2(\partial\Omega); \end{aligned}$$

2. introduce a mesh $\mathcal{T}_h$ on Ω;

3. multiply the Helmholtz equation with a test function v and integrate by parts on a single element $K \in \mathcal{T}_h$:

$$\int_K (\nabla u \cdot \nabla \overline{v} - \kappa^2 u \overline{v}) \,\mathrm{d}V - \int_{\partial K} (\mathbf{n} \cdot \nabla u) \overline{v} \,\mathrm{d}S = 0;$$

4. integrate by parts again: ultraweak step

$$\int_K (-u \Delta \overline{v} - \kappa^2 u \overline{v}) \,\mathrm{d}V + \int_{\partial K} (-\mathbf{n} \cdot \nabla u \, \overline{v} + u \, \mathbf{n} \cdot \nabla \overline{v}) \,\mathrm{d}S = 0;$$

5. choose a discrete Trefftz space $V_p(K)$,

   denote u_p the discrete solution;

TDG: derivation — II

⑥ replace traces on ∂K with numerical fluxes $\widehat{u}_p$ and $\widehat{\boldsymbol{\sigma}}_p$:

$$u \to \widehat{u}_p, \qquad \frac{\nabla u}{\mathrm{i}\kappa} \to \widehat{\boldsymbol{\sigma}}_p \qquad\qquad \text{on } \partial K;$$

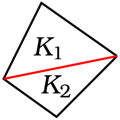
⑦ use the Trefftz property: $\forall\, v_p \in V_p(K)$

$$\int_K u_p \underbrace{\overline{(-\Delta v_p - \kappa^2 v_p)}}_{=0} \mathrm{d}V + \underbrace{\int_{\partial K} \widehat{u}_p\, \overline{\nabla v_p \cdot \mathbf{n}}\, \mathrm{d}S - \int_{\partial K} \mathrm{i}\kappa \widehat{\boldsymbol{\sigma}}_p \cdot \mathbf{n}\, \overline{v}_p\, \mathrm{d}S = 0}_{\text{TDG eq. on 1 element}};$$

⑧ Sum this equation over the elements $K \in \mathcal{T}_h$.

TDG numerical fluxes on interior faces:

$$\begin{cases} \widehat{\boldsymbol{\sigma}}_p = \frac{1}{\mathrm{i}\kappa}\{\!\{\nabla_h u_p\}\!\} - \alpha\, [\![u_p]\!]_N \\ \widehat{u}_p = \{\!\{u_p\}\!\} - \beta\, \frac{1}{\mathrm{i}\kappa} [\![\nabla_h u_p]\!]_N \end{cases}$$



$\{\!\{\cdot\}\!\}$ = averages, $[\![\cdot]\!]_N$ = normal jumps on the interfaces, $\alpha, \beta > 0$.

Variational formulation of the TDG

The TDG method reads: find $u_p \in V_p(\mathcal{T}_h)$ s.t.

$$\mathcal{A}_h(u_p, v_p) \;=\; \mathrm{i}\kappa^{-1}\int_{\partial\Omega} \delta\, g\,\overline{\nabla_h v_p \cdot \mathbf{n}}\,\mathrm{d}S + \int_{\partial\Omega} (1-\delta) g\,\overline{v_p}\,\mathrm{d}S,$$

$\forall\, v_p \in V_p(\mathcal{T}_h)$where ($\mathcal{F}_h^I$ = interior skeleton)

$$\begin{aligned}
\mathcal{A}_h(u,v) := &\int_{\mathcal{F}_h^I} \{\!\{u\}\!\}[\![\overline{\nabla_h v}]\!]_N\,\mathrm{d}S &&+\mathrm{i}\,\kappa^{-1}\int_{\mathcal{F}_h^I} \beta\,[\![\nabla_h u]\!]_N [\![\overline{\nabla_h v}]\!]_N\,\mathrm{d}S\\
&-\int_{\mathcal{F}_h^I} \{\!\{\nabla_h u\}\!\}\cdot[\![\overline{v}]\!]_N\,\mathrm{d}S &&+\mathrm{i}\,\kappa\int_{\mathcal{F}_h^I} \alpha\,[\![u]\!]_N\cdot[\![\overline{v}]\!]_N\,\mathrm{d}S\\
&+\int_{\partial\Omega}(1-\delta)\,u\,\overline{\nabla_h v\cdot\mathbf{n}}\,\mathrm{d}S &&+\mathrm{i}\,\kappa^{-1}\int_{\partial\Omega}\delta\,\nabla_h u\cdot\mathbf{n}\,\overline{\nabla_h v\cdot\mathbf{n}}\,\mathrm{d}S\\
&-\int_{\partial\Omega}\delta\,\nabla_h u\cdot\mathbf{n}\,\overline{v}\,\mathrm{d}S &&+\mathrm{i}\,\kappa\int_{\partial\Omega}(1-\delta)u\,\overline{v}\,\mathrm{d}S.
\end{aligned}$$

$\alpha, \beta > 0$, $0 < \delta < 1$ are parameter functions.

Notation: $\{\!\{\cdot\}\!\}$ = averages, $[\![\cdot]\!]_N$ = normal jumps on the interfaces

$u_p \mapsto (\mathrm{Im}\,\mathcal{A}_h(u_p,u_p))^{\frac{1}{2}}$ is a norm on the Trefftz space $\Rightarrow$ $\exists !\, u_p$.

Evanescent plane waves

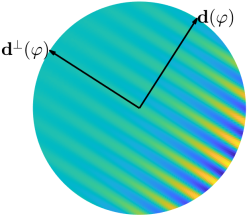
$$e^{i\kappa \mathbf{d}\cdot\mathbf{x}} \qquad \mathbf{d}\in\mathbb{C}^2 \quad \mathbf{d}\cdot\mathbf{d}=1$$

Parametrised by φ = direction, ζ = "evanescence".

Parametric cylinder: $\mathbf{y} := (\varphi,\zeta) \in Y := [0,2\pi)\times\mathbb{R}$.

$$\mathbf{d}(\mathbf{y}) := \big(\cos(\varphi+i\zeta),\, \sin(\varphi+i\zeta)\big) \in \mathbb{C}^2$$

$$\mathrm{EW}_{\mathbf{y}}(\mathbf{x}) := e^{i\kappa\mathbf{d}(\mathbf{y})\cdot\mathbf{x}}$$
$$= e^{i\kappa(\cosh\zeta)\mathbf{x}\cdot\mathbf{d}(\varphi)}\; e^{-\kappa(\sinh\zeta)\mathbf{x}\cdot\mathbf{d}^{\perp}(\varphi)},$$

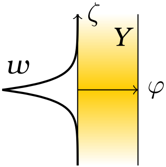


oscillations along $\mathbf{d}(\varphi) := (\cos\varphi,\, \sin\varphi)$

decay along $\mathbf{d}^{\perp}(\varphi) := (-\sin\varphi,\, \cos\varphi)$

Weighted $L^2(Y)$ space $\mathcal{A}$

Weighted L^2 space on parametric cylinder & orthonormal basis:



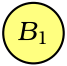
$$w(\mathbf{y}) := \mathrm{e}^{-\kappa \sinh|\zeta| + \frac{1}{4}|\zeta|} \qquad \mathbf{y} = (\varphi, \zeta) \in Y$$

$$\|v\|^2_{\mathcal{A}} := \|v\|^2_{L^2(Y;w^2)} = \int_Y |v(\mathbf{y})|^2 w^2(\mathbf{y})\,\mathrm{d}\mathbf{y}$$

$$a_p(\mathbf{y}) := \alpha_p\, \mathrm{e}^{p(\zeta + \mathrm{i}\varphi)}$$ $\alpha_p > 0$ normalization in $\|\cdot\|_{\mathcal{A}}$, $p \in \mathbb{Z}$

$$\mathcal{A} := \overline{\mathrm{span}\{a_p\}_{p\in\mathbb{Z}}}^{\|\cdot\|_{\mathcal{A}}} \subsetneq L^2(Y; w^2)$$

Jacobi–Anger: $\mathbf{x} \in$



$\mathbf{y} \in$

$$\mathrm{EW}_{\mathbf{y}}(\mathbf{x}) = \sum_{p\in\mathbb{Z}} \mathrm{i}^p J_p(\kappa r) \mathrm{e}^{\mathrm{i}p(\theta - [\varphi + \mathrm{i}\zeta])} = \sum_{p\in\mathbb{Z}} \tau_p \overline{a_p(\mathbf{y})}\, b_p(\mathbf{x}), \qquad \tau_p := \frac{\mathrm{i}^p}{\alpha_p \beta_p}.$$

From asymptotics & choice of w: $0 < \tau_- \leq |\tau_p| \leq \tau_+ < \infty \quad \forall p \in \mathbb{Z}$.

$$\forall \mathbf{x} \in B_1, \qquad \mathbf{y} \mapsto \mathrm{EW}_{\mathbf{y}}(\mathbf{x}) \in \mathcal{A} \qquad \text{(not true for } \mathbf{x} \in \partial B_1\text{)}$$

Boundary sampling method

Given (PPW, EPW,. . .) approximation set $\mathrm{span}\{\phi_m\}_{m=1,\dots,M}$,
how do we approximate $u \in \mathcal{B}$ in practice?

We use boundary sampling on $\left\{\mathbf{x}_s = \left(\substack{r=1\\ \theta_s=\frac{2\pi s}{S}}\right)\right\}_{s=1,\dots,S} \subset \partial B_1$:

$$A\boldsymbol{\xi} = \mathbf{c} \qquad \text{with} \qquad \begin{matrix} A_{s,m} := \phi_m(\mathbf{x}_s), \\ c_s := u(\mathbf{x}_s) \end{matrix} \quad \substack{s=1,\dots,S\\ m=1,\dots,M} \quad \to \quad u_M = \sum_m \xi_m \phi_m \approx u.$$

Choose $\kappa^2 \neq$ Laplace–Dirichlet eigenvalue on B_1.

Could use instead: $\left\{\begin{array}{l}\text{sampling in the bulk of } B_1, \\ \text{impedance trace,} \\ \mathcal{B} \;/\; L^2(B_1) \;/\; L^2(\partial B_1) \text{ projection...}\end{array}\right.$

- Oversampling: $S > M$
- SVD regularization, threshold ϵ:

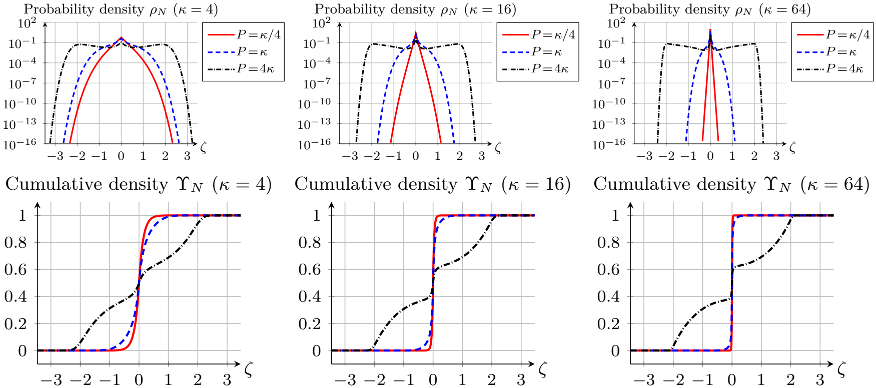
} required by Adcock–Huybrechs

$$A = U \,\mathrm{diag}(\sigma_1, \dots, \sigma_M)\; V^*, \qquad \Sigma_\epsilon := \mathrm{diag}(\{\sigma_m > \epsilon \max_{m'} \sigma_{m'}\}),$$

$$\boxed{\boldsymbol{\xi}_\epsilon = V \Sigma_\epsilon^\dagger U^* \mathbf{c}}$$

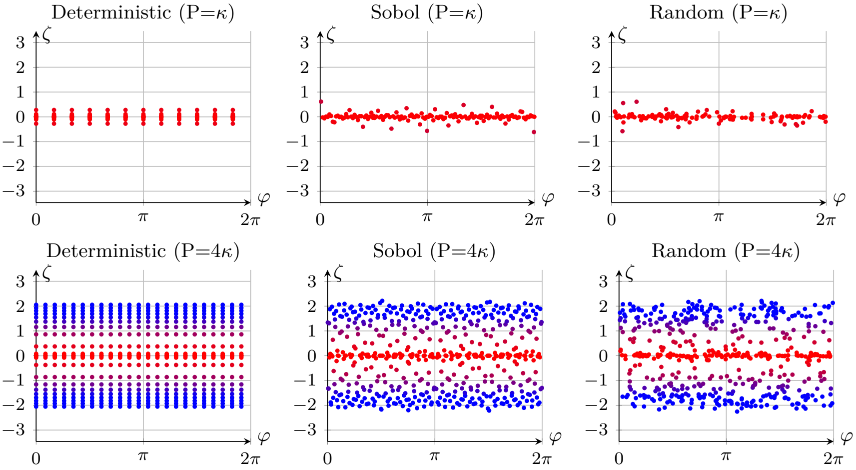
EPW approximation: probability measure on Y

Probability density ρ & cumulative d.f. as functions of evanescence ζ:



They depend on P: target functions in $\mathrm{span}\{b_p\}_{|p|\le P}$.
Modes at $\zeta \approx \pm\log(2P/\kappa)$.
Computation of ρ requires κ-dependent normalisation factors α_p.

Parameter samples in the cylinder Y

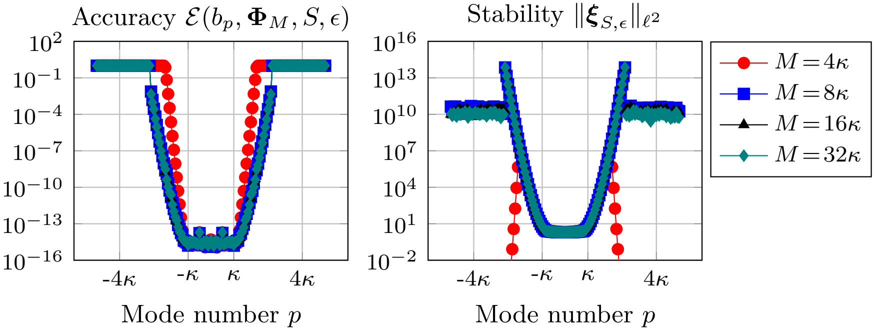


Samples computed on $(0, 1)^2$ & uniform prob., mapped to Y by Υ^{-1}.

Approximation by PPWs

Approximation of circular waves $\{b_p\}_p$ by equispaced PPWs

$\kappa = 16$, $\epsilon = 10^{-14}$, $S = \max\{2M, 2|p|\}$, residual $\mathcal{E} = \frac{\|A\boldsymbol{\xi}_\epsilon - \mathbf{c}\|}{\|\mathbf{c}\|}$

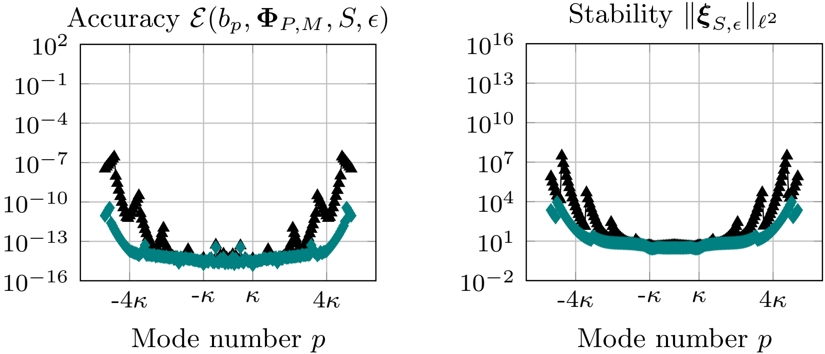


- Propagative modes $|p| \lesssim \kappa$: $\mathcal{O}(\epsilon)$ error $\forall M$, $\mathcal{O}(1)$ coeff.'s
- Evanescent modes $|p| \gtrsim 3\kappa$: $\mathcal{O}(1)$ error $\forall M$, large coeff.'s

Condition number is irrelevant!

Approximation by EPWs

Approximation of $\{\color{red}{b_p}\}$, $\boxed{P = 4\kappa}$, $\kappa = 16$, ▲ $M = 4P$, ♦ $M = 8P$



Accuracy $\mathcal{E}(b_p, \mathbf{\Phi}_{P,M}, S, \epsilon)$

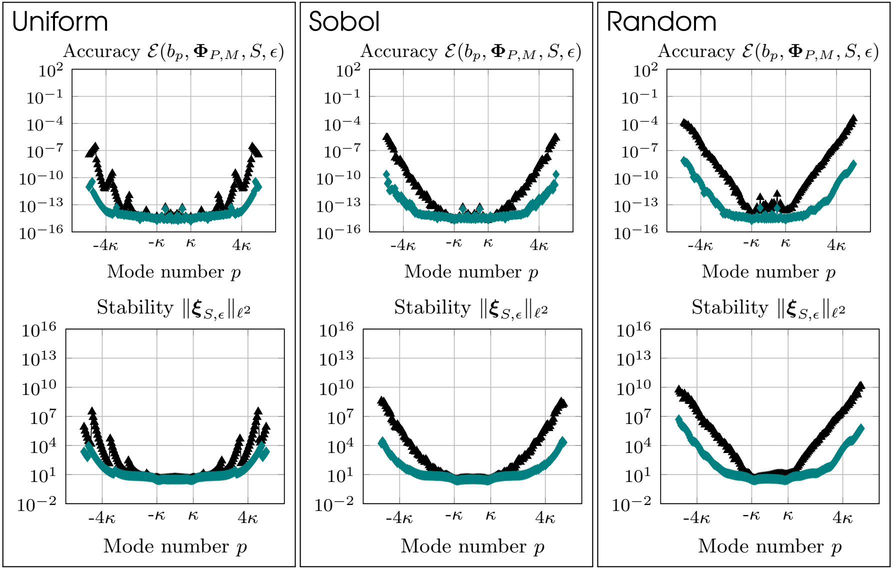
Stability $\|\boldsymbol{\xi}_{S,\epsilon}\|_{\ell^2}$

Discrete EPW space approximates all b_ps for $|p| \leq P$!

Approximation by EPWs

Approximation of $\{b_p\}$, ▲ $M = 4P$, ◆ $M = 8P$

$P = 4\kappa,\ \kappa = 16$



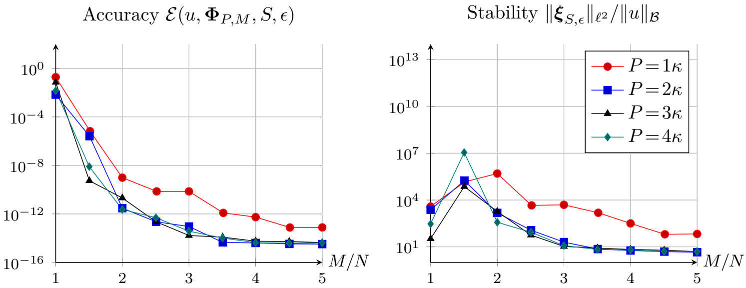
Approximation of general (truncated) u

Evanescent PW approximation of rough u: $(S = 2M, \kappa = 16)$

$$u = \sum_{|p| \le P} \hat{u}_p b_p, \qquad \hat{u}_p \sim (\max\{1, |p| - \kappa\})^{-1/2}$$

EPWs constructed assuming that P is known. Deterministic sampling.

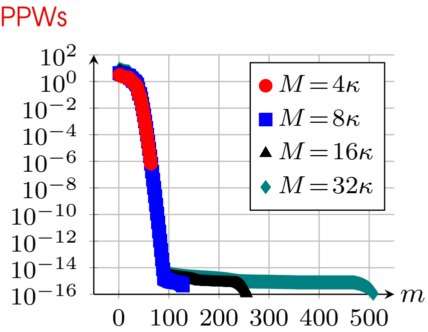
Convergence for $M \nearrow$ plotted against $\frac{M}{2P+1} = \frac{\dim(\text{approx. space})}{\dim(\text{solution space})}$:

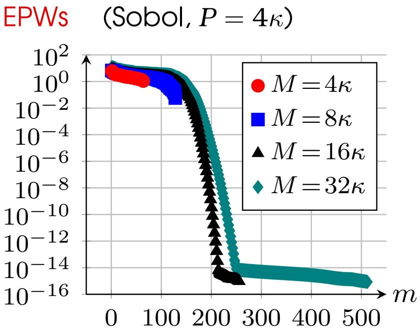


Error is P-independent.

Singular values of the matrix A

$\kappa = 16$





Comparable condition numbers, larger ϵ-rank for EPWs.
Can further increase ϵ-rank by raising P.