Are Absorbing Boundary Conditions and Perfectly Matched Layers Really so Different?

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Joint work with Achim Schädle
History of Absorbing Boundary Conditions

Engquist and Majda (1977): Wave Propagation: “In practical calculations, it is often essential to introduce artificial boundaries to limit the area of computation. Unfortunately [transparent boundary conditions] necessarily have to be non-local in both space and time and thus are not useful for practical calculations”

Bayliss Turkel (1980): Wave-Like Equations: “In the numerical computation of hyperbolic equations it is not practical to use infinite domains. Instead, one truncates the domain with an artificial boundary“

Halpern (Wave Propagation 1982, Diffusion 1987): “…one often introduces artificial boundaries with boundary conditions chosen so that the problem one gets is well-posed and the solution is ’as close as possible’ to that of the original problem”
Truncation of the unbounded domain using
- A transparent (or exact) boundary condition (TBC) or an absorbing (or inexact) boundary condition (ABC)
- A perfectly matched layer (PML)
Interest for Domain Decomposition Methods

Computation performed with an optimized Schwarz method on 16 subdomains

An optimized Schwarz method with two-sided Robin transmission conditions for the Helmholtz equation (G, Halpern and Magoules, 2006)
An Advice from the Past

Émile Picard (1893): Sur l’application des méthodes d’approximations successives à l’étude de certaines équations différentielles ordinaires

Les méthodes d’approximation dont nous faisons usage sont théoriquement susceptibles de s’appliquer à toute équation, mais elles ne deviennent vraiment intéressantes pour l’étude des propriétés des fonctions définies par les équations différentielles que si l’on ne reste pas dans les généralités et si l’on envisage certaines classes d’équations.
Construction of Transparent Boundary Conditions

We consider the model problem

\[(\eta - \Delta)u = f \quad \text{in } \Omega = \mathbb{R} \times (0, \pi)\]
\[u(x, 0) = 0\]
\[u(x, \pi) = 0\]

with \(f\) compactly supported in \(\Omega_{int} = (0, 1) \times (0, \pi)\), and \(u\) bounded at infinity.

In order to solve this problem on a computer, the computational domain needs to be truncated in \(x\), and an artificial boundary condition needs to be imposed at \(x = 0\) and \(x = 1\).
Construction of Transparent Boundary Conditions

Based on the decomposition of \( \Omega = \overline{\Omega}^- \cup \overline{\Omega}_{int} \cup \overline{\Omega}^+ \)

and the equivalent coupled problems

\[
\begin{align*}
(\eta - \Delta)v^- &= 0 \quad \text{in } \Omega^- \\
v^- &= v \quad \text{on } \Gamma_0 \\
\partial_n v &= \partial_n v^- \quad \text{on } \Gamma_0 \\
(\eta - \Delta)v &= f \quad \text{in } \Omega_{int} \\
\partial_n v &= \partial_n v^+ \quad \text{on } \Gamma_1 \\
v^+ &= v \quad \text{on } \Gamma_1 \\
(\eta - \Delta)v^+ &= 0 \quad \text{in } \Omega^+
\end{align*}
\]

with homogeneous conditions at \( y = 0 \) and \( y = \pi \).
Solution of Exterior Problems

The exterior problems are independent of the data $f$ and can be readily solved using Fourier series in $y$: for example on $\Omega_+$ we have

$$(\eta + k^2 - \partial_{xx})\hat{v}^+ = 0$$

an ordinary differential equation, whose solution is

$$\hat{v}^+(x, k) = A(k)e^{\sqrt{\eta+k^2}x} + B(k)e^{-\sqrt{\eta+k^2}x}$$

Since $v^+$ needs to stay bounded for $x \to +\infty$, we have $A(k) = 0$ and using the Dirichlet data $v^+ = v$ at $x = 1$ we obtain

$$\hat{v}^+(x, k) = \hat{v}(1, k)e^{-\sqrt{\eta+k^2}(x-1)}$$

This implies

$$\partial_x \hat{v}^+(x, k)|_{x=1} = -\sqrt{\eta + k^2}\hat{v}(x, k)|_{x=1}$$

and similarly on the left boundary $\Gamma_0$, we obtain

$$-\partial_x \hat{v}^-(x, k)|_{x=0} = -\sqrt{\eta + k^2}\hat{v}(x, k)|_{x=0}$$
Closing the Interior Problem

Using these solutions for the interior problem, we get

\[
(\eta - \Delta)v = f \quad \text{in } \Omega_{int} \\
\partial_n v = \mathcal{F}^{-1}(-\sqrt{\eta + k^2} \hat{v}) \quad \text{on } \Gamma_0 \\
\partial_n v = \mathcal{F}^{-1}(-\sqrt{\eta + k^2} \hat{v}) \quad \text{on } \Gamma_1
\]

where the inverse transform in general is a convolution:

\[
\mathcal{F}^{-1}(-\sqrt{\eta + k^2} \hat{v}) = \int_{-\infty}^{\infty} f(y - \xi)v(\cdot, \xi)d\xi
\]

with

\[
\mathcal{F}(f(y)) = -\sqrt{\eta + k^2}.
\]

By construction, \(v\) coincides with \(u\) in \(\Omega_{int}\), and the conditions obtained are called transparent boundary conditions (TBCs). They require a non-local convolution boundary condition.
Using Transparent Boundary Conditions

Because of their non-local nature, one often approximates TBCs and obtains **Absorbing Boundary Conditions (ABCs)**:

- by polynomial or rational approximations of the symbol (Enquist, Majda, Halpern, Bruneau-Di Menza, Nataf, Japhet, Szeftel, Shibata ...)
- by approximation of the convolution kernel (Hairer, Lubich, Schlichte, Greengard, Strain, Schädle ...)
- using quadrature rules (Mayfield, Baskakov and Popov, ...)

**Remark:** To couple an incoming field $u_{in}$ from $\Omega^+$:

$$\partial_x (v - u_{in}) = \mathcal{F}^{-1}(-\sqrt{\eta + k^2(\hat{v} - \hat{u}_{in}))} \quad \text{on } \Gamma_1$$

which by linearity is equivalent to

$$\partial_x v - \mathcal{F}^{-1}(-\sqrt{\eta + k^2\hat{v})} = \partial_x u_{in} - \mathcal{F}^{-1}(-\sqrt{\eta + k^2\hat{u}_{in})} \quad \text{on } \Gamma_1$$
Perfectly Matched Layers

**J. Berenger (1994):** A perfectly matched layer for the absorption of electromagnetic waves

*Split-Field PML:* Original idea, split the electromagnetic fields into two unphysical fields in the PML region

![Diagram of PML region with coordinates](image)

**S.D. Gedney (1996):** An anisotropic perfectly matched layer absorbing media for the truncation of FDTD latices

*Uniaxial PML (UPML):* The PML is described as an artificial anisotropic absorbing material
Stretched-Coordinate PML

**W.C. Chew and W. H. Weedon (1994):** A 3d perfectly matched medium from modified Maxwell’s equations with stretched coordinates

**F.L. Teixeira and W.C. Chew (1998):** General closed-form PML constitutive tensors to match arbitrary bianisotropic and dispersive linear media

**Idea:** Analytic continuation of the solution and equation to a complex $x$ contour which changes oscillating waves into exponentially decaying waves outside the region of interest:

$$e^{ikx} \rightarrow e^{ik(\Re(x)+i\Im(x))} = e^{ik\Re(x)}e^{-k\Im(x)}$$

Then perform a coordinate transform to express the complex $x$ as a function of a real coordinate, which leads to complex materials:

$$\frac{\partial}{\partial x} \rightarrow \frac{1}{1 + \frac{i\sigma(x)}{k}} \frac{\partial}{\partial x}$$
Example of a Coordinate Stretching

- **ABS and PML**
- **Martin J. Gander**
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Alternative Formulation: the Pole Condition


“The pole condition is a general concept for the theoretical analysis and the numerical solution of a variety of wave propagation problems. It says that the Laplace transform of the physical solution in the radial direction has no poles in the lower complex halfplane.”

\[ \Gamma \]

\[ \Omega_{int} \]
The Pole Condition for our Model Problem

On \( \Omega_+ \) we had after a Fourier transform

\[
(\eta + k^2 - \partial_{xx})\hat{v}^+ = 0
\]

Applying a Laplace transform in the radial, i.e. \( x \) direction, we obtain

\[
(\eta + k^2 - s^2)\tilde{v}^+(s, k) - \partial_n\hat{v}^+(1, k) - s\hat{v}^+(1, k) = 0
\]

Hence

\[
\tilde{v}^+(s, k) = \frac{\partial_n\hat{v}^+(1, k) + s\hat{v}^+(1, k)}{\eta + k^2 - s^2}
\]

This solution has poles at \( s = \pm \sqrt{\eta + k^2} \), and a partial fraction expansion gives

\[
\tilde{v}^+(s, k) = \frac{\hat{v}^+(1, k) - \frac{\partial_n\hat{v}^+(1,k)}{\sqrt{\eta+k^2}}}{2(s + \sqrt{\eta + k^2})} + \frac{\hat{v}^+(1, k) + \frac{\partial_n\hat{v}^+(1,k)}{\sqrt{\eta+k^2}}}{2(s - \sqrt{\eta + k^2})}
\]
The Meaning of the Pole Condition

Now the pole condition states that this solution

\[ \tilde{\nu}^+(s, k) = \frac{\hat{\nu}^+(1, k) - \frac{\partial_n \hat{\nu}^+(1,k)}{\sqrt{\eta+k^2}}}{2(s + \sqrt{\eta + k^2})} + \frac{\hat{\nu}^+(1, k) + \frac{\partial_n \hat{\nu}^+(1,k)}{\sqrt{\eta+k^2}}}{2(s - \sqrt{\eta + k^2})} \]

can not have any poles in the right half of the complex plane, \( \Re(s) \geq 0 \), and since \( \sqrt{\eta + k^2} > 0 \), the second term can not be present, which means that

\[ \hat{\nu}^+(1, k) + \frac{\partial_n \hat{\nu}^+(1,k)}{\sqrt{\eta + k^2}} = 0 \]

which is equivalent to

\[ \partial_n \hat{\nu}^+(1, k) = -\sqrt{\eta + k^2} \hat{\nu}^+(1, k) \]

as we found before choosing the bounded solution in the right outer domain.
Approximations from the Pole Condition

In order to satisfy the pole condition approximately, it is natural to expand the desired analytic function in the right half plane into a power series. To do so, we first map the right half plane into the unit disk using the Möbius transform

\[ \tilde{s} = \frac{s - s_0}{s + s_0} \quad \iff \quad s = -s_0 \frac{\tilde{s} + 1}{\tilde{s} - 1} \]

and expand \( \tilde{\nu}^+(\tilde{s}, k) \) into a power series about \( \tilde{s} = 0 \).
An Educated Guess

We use a particular Ansatz for the power series (Schädle 2008):

\[
\tilde{v}^+(\tilde{s}, k) = (\tilde{s} - 1) \left( (\tilde{s} - 1) \sum_{n=0}^{\infty} a_n \tilde{s}^n - \frac{\hat{v}^+(1, k)}{2s_0} \right)
\]

because then \( \tilde{v}^+(\tilde{s}, k) \) satisfies already the limit property of Laplace transforms

\[
\lim_{s \to \infty} s\tilde{v}^+(s, k) = \hat{v}^+(1, k)
\]

as one can see from (recall that \( s = -s_0 \frac{\tilde{s} + 1}{\tilde{s} - 1} \))

\[
\lim_{\tilde{s} \to 1} -s_0 \frac{\tilde{s} + 1}{\tilde{s} - 1} \tilde{v}^+(\tilde{s}, k) = \hat{v}^+(1, k).
\]
Determination of the Coefficients

Inserting this power series Ansatz into the equation

$$(\eta + k^2 - s^2)\tilde{v}^+(s, k) - \partial_n \hat{v}^+(1, k) - s\hat{v}^+(1, k) = 0$$

satisfied by $\tilde{v}^+(\tilde{s}, k)$ and comparing coefficients of powers of $\tilde{s}$, we find

$$\tilde{s}^0 : (\eta + k^2)a_0 + (\eta + k^2)\frac{\hat{v}^+(1,k)}{2s_0} - s_0^2 a_0 + \frac{s_0}{2} \hat{v}^+(1, k) = -\partial_n \hat{v}^+(1,k)$$

$$\tilde{s}^1 : (\eta + k^2)(a_1 - 2a_0) - (\eta + k^2)\frac{\hat{v}^+(1,k)}{2s_0} - s_0^2 (a_1 + 2a_0) + \frac{s_0}{2} \hat{v}^+(1,k) = 0$$

$$\vdots$$

$$\tilde{s}^i : (\eta + k^2)(a_i - 2a_{i-1} + a_{i-2}) - s_0^2 (a_i + 2a_{i-1} + a_{i-2}) = 0$$

for $i = 2, \ldots$. Truncating this recurrence relation for $a_i$ at some $i = I$, and setting $a_i = 0$ for $i \geq I$ we obtain a linear system for the unknowns $a_i$, and an approximate relation between $\hat{v}^+(1, k)$ and $\partial_n \hat{v}^+(1, k)$. 
A Simple Example

For $l = 0$, all coefficients $a_i = 0$, and only the relation from the $s^0$ term remains:

$$\partial_n \hat{v}^+(1, k) + \left( \frac{\eta}{2s_0} + \frac{s_0}{2} + \frac{k^2}{2s_0} \right) \hat{v}^+(1, k) = 0$$

It remains to choose the expansion point $s_0$:

The spectrum we try to approximate is at $s = \sqrt{\eta + k^2}$, $k \in \{k_{\text{min}}, \ldots, k_{\text{max}}\}$. If we choose $s_0 = \sqrt{\eta}$, we get

$$\partial_n \hat{v}^+(1, k) + \left( \sqrt{\eta} + \frac{k^2}{2\sqrt{\eta}} \right) \hat{v}^+(1, k) = 0$$

a second order Taylor condition.
Formulation for the More General Case

Discretization of $v^+$ in $x$ using finite differences:

$$(\eta - D_{yy})v_{ij}^+ - \frac{1}{h^2}(v_{i+1,j}^+ - 2v_{ij}^+ + v_{i-1,j}^+) = f_{n,j}$$

Representation of the recurrence relation $a_i$ on the same grid:

$$(\eta - D_{yy} - s_0^2)a_{0j} + \left(\frac{s_0}{2} + \frac{\eta-D_{yy}}{2s_0}\right)v_{nj}^+ + D_n v_{nj}^+ = 0$$
$$(\eta - D_{yy})(a_{1j} - 2a_{0j}) - s_0^2(a_{1j} + 2a_{0j}) + \left(\frac{s_0}{2} - \frac{\eta-D_{yy}}{2s_0}\right)v_{nj}^+ = 0$$
$$\vdots$$
$$(\eta - D_{yy})(a_{i+1,j} - 2a_{i,j} + a_{i-1,j}) - s_0^2(a_{i+1,j} + 2a_{i,j} + a_{i-1,j}) = 0$$
Equivalence With Stretched-Coordinate PML

A general finite difference discretization of the PML layer equation with the coordinate stretching $\gamma$

$$\partial_x \gamma(x) \partial_x u - (\eta - D_{yy}) u = 0$$

is given by

$$\gamma_j \frac{u_{j+1} - u_j}{h_j} - \gamma_{j-1} \frac{u_j - u_{j-1}}{h_{j-1}} \frac{h^*}{h_j} = (\eta - D_{yy}) u_j = 0$$

Result (G, Schädle 2010)

The Pole condition gives a recurrence relation which can be identified with a geometrically stretched-coordinate PML.
Operator in the General Case

Need to understand the general recurrence relation

$$(\eta + k^2)(a_i - 2a_{i-1} + a_{i-2}) - s_0^2(a_i + 2a_{i-1} + a_{i-2}) = 0$$

which is equivalent to

$$(\eta + k^2 - s_0^2)a_{i-1} - 2(\eta + k^2 + s_0^2)a_i + (\eta + k^2 - s_0^2)a_{i+1} = 0$$

or with

$$b := \frac{\eta + k^2 + s_0^2}{\eta + k^2 - s_0^2}$$

we have the simple recursion

$$a_{i-1} - 2ba_i + a_{i+1} = 0$$

which will be truncated for some $i = I$,

$$a_{I-1} - 2ba_I = 0.$$
Equivalence with Absorbing Boundary Conditions

Result (G, Schädle 2010)

The recurrence relation is equivalent to the continued fraction expansion

\[
\frac{1}{4s_0} \left( \frac{2b - 2}{2b - \frac{1}{2b - \ldots}} \right) \hat{v}^+(1, k) = -\frac{\partial_n \hat{v}^+(1, k)}{\eta + k^2 - s_0^2}.
\]

In the limit, independently of \(s_0\), we recover the DtN operator:

\[
\sqrt{\eta + k^2} \hat{v}^+(1, k) = -\partial_n \hat{v}^+(1, k).
\]

Result (G, Schädle 2010)

The Pole condition truncated at step \(I\) gives an absorbing boundary condition which is the \((2I+2, 2I)\) Padé approximation at \(s_0\) of the symbol of the DtN operator.
Pole Condition as ABC

\[ \Omega = (0.5, 1) \times (0, 1) \] with truncation at \( x = 0.5 \),

\[ u_{\text{ex}} = \sin(\pi ky) e^{\sqrt{\pi^2 k^2 + \eta(x-1)}}, \ \eta = 0, \ s_0 = 1.5, \ l = 0 \]
Error Level of the ABC

\[ I = 0, \ s_0 = 1.5 \]

\[ I = 2, \ s_0 = 1.5 \]

\[ I = 0, \ s_0 = 2 \]

\[ I = 2, \ s_0 = 3 \]
Varying $s_0$: $s_0 = \sqrt{\eta + k_{\text{min}}^2}$

\[ u \begin{array}{cccc}
0 & 0.5 & 1 & 1 \\
0.5 & 0.8 & 0.9 & 0.95 \\
0.8 & 0.9 & 0.95 & 1 \\
1 & 1 & 1 & 1 \\
\end{array} \]

\[ \text{error} \begin{array}{cccc}
0 & 0.5 & 1 & 1 \\
0.5 & 0.8 & 0.9 & 0.95 \\
0.8 & 0.9 & 0.95 & 1 \\
1 & 1 & 1 & 1 \\
\end{array} \]
Varying $s_0$: $s_0 = \sqrt{\eta + k^2}$
Varying $s_0$: $s_0 = \sqrt{\eta + k^2}$
Varying $s_0$: $s_0 = \sqrt{\eta + k_4^2}$
Varying $s_0$: $s_0 = \sqrt{\eta + k^2}$
Varying $s_0$: $s_0 = \sqrt{\eta + k_0^2}$
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Varying $s_0$: $s_0 = \sqrt{\eta + k_0^2}$
Varying $s_0$: Error Levels Attained

![Graph showing the error levels as a function of $k_m$. The x-axis represents $k_m$ ranging from 0 to 18, and the y-axis represents the error ranging from $10^{-2}$ to $10^0$. The dashed line shows a minimum error around $k_m = 6$.](image)
Optimization of $s_0$

Result (G, Schädle 2010)

Let \( \frac{P_j(k,s_0)}{Q_j(k,s_0)} \) be the \((2j + 2, 2j)\) Padé approximation at $s_0$ of the symbol of the DtN operator.

Then the reflection coefficient of the $j$th pole condition approximation,

\[
\rho(k, s_0) = \frac{\sqrt{\eta + k^2} - \frac{P_j(k,s_0)}{Q_j(k,s_0)}}{\sqrt{\eta + k^2} + \frac{P_j(k,s_0)}{Q_j(k,s_0)}},
\]

is minimized for $k \in [0, k_{\max}]$, $k_{\max}$ large, if the expansion point is chosen to be

\[
s_0^2 = \eta^{1/2} (\eta + k_{\max}^{2})^{1/2}.
\]
Conclusions

- The **Pole Condition** leads to Padé approximations of the symbol of the DtN operator, and hence gives an **Absorbing Boundary Condition**
- The **Pole Condition** also leads to a geometrically stretched-coordinate **Perfectly Matched Layer**
- Complete **error estimates for the Helmholtz case**, including optimal choice of $s_0$ for any order.

Current efforts:

- An improved Pole Condition would use collocation in order to obtain best approximation. For example:

  $$
  s_0 = (\eta + k_{\text{min}}^2)^{1/4}(\eta + k_{\text{max}}^2)^{1/4}
  s_1 = \frac{1}{2}(\eta + k_{\text{min}}^2)^{5/12}(\eta + k_{\text{max}}^2)^{1/12}
  s_2 = 2(\eta + k_{\text{min}}^2)^{1/12}(\eta + k_{\text{max}}^2)^{5/12}
  \Rightarrow R = 1 - 4 \frac{(\eta + k_{\text{min}}^2)^{1/12}}{(\eta + k_{\text{max}}^2)^{1/12}}
  $$

- Use of the Pole Condition in Domain Decomposition