Perfectly Matched Layers for Wave-Like Time-Dependent Problems Design, Discretization and Optimization

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Introduction. Context

Wave-like phenomena occuring in large areas







(Aero)acoustics

Electromagnetic compatibility Regional oceanic modeling

Finite difference/finite volume/finite element numerical simulations require a limited computational domain

Need for a domain truncation strategy

Introduction. Domain truncation

Original problem



Artificial boundary conditions

Radiation conditions Sommerfeld, Silver-Muller, Flather, Bayliss-Turkel, ... Hierarchical conditions Exact conditions

Modified problem



Introduction. Domain truncation

Original problem



Modified problem



Artificial boundary conditions

Radiation conditions Sommerfeld, Silver-Muller, Flather, Bayliss-Turkel, ... Hierarchical conditions Exact conditions

Artificial layers

Absorbing/Sponge layers Perfectly matched layers (PMLs)

Interesting properties of PMLs:

- \rightarrow dissipative medium
- \rightarrow perfect matching
- \rightarrow perfect absorption

Original equations

$$\partial_t p + \rho c^2 (\partial_x u + \partial_y v + \partial_z w) = 0$$

$$\partial_t u + \rho^{-1} \partial_x p = 0$$

$$\partial_t v + \rho^{-1} \partial_y p = 0$$

$$\partial_t w + \rho^{-1} \partial_z p = 0$$

Bérenger's PML equations

$$\partial_t p_x + \rho c^2 \partial_x u = -\sigma_x p_x$$
$$\partial_t p_y + \rho c^2 \partial_y v = -\sigma_y p_y$$
$$\partial_t p_z + \rho c^2 \partial_z w = -\sigma_z p_z$$
$$\partial_t u + \rho^{-1} \partial_x p = -\sigma_x u$$
$$\partial_t v + \rho^{-1} \partial_y p = -\sigma_y v$$
$$\partial_t w + \rho^{-1} \partial_z p = -\sigma_z w$$



Original equations

$$\partial_t p + \rho c^2 (\partial_x u + \partial_y v + \partial_z w) = 0$$

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$$\partial_t v + \rho^{-1} \partial_y p = 0$$

$$\partial_t w + \rho^{-1} \partial_z p = 0$$

Bérenger's PML equations

$$\partial_t p + \rho c^2 (\partial_x u + \partial_y v + \partial_z w) = -\cdots$$
$$\partial_t p_x + \rho c^2 \partial_x w = -\sigma_x p_z$$
$$\partial_t p_y + \rho c^2 \partial_y v = -\sigma_y p_y$$
$$\partial_t u + \rho^{-1} \partial_x p = -\sigma_x u$$
$$\partial_t v + \rho^{-1} \partial_y p = -\sigma_y v$$
$$\partial_t w + \rho^{-1} \partial_z p = -\sigma_z w$$

 $e_x \xrightarrow{(\sigma_x, 0, \sigma_z)} (\sigma_x, 0, \sigma_z) \xrightarrow{(\sigma_x, 0, \sigma_z)} (\sigma_x, \sigma_y, \sigma_z) \xrightarrow{(\sigma_x, 0, \sigma_z)} (\sigma_x, \sigma_y, \sigma_z) \xrightarrow{(\sigma_x, 0, \sigma_z)} (\sigma_x, \sigma_y, \sigma_z) \xrightarrow{(\sigma_x, 0, \sigma_y, 0)} (\sigma_x, \sigma_y, \sigma_z) \xrightarrow{(\sigma_x, \sigma_y, \sigma_z)} (\sigma_x, \sigma_y, \sigma_z) \xrightarrow{(\sigma_x, \sigma_y, \sigma_z)} (\sigma_x, \sigma_y, 0)$

with $p_x = p - p_y - p_z$

Original system + Source terms + 2 additionnal PDEs

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\sigma_x(x), \sigma_y(y) \text{ and } \sigma_z(z)
Absorption functions
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Introduction. Some goals/requirements for novel PMLs

1. Mathematical/numerical features

- (strong) Well-posedness
- (strong) Stability
- Accuracy at both continuous and discrete levels
- 2. General geometry
 - Cuboidal truncated domains
 - · Cylindrical or spherical truncated domains
 - Convex truncated domains

3. Complicated physics

- · Dispersive waves
- · Heterogeneous and anisotropic media
- Multiple wave modes
- Nonlinear dynamics

4. Scheme compatibility / Ease of implementation / Computational efficiency

In this talk:

- Optimization (accuracy) at the discrete level
- PMLs for generally-shaped truncated domains

[adapted from Givoli, 2008]

Optimization in discrete contexts

Two PMLs for generally-shaped domains Numerical simulations

Optimization. Plane-wave analysis in 1D at the continuous level

Consider a plane-wave solution with an incident (A_i) and a reflected wave (A_r)



▶ The effectiveness of the layer is quantified with the reflection coefficient

$$r = \left|\frac{A_r}{A_i}\right|$$

with $\begin{vmatrix} r = 0 \text{ for a perfectly absorbing boundary} \\ r = 1 \text{ for a perfectly reflecting boundary (wall)} \end{vmatrix}$

The reflection coefficients are

$$\begin{split} r_{interf} &= 0 & (infinite \ PML) \\ r_{pml} &= \exp\left\{-\frac{2}{c}\int_{0}^{\delta}\sigma(x')dx'\right\} & (finite \ PML \ of \ thickness \ \delta) \end{split}$$

The interface domain/layer is perfectly matched A finite layer is perfectly absorbing if the integral of $\sigma(x)$ is infinite



Goal: The solution of the discrete problem must be close to the solution of the original continuous problem

Two complementary viewpoints:

- Minimize the modeling error and the numerical error
- Minimize the reflection of discrete waves

Optimization. Plane-wave analysis in 1D at a discrete level (constant σ)

Discretization of the problem with a finite difference scheme Constant absorption function $\boldsymbol{\sigma}$



The discrete harmonic plane-wave solution is

in
$$\Omega$$
: $e^{i(kx_i - \omega t)}$ with $k = \pm \frac{2}{\Delta x} \arcsin\left(\frac{\omega \Delta x}{2c}\right)$
in Σ : $e^{i(\beta x_i - \omega t)}$ with $\beta = \pm \frac{2}{\Delta x} \arcsin\left(\frac{\omega \Delta x}{2c} - i\frac{\sigma \Delta x}{2c}\right)$

where h is the spatial step.

The discrete reflection coefficients are

 $\begin{aligned} r_{interf}^{\star} &= \left| \frac{e^{-\imath\beta\Delta x/2} - e^{-\imath k\Delta x/2}}{e^{-\imath\beta\Delta x/2} + e^{\imath k\Delta x/2}} \right| & \text{(infinite PML)} \\ r_{pml}^{\star} &= \left| \frac{\imath\cos(\beta\delta + \beta\Delta x/2) - \sin(\beta\delta) e^{-\imath k\Delta x/2}}{\imath\cos(\beta\delta + \beta\Delta x/2) + \sin(\beta\delta) e^{\imath k\Delta x/2}} \right| & \text{(finite PML)} \end{aligned}$



Small σ : Same behavior in continuous and discrete context *Large* σ : Different behavior – Discrete PML are reflective

Interpretation



Too small σ : The outgoing waves are not enough damped in the PML ($\varepsilon > \delta$). The continuous reflection coefficient is recovered (modeling error)

Too large σ : The characteristic scale of the exponential decay ε is too small ($\varepsilon < \Delta x$) The discretization cannot represent the solution (*numerical error*)

$$\Delta x < \varepsilon < \delta$$



Optimization. Numerical optimization in 1D (constant σ)

Description of the 1D time-dependent benchmark

A Gaussian-shaped pulse moves to the right At the end of the simulation $(t = t_f)$, if the layer is perfectly reflecting, the pulse is back at its initial position



The effectiveness of the layer is quantified with the relative error ξ_r

$$\xi_r = \sqrt{\frac{E_{\text{with pml}}}{E_{\text{with wall}}}}$$

where
$$E = \int_{-L}^{0} \left(\frac{1}{2a} \left| p \right|^2 + \frac{1}{2b} \left| u \right|^2 \right) d\Omega$$

with $\begin{cases} \xi_r = 0 \text{ for a perfectly absorbing boundary} \\ \xi_r = 1 \text{ for a perfectly reflecting boundary (wall)} \end{cases}$

Numerical results



Optimization. Numerical optimization in 1D (constant σ)

Numerical results



Optimization. Spatially varying $\sigma(x)$

Exponential decay of the solution

 $\sigma(x)$ such that progressive decay of the solution





Bermúdez et al., 2007 Modave et al., 2010

Numerical results



(figures for CG scheme - similar figures for other schemes)

Comparison

• Optimum value of α

 σ_2 and σ_3 : ?

- σ_h and σ_{sh} : approx. propagation velocity c
- Best absorption function

FD scheme: optimized σ_2 and σ_3 better than σ_{sh} ,

optimized σ_h the worst

CG and DG schemes: optimized σ_h equivalent or slightly better than others

Optimization. Interpretation



Linear decay Discontinuous derivative at the interface OK with finite element schemes NO with finite difference schemes Bater soution *Domain* Ω LayerΣ Spatial coordinate x

 σ_{sh} with $\alpha = c$

Exponential-linear decay Continuous derivative at the interface OK with all schemes

For oblique plane-wave solution (2D/3D), the shape of decay changes!

[Modave et al., ODyn, 2010]

Optimization. Numerical optimization in 2D (spatially varying σ)

Description of the 2D time-dependent benchmark



The effectiveness of the layer is now quantified with the relative error

$$\xi_r = \sqrt{\frac{E_{\text{error with pml}}(t_f)}{E_{\text{error with wall}}(t_f)}}$$

where
$$E_{\text{error}} = \int_{\Omega} \left(|p - p_{ref}|^2 + |\mathbf{u} - \mathbf{u}_{ref}|^2 \right) d\Omega$$

with $\begin{cases} \xi_r = 0 \text{ for a perfectly absorbing boundary} \\ \xi_r = 1 \text{ for a perfectly reflecting boundary (wall)} \end{cases}$

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Numerical results



With all the considered schemes:

Optimized $\sigma_{\rm 2},\,\sigma_{\rm 3}$ and σ_{sh} are nearly equivalent, far better than σ_h

The optimum α remains close to c for σ_{sh}

The absorption function σ_{sh} with $\alpha = c$ is the most convenient choice

[Modave et al., IJNME, 201X]

Optimization in discrete contexts

Two PMLs for generally-shaped domains

Numerical simulations

Design. Definition of the problem

Original domain \mathbb{R}^d



Scalar wave problem

Find $p(t, \mathbf{x})$ and $\mathbf{u}(t, \mathbf{x})$ such that:

$$\begin{cases} rac{\partial oldsymbol{
ho}}{\partial t} +
ho c^2
abla \cdot \mathbf{u} = 0, & \forall \, \mathbf{x} \in \mathbb{R}^d, t > 0 \\ rac{\partial oldsymbol{u}}{\partial t} + rac{1}{
ho}
abla oldsymbol{p} = 0, & \forall \, \mathbf{x} \in \mathbb{R}^d, t > 0 \end{cases}$$

with initial conditions on p and \mathbf{u} at t = 0

p and u have initially a compact support in Ω

Design. Definition of the problem

Convex truncated domain Ω with regular boundary surrounded with a PML Σ



(Conformal PML)

Scalar wave problem with PML

Find $p(t, \mathbf{x})$ and $\mathbf{u}(t, \mathbf{x})$ such that:

$$\begin{split} \frac{\partial \boldsymbol{\rho}}{\partial t} &+ \rho c^2 \nabla \cdot \mathbf{u} = 0, \quad \forall \, \mathbf{x} \in \Omega, \, t > 0 \\ \frac{\partial \mathbf{u}}{\partial t} &+ \frac{1}{\rho} \nabla \boldsymbol{\rho} = 0, \quad \forall \, \mathbf{x} \in \Omega, \, t > 0 \end{split}$$

with initial conditions on p and \mathbf{u} at t = 0

Equations in Σ ? Conditions at Υ and Γ ?

Design. Procedure with a convex truncated domain (coordinate stretch)



Consider the time-harmonic equations

$$-\imath \omega p + \rho c^2 \nabla \cdot \mathbf{u} = 0$$
$$-\imath \omega \mathbf{u} + \frac{1}{\rho} \nabla \rho = 0$$

Use the complex substitution

$$\mathbf{x} \quad o \quad \mathbf{ ilde{x}}(\mathbf{x}) = \mathbf{x} - rac{\mathbf{e}_s}{\imath \omega} \int_0^s \sigma(s') \, \mathrm{d}s'$$

Lassas & Somersalo, 1999 Teixeira & Chew, 2000 Mouysset, 2006 Laurens, 2010

where $\begin{array}{|c|c|} \tilde{\mathbf{x}} \in \mathcal{U} \subset \mathbb{C}^d \\ \mathbf{e}_s \text{ is the stretching direction} \\ s \text{ is the curvilinear coordinate in the direction } \mathbf{e}_s \\ \sigma(s) \text{ is the (positive) absorption function} \end{array}$

As a consequence, the elementary time-harmonic plane-wave solution changes:

$$e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} \rightarrow e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} e^{-\frac{\mathbf{k}\cdot\mathbf{e}_{s}}{\omega}\int_{0}^{s}\sigma(s')\,\mathrm{d}s'}$$
Propagation Damping

Local orthogonal coordinates (s, φ, θ) Local orthonormal frame $(\mathbf{e}_s, \mathbf{e}_{\varphi}, \mathbf{e}_{\theta})$ Darboux's frame

The original system reads

$$\begin{cases} -\imath\omega\hat{p} + \rho c^2 \left(\frac{\partial u_s}{\partial s} + \frac{1}{1 + \kappa_{\varphi} s}\frac{\partial u_{\varphi}}{\partial \varphi} + \frac{1}{1 + \kappa_{\theta} s}\frac{\partial u_{\theta}}{\partial \theta}\right) = 0\\ -\imath\omega\hat{\mathbf{u}} + \frac{1}{\rho} \left(\mathbf{e}_s \frac{\partial p}{\partial s} + \frac{\mathbf{e}_{\varphi}}{1 + \kappa_{\varphi} s}\frac{\partial p}{\partial \varphi} + \frac{\mathbf{e}_{\theta}}{1 + \kappa_{\theta} s}\frac{\partial p}{\partial \theta}\right) = 0\end{cases}$$



After the complex substitution and the parametrization

$$s \quad o \quad ilde{s}(s) = s - rac{1}{\imath \omega} \int_0^s \sigma(s') \, \mathrm{d} s'$$

the system becomes

$$\begin{cases} -\imath\omega\hat{p} + \rho c^{2} \left(\frac{\imath\omega}{\imath\omega - \sigma} \frac{\partial u_{s}}{\partial s} + \frac{1}{1 + \kappa_{\varphi}\tilde{s}} \frac{\partial u_{\varphi}}{\partial \varphi} + \frac{1}{1 + \kappa_{\theta}\tilde{s}} \frac{\partial u_{\theta}}{\partial \theta}\right) = 0\\ -\imath\omega\hat{\mathbf{u}} + \frac{1}{\rho} \left(\frac{\imath\omega \mathbf{e}_{s}}{\imath\omega - \sigma} \frac{\partial p}{\partial s} + \frac{\mathbf{e}_{\varphi}}{1 + \kappa_{\varphi}\tilde{s}} \frac{\partial p}{\partial \varphi} + \frac{\mathbf{e}_{\theta}}{1 + \kappa_{\theta}\tilde{s}} \frac{\partial p}{\partial \theta}\right) = 0\end{cases}$$

where κ_φ and κ_θ are the main curvatures of the interface Υ at its point closest to ${\bf x}$

Design. Procedure with a convex truncated domain (1st method)

The time-harmonic PML equations can be written

$$\begin{aligned} & \int -\imath\omega p +
ho c^2 \tilde{
abla} \cdot \mathbf{u} = 0 \\ & -\imath\omega \mathbf{u} + rac{1}{
ho} \tilde{
abla} p = 0 \end{aligned}$$

with the differential operator $\tilde{\nabla}$

$$\tilde{\nabla} = \nabla - \frac{\sigma}{\sigma - i\omega} [\mathbf{e}_{\mathsf{s}}(\mathbf{e}_{\mathsf{s}} \cdot \nabla)] - \frac{\bar{\kappa}_{\varphi}\bar{\sigma}}{\bar{\kappa}_{\varphi}\bar{\sigma} - i\omega} [\mathbf{e}_{\varphi}(\mathbf{e}_{\varphi} \cdot \nabla)] - \frac{\bar{\kappa}_{\theta}\bar{\sigma}}{\bar{\kappa}_{\theta}\bar{\sigma} - i\omega} [\mathbf{e}_{\theta}(\mathbf{e}_{\theta} \cdot \nabla)]$$

where $\bar{\kappa}_{\varphi} = (\kappa_{\varphi}^{-1} + s)^{-1}$, $\bar{\kappa}_{\theta} = (\kappa_{\theta}^{-1} + s)^{-1}$ and $\bar{\sigma} = \int_{0}^{s} \sigma(s') dx'_{s}$

PML's equations (PML "with PDEs")

In the layer Σ , the fields p and u and two additional fields p_s and p_{φ} are governed by

$$\begin{cases} \frac{\partial p}{\partial t} + \rho c^2 \nabla \cdot \mathbf{u} = -\sigma p_s - \bar{\kappa}_{\varphi} \bar{\sigma} p_{\varphi} - \bar{\kappa}_{\theta} \bar{\sigma} (p - p_s - p_{\varphi}) \\ \frac{\partial \mathbf{u}}{\partial t} + \frac{1}{\rho} \nabla p = -\sigma \mathbf{e}_s (\mathbf{e}_s \cdot \mathbf{u}) - \bar{\kappa}_{\varphi} \bar{\sigma} \mathbf{e}_{\varphi} (\mathbf{e}_{\varphi} \cdot \mathbf{u}) - \bar{\kappa}_{\theta} \bar{\sigma} \mathbf{e}_{\theta} (\mathbf{e}_{\theta} \cdot \mathbf{u}) \\ \frac{\partial p_s}{\partial t} + \rho c^2 [\mathbf{e}_s (\mathbf{e}_s \cdot \nabla)] \cdot \mathbf{u} = -\sigma p_s \\ \frac{\partial p_{\varphi}}{\partial t} + \rho c^2 [\mathbf{e}_{\varphi} (\mathbf{e}_{\varphi} \cdot \nabla)] \cdot \mathbf{u} = -\bar{\kappa}_{\varphi} \bar{\sigma} p_{\varphi} \end{cases}$$

Cartesian case \rightarrow Bérenger's PML system

Well-posedness [Kreiss and Lorenz, 1989]

The Cauchy problem is *weakly/strongly well-posed* if there exists K > 0 and $\alpha \in \mathbb{R}$ such that the solution U(t) satisfies an estimate on the type

 $\begin{aligned} \|U(.,t)\|_{L^{2}} &\leq K e^{\alpha t} \|U(.,0)\|_{H^{s}} & \text{with } s > 0 \qquad (weak) \\ \|U(.,t)\|_{L^{2}} &\leq K e^{\alpha t} \|U(.,0)\|_{L^{2}} & (strong) \end{aligned}$

Stability [Bécache and Joly, 2002]

A system that is a 0th-order perturbation of a 1st-order hyperbolic system is weakly/strongly stable if there exists K > 0 and $A \in \mathbb{R}$ such that the solution U(t)satisfies an estimate on the type

 $\begin{aligned} \|U(.,t)\|_{L^2} &\leq K(1+At)^s \|U(.,0)\|_{H^s} \quad \text{with } s > 0 \qquad (weak) \\ \|U(.,t)\|_{L^2} &\leq K \|U(.,0)\|_{L^2} \qquad (strong) \end{aligned}$

Optimization in discrete contexts Two PMLs for generally-shaped domains Numerical simulations

Description of the 2D time-dependent benchmark

Initial pulse — Elliptical truncated domain DG finite element scheme with piecewise linear basis functions ($\mathfrak{p} = 1$) About 230/310.000 discrete unknowns ($\sim 17 - 25\%$ in the PML for $\delta = 5\ell$)



Wall BC case



Pressure at $t = t_{fin}$ Colorbar [-0.35, 0.35]

Absorbing BC case



Pressure at $t = t_{fin}$ Colorbar [-0.1, 0.1]

PML with PDEs and $\delta = 1h$



Pressure at $t = t_{fin}$ Colorbar [-0.1, 0.1]

PML with ODEs and $\delta = 1h$



Pressure at $t = t_{fin}$ Colorbar [-0.1, 0.1]

PML with PDEs and $\delta = 3h$



PML with ODEs and $\delta = 3h$



PML with PDEs and $\delta = 5h$



PML with ODEs and $\delta = 5h$



Description of the 3D time-dependent benchmark

Initial pulse in the front of a submarine — Ellipsoidal truncated domain DG finite element scheme with piecewise linear basis functions ($\mathfrak{p} = 1$) About 17.8 millions discrete unknowns ($\sim 50\%$ in the PML for $\delta = 5\ell$)



Iso-surfaces of the pressure at t = 0.



An ABC termination improves a poorly efficient PML

[see also Petropoulos, 1998]



Shielding effectiveness of a cavity

$$\mathsf{SE}_{\mathsf{dB}} = 20 \log_{10} \left| \frac{\textit{E}^{\mathsf{inc}}}{\textit{E}^{\mathsf{trans}}} \right|$$

where E^{inc} and E^{inc} are the wave amplitudes at the center of the cavity.

Time-domain simulation with the modulated transverse-magnetic incident field.







 E^{total} (in the domain) $E^{\text{scattered}}$ (in the layer)



Shielding effectiveness of a cavity

$$\mathsf{SE}_{\mathsf{dB}} = 20 \log_{10} \left| \frac{\textit{E}^{\mathsf{inc}}}{\textit{E}^{\mathsf{trans}}} \right|$$

where E^{inc} and E^{inc} are the wave amplitudes at the center of the cavity.

Time-domain simulation with the modulated transverse-magnetic incident field.



Benchmark. PML for other wave-like systems (preliminary results)

PML for elastic waves



Velocity at the beginning of the simulation

PML for elastic waves





Velocity ... later ...

Optimization in discrete contexts Two PMLs for generally-shaped domains Numerical simulations

$\mathsf{PML} \rightarrow \mathsf{An}$ efficient way for domain truncation

Choice of the parameters in discrete context

Effectiveness of the shifted hyperbolic function σ_{sh}

 \rightarrow Does not require a costly optimization procedure

 \rightarrow Interpretation of the optimum value of the free parameter

Improving the effectiveness by increasing the layer thickness δ

Design of PML time-dependent formulations

Valid for convex truncated domains with regular boundary

Easy to implement in existing codes

Good framework for further developments

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