volume-based methods for the Helmholtz equations

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outline:

1. classical FEM for Helmholtz problems on bounded domains

2. methods based on plane waves for solving Helmholtz problems (on bounded domains)

3. Helmholtz equations on unbounded domains: (local and non-local) absorbing boundary conditions

4. Helmholtz equations on unbounded domains: absorbing layers (PML)

abstract Galerkin(-Petrov) methods

X, Y Hilbert spaces, $B : X \times Y \to \mathbb{C}$ sesquilinear form, $l \in Y'$.

continuous form:

$$\text{find } u \in X \text{ s.t.} \qquad B(u, v) = l(v) \qquad \forall v \in Y \tag{1}$$

discretized form:

Let $X_N \subset X$, $Y_N \subset Y$ be both of dimension $N \in \mathbb{N}$.

$$\text{find } u_N \in X_N \text{ s.t.} \qquad B(u_N, v) = l(v) \qquad \forall v \in Y_N \tag{2}$$

By linearity/anti-linearity, (2) represent a linear system of equations:

- Choose basis $(\varphi_j)_{j=1}^N$ of X_N and basis $(\psi_i)_{i=1}^N$ of Y_N,
- expand $u_N = \sum_{j=1}^N \mathbf{u}_j \varphi_i \implies$ (2) is equivalent to

$$\boxed{\text{Find } \mathbf{u} \in \mathbb{C}^N \text{ s.t.} \quad \mathbf{B}\mathbf{u} = \mathbf{l}}$$

- $\mathbf{B} \in \mathbb{C}^{N \times N}$ given by $\mathbf{B}_{ij} = B(\varphi_j, \psi_i)$ is called the stiffness matrix;
- $\mathbf{l} \in \mathbb{C}^N$ given by $\mathbf{l}_i = l(\psi_i)$ is called the load vector

abstract Galerkin methods: X-elliptic case

Thm. 1. [Lax-Milgram] Let X be a Hilbert space, $B : X \times X \to \mathbb{C}$ an X-elliptic, continuous sesquilinear form:

$$\underline{\alpha}\|u\|^2 \leq |B(u,u)| \quad \text{and} \quad |B(u,v)| \leq M\|u\|\,\|v\| \qquad \forall u, v \in X.$$

Let $l \in X'$. Then the problem:

$$\text{find } u \in X \text{ s.t. } B(u,v) = l(v) \qquad \forall v \in X$$

has a unique solution and $\|u\| \leq \frac{\|l\|_{X'}}{\underline{\alpha}}$.

Thm. 2. [Céa's Lemma/Galerkin orthogonality] Assume the hypotheses of Thm. 1. Let $X_N \subset X$. Then the problem

$$\text{find } u_N \in X_N \text{ s.t. } B(u_N,v) = l(v) \qquad \forall v \in X_N$$

has a unique solution and

Galerkin orthogonality: $\quad B(u - u_N, v) = 0 \qquad \forall v \in X_N$

best approximation property: $\quad \|u - u_N\| \leq \dfrac{M}{\underline{\alpha}} \inf\limits_{v \in X_N} \|u - v\|$

abstract Galerkin methods: inf-sup conditions

Thm. 3. [Babuška-Brezzi] Let X, Y be a Hilbert spaces, $B : X \times Y \to \mathbb{C}$ be a continuous sesquilinear form.

Let $\mathbf{B} : X \to Y'$ be the linear operator given by

$$\langle \mathbf{B}u, v\rangle_{Y' \times Y} = B(u, v) \qquad \forall u \in X,\ v \in Y.$$

Then the following are equivalent:

(i) $$\inf_{0 \neq u \in X} \sup_{0 \neq v \in Y} \frac{|B(u,v)|}{\|u\|_X \|v\|_Y} \geq \gamma > 0, \qquad \text{(inf-sup)} \tag{3}$$

$$\forall 0 \neq v \in Y : \qquad \sup_{u \in X} |B(u,v)| > 0 \qquad \text{(non-degeneracy, } N(\mathbf{B}') = \{0\}\text{)} \tag{4}$$

(ii) $\mathbf{B} : X \to Y'$ is invertible and $\|\mathbf{B}^{-1}\|_{X \leftarrow Y'} \leq \frac{1}{\gamma}$

(iii) the adjoint $\mathbf{B}' : Y \to X'$ is invertible and $\|\mathbf{B}'^{-1}\|_{Y \leftarrow X'} \leq \frac{1}{\gamma}$.

inf-sup conditions: discrete case

Let $X_N \subset X$, $Y_N \subset Y$, $\quad l \in Y'$.

$$\text{continuous case:} \quad \text{Find } u \in X \text{ s.t.} \quad B(u,v) = l(v) \quad \forall v \in Y \tag{5}$$

$$\text{Galerkin discretization:} \quad \text{Find } u_N \in X_N \text{ s.t. } B(u_N,v) = l(v) \quad \forall v \in Y_N \tag{6}$$

Thm. 4. [quasi-optimality] Assume $\dim X_N = \dim Y_N$ and

$$\inf_{0 \neq u \in X_N} \sup_{0 \neq v \in Y_N} \frac{|B(u,v)|}{\|u\|_X \|v\|_Y} \geq \gamma_N > 0. \tag{7}$$

Then a unique solution $u_N \in X_N$ of (6) exists and

$$\text{Galerkin orthogonality:} \quad B(u - u_N, v) = 0 \quad \forall v \in Y_N \tag{8}$$

$$\text{quasi-optimality} \quad \|u - u_N\|_X \leq \left(1 + \frac{\|\mathbf{B}\|}{\gamma_N}\right) \inf_{v \in X_N} \|u - v\|_X. \tag{9}$$

compact perturbations of X-elliptic operators—Gårding inequality

Thm. 5. Let X, $\widetilde{X}$ be Hilbert spaces and the embedding $X \subset \widetilde{X}$ be compact. Let the continuous sesquilinear form $B : X \times X \to \mathbb{C}$ satisfy

$$\operatorname{Re} B(u,u) \geq \gamma \|u\|_X^2 - \gamma' \|u\|_{\widetilde{X}}^2 \qquad \forall u \in X. \tag{10}$$

Then the Fredholm alternative holds:

Either the operator $\mathbf{B} : X \to X'$ is invertible

or the homogeneous equation

$$B(u,v) = 0 \qquad \forall v \in X$$

has non-trivial solutions and the kernel $N(\mathbf{B})$ has finite dimension.

compact perturbations of X-elliptic operators—discrete case

Thm. 6. Let X, $\widetilde{X}$ be Hilbert spaces and the embedding $X \subset \widetilde{X}$ be compact. Assume:

- $\operatorname{Re} B(u,u) \geq \gamma \|u\|_X^2 - \gamma' \|u\|_{\widetilde{X}}^2 \qquad \forall u \in X.$
- $\mathbf{B}$ is injective (i.e., $B(u,v) = 0 \quad \forall v \in X$ implies $u = 0$)
- $(X_N)_{N\in\mathbb{N}} \subset X$ satisfies $\lim\limits_{N\to\infty} \inf\limits_{v\in X_N} \|u - v\|_X = 0$ for all $u \in X$

Then there exist $\widetilde{\gamma} > 0$ and N_0 s.t. for all $N \geq N_0$:

$$\inf_{0\neq u\in X_N} \sup_{0\neq v\in X_N} \frac{|B(u,v)|}{\|u\|_X \|v\|_X} \geq \widetilde{\gamma} > 0$$

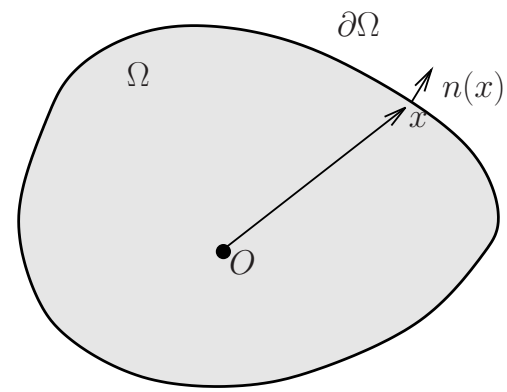
Cor. 7. [asymptotic quasi-optimality] For $N \geq N_0$ there holds

$$\|u - u_N\|_X \leq \left(1 + \frac{\|\mathbf{B}\|}{\widetilde{\gamma}}\right) \inf_{v\in X_N} \|u - v\|_X$$

bounded domain model problem

$$-\Delta u - k^2 u = f \quad \text{on } \Omega, \tag{11a}$$

$$\partial_n u \pm \mathbf{i} k u = g \quad \text{on } \partial\Omega \tag{11b}$$



weak formulation:

$$\text{Find } u \in H^1(\Omega) \text{ s.t.} B(u,v) = l(v) \qquad \forall v \in H^1(\Omega) \tag{12}$$

$$B(u,v) = \int_\Omega \nabla u \cdot \nabla \overline{v} - k^2 \int_\Omega u\overline{v} \pm \mathbf{i}k \int_{\partial\Omega} u\overline{v}$$

$$l(v) = \int_\Omega f\overline{v} + \int_{\partial\Omega} g\overline{v}$$

notation

Let $\mathbf{B} : H^1(\Omega) \to (H^1(\Omega))'$ be defined by $\langle \mathbf{B}u, v\rangle = B(u,v)$.

weighted H^1-norm: $\|u\|_{1,k}^2 := \|\nabla u\|_{L^2(\Omega)}^2 + k^2\|u\|_{L^2(\Omega)}^2$

note: $|B(u,v)| \le C\|u\|_{1,k}\|v\|_{1,k}$, C indep. of k

invertibility of $\mathbf{B}$

Thm. 8. The operator $\mathbf{B}$ is invertible and $\exists$ a constant $C(\Omega, k) > 0$ s.t.

$$\inf_{u \in H^1(\Omega)} \sup_{v \in H^1(\Omega)} \frac{|B(u,v)|}{\|u\|_{1,k} \|v\|_{1,k}} \geq C(\Omega, k)$$

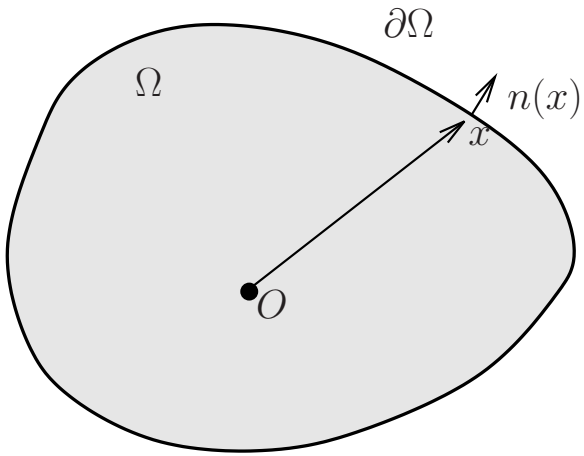
Proof:

- **Gårding inequality**: $\operatorname{Re} B(u,u) = \|\nabla u\|^2_{L^2(\Omega)} - k^2 \|u\|^2_{L^2(\Omega)}$
- **injectivity of** B

k-explicit inf-sup condition

$$-\Delta u - k^2 u = f \quad \text{on } \Omega, \tag{13a}$$

$$\partial_n u \pm \mathbf{i} k u = g \quad \text{on } \partial\Omega \tag{13b}$$



Ass. 1. 1. Ω is a bounded Lipschitz domain,

2. $x \cdot n(x) \geq \gamma > 0$ for all $x \in \partial\Omega$

3. Ω allows H^2-regularity for $-\Delta$ (e.g., $\partial\Omega$ smooth)

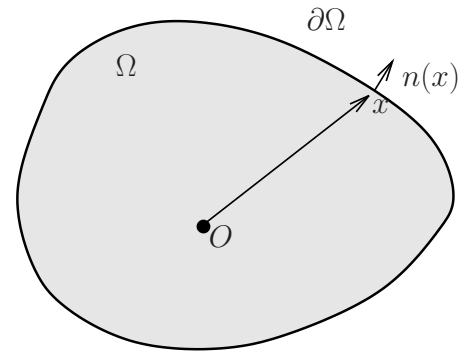
Thm. 9. Under Ass. 1 the operator $\mathbf{B}$ is invertible and $\exists\, C(\Omega) > 0$ s.t.

$$\inf_{u \in H^1(\Omega)} \sup_{v \in H^1(\Omega)} \frac{|B(u,v)|}{\|u\|_{1,k} \|v\|_{1,k}} \geq \frac{C(\Omega)}{k}$$

k-explicit bounds

$$-\Delta u - k^2 u = f \quad \text{on } \Omega, \tag{14a}$$

$$\partial_n u \pm \mathbf{i} k u = g \quad \text{on } \partial\Omega \tag{14b}$$



Thm. 10. Under Ass. 1 $\exists$ a constant $C(\Omega) > 0$ s.t.

$$\begin{aligned} \|u\|_{1,k} &\leq C(\Omega)\left[\|f\|_{L^2(\Omega)} + \|g\|_{L^2(\partial\Omega)}\right], \\ |u|_{H^2(\Omega)} &\leq C(\Omega)k\left[\|f\|_{L^2(\Omega)} + \|g\|_{L^2(\partial\Omega)}\right] + C(\Omega)\|g\|_{H^{1/2}(\partial\Omega)} \end{aligned}$$

key ingredient of the proof: choose $v := x \cdot \nabla u$ as a test function in variational formulation $B(u,v) = \int_\Omega f\overline{v} + \int_{\partial\Omega} g\overline{v}$

asymptotic quasi-optimality of the FEM

Thm. 11. Let Ω satisfy Ass. 1. Let the FE-space X_N satisfy:

$$\inf_{v\in X_N} \|z-v\|_{L^2(\Omega)} + \frac{h}{p}\|\nabla(z-v)\|_{L^2(\Omega)} \leq C\left(\frac{h}{p}\right)^2 |z|_{H^2(\Omega)} \qquad \forall z \in H^2(\Omega).$$

Then $\exists C_1$, $C_2 > 0$ depending solely on Ω s.t. for $k^2\frac{h}{p} \leq C_1$ there holds

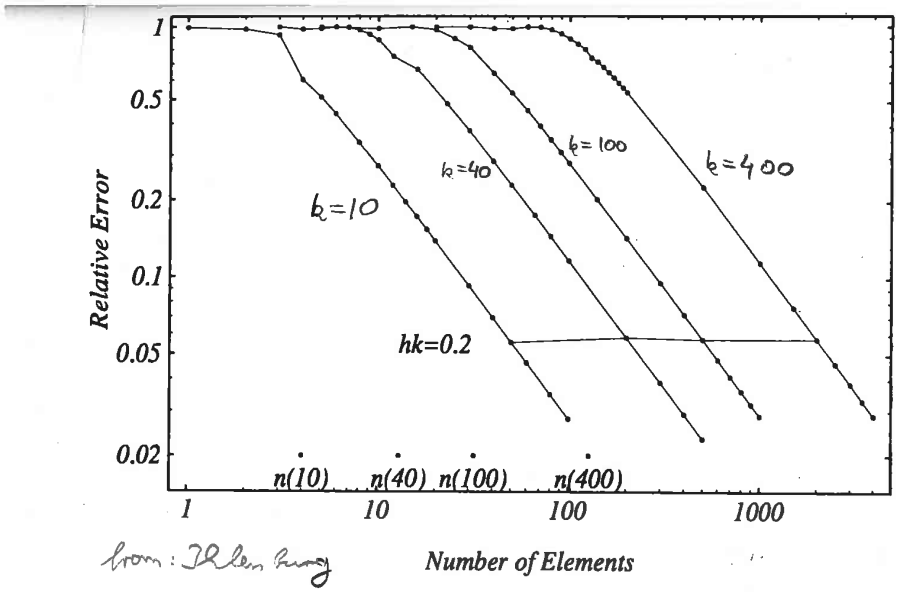
$$\inf_{u\in X_N} \sup_{v\in X_N} \frac{|B(u,v)|}{\|u\|_{1,k}\|v\|_{1,k}} \geq \frac{C_2}{k}$$

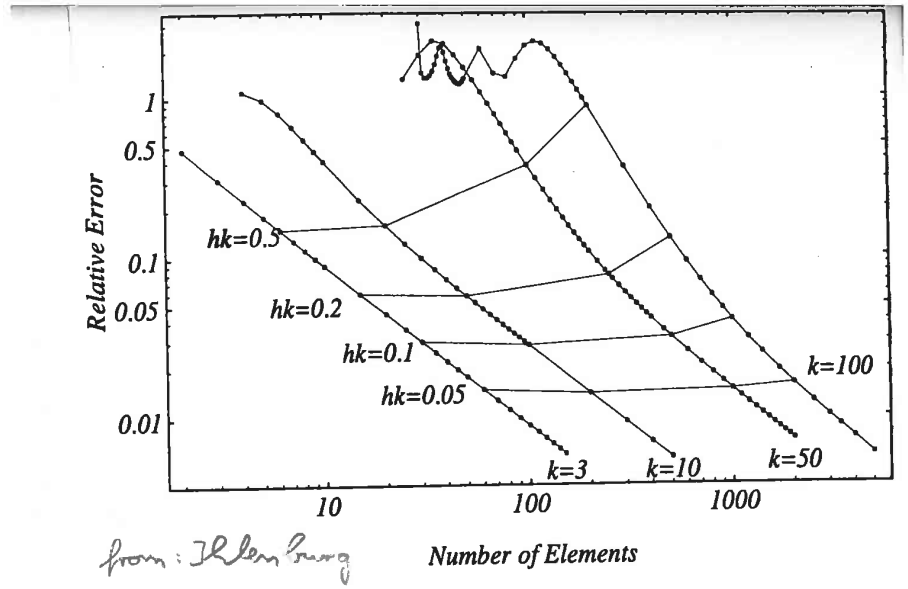
$$\|u-u_N\|_{1,k} \leq C_2 \inf_{v\in X_N} \|u-v\|_{1,k}.$$

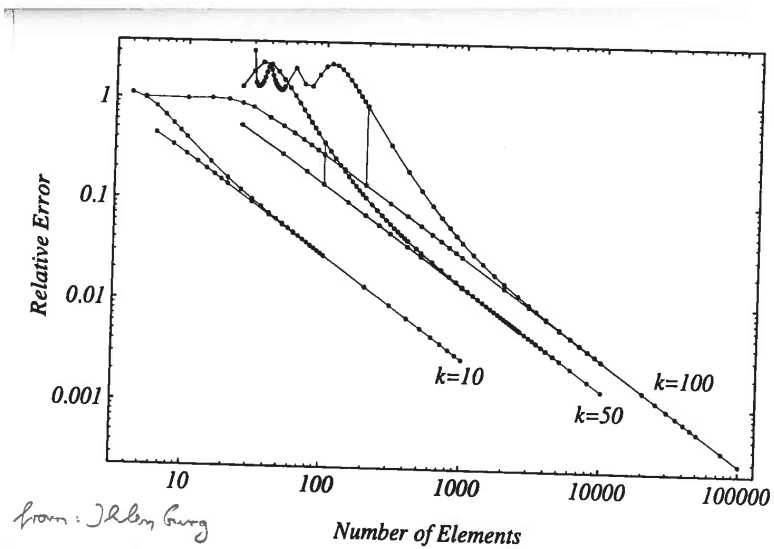
Cor. 12. If $u \in H^2(\Omega)$ and $\|u\|_{H^m(\Omega)} \sim k^m$ for $m \in \{0,1,2\}$, then for k^2h/p sufficiently small:

$$\frac{\|u-u_N\|_{1,k}}{\|u\|_{1,k}} \leq C\left(\frac{hk}{p}\right).$$

$$-u'' - k^2 u = 1, \qquad u(0) = 0, \quad u'(1) - \mathbf{i}ku(1) = 0$$







uniform mesh of size h

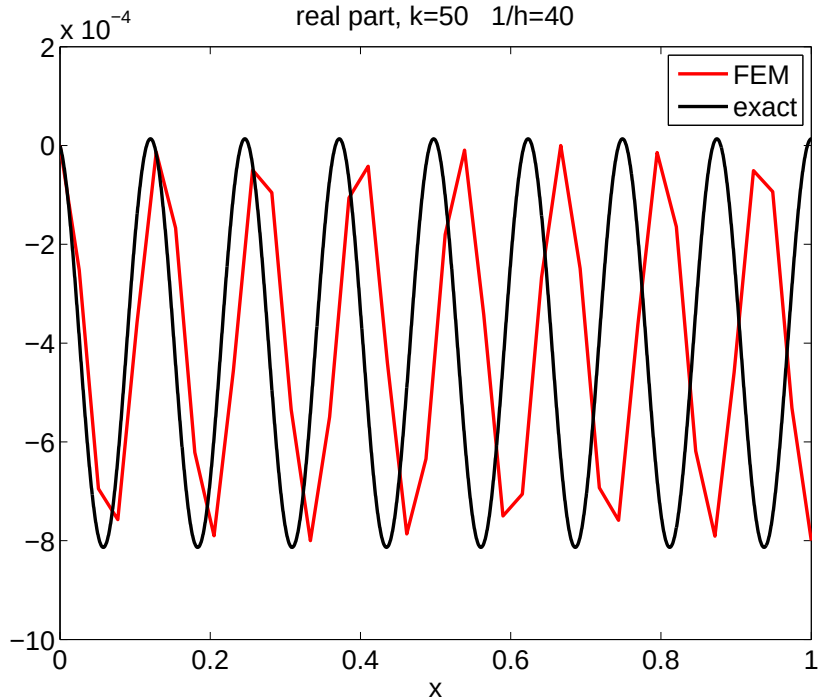
$p = 1$

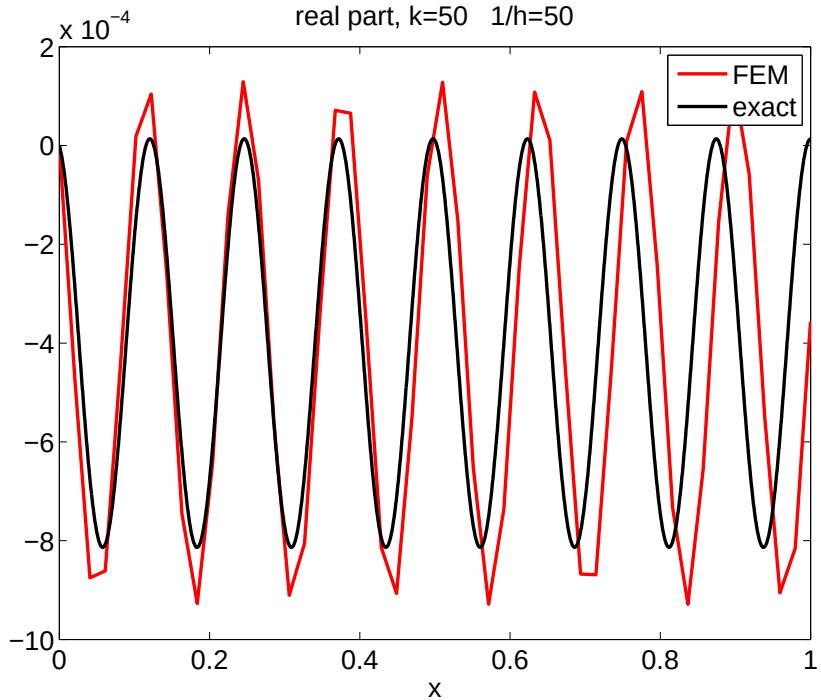
top left: best approximation error top right: FEM error

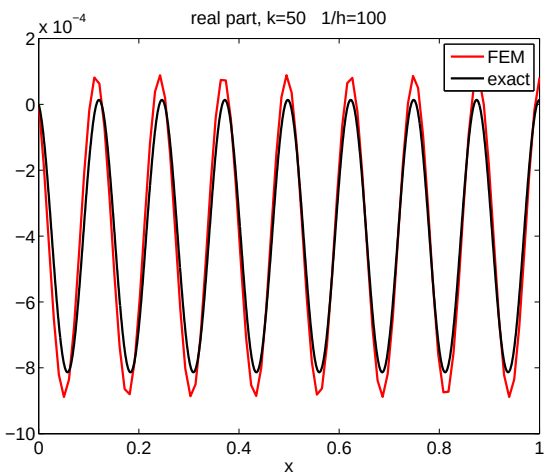
bottom left: FEM error together with best approximation error

1D-FEM: phase error

$$-u'' - k^2 u = 1 \quad \text{on } (0,1), \qquad u(0) = 0, \qquad u'(1) - \mathbf{i}ku(1) = 0$$







phase error for piecewise linear approximation on uniform mesh

problem: $-u'' - k^2 u = f, \qquad u(0) = 0, \quad u'(1) - \mathbf{i}ku(1) = 0$

cont. Green's fct: $$G(x,y) = k^{-1} \begin{cases} \sin kx e^{\mathbf{i}ky} & 0 < x < y \\ \sin ks e^{\mathbf{i}kx} & y < x < 1 \end{cases}$$

disc. Green's fct: $$G_h(x,y) = \frac{1}{h \sin k'h} \begin{cases} \sin k'x \, (A \sin k'y + \cos k'y) & 0 < x < y \\ \sin k'y \, (A \sin k'x + \cos k'x) & y < x < 1 \end{cases}$$

where $A = A(k, k', h) \in \mathbb{C}$ is a constant and k' is the discrete wave number satisfying the dispersion relation

$$\cos k'h = \cos \frac{6 - 2k^2h^2}{6 + k^2h^2} \tag{15}$$

For kh small, we get $k'h = kh - \frac{1}{24}(kh)^3 + \cdots$ and therefore

$$k' = k - \frac{1}{24}k^3h^2 + \cdots$$

higher order elements to combat phase error

Thm. 13. [Babuška & Ihlenburg, Ainsworth]

- if kh is small, then for fixed p

$$k'h - kh = -\frac{1}{2}\left[\frac{p!}{(2p)!}\right]^2 \frac{(kh)^{2p+1}}{2p+1} + O((kh)^{2p+3})$$

- if kh is large and $2p+1 > kh + o((kh)^{1/3})$ then

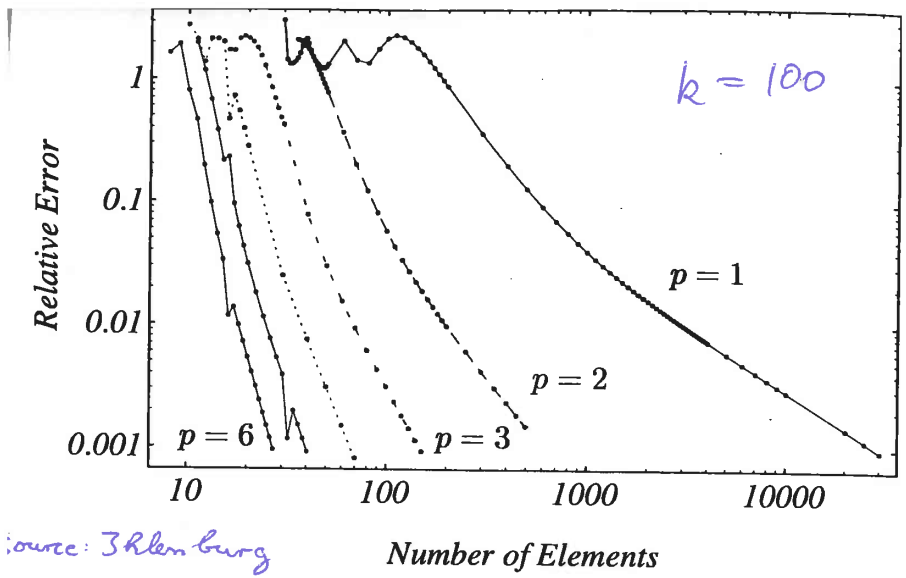
$$\cos k'h - \cos kh \approx \frac{\sin kh}{2}\left[\frac{khe}{2(2p+1)}\right]^{2p+1}$$

Thm. 14. [Babuska & Ihlenburg] For the 1D model problem and piecewise polynomial approximation of degree p, there holds for $kh < \pi$ and solution $u \in H^{l+1}(0,1)$:

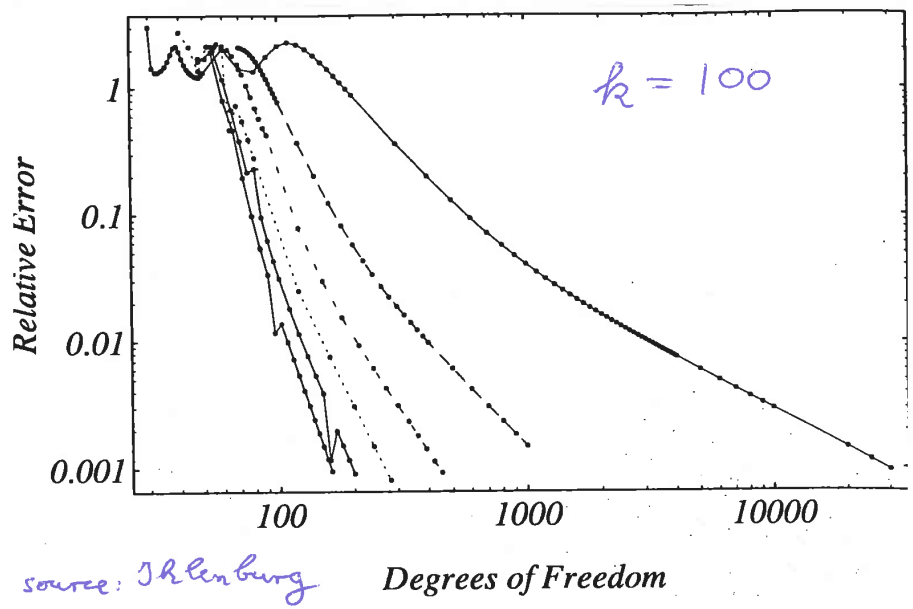
$$\|u - u_N\|_{H^1(0,1)} \leq C_p \left[1 + k\left(\frac{kh}{2p}\right)^p\right]\left(\frac{h}{2p}\right)^l |u|_{H^{l+1}(0,1)}.$$

conclusion: the phase error is not as pronounced for higher order elements as for lower order elements.

performance of higher order methods in 1D ($k = 100$)



source: Ihlenburg



source: Ihlenburg

p	1	2	3	4	5	6
rel. error	0.49	0.51	0.54	0.55	0.58	0.72
n_{ele}	211	48	25	16	12	10
DOF	211	96	75	64	60	60
rel. error	0.1	0.1	0.1	0.09	0.08	0.1
n_{ele}	499	76	35	22	16	12
DOF	499	152	105	88	80	72
rel. error	0.01	0.01	0.01	0.01	0.01	0.01
n_{ele}	2813	180	64	35	23	17
DOF	2813	360	192	140	115	102

two effects:

1. for smooth solutions, the use of higher order elements improves the rate of convergence
2. use of higher order elements mitigates the phase error, i.e., the onset of convergence is at smaller problem sizes

robust quasi-optimal methods in 1D

Let $\mathcal{T}$ be a mesh with nodes x_i, $i = 0, \ldots, N$. For each node x_i of the mesh define the shape function ψ_i by

$$\psi_i(x_j) = \delta_{ij}, \qquad (-\psi_i'' - k^2\psi_i)|_K = 0 \qquad \text{for each element } K \in \mathcal{T}$$

Set $\widetilde{X}_N := \operatorname{span}\{\psi_i \,|\, i = 1, \ldots, N\}$

Prop. 15. There exist C_1, $C_2 > 0$ with the following property: Let $u \in H^1_{(0}(0,1)$ satisfy $-u'' - k^2 u = f$ on $(0,1)$ and $u'(1) - \mathbf{i}ku(1) = 0$. Let $\widetilde{u}_N \in \widetilde{X}_N$ be its Galerkin approximation. If $kh < C_1$ then $\widetilde{u}_N$ exists and satisfies

$$\|u - \widetilde{u}_N\|_{1,k} \leq C_2 h \|f\|_{L^2(0,1)}.$$

Furthermore, the Galerkin method is nodally exact, i.e., $u(x_i) = \widetilde{u}_N(x_i)$ for all nodes x_i, $i = 0, \ldots, N$.

Comments on 1D case

1. key feature of 1D: the fundamental system for differential operator $L := -\partial_x^2 - k^2$ is finite dimensional (it is: $\{e^{\mathbf{i}kx}, e^{-\mathbf{i}kx}\}$)
2. there exist different ways to "derive" the stiffness matrix $\widetilde{\mathbf{B}}$ of of the Galerkin method based on $\widetilde{V}_N$. For example, it is also the stiffness matrix for a stabilized method with bilinear form $B^{stab}(u,v) := \int_0^1 u'\overline{v}' - k^2 u\overline{v} + \sum_{K\in\mathcal{T}} \tau_K \int_K LuL\overline{v}$ for suitably chosen τ_K.
3. improved performance of higher order elements can be understood through the limiting process $p \to \infty$: static condensation of the (elementwise) "bubble" modes leads to a condensed (tridiagonal) stiffness matrix $\mathbf{B}^{c,p}$ and condensed load vector $\mathbf{l}^{c,p}$ with

$$\lim_{p\to\infty} \mathbf{B}^{c,p} = \widetilde{\mathbf{B}}, \qquad \lim_{p\to\infty} \mathbf{l}^{c,p} = \widetilde{\mathbf{l}}.$$

   Hence: as $p \to \infty$, the nodal values of the p-FEM approximation converge to the nodal values of $\widetilde{u}_N$.
4. Babuška & Sauter on 2D problems: there does not exist a 9-point stencil that is robust with respect to k (error measure: L^2).

special shape functions for multi-d problems

idea: approximate solutions of $-\Delta u - k^2 u = 0$ with functions that solve the equation as well.

examples (2D):

$$
\begin{aligned}
W(p) &:= \operatorname{span}\{e^{\mathbf{i}k\omega_n\cdot(x,y)} \,|\, n = 0,\ldots,p\}, \qquad \omega_n = (\cos\frac{2\pi n}{p}, \sin\frac{2\pi n}{p}) \\
V(p) &:= \operatorname{span}\{J_n(kr)\sin(n\varphi),\ J_n(kr)\cos(n\varphi) \,|\, n = 0,\ldots,p\}
\end{aligned}
$$

reasons:

- improved approximation properties (error vs. DOF)
- hope of improved stability properties in the preasymptotic range

Approximation properties of systems of plane waves for the approximation of u satisfying $-\Delta u - k^2 u = 0$ on $\Omega \subset \mathbb{R}^2$

$$W(p) \quad := \quad \mathrm{span}\{e^{\mathbf{i}k\omega_n\cdot(x,y)} \,|\, n = 0, \ldots, p\}, \qquad \omega_n = (\cos\frac{2\pi n}{p}, \sin\frac{2\pi n}{p})$$

Thm. 16. [Cessenat & Després] Let Ω be a shape regular element with diameter h. Then:

$$\inf_{v\in W(2n)} \|u - v\|_{L^\infty(\Omega)} + h\|\nabla(u - v)\|_{L^\infty(\Omega)} \leq C_n h^{n+1}\|u\|_{C^{n+1}(\overline{\Omega})}$$

Thm. 17. [p-version, exponential convergence] Let $\Omega \subset \mathbb{R}^2$, $\Omega' \subset\subset \Omega$. Then:

$$\inf_{v\in W(p)} \|u - v\|_{H^1(\Omega')} \leq Ce^{-bp/\log p},$$

Thm. 18. [p-version, alg. conv.] Let Ω be star shaped with respect to a ball and satisfy an exterior cone condition with angle $\lambda\pi$. Let $u \in H^k(\Omega)$, $k \geq 1$. Then:

$$\inf_{v\in W(p)} \|u - v\|_{H^1(\Omega)} \quad \leq \quad C\left(\frac{\log^2(p+2)}{p+2}\right)^{\lambda(k-1)}.$$

approximation methods using special ansatz functions (plane waves)

1. partition-of-unity methods (Babuška & Melenk, Bettes & Laghrouche, Astley, etc.) employ "standard" variational formulation and construct H^1-conforming ansatz spaces based on the chosen ansatz function

2. Least squares method: approximate with plane wave elmentwise and penalize jumps across interelement boundaries (Trefftz, Monk & Wang, Desmet)

3. Discontinuous enrichement method (Farhat et al.): approximate with plane waves elementwise and enforce interelement continuity by a Lagrange multiplier

4. ultra weak formulation: (Cessenat & Deprés, Monk & Huttunen) use a new variational formulation that is only posed on the "skeleton" and defined by L-harmonic extension into the domain. Ansatz functions on the skeleton are the traces of plane waves

Remark: the idea to employ adapted shape functions in integral equations has also been pursued: Darrigrand, Perrey-Debain et al., Chandler-Wilde & Langdon, Graham et al.,...

Partition of Unity Method/Generalized FEM

Thm. 19. Let $\Omega \subset \mathbb{R}^d$ be a domain, and let $(\varphi_i)_{i=1}^N$ be a collection of Lipschitz continuous functions. Set $\Omega_i := (\mathbf{supp}\,\varphi_i)^\circ$ and assume

$$\|\varphi_i\|_{L^\infty(\mathbb{R}^d)} \le C_\infty, \qquad \|\nabla\varphi_i\|_{L^\infty(\mathbb{R}^d)} \le \frac{C_G}{\operatorname{diam}(\Omega_i)},$$

$$\sum_{i=1}^N \varphi_i \equiv 1 \quad \text{on } \Omega, \qquad \sup_{x\in\Omega} \mathbf{card}\{i \mid x \in \Omega_i\} \le M.$$

For each $i = 1, \ldots, N$, let $V_i \subset H^1(\Omega_i \cap \Omega)$ be given and set

$$V := \sum_{i=1}^N \varphi_i V_i = \left\{ \sum_{i=1}^N \varphi_i v_i \mid v_i \in V_i \right\}$$

local approximation property: given $u \in H^1(\Omega)$, assume that for $i = 1, \ldots, N$

$$\exists v_i \in V_i \quad \text{s.t. } \|u - v_i\|_{L^2(\Omega_i\cap\Omega)} = \varepsilon_1(i), \qquad \|\nabla(u - v_i)\|_{L^2(\Omega_i\cap\Omega)} = \varepsilon_2(i),$$

Then the function $v := \sum_{i=1}^{N} \varphi_i v_i \in V$ satisfies

$$\|u - v\|^2_{L^2(\Omega)} \leq M C_\infty^2 \sum_{i=1}^{N} |\varepsilon_1(i)|^2 ,$$

$$\|\nabla(u - v)\|^2_{L^2(\Omega)} \leq 2M \sum_{i=1}^{N} \left[\left(\frac{C_G}{\operatorname{diam} \Omega_i} \right)^2 |\varepsilon_1(i)|^2 + C_\infty^2 \, |\varepsilon_2(i)|^2 \right]$$

- PUM provides a framework for constructing conforming ansatz spaces with user specified local approximation properties
- the global space V inherits the approximation properties of the local spaces V_i

Example: reproducing the approximation properties of the classical FEM

Cor. 20. Let $V_i := \mathcal{P}_p$ for each $i = 1, \ldots, N$. Let B_i be a ball of diameter $h_i := \operatorname{diam} \Omega_i$ s.t. $\Omega_i \subset B_i$. Then $v \in V$ can be chosen such that

$$\|u - v\|^2_{L^2(\Omega)} \leq C \sum_{i=1}^{N} h_i^{2\min\{p+1,k\}} \|u\|^2_{H^k(B_i)},$$

$$\|\nabla(u - v)\|^2_{L^2(\Omega)} \leq C \sum_{i=1}^{N} h_i^{2(\min\{p+1,k\}-1)} \|u\|^2_{H^k(B_i)}.$$

In particular, if the balls B_i satisfy the overlap property

$$\sup_{x \in \mathbb{R}^d} \{i \mid x \in B_i\} \leq M < \infty$$

then $\quad \|u - v\|_{H^s(\Omega)} \leq C h^{\min\{p+1,k\}-s} \|u\|_{H^k(\Omega)}, \qquad s = 0, 1 \qquad (h = \max_i h_i)$

Comments on the PUM

1. classical linear/bilinear FE functions on a mesh $\mathcal{T}$ are a POU $(\varphi_i)_{i=1}^N$ of the above form

2. Choosing the POU $(\varphi_i)_i$ smooth $\rightarrow$ constructing $V \subset H^k(\Omega)$ for arbitrary k is easily possible.

3. Analogous approximation results can be obtained in other norms.

4. PUM can be viewed as a meshfree method

how to choose the spaces V_i?

1. choose V_i based on analytic knowledge about the problem
   $\rightarrow$ operator adapted spaces
2. compute V_i numerically in a preprocessing step

Approximation of the Helmholtz equation

$$\begin{aligned} W(p) &:= \operatorname{span}\{e^{\mathbf{i}k\omega_n\cdot(x,y)} \,|\, n=0,\dots,p\}, \qquad \omega_n = (\cos\frac{2\pi n}{p}, \sin\frac{2\pi n}{p}) \\ V(p) &:= \operatorname{span}\{J_n(kr)\sin(n\varphi),\ J_n(kr)\cos(n\varphi) \,|\, n=0,\dots,p\} \end{aligned}$$

Thm. 21. Let $\Omega \subset \mathbb{R}^2$, $\Omega' \subset\subset \Omega$. Let u solve $-\Delta u - k^2 u = 0$ on Ω'. Then there exist C, $b > 0$ s.t.

$$\inf_{v\in V(p)} \|u-v\|_{H^1(\Omega')} \le Ce^{-bp}, \qquad \inf_{v\in W(p)} \|u-v\|_{H^1(\Omega')} \le Ce^{-bp/\log p},$$

Thm. 22. Let $\Omega \subset \mathbb{R}^2$ be star shaped with respect to a ball. Let Ω satisfy an exterior cone condition with angle $\lambda\pi$. Let $u \in H^k(\Omega)$, $k \ge 1$, solve $-\Delta u - k^2 u = 0$ on Ω. Then

$$\begin{aligned} \inf_{v\in V(p)} \|u-v\|_{H^1(\Omega)} &\le C\left(\frac{\log(p+2)}{p+2}\right)^{\lambda(k-1)}, \\ \inf_{v\in W(p)} \|u-v\|_{H^1(\Omega)} &\le C\left(\frac{\log^2(p+2)}{p+2}\right)^{\lambda(k-1)}. \end{aligned}$$

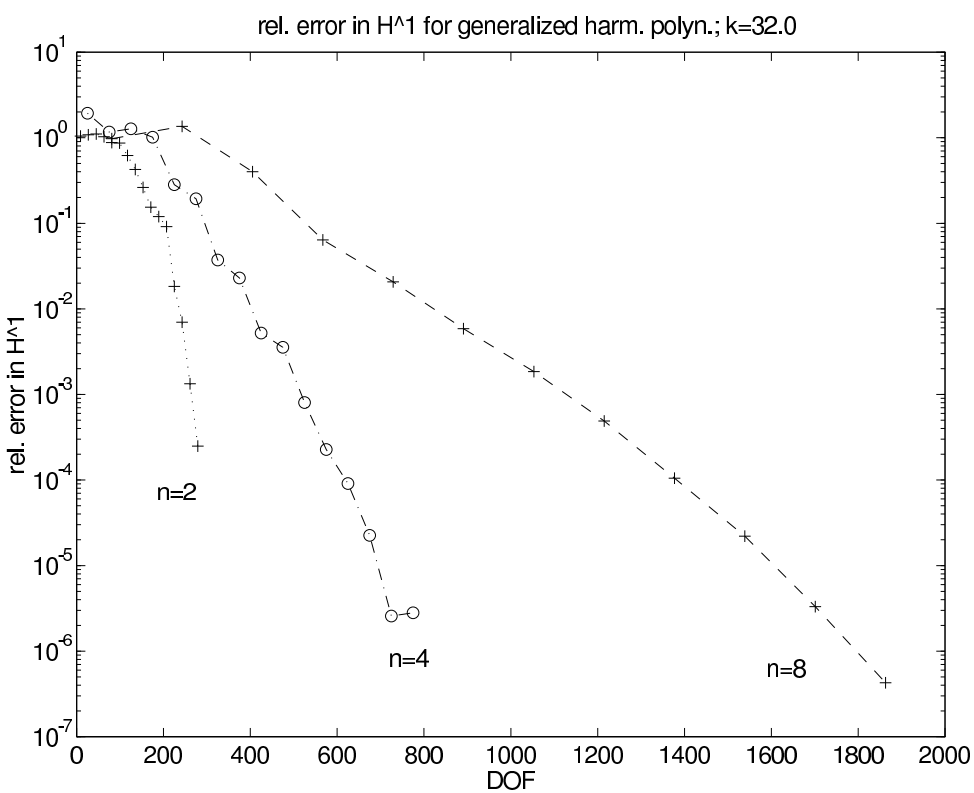
Approximation of the Helmholtz equation

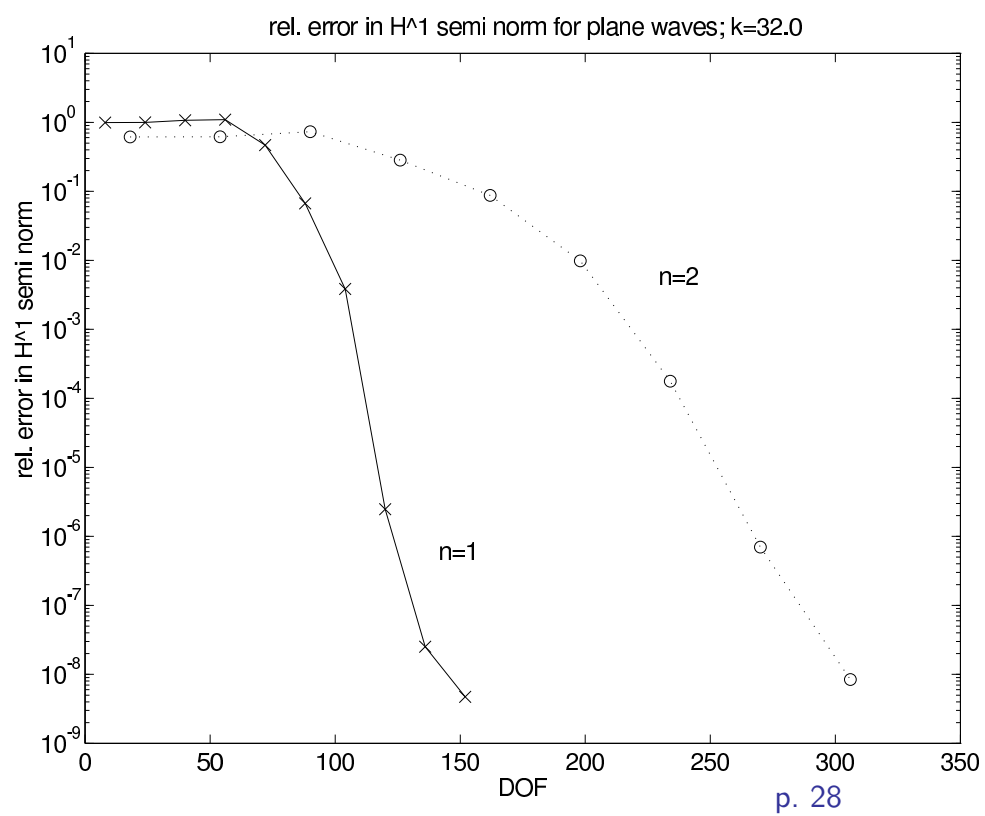
$$-\Delta u - k^2 u = 0 \quad \text{on } \Omega = (0,1)^2, \qquad \partial_n u + \mathbf{i}ku = g, \quad \text{on } \partial\Omega$$

$$\text{exact solution:} \quad u(x,y) = e^{\mathbf{i}k(\cos\theta,\sin\theta)\cdot(x,y)}, \quad \theta = \frac{\pi}{16}.$$

POU: bilinears φ_i on uniform $n \times n$ grid

Note: $\dim V(p) = 2p+1, \quad \dim W(p) = p+1$





performance of PUM: scattering by a sphere

- scattering by a sphere B_1 (radius 1) of an incident plane wave
- sound hard b.c. on $\Gamma = \partial B_1$ (i.e., Neumann b.c.)
- computational domain: ball of diameter $1 + 4\lambda$ ($\lambda = 2\pi/k$ = wave length)
- b.c. $\partial_n u^s + (\frac{1}{r} - \mathbf{i}\kappa)u^s = 0$ on outer boundary
- mesh: 4 layers in rad. dir., 8×5 elem./layers; $\rightarrow$ 160 elements; 170 nodes

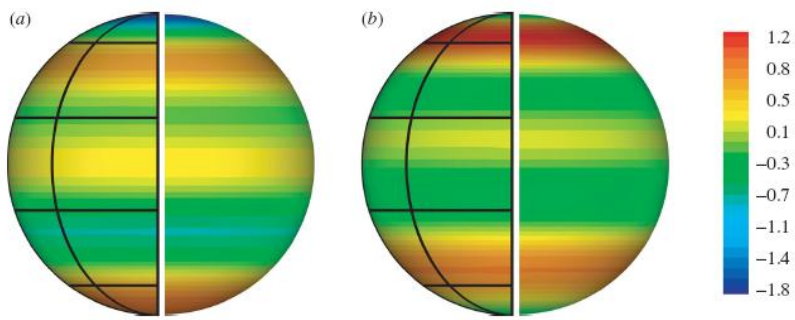


Figure 3. Scattered potential around the sphere, $\kappa = 2\pi$: (a) real part, (b) imaginary part.

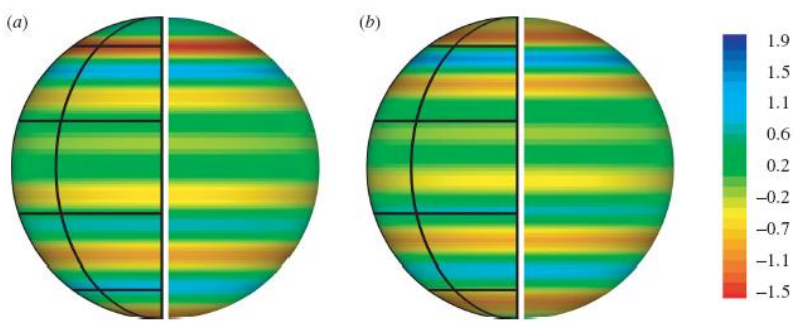


Figure 4. Scattered potential around the sphere, $\kappa = 5\pi$: (a) real part, (b) imaginary part.

k	number waves per node	DOF	$L^2(\Gamma)$ error	DOF per wave length
π	58	9860	0.1%	2.95
2π	58	9860	0.8%	2.66
3π	58	9860	2.1%	2.43
4π	98	16660	0.9%	2.67
5π	98	16660	2.7%	2.48

taken from: Perrey-Debain, Laghrouche, Bettess, Trevelyan, '03

Lagrange multiplier technique to enforce interelement continuity

original problem: find $u \in H^1(\Omega)$ s.t. $B(u,v) = l(v) \qquad \forall v \in H^1(\Omega)$

notation: $\mathcal{T}$ = mesh, $\mathcal{E}$ = set of internal edges/faces

spaces: $X = \{u \in L^2(\Omega) \,|\, u|_K \in H^1(K) \quad \forall K \in \mathcal{T}\}, \qquad M = \prod_{E \in \mathcal{E}} \left(H^{1/2}(E)\right)',$

define $b(u,\mu) = \sum_{E \in \mathcal{E}} \langle [u], \mu \rangle$

define $B_{\mathcal{T}}(u,\mu) = \sum_{K \in \mathcal{T}} B_K(u,v), \qquad B_K(u,v) = \int_K \nabla u \cdot \nabla \overline{v} - k^2 u \overline{v} \pm \mathbf{i}k \int_{\partial K \cap \partial \Omega} u \overline{v}$

continuous version

find $(u,\lambda) \in X \times M$ s.t.

$$\begin{aligned} B_{\mathcal{T}}(u,v) + b(v,\lambda) &= l(v) \quad \forall v \in X \\ b(u,\mu) &= 0 \quad \forall \mu \in M \end{aligned}$$

discrete version

Let $X_N \subset X$, $M_N \subset M$:
Find $(u_N, \lambda_N) \in X_N \times M_N$ s.t.

$$\begin{aligned} B_{\mathcal{T}}(u_N,v) + b(v,\lambda_N) &= l(v) \quad \forall v \in X_N \\ b(u_N,\mu) &= 0 \quad \forall \mu \in M_N \end{aligned}$$

"Discontinuous enrichement method" of Farhat et al. (IJNME '06)

Ansatz space for solution u:

$$X_N := \prod_{K \in \mathcal{T}} W_K,$$

$$W_K := \operatorname{span}\{e^{\mathbf{i}k\mathbf{d}_n \cdot \mathbf{x}} \,|\, n = 1, \ldots, N_u\}$$

Ansatz space for Lagrange multiplier

$$M_N := \prod_{E \in \mathcal{E}} \widetilde{W}_E,$$

$$\widetilde{W}_E := \operatorname{span}\{e^{\mathbf{i}kc_n\omega_n \cdot \mathbf{t}} \,|\, n = 1, \ldots, N_\lambda\}$$

where the parameters c_n are between 0.4 and 0.8 and are obtained from a numerical study of a test problem

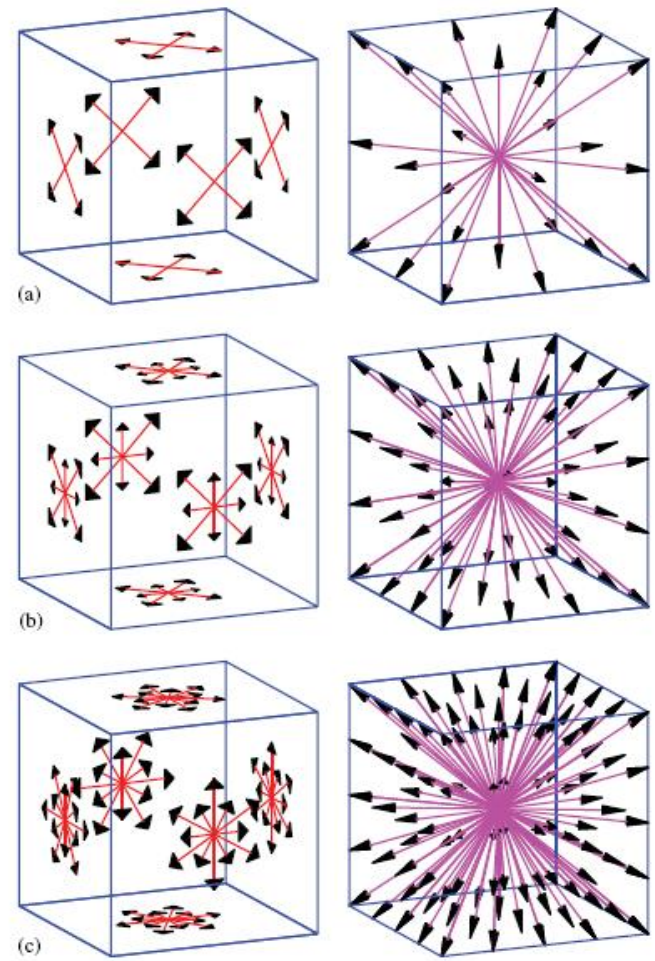


Figure 1. 3D DGMH elements: directions of the Lagrange multipliers (left), directions of the element basis functions (right): (a) DGMH-26-4; (b) DGMH-56-8; and (c) DGMH-98-12.

performance of DEM: scattering by a sphere

- scattering by a sphere B_1 (radius 1) of an incident plane wave
- sound hard b.c. on $\Gamma = \partial B_1$ (i.e., Neumann b.c.)
- computational domain: ball of diameter 2
- b.c. $\partial_n u^s - \mathbf{i}\kappa u^s = 0$ on outer boundary

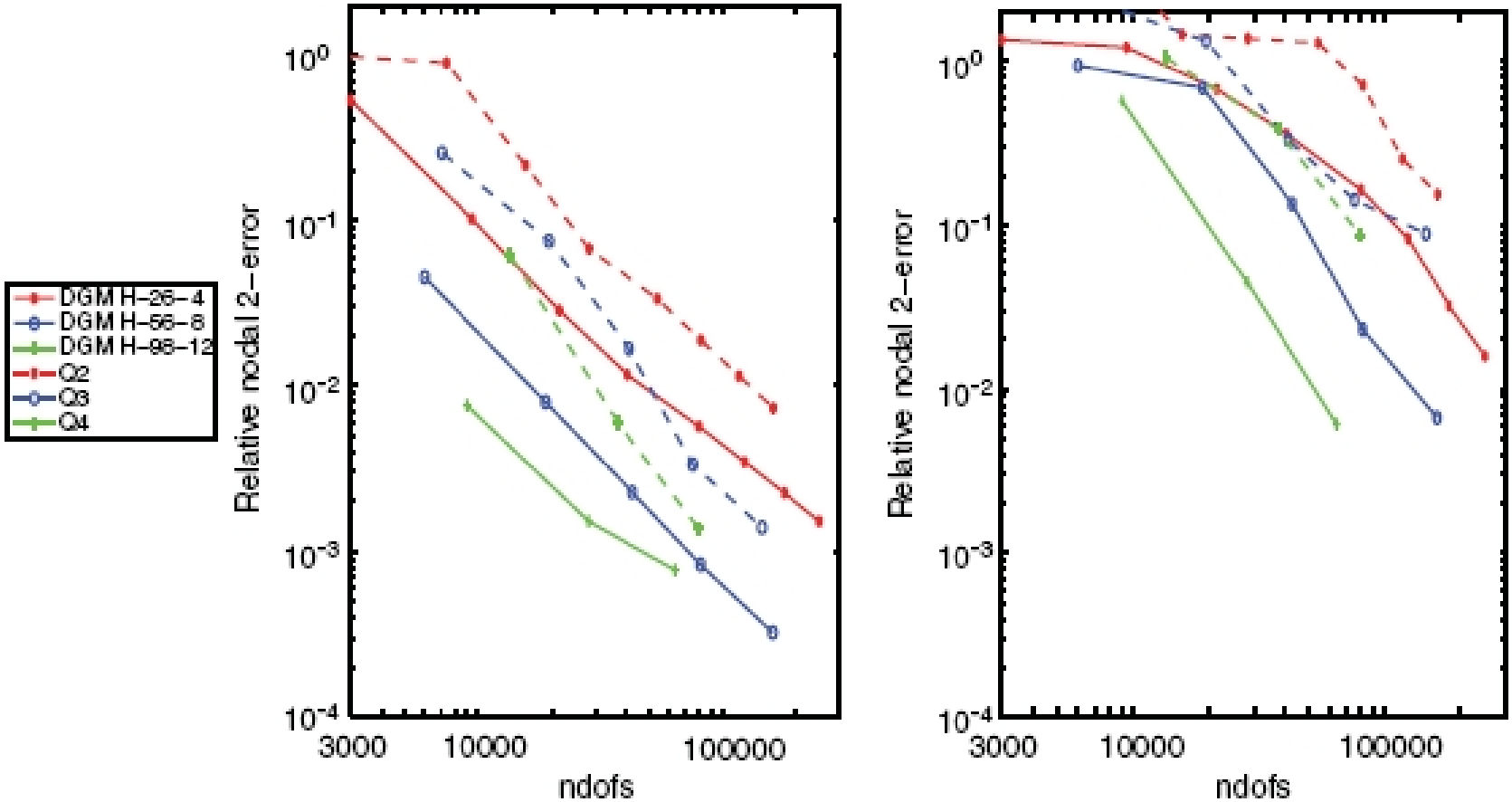


Figure 6. Convergence of the Galerkin and DGM elements for the problem of sound-hard scattering by a sphere: $R_1 = 1$, $R_2 = 2$, $kR_1 = 12$ (left) and $kR_1 = 24$ (right).

legend: dashed lines = standard Q_2, Q_3, Q_4 elements; solid lines = new elements; taken from Tezaur & Farhat, IJNME '06

ultra weak variational formulation (Cessenat & Després)

model problem:

$$-\Delta u - k^2 u = f \in L^2(\Omega) \qquad \text{in } \Omega \tag{16a}$$

$$\partial_n u + \mathbf{i}ku = t(-\partial_n + \mathbf{i}u) + g \qquad \text{on } \partial\Omega, \qquad t \in \mathbb{C}, \qquad |t| < 1. \tag{16b}$$

goal: given a mesh $\mathcal{T}$ construct a variational formulation for the functions

$$x_K := -\partial_n u_K + \mathbf{i}ku_K \qquad \text{(here: } u_K = u|_K \text{ for } K \in \mathcal{T}\text{)}.$$

reconstruction of u_K:

for each $K \in \mathcal{T}$, the fct u_K is the well-defined solution of

$$-\Delta u_K - k^2 u_K = f|_K, \quad \text{on } K, \qquad -\partial_n u_K + \mathbf{i}ku_K = x_K \quad \text{on } \partial K.$$

regularity assumption: $\partial_n u_K \in L^2(\partial K)$ for every $K \in \mathcal{T}$

ultra weak variational formulation II

extension operator $E_K : L^2(\partial K) \to H^1(K)$

$$\boxed{-\Delta(E_K y) - k^2(E_K y) = 0 \quad \text{on } K, \qquad\qquad -\partial_n(E_K y) + \mathbf{i}k(E_K y) = y \quad \text{on } \partial K.}$$

twisting operator $T_K : L^2(\partial K) \to L^2(\partial K)$

$$\boxed{T_K y := \partial_n(E_K y) + \mathbf{i}k(E_K y).}$$

Define: $\quad X := \prod_{K \in \mathcal{T}} L^2(\partial K), \qquad \Gamma_{K,K'} := \overline{K} \cap \overline{K'}, \qquad \Gamma_K := \partial K \cap \partial\Omega$

On X define the sesquilinear form C and $l \in X'$ by:

$$\begin{aligned} C(x,y) &:= \sum_{K \in \mathcal{T}} \int_{\partial K} x_K \overline{y}_K - \sum_{K,K' \in \mathcal{T}} \int_{\Gamma_{K,K'}} x_K \overline{T_{K'} y} \qquad - \sum_{K \in \mathcal{T}} t \int_{\Gamma_K} x_K \overline{T_K y} \\ l(y) &:= -2\mathbf{i}k \sum_{K \in \mathcal{T}} \int_K f \overline{E_K y} + \sum_{K \in \mathcal{T}} \int_{\Gamma_K} g \overline{T_K y} \end{aligned}$$

ultra weak variational formulation III

$$
\begin{aligned}
C(x,y) &:= \sum_{K\in\mathcal{T}} \int_{\partial K} x_K \overline{y}_K - \sum_{K,K'\in\mathcal{T}} \int_{\Gamma_{K,K'}} x_K \overline{T_{K'} y} \qquad - \sum_{K\in\mathcal{T}} t \int_{\Gamma_K} x_K \overline{T_K y} \\
l(y) &:= -2\mathbf{i}k \sum_{K\in\mathcal{T}} \int_K f \overline{E_K y} + \sum_{K\in\mathcal{T}} \int_{\Gamma_K} g \overline{T_K y}
\end{aligned}
$$

Thm. 23. [Cessenat & Després] Assume that $\partial_n u \in L^2(\partial K)$ for all $K \in \mathcal{T}$. Define $x \in X$ by $x_K := -\partial_n u_K + \mathbf{i}k u_K$ with $u_K := u|_K$. Then x satisfies

$$C(x,y) = l(y) \qquad \forall y \in X. \tag{17}$$

Conversely, let $x \in X$ solve (17). Then the function u defined elementwise by $u_K := E_K x$ is in $H^1(\Omega)$ and solves (16).

Remark: key observation for interelement continuity is that it is equivalent to

$$\partial_{n_K} u_K + \mathbf{i}k u_K = -\partial_{n_{K'}} u_{K'} + \mathbf{i}k u_{K'} \quad \text{on } \Gamma_{K,K'}$$

ultra weak variational formulation IV

Thm. 24. [Cessenat & Després] Let $X_N \subset X$ be arbitrary. Then the problem:

$$\text{Find } x_N \in X_N \text{ s.t.} \quad C(x_N, v) = l(v) \qquad \forall v \in X_N$$

has a unique solution.

Choice of the discrete space X_N:

1. $\forall K \in \mathcal{T}$ let $W_K = \text{span}\{w_{n,K} \,|\, n = 1, \ldots, p\}$ be a space of plane waves
2. set $X_N := \prod_{K \in \mathcal{T}} \widetilde{X}_K$, where

$$\widetilde{X}_K := \text{span}\{-\partial_n w_{n,K} + \mathbf{i}k w_{n,K} \,|\, n = 1, \ldots, p\}$$

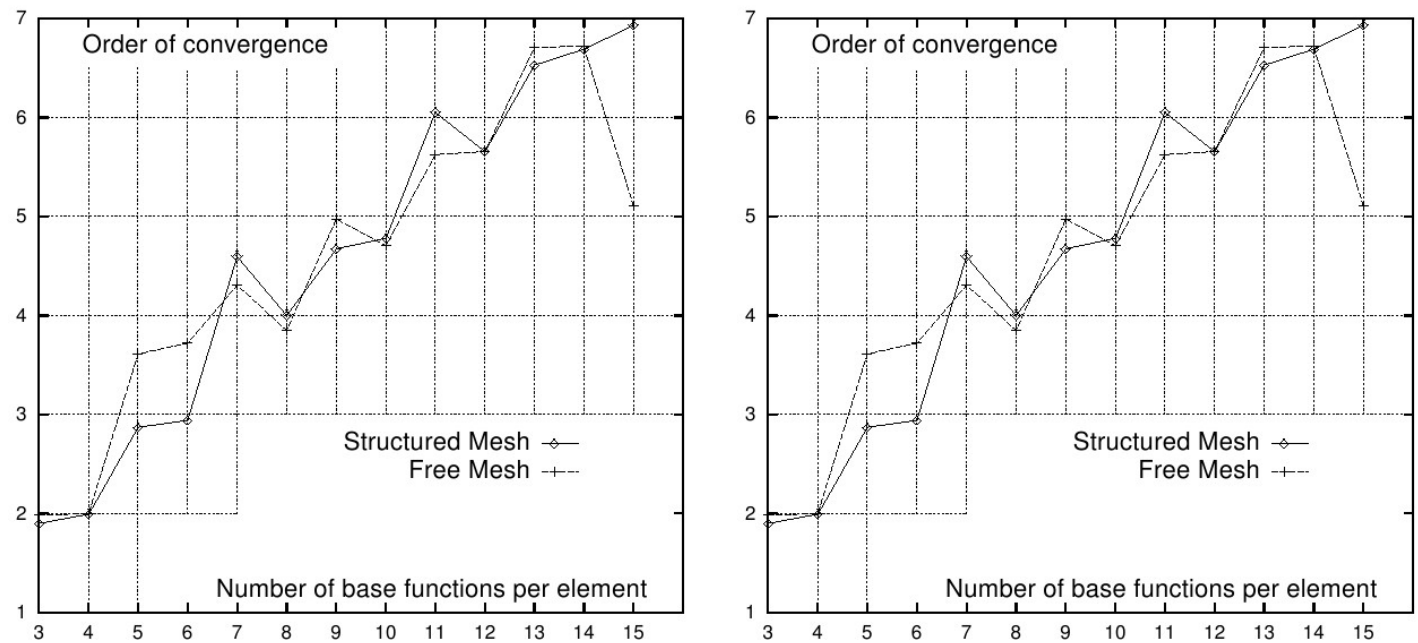
note: sesq. form C is easily evalulated by observing for the twisting operator T_K:

$$T_K(-\partial_n w_{n,K} + \mathbf{i}k w_{n,K}) \quad = \quad +\partial_n w_{n,K} + \mathbf{i}k w_{n,K}$$

ultra weak variational formulation V

Thm. 25. [Cessenat & Després] Let $\Omega \subset \mathbb{R}^2$, $f = 0$ and the solution u of (16) be in $C^{\mu+1}(\overline{\Omega})$. Assume that $|t| < 1$. Assume that $p = 2\mu + 1$ plane waves are employed for each element. Then the approximation x_N to $x = -\partial_n u + \mathbf{i}ku$ satisfies

$$\|x - x_N\|_{L^2(\partial\Omega)} \leq Ch^{\mu-1/2}\|u\|_{C^{\mu-1/2}(\overline{\Omega})}.$$



- smooth solution
- $t = 0$
- $f = 0$

left: $L^2(\Omega)$-error

right: $L^2(\partial\Omega)$-error

source:
Cessenat & Després '98

Remark: If $f = 0$, the reconstruction of u_K on the elements is particularly simple.

robust method as limit $p \to \infty$ p-FEM

For a fixed mesh $\mathcal{T}$, define the L-harmonic shape functions ψ_i and the discrete harmonic shape functions $\psi_i^p \in S^p(\mathcal{T})$ by

$$\begin{aligned} \psi_i(x_j) &= \delta_{ij} \qquad B(\psi_i, v) = 0 \qquad \forall v \in H_0^1(K) \quad \forall K \in \mathcal{T} \\ \psi_i^p(x_j) &= \delta_{ij} \qquad B(\psi_i, v) = 0 \qquad \forall v \in H_0^1(K) \cap S^p(\mathcal{T}) \quad \forall K \in \mathcal{T} \end{aligned}$$

Then:

$$\lim_{p\to\infty} \psi_i^p = \psi_i \qquad \text{(convergence in } H^1\text{)}$$

Let $\widetilde{X}_N := \operatorname{span}\{\psi_i \,|\, i = 1, \ldots, N\}$ and $\widetilde{X}_N^p := \operatorname{span}\{\psi_i^p \,|\, i = 1, \ldots, N\}$.

Let $\widetilde{\mathbf{B}}$, $\widetilde{\mathbf{l}}$, $\widetilde{\mathbf{B}}^p$, $\widetilde{\mathbf{l}}^p$ be the corresponding stiffness matrices and load vectors. Then:

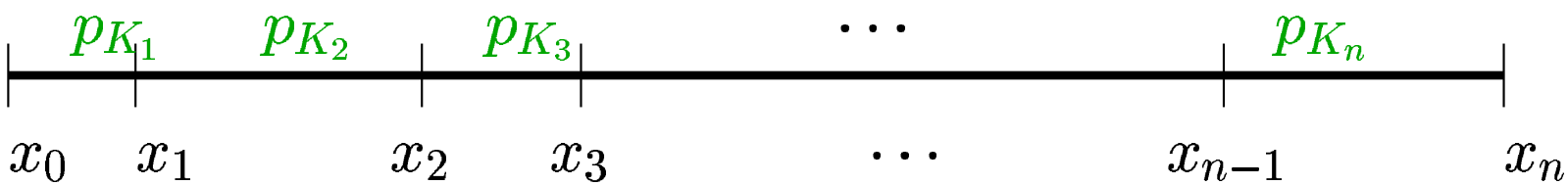
$$\lim_{p\to\infty} \widetilde{\mathbf{B}}^p = \widetilde{\mathbf{B}}, \qquad \lim_{p\to\infty} \widetilde{\mathbf{l}}^p = \widetilde{\mathbf{l}}.$$

It remains to see that $\widetilde{\mathbf{B}}^p$ and $\widetilde{\mathbf{l}}^p$ are obtained by condensing out the "bubble modes" from the full problem posed on $S^p(\mathcal{T})$.

back

high order FEM in 1D

- mesh $\mathcal{T}$: consists of elements K_i, $i = 1, \ldots, n$
- for each $K \in \mathcal{T}$ choose a polynomial degree $p_K \in \mathbb{N}$



$$X_N := S^{\mathbf{p}}(\mathcal{T}) := \{u \in H^1(\Omega) \,|\, u|_K \in \mathcal{P}_{p_K} \quad \forall K \in \mathcal{T}\}.$$

classical basis of $S^{\mathbf{p}}(\mathcal{T})$:

- piecewise linears associated with the nodes
- for each $K \in \mathcal{T}$ $p_K - 1$ "bubble" shape fct $\{b_{K,i} \,|\, i = 1, \ldots, p_K - 1\}$ with:
  - $\operatorname{supp} b_{K,i} \subset \overline{K}$ for $i = 1, \ldots, p_K - 1$ and $K \in \mathcal{T}$
  - for each $K \in \mathcal{T}$: $\operatorname{span}\{b_{K,i} \,|\, i = 1, \ldots, p_K - 1\} = \{u \in \mathcal{P}_{p_K} \,|\, u(a_K) = u(b_K) = 0\}$, where a_K, , b_K denote the endpoints of K

back

remarks on quadrature

methods based on plane waves require the evaluation of oscillatory integrals of the form

$$\int_a^b e^{\mathbf{i}k\alpha x} f(x)\,dx \quad (d=1), \qquad\qquad \int_a^b \int_{a'}^{b'} e^{\mathbf{i}k(\alpha x+\beta y)} f(x,y)\,dx \quad (d=2),$$

for some parameters α, $\beta \in \mathbb{R}$.

Possible techniques are (for the case of large $|\alpha|$, $|\beta|$):

1. asymptotic methods

2. specialized quadrature: require that quadrature formula be exact for polynomials f up to a given order

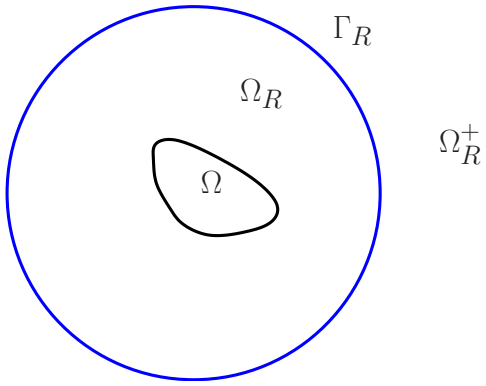
infinite elements for exterior domain problems I: variational formulation

$$-\Delta u - k^2 u = f \quad \text{on } \Omega^+ = \mathbb{R}^d \setminus \overline{\Omega}, \tag{18a}$$

Neumann b.c. on $\partial\Omega$ (18b)

Sommerfeld radiation cond. (18c)

$\text{supp} f \subset B_R(0)$



- solution u satisfies
$$B(u,v) := \int_{\Omega^+} \nabla u \cdot \nabla \overline{v} - k^2 u \overline{v} = l(v) := \int_{\Omega^+} f\overline{v} + \int_{\partial\Omega} g\overline{v} \qquad \forall v \in C^\infty(\mathbb{R}^d).$$
- ($d = 3$:) outside $B_R(0)$, solution u has the form
$$u(r,\varphi,\theta) = \sum_{n \in \mathbb{N}_0} A_n(\varphi,\theta) h_n^{(1)}(kr)$$
- from $h_n^{(1)}(kr) \sim e^{\mathbf{i}kr}/r$ as $r \to \infty$ we conclude $u \notin L^2(\Omega^+)$ and $\nabla u \notin L^2(\omega^+)$. However, one can show that u and $\nabla u \in L^2_w(\Omega^+)$, where the weight function $w(r) = (1+r)^{-1}$.

infinite elements for exterior domain problems II: variational formulation cont'd

- for $w(r) := (1+r)^{-1}$ def. the weighted spaces $H^1_w(\Omega^+)$, $H^1_{1/w}(\Omega^+)$ by

$$\begin{aligned} \|u\|^2_{H^1_w(\Omega^+)} &:= \int_{\Omega^+} |\nabla u|^2 w(r)\,dx + \int_{\Omega^+} |u|^2 w(r)\,dx \\ \|u\|^2_{H^1_{1/w}(\Omega^+)} &:= \int_{\Omega^+} |\nabla u|^2 \frac{1}{w(r)}\,dx + \int_{\Omega^+} |u|^2 \frac{1}{w(r)}\,dx, \end{aligned}$$

- we have: the solution u is a solution of the variational problem:

$$\text{find } u \in H^1_w(\Omega^+) \text{ s.t.} \qquad B(u,v) = l(v) \qquad \forall v \in H^1_{1/w}(\Omega^+) \tag{19}$$

- (19) does not enforce Sommerfeld radiation condition. This has to be built explicitly into the spaces:

$$\begin{aligned} \|u\|^2_{w,+} &:= \|u\|^2_{H^1_w(\Omega^+)} + \int_{\Omega^+} |\partial_r - \mathbf{i}ku|^2\,dx \\ \|u\|^2_{1/w,+} &:= \|u\|^2_{H^1_w(\Omega^+)} + \int_{\Omega^+} |\partial_r - \mathbf{i}ku|^2\,dx \end{aligned}$$

infinite elements for exterior domain problems III

Thm. 26. [Leis] The solution u of (25) is the unique solution of the problem:

$$\text{find } u \in H^1_{w,+}(\Omega^+) \text{ s.t.} \qquad B(u,v) = l(v) \qquad \forall v \in H^1_{1/w,+}(\Omega^+). \tag{20}$$

---

(20) leads to numerical methods by choosing $X_N \subset H^1_{w,+}(\Omega^+)$ and $Y_N \subset H^1_{1/w,+}(\Omega^+)$.

Lemma 27. $\exists$ unique functions $u_n \in H^1(\Omega_R)$ s.t. the solution u has the form

$$u(x) = \sum_{n=0}^{N} (E_n u_n)(x)$$

where

$$(E_n v)(x) := \begin{cases} v(x) & |x| < R \\ v(x/r)\frac{h_n^{(1)}(kr)}{h_n^{(1)}(kR)} & |x| \geq R \end{cases}$$

Proof: follows from the representation formula $u = \sum_n A_n(\varphi,\theta) h_n^{(1)}(kr)$ valid for $r \geq R$

infinite elements for exterior domain problems IV

semi-discrete method: Let $X_N := \{\sum_{n=0}^{N} E_n u_n \,|\, u_n \in H^1(\Omega_R)\}$, $Y_N := \{\frac{1}{r^2}\sum_{n=0}^{N} E_n v_n \,|\, v_n \in H^1(\Omega_R)\}$.

$$\text{Find } u \in X_N \text{ s.t.} B(u,v) = l(v) \qquad \forall v \in Y_N. \tag{21}$$

1. (21) is a coupled system of $N+1$ elliptic equations. A fully discrete problem is obtained by approximating the functions u_n by the classical FEM.
2. the factor $1/r^2$ in the definition of Y_N ensures that $Y_N \subset H^1_{1/w,+}(\Omega^+)$.
3. semi-analytic evaluation of the integrals. Example:

$$\int_{\Omega^+} E_n u \overline{E_m v} r^{-2} = \int_{\Omega_R} u\overline{v} r^{-2} + \int_{\omega\in\partial B_R(0)} u(\omega)\overline{v}(\omega) \underbrace{\int_{r=R}^{\infty} r^{-2} h_n^{(1)}(kr)\overline{h^{(1)}}_m(kr) r^2\, dr}_{=:a_{nm}}$$

   and the coefficients a_{nm} can be computed analytically.
4. observation in practice: $N \geq k$ needed for good results.
5. infinite elements can also be defined for the exterior of ellipsoids etc.

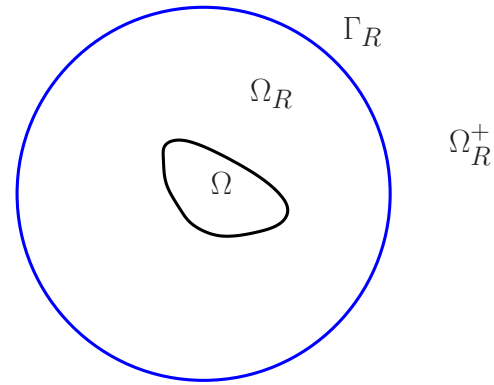
truncating infinite domains and local b.c.

$$-\Delta u - k^2 u = f \quad \text{on } \Omega^+ = \mathbb{R}^d \setminus \overline{\Omega}, \tag{22a}$$

$$u = 0 \text{ on } \partial\Omega \tag{22b}$$

$$\text{Sommerfeld radiation cond.} \tag{22c}$$

$$\text{supp} f \subset B.$$



approximate solution u_R:

$$-\Delta u_R - k^2 u_R = f \qquad \text{on } \Omega_R \tag{23a}$$

$$u_R = 0 \quad \text{on } \partial\Omega \tag{23b}$$

$$B_1 u_R := (\partial_r - \mathbf{i}k + R^{-1}) u_R = 0. \tag{23c}$$

Thm. 28. [Goldstein] Let B be fixed. Then $\exists\, C > 0$ s.t. the error $u - u_R$ satisfies

$$\|u - u_R\|_{L^2(B)} \leq C R^{-2} \|f\|_{L^2(B)}.$$

truncating infinite domains and local b.c. II

Lemma 29. [Atkinson-Wilcox expansion] Let $B \subset B_{r_0}(0)$. Then the solution u can be expanded as a convergent series

$$u = \frac{e^{\mathbf{i}kr}}{r} \sum_{n=0}^{\infty} \frac{A_n(\varphi, \theta)}{r^n}, \qquad r > r_0 \tag{24}$$

The function $U := ue^{-\mathbf{i}kr}$ satisfies

1. $|D^\alpha U(x)| \leq C_\alpha r^{-(|\alpha|+1)} \|f\|_{L^2(B)}$
2. $|\partial_r U(x) + r^{-1} U(x)| \leq C r^{-3} \|f\|_{L^2(B)}$

Therefore, u satisfies on Γ_R: $|B_1 u| \leq C R^{-3} \|f\|_{L^2(B)}$.

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key ingredient of proof:

- Green's theorem: $u(x) = \dfrac{1}{4\pi} \displaystyle\int_{\partial\Omega} \frac{e^{\mathbf{i}k\rho(x')}}{\rho(x')} \partial_n u(x')\, ds_{x'} - \int_B \frac{e^{\mathbf{i}k\rho(x')}}{\rho(x')} f(x')\, dx'$
- a priori estimate $\|\partial_n u\|_{L^2(\partial\Omega)} \leq C \|f\|_{L^2(B)}$.

truncating infinite domains and local b.c. III

A theorem analogous to Lemma 29 holds for incoming b.c. as well:

Lemma 30. Let $B \subset B_{r_0}(0)$. Then the solution Φ of

$$\begin{aligned} &-\Delta\Phi - k^2\Phi = \varphi \in L^2(B) \qquad \text{on } \Omega^+, \\ &\Phi = 0 \qquad \text{on } \partial\Omega, \\ &(\partial_r + \mathbf{i}k)\Phi = o(r^{-1}) \qquad \text{as } r \to \infty \end{aligned}$$

has an expansion $\Phi = \dfrac{e^{-\mathbf{i}kr}}{r} \displaystyle\sum_{n=0}^{\infty} \frac{\widetilde{A}_n(\varphi,\theta)}{r^n}$ (for $r > r_0$)

The function $\widetilde{\Phi} := e^{\mathbf{i}kr}\Phi$ satisfies

1. $|D^\alpha \widetilde{\Phi}(x)| \le C_\alpha r^{-(|\alpha|+1)} \|\varphi\|_{L^2(B)}$
2. $|\partial_r \widetilde{\Phi}(x) + r^{-1}\widetilde{\Phi}(x)| \le C r^{-3} \|f\|_{L^2(B)}$

Therefore, Φ satisfies on Γ_R: $|B_1'\Phi| \le CR^{-3}\|\varphi\|_{L^2(B)}$ where

$$B_1'\Phi := \partial_r\Phi + \left(\frac{1}{R} + \mathbf{i}k\right)\Phi$$

local b.c. of higher order (BGT)

The boundary condition $B_1 u = 0$ on Γ_R can be motivated as follows: From the Atkinson-Wilcox expansion we have

$$u = \frac{e^{\mathbf{i}kr}}{r} \sum_{n=0}^{\infty} \frac{A_n(\varphi, \theta)}{r^n}.$$

It can be checked that $B_1 := \partial_r - \mathbf{i}k + r^{-1}$ satisfies

$$B_1 u = \sum_{n=1+1}^{\infty} A_n^{(1)} r^{-(n+1)}, \qquad \text{suitable } A_n^{(1)}$$

More generally, for $L := \partial_r - \mathbf{i}k$, we can define recursively

$$B_1 := L + \frac{1}{r}, \qquad B_2 := (L + \frac{3}{r})(L + \frac{1}{r}), \cdots, B_N := (L + \frac{2N-1}{r}) B_{N-1}$$

and get

$$B_N u = \sum_{n=N+1}^{\infty} A_n^{(N)} r^{-n-N}, \qquad \text{suitable } A_n^{(N)}$$

Hence, $B_N u = O(R^{-(2N+1)})$ on Γ_R.

local b.c. of higher order (BGT)

- Choosing the artificial boundary condition on Γ_R to be $B_N u_R = 0$, we expect faster convergence (as $R \to \infty$) than for the case $N = 1$ analyzed above.
- for $N \geq 2$, B_N contains higher order derivatives in ∂_r. Since the exact solution solves $-\Delta u - k^2 u = 0$ near Γ_R, the derivatives ∂_r^j for $j \geq 2$ can be expressed in terms of $\partial_\varphi^\alpha \partial_\theta^\beta$ and $\partial_\varphi^\alpha \partial_\theta^\beta \partial_r$.

  For example, in $2D$ the operator $B_2 = (\partial_r - \mathbf{i}k + \frac{3}{r})(\partial_r - \mathbf{i}k + \frac{1}{r})$ is expanded as $B_2 = \partial_r^2 + \left(\frac{4}{r} - 2\mathbf{i}k\right) + \left(\frac{2}{r} - 4\mathbf{i}k\right)\frac{1}{r} - k^2$; using the differential equation $0 = \Delta u + k^2 u = \frac{1}{r}\partial_r(r\partial_r u) + \frac{1}{r^2}\partial_\varphi^2 u + k^2 u = 0$, the term $\partial_r^2 u$ can expressed in terms of u, $\partial_\varphi u$, $\partial_\varphi^2 u$, $\partial_\varphi \partial_r u$.
- higher order differential operators are not easily implemented in FEM. One possible option: introduce auxiliary variables for the boundary derivatives.

Further methods for deriving local boundary conditions of higher order exist, notably those of Engquist & Majda and Higdon.

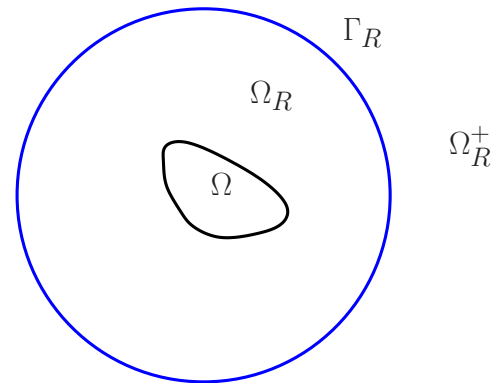
DtN operators

$$-\Delta u - k^2 u = f \quad \text{on } \Omega^+ = \mathbb{R}^d \setminus \overline{\Omega}, \tag{25a}$$

$$u = 0 \text{ on } \partial\Omega \tag{25b}$$

$$\text{Sommerfeld radiation cond.} \tag{25c}$$

$$\text{supp} f \subset B.$$



- fix R
- define the **DtN operator** $T : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R)$ by $Tu := \partial_r U|_{\Gamma_R}$, where U solves the exterior problem

$$-\Delta U - k^2 U = 0 \qquad \text{on } \Omega_R^+$$

$$U = u \qquad \text{on } \Gamma_R, \qquad\qquad U \text{ satisfies Sommerfeld radiation cond.}$$

- weak formulational for $u|_{\Gamma_R}$:

$$\text{find } u \in H_D^1 \text{ s.t. } \int_{\Omega_R} \nabla u \cdot \nabla \overline{v} - k^2 \int_{\Omega_R} u\overline{v} - \int_{\Gamma_R} Tu\overline{v} = \int_{\Omega_R} f\overline{v} \qquad \forall v \in H_D^1$$

where $H_D^1 := \{v \in H^1(\Omega_R) \,|\, v|_{\partial\Omega} = 0\}$

numerical realization of DtN operator T

- T can be realized numerically by the boundary element method. "Fast BEM" (multipole, panel clustering, $\mathcal{H}$-matrix techniques,...) can be brought to bear.
- simple geometries (circles/spheres, ellipsoids): DtN-operator can be written down explicitly. For example, in 2D the DtN operator on $\Gamma_R = \partial B_R(0)$ takes the form

$$(Tu)(R,\varphi) = \sum_{n\in\mathbb{Z}} \frac{1}{2\pi} k \frac{H_n'(kR)}{H_n(kR)} e^{\mathrm{i}n\varphi} \int_0^{2\pi} u(R,\varphi') e^{-\mathrm{i}n\varphi'}\, d\varphi', \qquad H_n = H_n^{(1)}$$

One possibility to approximate T is by truncation:

$$(T_N u) := \sum_{|n|\le N} \frac{1}{2\pi} k \frac{H_n'(kR)}{H_n(kR)} e^{\mathrm{i}n\varphi} \int_0^{2\pi} u(R,\varphi') e^{-\mathrm{i}n\varphi'}\, d\varphi',$$

– the approximate problem is:

$$\text{find } u \in H_D^1 \text{ s.t. } \int_{\Omega_R} \nabla u \cdot \nabla \overline{v} - k^2 \int_{\Omega_R} u\overline{v} - \int_{\Gamma_R} T_N u \overline{v} = \int_{\Omega_R} f\overline{v}$$

– approximate problem is only well-posed if $kR < N$ ($\rightarrow$ many terms!)
– "stabilization" possible (Grote & Keller)