An adaptive PML technique for time-harmonic scattering problems

Following a paper by Zhiming Chen and Xuezhe Liu

Manuel Largo
Overview

- Introduction, Hankel functions
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- PML formulation
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- Finite Elements and the Main Theorem
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- Introduction, Hankel functions
- PML formulation
- Finite Elements and the Main Theorem
- Implementation and Examples
First Part

INTRODUCTION AND HANKEL FUNCTIONS
Task

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To do so, we need an a posteriori error estimate to control the error we make when discretizing space.

We extend the idea of using a posteriori error estimates to determine the PML parameters and propose an adaptive PML technique for solving the Helmholtz-type scattering problem.

We will first introduce and prove some error estimates, later construct an algorithm to adapt mesh size with a posteriori error control.
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Let $D \in \mathbb{R}^2$ denote the bounded domain (scatterer) with boundary $\Gamma_D$, $g \in H^{-1/2}(\Gamma_D)$ determined by the incoming wave, $\mathbf{n}$ the unit outer normal to $\Gamma_D$. 
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Helmholtz-type scattering problem (constant $k$):

$$\Delta u + k^2 u = 0 \quad \text{in} \quad \mathbb{R}^2 \setminus \bar{D}$$

$$\frac{\partial u}{\partial \mathbf{n}} = -g \quad \text{on} \quad \Gamma_D$$

$$\sqrt{r} \left( \frac{\partial u}{\partial r} - iku \right) \to 0 \quad \text{as} \quad r = |x| \to \infty$$
Hankel functions

First, consider the Bessel equation for functions of order $\nu$:

$$z^2 \frac{d^2 y}{dz^2} + z \frac{dy}{dz} + (z^2 - \nu^2)y = 0, \quad \nu \in \mathbb{C}.$$
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We introduce now the Hankel function of the first kind and order $\nu$

$H^{(1)}_{\nu}(z), \ z \in \mathbb{C},$ and the Hankel function of the second kind and order $\nu$

$H^{(2)}_{\nu}(z), \ z \in \mathbb{C},$ are defined by

\[
H^{(1)}_{\nu}(z) \equiv J_{\nu}(z) + iY_{\nu}(z), \\
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Asymptotic behaviour:

$$H^{(1)}_{\nu}(z) \sim \sqrt{\frac{2}{\pi z}}e^{i(z - \frac{1}{2}\nu\pi - \frac{1}{4}\pi)},$$
$$H^{(2)}_{\nu}(z) \sim \sqrt{\frac{2}{\pi z}}e^{-i(z - \frac{1}{2}\nu\pi - \frac{1}{4}\pi)}.$$
Hankel functions, $H_0^{(1)}$
Hankel functions, $H^{(1)}_1$
Hankel functions, $H_{-1}^{(1)}$
Lemma 1:
For any $\nu \in \mathbb{R}, z \in \mathbb{C}_{++} = \{ z \in \mathbb{C} : \Im(z) \geq 0, \Re(z) \geq 0 \}$, and $\Theta \in \mathbb{R}$ such that $0 < \Theta \leq |z|$, we have

$$|H_{\nu}^{(1)}(z)| \leq e^{-\Im(z)\sqrt{1-\frac{\Theta^2}{|z|^2}}} |H_{\nu}^{(1)}(\Theta)|$$
Lemma 1:

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Lemma 1 (cont.)
Second Part

PML FORMULATION
Setup

Let the scatterer $D$ be contained in the interior of the circle $B_R = \{ x \in \mathbb{R}^2 : |x| < R \}$, and $\Omega_R = B_R \setminus \bar{D}$.

We now surround the domain $\Omega_R$ with a PML layer $\Omega_{\text{PML}} = \{ x \in \mathbb{R}^2 : R < |x| < \rho \}$. 
The PML formulation

Look at the domain $\mathbb{R}^2 \setminus \bar{B}_R$. The solution $u$ of the scattering problem can be written under the polar coordinates as follows:

$$u(r, \theta) = \sum_{n \in \mathbb{Z}} \frac{H_n^{(1)}(kr)}{H_n^{(1)}(kR)} \hat{u}_n e^{in\theta}, \quad \hat{u}_n = \frac{1}{2\pi} \int_0^{2\pi} u(R, \theta) e^{-in\theta} d\theta.$$  

$H_n^{(1)}$ denotes the just discussed Hankel function of the first kind and order $n$. It can be shown that this series converges uniformly for $r > R$. 
We now introduce the so called Dirichlet-to-Neumann operator $T : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R)$, where $\Gamma_R = \partial B_R$. It is defined as follows: for any $f \in H^{1/2}(\Gamma_R)$,

$$Tf = \sum_{n \in \mathbb{Z}} k \frac{H_n^{(1)'}(kR)}{H_n^{(1)}(kR)} \hat{f}_n e^{in\theta}, \quad \hat{f}_n = \frac{1}{2\pi} \int_0^{2\pi} f e^{-in\theta} d\theta.$$
Dirichlet-to-Neumann operator

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$$Tf = \sum_{n \in \mathbb{Z}} k \frac{H_n^{(1)'}(kR)}{H_n^{(1)}(kR)} \hat{f}_n e^{i n \theta}, \quad \hat{f}_n = \frac{1}{2\pi} \int_0^{2\pi} f e^{-i n \theta} d\theta.$$

Looking at the representation of the solution $u$ in polar coordinates:

$$u(r, \theta) = \sum_{n \in \mathbb{Z}} \frac{H_n^{(1)}(kr)}{H_n^{(1)}(kR)} \hat{u}_n e^{i n \theta}, \quad \hat{u}_n = \frac{1}{2\pi} \int_0^{2\pi} u(R, \theta)e^{-i n \theta} d\theta,$$

it is obvious that it satisfies

$$\frac{\partial u}{\partial n}\bigg|_{\Gamma_R} = Tu.$$
Let $a : H^1(\Omega_R) \times H^1(\Omega_R) \to \mathbb{C}$ be the sesquilinear form

$$a(\varphi, \psi) = \int_{\Omega_R} \left( \nabla \varphi \cdot \nabla \bar{\psi} - k^2 \varphi \bar{\psi} \right) dx - \langle T \varphi, \psi \rangle_{\Gamma_R}.$$
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Given $g \in H^{-1/2}(\Gamma_R)$, find $u \in H^1(\Gamma_R)$ such that

$$a(u, \psi) = \langle g, \psi \rangle_{\Gamma_D} \quad \forall \psi \in H^1(\Omega_R), \mu > 0.$$
Reformulation

Let $a : H^1(\Omega_R) \times H^1(\Omega_R) \rightarrow \mathbb{C}$ be the sesquilinear form

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$$a(u, \psi) = \langle g, \psi \rangle_{\Gamma_D} \quad \forall \psi \in H^1(\Omega_R), \mu > 0.$$ 

$$\sup_{0 \neq \psi \in H^1(\Omega_R)} \frac{|a(\varphi, \psi)|}{\|\psi\|_{H^1(\Omega_R)}} \geq \mu \|\varphi\|_{H^1(\Omega_R)} \quad \forall \varphi \in H^1(\Omega_R).$$
Let $\alpha(r) = 1 + i\sigma(r)$ be the PML model medium property with

$$\sigma \in C(\mathbb{R}), \quad \sigma \geq 0, \quad \text{and} \quad \sigma = 0 \text{ for } r \leq R.$$ 

We denote by $\tilde{r}$ the complex radius defined by

$$\tilde{r} = \tilde{r}(r) = \begin{cases} 
  r & \text{if } r \leq R, \\
  \int_0^r \alpha(t)dt = r\beta(r) & \text{if } r \geq R.
\end{cases}$$
PML formulation

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\end{cases}$$

Let’s introduce now the PML equation:

$$\nabla \cdot (A \nabla w) + \alpha\beta k^2 w = 0 \quad \text{in } \Omega^{\text{PML}},$$

where $A = A(x)$ is a matrix which satisfies, in polar coordinates,

$$\nabla \cdot (A \nabla) = \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\beta r}{\alpha} \frac{\partial}{\partial r} \right) + \frac{\alpha}{\beta r^2} \frac{\partial^2}{\partial \theta^2}.$$
Now, the PML solution $\hat{u}$ in $\Omega_\rho = B_\rho \setminus \bar{D}$ is defined as the solution of the system

$$\nabla \cdot (A\nabla \hat{u}) + \alpha \beta k^2 \hat{u} = 0 \quad \text{in } \Omega_\rho,$$

$$\frac{\partial \hat{u}}{\partial n} = -g \quad \text{on } \Gamma_D,$$

$$\hat{u} = 0 \quad \text{on } \Gamma_\rho.$$
PML formulation (cont)

Now, the PML solution $\hat{u}$ in $\Omega_\rho = B_\rho \setminus \tilde{D}$ is defined as the solution of the system

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$$\frac{\partial \hat{u}}{\partial n} = -g \quad \text{on} \quad \Gamma_D,$$

$$\hat{u} = 0 \quad \text{on} \quad \Gamma_\rho.$$

Again, we introduce the sesquilinear form $\hat{a} : H^1(\Omega_R) \times H^1(\Omega_R) \to \mathbb{C}$ by

$$\hat{a}(\varphi, \psi) = \int_{\Omega_R} (A \nabla \varphi \cdot \nabla \bar{\psi} - k^2 \alpha \beta \varphi \bar{\psi}) \, dx - \langle \hat{T} \varphi, \psi \rangle_{\Gamma_R},$$

and

$$\hat{a}(\hat{u}, \psi) = \langle g, \psi \rangle_{\Gamma_D} \quad \forall \psi \in H^1(\Omega_R).$$
Similar to the previous problem, we can reformulate the problem in the bounded domain $\Omega_R$ by imposing the boundary condition

$$\frac{\partial \hat{u}}{\partial n} \bigg|_{\Gamma_R} = \hat{T} \hat{u},$$

where $\hat{T} : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R)$ is defined as follows: given $f \in H^{1/2}(\Gamma_R)$,

$$\hat{T} f = \frac{\partial \zeta}{\partial n} \bigg|_{\Gamma_R},$$

where $\zeta \in H^1(\Omega^{\text{PML}})$ satisfies

$$\nabla \cdot (A \nabla \zeta) + \alpha \beta k^2 \zeta = 0 \quad \text{in} \quad \Omega^{\text{PML}},$$

$$\zeta = f \quad \text{on} \quad \Gamma_R,$$

$$\zeta = 0 \quad \text{on} \quad \Gamma_\rho.$$
The PML equation in the layer

Lets look now at the Dirichlet problem in the PML layer $\Omega^{PML}$ only: The solution $w$ solves

$$\nabla \cdot (A \nabla w) + \alpha \beta k^2 w = 0 \quad \text{in } \Omega^{PML},$$

$$w = 0 \quad \text{on } \Gamma_R,$$

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where $q \in H^{1/2}(\Gamma_\rho)$. With $\hat{b} : H^1(\Omega^{\text{PML}}) \times H^1(\Omega^{\text{PML}}) \to \mathbb{C}$ defined to be

$$\hat{b}(\varphi, \psi) = \int_{\Gamma_\rho} \int_0^{2\pi} \left( \frac{\beta r}{\alpha} \frac{\partial \varphi}{\partial r} \frac{\partial \bar{\psi}}{\partial r} + \frac{\alpha}{\beta r} \frac{\partial \varphi}{\partial \theta} \frac{\partial \bar{\psi}}{\partial \theta} - \alpha \beta k^2 r \varphi \bar{\psi} \right) dr d\theta,$$

we can write down the weak formulation for this problem: given $q \in H^{1/2}(\Gamma_\rho)$, find $w \in H^1(\Omega^{\text{PML}})$ such that $w = 0$ on $\Gamma_R$, $w = q$ on $\Gamma_\rho$, and

$$\hat{b}(w, \varphi) = 0 \quad \forall \varphi \in H^1_0(\Omega^{\text{PML}}).$$
Medium property

We make the following assumption for the fictitious medium property $\sigma$:

\[(H1): \quad \sigma = \sigma_0 \left( \frac{r - R}{\rho - R} \right)^m \quad \text{for some } \sigma_0 > 0 \text{ and } m \in \mathbb{N}.\]
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(H1): $\sigma = \sigma_0 \left( \frac{r-R}{\rho-R} \right)^m$ for some $\sigma_0 > 0$ and $m \in \mathbb{N}$.

We know that $\beta(r) = r^{-1} \int_0^r \alpha(t) dt$, and therefore $\beta(r) = 1 + i\hat{\sigma}(r)$, where

$$\hat{\sigma}(r) = \frac{1}{r} \int_R^r \sigma(t) dt = \frac{\sigma_0}{m + 1} \frac{r - R}{r} \left( \frac{r - R}{\rho - R} \right)^m.$$

Therefore, $\hat{\sigma} \leq \sigma \ \forall r \geq R$. 


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Therefore, $\hat{\sigma} \leq \sigma \ \forall r \geq R$.

**\( \text{H2} \)** There exists a unique solution to the Dirichlet PML problem in the PML layer $\Omega^{\text{PML}}$. 
Theorem 1

We give the following theorem (without proof) as the main objective of this subsection:

**Theorem 1**

Let (H1)-(H2) be satisfied. There exists a constant $C > 0$ independent of $k, R, \rho,$ and $\sigma_0$ such that the following estimates hold:

\[
\| \| \alpha \|^{-1} \nabla w \|_{L^2(\Omega_{\text{PML}})} \leq C \hat{C}^{-1} (1 + kR) |\alpha_0| \| q \|_{H^{1/2}(\Gamma_\rho)},
\]

\[
\left\| \frac{\partial w}{\partial n} \right\|_{H^{-1/2}(\Gamma_R)} \leq C \hat{C}^{-1} (1 + kR)^2 |\alpha_0|^2 \| q \|_{H^{1/2}(\Gamma_\rho)}.
\]

where $\alpha_0 = 1 + i\sigma_0$. 
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\left\| \alpha^{-1}\nabla w \right\|_{L^2(\Omega_{PML})} \leq C\hat{C}^{-1}(1 + kR)|\alpha_0|\|q\|_{H^{1/2}(\Gamma_\rho)},
$$

$$
\left\| \frac{\partial w}{\partial n} \right\|_{H^{-1/2}(\Gamma_R)} \leq C\hat{C}^{-1}(1 + kR)^2|\alpha_0|^2\|q\|_{H^{1/2}(\Gamma_\rho)}.
$$

where $\alpha_0 = 1 + i\sigma_0$.

We will need these estimates later to prove the main theorem of this talk …
Propagation operator

To prove the convergence of the just considered PML problem to the original scattering problem, we need to introduce the propagation operator $P : H^{1/2}(\Gamma_R) \rightarrow H^{1/2}(\Gamma_\rho)$ defined as (Lassas and Somersalo):

$$P(f) = \sum_{n \in \mathbb{Z}} \frac{H_n^{(1)}(k\tilde{\rho})}{H_n^{(1)}(kR)} \hat{f}_n e^{in\theta}, \quad \hat{f}_n = \frac{1}{2\pi} \int_0^{2\pi} f e^{-in\theta} d\theta.$$
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One can also show that

$$\|P(f)\|_{H^{1/2}(\Gamma_\rho)} \leq e^{-k\Im(\tilde{\rho})\sqrt{1 - \frac{R^2}{|\tilde{\rho}|^2}}} \|f\|_{H^{1/2}(\Gamma_R)}, \quad \forall r \geq R.$$

**Lemma 2:**
Let (H1)-(H2) be satisfied. Then, we have

\[ \| Tf - \hat{T}f \|_{H^{-1/2}(\Gamma_R)} \leq C\hat{C}^{-1}(1 + kR)^2|\alpha_0|^2e^{-k\Im(\bar{\rho})}\sqrt{1 - \frac{R^2}{|\bar{\rho}|^2}} \| f \|_{H^{1/2}(\Gamma_R)}. \]
Lemma 2:
Let (H1)-(H2) be satisfied. Then, we have

\[ \|Tf - \hat{T}f\|_{H^{-1/2}(\Gamma_R)} \leq C\hat{C}^{-1}(1 + kR)^2|\alpha_0|^2e^{-k\Im(\tilde{\rho})}\sqrt{1 - \frac{R^2}{|\tilde{\rho}|^2}} \|f\|_{H^{1/2}(\Gamma_R)}. \]

Theorem 2:
Let again (H1)-(H2) be satisfied. Then, for sufficiently large \( \sigma_0 > 0 \), the PML problem has a unique solution \( \hat{u} \in H^1(\Omega_\rho) \). Moreover, we have the following estimate:

\[ \|u - \hat{u}\|_{H^1(\Omega_R)} \leq C\hat{C}^{-1}(1 + kR)^2|\alpha_0|^2e^{-k\Im(\tilde{\rho})}\sqrt{1 - \frac{R^2}{|\tilde{\rho}|^2}} \|\hat{u}\|_{H^{1/2}(\Gamma_R)}. \]
Third Part

FINITE ELEMENTS AND
THE MAIN THEOREM
The Finite Element Method (FEM)

**Task:** By discretization, transform a variational boundary value problem to a system of finite number of equations for real unknowns. I.e. transform the linear variational problem

\[ u \in V : a(u, v) = f(v) \quad \forall v \in V \]

to

\[ u_N \in V_h : a(u_N, v_N) = f(v_N) \quad \forall v_N \in V_h. \]
The Finite Element Method (FEM)

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Do it by **tria**ngulation of space \( \Omega \):
Basis functions $\phi_1, \ldots, \phi_N$ for a finite element space $V_h$ built on a mesh $\mathcal{M}_h$ satisfy:

1. each $\phi_i$ associated with a single cell/edge/face/vertex of $\mathcal{M}_h$,
2. $\text{supp}(\phi_i) = \bigcup\{\bar{K} : K \in \mathcal{M}_h, p \subset \bar{K}\}$, if $\phi_i$ associated with cell/edge/face/vertex $p$. 
FEM basis functions

Basis functions $\phi_1, \ldots, \phi_N$ for a finite element space $V_h$ built on a mesh $\mathcal{M}_h$ satisfy:

- each $\phi_i$ associated with a single cell/edge/face/vertex of $\mathcal{M}_h$,
- $\text{supp}(\phi_i) = \bigcup\{\bar{K} : K \in \mathcal{M}_h, p \subset \bar{K}\}$, if $\phi_i$ associated with cell/edge/face/vertex $p$. 
Let $V_h(\mathcal{M}_h) = \mathcal{N}_h := \text{set of nodes of } \mathcal{M}_h$. Then, the nodal basis is defined as: If $\mathcal{N}_h = \{a_1, \ldots, a_N\}$, nodal basis $\Phi_h := \{\phi_1, \ldots, \phi_N\}$ defined by $\phi_i(a_j) = \delta_{ij}$. 
Let $V_h(M_h) = N_h := \text{set of nodes of } M_h$.
Then, the nodal basis is defined as: If $N_h = \{a_1, \ldots, a_N\}$, nodal basis $\Phi_h := \{\phi_1, \ldots, \phi_N\}$ defined by $\phi_i(a_j) = \delta_{ij}$.
Now, we introduce the finite element approximation of the PML problem. From now on, we assume $g \in L^2(\Gamma_D)$. Let $b : H^1(\Omega_\rho) \times H^1(\Omega_\rho) \to \mathbb{C}$ be the sesquilinear form given by

$$b(\varphi, \psi) = \int_{\Omega_\rho} (A \nabla \varphi \cdot \nabla \psi - \alpha \beta k^2 \varphi \overline{\psi}) dx.$$
Finite element approximation

Now, we introduce the finite element approximation of the PML problem. From now on, we assume \( g \in L^2(\Gamma_D) \). Let \( b : H^1(\Omega_\rho) \times H^1(\Omega_\rho) \to \mathbb{C} \) be the sesquilinear form given by

\[
b(\varphi, \psi) = \int_{\Omega_\rho} (A \nabla \varphi \cdot \nabla \psi - \alpha \beta k^2 \varphi \overline{\psi}) \, dx.
\]

Furthermore, denote by \( H^1_{(0)}(\Omega_\rho) = \{ v \in H^1(\Omega_\rho) : v = 0 \text{ on } \Gamma_\rho \} \). Then, we can write down the weak formulation for the PML problem: given \( g \in L^2(\Gamma_D) \), find \( \hat{u} \in H^1_{(0)}(\Omega_\rho) \) such that

\[
b(\hat{u}, \psi) = \int_{\Gamma_D} g \overline{\psi} \, ds \quad \forall \psi \in H^1_{(0)}(\Omega_\rho).
\]
Finite element notation

Let $\Gamma^h_\rho$, which consists of piecewise segments whose vertices lie on $\Gamma_\rho$, be an approximation of $\Gamma_\rho$. 
Finite element notation

- Let $\Gamma_h^\rho$, which consists of piecewise segments whose vertices lie on $\Gamma_\rho$, be an approximation of $\Gamma_\rho$.

- Let $M_h$ be a regular triangulation of the domain $\Omega_h^\rho$. 
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- Let $\mathcal{M}_h$ be a regular triangulation of the domain $\Omega^h_\rho$.

- Assume the elements $K \in \mathcal{M}_h$ may have one curved edge align with $\Gamma_D$, such that $\Omega^h_\rho = \bigcup_{K \in \mathcal{M}_h} K$. 
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- Let $\mathcal{M}_h$ be a regular triangulation of the domain $\Omega^h_\rho$.

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- Let $V_h \subset H^1(\Omega^h_\rho)$ be the conforming linear finite element space over $\Omega^h_\rho$, and $V^0_h = \{v_h \in V_h : v_h = 0 \text{ on } \Gamma^h_\rho\}$.
Now, we can formulate the finite element approximation to the variational PML problem: find $u_h \in V_h^0$ such that

$$b(u_h, \psi_h) = \int_{\Gamma_D} g \bar{\psi}_h ds \quad \forall \psi_h \in V_h^0.$$ 

and the discrete inf-sup condition

$$\sup_{0 \neq \psi_h \in V_h^0} \frac{|b(\varphi_h, \psi_h)|}{\|\psi_h\|_{H^1(\Omega_\rho)}} \geq \hat{\mu} \|\varphi_h\|_{H^1(\Omega_\rho)} \quad \forall \varphi_h \in V_h^0, \hat{\mu} > 0.$$
Finite elements

Now, we can formulate the finite element approximation to the variational PML problem: find $u_h \in V_h^0$ such that

$$b(u_h, \psi_h) = \int_{\Gamma_D} g \overline{\psi_h} ds \quad \forall \psi_h \in V_h^0.$$ 

and the discrete inf-sup condition

$$\sup_{0 \neq \psi_h \in V_h^0} \frac{|b(\varphi_h, \psi_h)|}{\|\psi_h\|_{H^1(\Omega)}} \geq \hat{\mu} \|\varphi_h\|_{H^1(\Omega)} \quad \forall \varphi_h \in V_h^0, \hat{\mu} > 0.$$ 

Since we are interested in a posterior error estimates and the associated adaptive algorithm, we simply assume that the discrete problem has a unique solution $u_h \in V_h^0$. 
For any $K \in \mathcal{M}_h$, denote by $h_K$ its diameter.
Finite elements, definitions

- For any $K \in \mathcal{M}_h$, denote by $h_K$ its diameter.
- Let $\mathcal{B}_h$ denote the set of all sides that do not lie on $\Gamma_D$ and $\Gamma^h_{\rho}$.
Finite elements, definitions

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- For any $e \in \mathcal{B}_h$, $h_e$ stands for its length.
- For any $K \in \mathcal{M}_h$, introduce the residual

$$R_h := \nabla \cdot (A\nabla u_h|_K) + \alpha \beta k^2 u_h|_K.$$
Finite elements, definitions

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  \[ R_h := \nabla \cdot (A \nabla u_h|_K) + \alpha \beta k^2 u_h|_K. \]
- For any interior side $e \in \mathcal{B}_h$, which is the common side of $K_1$ and $K_2 \in \mathcal{M}_h$, define the jump residual across $e$:
  \[ J_e := (A \nabla u_h|_{K_1} - A \nabla u_h|_{K_2}) \cdot \nu_e, \]
  where the unit normal vector $\nu_e$ to $e$ points from $K_2$ to $K_1$. 

Finite elements, definitions

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  \[ J_e := (A\nabla u_h|_{K_1} - A\nabla u_h|_{K_2}) \cdot \nu_e, \]
  where the unit normal vector $\nu_e$ to $e$ points from $K_2$ to $K_1$.

- If $e = \Gamma_D \cap \partial K$ for some element $K \in \mathcal{M}_h$, then we define the jump residual to be:
  \[ J_e := 2(\nabla u_h|_K \cdot \mathbf{n} + g). \]
Finite elements, definitions (cont)

For any $K \in \mathcal{M}_h$, denote by $\eta_K$ the local error estimator which is defined by

$$
\eta_K = \max_{x \in \tilde{K}} w(x) \cdot \left( \| h_K R_h \|_{L^2(K)}^2 + \frac{1}{2} \sum_{e \subset \partial K} h_e \| J_e \|_{L^2(e)}^2 \right)^{1/2},
$$

where $\tilde{K}$ is the union of all elements having nonempty intersection with $K$, and

$$
w(x) = \begin{cases} 
1 & \text{if } x \in \tilde{\Omega}_R, \\
|\alpha_0\alpha| e^{-k\Im(\tilde{r})} \sqrt{1 - \frac{r^2}{|\tilde{r}|^2}} & \text{if } x \in \Omega^{PML}.
\end{cases}
$$
Theorem 3:
There exists a constant $C$ depending only on the minimum angle of the mesh $\mathcal{M}_h$ such that the following a posterior error estimate is valid:

$$
\| u - u_h \|_{H^1(\Omega_R)} \leq C \hat{C}^{-1} \sqrt{\Lambda(kR)(1 + kR)} \left( \sum_{K \in \mathcal{M}_h} \eta_K^2 \right)^{1/2} \\
+ C \hat{C}^{-1} (1 + kR)^2 |\alpha_0|^2 e^{-k\Im(\bar{\rho})} \sqrt{1 - \frac{R^2}{|\rho|^2}} \| u_h \|_{H^{1/2}(\Gamma_R)},
$$

where $\Lambda(kR) = \max \left( 1, \frac{|H_0^{(1)'}(kR)|}{|H_0^{(1)}(kR)|} \right)$. 
Main Theorem

Theorem 3:
There exists a constant $C$ depending only on the minimum angle of the mesh $\mathcal{M}_h$ such that the following a posterior error estimate is valid:

$$
\| u - u_h \|_{H^1(\Omega_R)} \leq C \hat{C}^{-1} \sqrt{\Lambda(kR)(1 + kR)} \left( \sum_{K \in \mathcal{M}_h} \eta^2_K \right)^{1/2}
$$

$$
+ C \hat{C}^{-1} (1 + kR)^2 |\alpha_0|^2 e^{-k \Im(\tilde{\rho}) \sqrt{1 - \frac{r^2}{|\tilde{\rho}|^2}}} \| u_h \|_{H^{1/2}(\Gamma_R)},
$$

where $\Lambda(kR) = \max \left( 1, \frac{|H_0^{(1)'}(kR)|}{|H_0^{(1)}(kR)|} \right)$.

The important exponentially decaying factor $e^{-k \Im(\tilde{\rho}) \sqrt{1 - \frac{r^2}{|\tilde{\rho}|^2}}}$ in the PML region $\Omega^{\text{PML}}$ allows us to take thicker PML layers without introducing unnecessary fine meshes away from the fixed domain $\Omega_R$. 
Symmetry in $\hat{T}$

For any $\varphi \in H^1(\Omega_R)$, let $\tilde{\varphi}$ be its extension in $\Omega^{\text{PML}}$ such that

\[
\nabla \cdot (\tilde{A} \nabla \tilde{\varphi}) + \alpha^2 \beta^2 \varphi = 0 \quad \text{in } \Omega^{\text{PML}},
\]

\[
\tilde{\varphi} = \varphi \quad \text{on } \Gamma_R,
\]

\[
\tilde{\varphi} = 0 \quad \text{on } \Gamma_\rho.
\]
Symmetry in $\hat{T}$

For any $\varphi \in H^1(\Omega_R)$, let $\tilde{\varphi}$ be its extension in $\Omega^{PML}$ such that

$$\nabla \cdot (\bar{A} \nabla \tilde{\varphi}) + \bar{\alpha} \bar{\beta} k^2 \tilde{\varphi} = 0 \quad \text{in } \Omega^{PML},$$

$$\tilde{\varphi} = \varphi \quad \text{on } \Gamma_R,$$

$$\tilde{\varphi} = 0 \quad \text{on } \Gamma_\rho.$$

Lemma 3:
Let (H2) be satisfied. For any $\varphi, \psi \in H^1(\Omega^{PML})$, we have

$$\langle \hat{T} \varphi, \psi \rangle_{\Gamma_R} = \langle \hat{T} \psi, \bar{\varphi} \rangle_{\Gamma_R}.$$
Symmetry in $\hat{T}$

For any $\varphi \in H^1(\Omega_R)$, let $\tilde{\varphi}$ be its extension in $\Omega^{\text{PML}}$ such that

\[
\nabla \cdot (\tilde{A} \nabla \tilde{\varphi}) + \tilde{\alpha} \beta k^2 \tilde{\varphi} = 0 \quad \text{in } \Omega^{\text{PML}},
\]

\[
\tilde{\varphi} = \varphi \quad \text{on } \Gamma_R,
\]

\[
\tilde{\varphi} = 0 \quad \text{on } \Gamma_\rho.
\]

**Lemma 3:**

Let (H2) be satisfied. For any $\varphi, \psi \in H^1(\Omega^{\text{PML}})$, we have

\[
\langle \hat{T} \varphi, \psi \rangle_{\Gamma_R} = \langle \hat{T} \tilde{\psi}, \tilde{\varphi} \rangle_{\Gamma_R}.
\]

Whenever no confusion of the notation incurred, we shall write in the following $\tilde{\varphi}$ as $\varphi$ in $\Omega^{\text{PML}}$. 
Lemma 4:
For any $\varphi \in H^1(\Omega_R)$, which is extended to be a function in $H^1(\Omega_\rho)$, and $\varphi_h \in V_h^0$, we have

$$a(u - u_h, \varphi) = \int_{\Gamma_D} g(\varphi - \varphi_h) - b(u_h, \varphi - \varphi_h) + \langle Tu_h - \hat{T}u_h, \varphi \rangle_{\Gamma_R}.$$
**Lemma 4:**

For any $\varphi \in H^1(\Omega_R)$, which is extended to be a function in $H^1(\Omega_\rho)$, and $\varphi_h \in V_h^0$, we have

$$a(u - u_h, \varphi) = \int_{\Gamma_D} g(\varphi - \varphi_h) - b(u_h, \varphi - \varphi_h) + \langle Tu_h - \hat{T}u_h, \varphi \rangle_{\Gamma_R}.$$ 

Let's now prove this important Lemma!
Interpolation Operator

Since we are going to interpolate nonsmooth functions satisfying boundary conditions, we resort to an interpolation operator
\[ \Pi_h : H^1_0(\Omega^h_{\rho}) \rightarrow V^0_h \] of Scott-Zhang.

Notation:

- Let \( \mathcal{N}_h = \{ a_i \}_{i=1}^N \) be the set of all nodes of \( \mathcal{M}_h \).
Interpolation Operator

Since we are going to interpolate nonsmooth functions satisfying boundary conditions, we resort to an interpolation operator
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Notation:

- Let \( \mathcal{N}_h = \{ a_i \}_{i=1}^{N} \) be the set of all nodes of \( \mathcal{M}_h \).
- Let \( \{ \phi_i \}_{i=1}^{N} \) be the corresponding nodal basis of \( V_h \).
Interpolation Operator

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Notation:

- Let \( \mathcal{N}_h = \{ a_i \}_{i=1}^{N} \) be the set of all nodes of \( \mathcal{M}_h \).
- Let \( \{ \phi_i \}_{i=1}^{N} \) be the corresponding nodal basis of \( V_h \).
- For any node \( a_i \) which is interior to \( \Omega^h_\rho \) or on the boundary \( \Gamma_R \), we take \( \sigma_i = e \), any side in \( \mathcal{B}_h \) having \( a_i \) as one of its vertex.
Interpolation Operator

Since we are going to interpolate nonsmooth functions satisfying boundary conditions, we resort to an interpolation operator $\Pi_h : H^1_{(0)}(\Omega^h_\rho) \to V^0_h$ of Scott-Zhang.

Notation:

- Let $\mathcal{N}_h = \{a_i\}_{i=1}^N$ be the set of all nodes of $\mathcal{M}_h$.
- Let $\{\phi_i\}_{i=1}^N$ be the corresponding nodal basis of $V_h$.
- For any node $a_i$ which is interior to $\Omega^h_\rho$ or on the boundary $\Gamma_R$, we take $\sigma_i = e$, any side in $\mathcal{B}_h$ having $a_i$ as one of its vertex.
- For any node $a_i$ which is on the boundary $\Gamma^h_\rho$, we take $\sigma_i$ as any side on $\Gamma^h_\rho$ with one vertex $a_i$. 
Let $a_{i,1} = a_i$, and $\{a_{i,j}\}_{j=1}^2$ the set of nodal points in $\sigma_i$ with nodal basis $\{\phi_{i,j}\}_{j=1}^2$. 
Let $a_{i,1} = a_i$, and $\{a_{i,j}\}_{j=1}^2$ the set of nodal points in $\sigma_i$ with nodal basis $\{\phi_{i,j}\}_{j=1}^2$.

Let $\{\psi_{i,j}\}_{j=1}^2$ be the $L^2(\sigma_i)$ dual basis:

$$\int_{\sigma_i} \psi_{i,j}(x) \phi_{i,k}(x) dx = \delta_{jk}, \quad j, k = 1, 2.$$
Interpolation Operator (cont)

We now define the interpolation operator $\Pi_h : H^1(\Omega^h_\rho) \rightarrow V_h$ to be

$$\Pi_h v(x) = \sum_{i=1}^{N} \phi_i(x) \int_{\sigma_i} \psi_i(x)v(x)dx.$$  

One can show the following properties of $\Pi_h$:

- $\Pi_h v \in V_h^0$ if $v \in H^1_{(0)}(\Omega^h_\rho)$.
- $\|v - \Pi_h v\|_{L^2(K)} \leq Ch_k\|\nabla v\|_{L^2(\tilde{K})}$,
- $\|v - \Pi_h v\|_{L^2(e)} \leq Ch^1/2_e\|\nabla v\|_{L^2(\tilde{e})}$.

$\tilde{K}$ and $\tilde{e}$ denote the union of all elements in $\mathcal{M}_h$ having non-empty intersection with $K \in \mathcal{M}_h$ and the side $e$, respectively.
Fourth Part

IMPLEMENTATION AND EXAMPLES
Implementation

We use the a posteriori error estimate in the main theorem to determine the PML parameters. Just as before, we choose the PML medium property to be a power function. So, only the thickness $\rho - R$ of the layer and the medium parameter $\sigma_0$ are left to be specified.
We use the a posteriori error estimate in the main theorem to determine the PML parameters. Just as before, we choose the PML medium property to be a power function. So, only the thickness $\rho - R$ of the layer and the medium parameter $\sigma_0$ are left to be specified.

First, we choose the exponentially decaying factor to be small such that it becomes negligible compared with the finite element discretization errors. Now, we set up an algorithm to adapt mesh size according to the a posteriori error estimate.
Algorithm

Let $TOL > 0$ be the tolerance for the error. Set $m = 2$. Now, the strategy is:

- Choose $\rho$ and $\sigma_0$ such that the exponentially decaying factor $\hat{\omega} \leq 10^{-8}$;
Let $TOL > 0$ be the tolerance for the error. Set $m = 2$. Now, the strategy is:

1. Choose $\rho$ and $\sigma_0$ such that the exponentially decaying factor $\hat{\omega} \leq 10^{-8}$;

2. Set the computational domain $\Omega_\rho = B_\rho \setminus \Gamma_D$ and generate an initial mesh $\mathcal{M}_h$ over $\Omega_\rho$;
Algorithm

Let $TOL > 0$ be the tolerance for the error. Set $m = 2$. Now, the strategy is:

- Choose $\rho$ and $\sigma_0$ such that the exponentially decaying factor $\hat{\omega} \leq 10^{-8}$;

- Set the computational domain $\Omega_\rho = B_\rho \setminus \overline{\Gamma}_D$ and generate an initial mesh $\mathcal{M}_h$ over $\Omega_\rho$;

- While $ERR > TOL$ do
  - refine the mesh $\mathcal{M}_h$: if $\eta_K > \frac{1}{2} \max_{\tilde{K} \in \mathcal{M}_h} \eta_{\tilde{K}}$, refine the element $K \in \mathcal{M}_h$;
  - solve the discrete problem (3.3) on $\mathcal{M}_h$;
  - compute error estimators on $\mathcal{M}_h$;
Let $TOL > 0$ be the tolerance for the error. Set $m = 2$. Now, the strategy is:

- Choose $\rho$ and $\sigma_0$ such that the exponentially decaying factor $\hat{\omega} \leq 10^{-8}$;

- Set the computational domain $\Omega_\rho = B_\rho \setminus \Gamma_D$ and generate an initial mesh $\mathcal{M}_h$ over $\Omega_\rho$;

- While $\text{ERR} > TOL$ do
  - refine the mesh $\mathcal{M}_h$: if $\eta_K > \frac{1}{2} \max_{K \in \mathcal{M}_h} \eta_K$, refine the element $K \in \mathcal{M}_h$;
  - solve the discrete problem (3.3) on $\mathcal{M}_h$;
  - compute error estimators on $\mathcal{M}_h$;

- End While.
Example 1: Unit circle

Let the scatterer $D$ be the unit circle. Let the exact solution be $u = H_0^{(1)}(kr)$, where $r = |x|$. Take $R = 2$, and $k = 1$. ($\rho = 4R$ and $\sigma_0 = 10$)
Example 1: Unit circle (cont)

Fig. 5.4. The mesh of 6668 nodes after 10 adaptive iterations when \( \rho = 4R \) for Example 1.
Example 2

![Diagram of a complex geometry](image)

**Fig. 5.1.** The geometry of the scatter for Example 2.
Example 2 (cont)

FIG. 5.3. Quasi-optimality of the adaptive mesh refinement of the a posteriori error estimator for Example 2.

FIG. 5.4. The real part of the far fields in the incident direction for Example 2.

FIG. 5.7. The real part of the far fields in the reflective direction for Example 2.
Example 2

Fig. 5.8. The mesh of 7048 nodes after 13 adaptive iterations when $\rho = 3R$ for Example 2.
Example 2

Fig. 5.9. The contour plot of the real part of the solution when $\rho = 3R$ for Example 2.
The End

Remarks / Questions