

A friendly review of absorbing boundary conditions and perfectly matched layers for classical and relativistic quantum waves equations.

Modeling Seminar Presentation
Study report

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UGA - MSIAM

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Outline

1 Preamble

② Seminar - Presentation of our study

- Problem and challenges
 - Proposed solutions
 - ABC
 - PML
 - ABC & PML
 - Conclusion

3 Conclusion

Context

- Who we are:

Linnea Hallin, Éloi Navet, Maxime Renard, Nicolas Roblet.

- Studied article [ALT17]:

By X. Antoine, E. Lorin, and Q. Tang,

A Friendly Review of Absorbing Boundary Conditions and Perfectly Matched Layers for Classical Relativistic Quantum Waves Equations

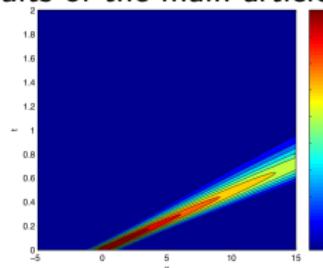
Molecular Physics, vol.115, no.5-16, pp.1861–1879, 2017.
DOI:10.1080/00268976.2017.1290834

- Under the supervision of:

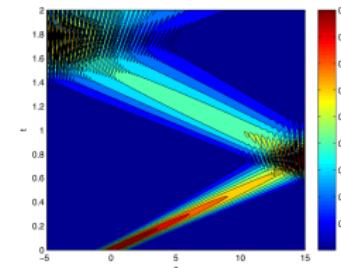
Brigitte Bidégaray-Fesquet (CNRS), Clément Jourdana (UGA).

The objectives of our study

- Retrieve the results of the main article



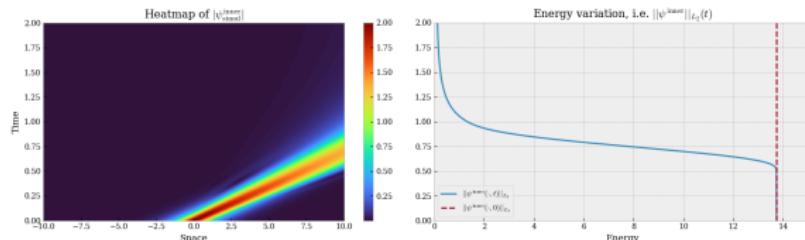
(a) Exact reference solution



(b) Numerical solution with a Dirichlet boundary condition

- Provide a deeper analysis

Schrodinger equation simulation with transparent potential BC and with PML. Focused on the area of interest.



- Cover all grey areas

Problem and challenges

Discrete wave propagation - Initial problem

Schrödinger equation

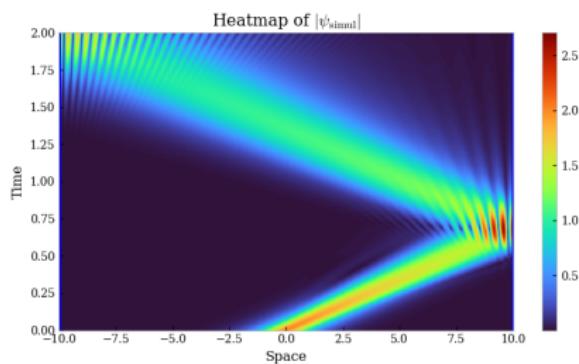


Figure: Neumann condition

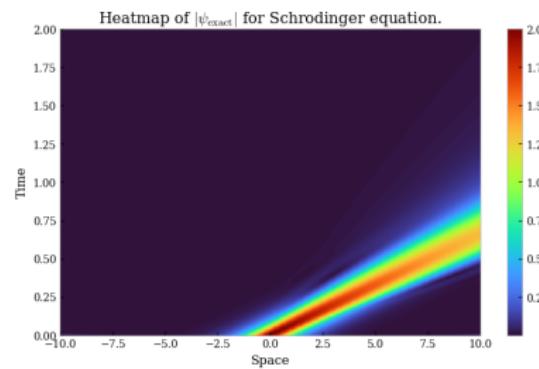


Figure: Exact solution

Issues :

- Reflections
 - Precision of the scheme

Problem and challenges

Ways of fixing the issue

Intuitive & rigorous methods

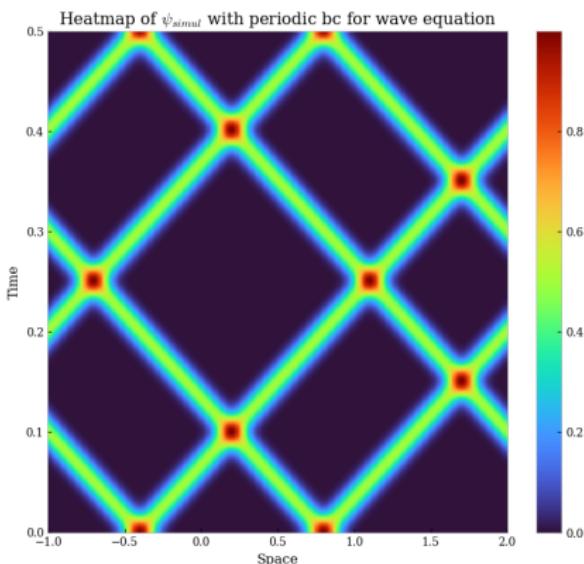


Figure: Wave equation, periodic BC.

Unsatisfying possibilities :

- No boundaries
 - ↳ Periodic condition
 - Larger domain & re-framing
 - ↳ Knowledge of exact solution
 - Extra wide domain
 - ↳ Computational cost

From article :

- **Absorbing Boundary Conditions (ABC):** change nature of boundary;
 - **Perfectly Matched Layers (PML):** change boundary localization.

Initial value problem for wave equation (1D)

System of equation: Initial Value Problem (IVP)

$$\begin{cases} \partial_{tt}\psi - c^2\partial_{xx}\psi = 0 & \text{in } \mathbb{R} \times (0, T), \\ \psi(\cdot, 0) = \psi_0, \quad \partial_t\psi(\cdot, 0) = \psi_{t,0} & \text{on } \mathbb{R}, \end{cases}$$



Figure: Wave illustration. Source: Wikipedia

Wave equation: ABCs idea

Exact solution: Alembert's formula, $\forall (x, t) \in \mathbb{R} \times [0, T]$

$$\begin{aligned}\psi(x, t) &= \frac{1}{2}[\psi_0(x + ct) + \psi_0(x - ct)] + \frac{1}{2c} \int_{x-ct}^{x+ct} \psi_{t,0}(y) dy \\ &= \psi^l(x + ct) + \psi^r(x - ct)\end{aligned}$$

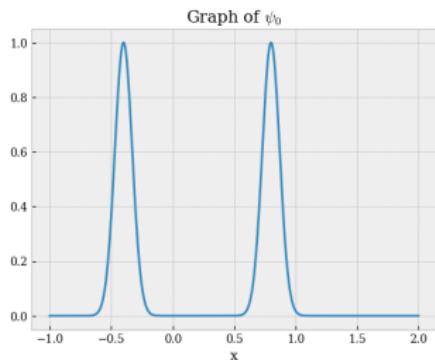


Figure: Example of initial condition compactly supported and bounded $\psi_0(x)$.

Key idea: Derive 'far' space conditions to mimic what's going on over there :

- Define left (resp. right) area s.t.:
 - ↳ Space set where right propagation term is null.
 - ↳ $\psi(x, t) = \psi'(x + ct)$
 - Derive a 'far' fluctuation behaviour:
 - ↳ $\partial_t \psi(x, t) = c \partial_x \psi(x, t)$
 - Deduce a general behaviour at boundary:
 - ↳ $\partial_n \psi + \frac{1}{c} \partial_t \psi = 0$

Wave equation: ABCs mathematical formulation for simulation

Complete simulated system: Initial Boundary Value Problem (IBVP : IVP + ABCs)

$$\begin{cases} \partial_{tt}\psi - c^2\partial_{xx}\psi = 0 & \text{in } \Omega \times (0, T), \\ \psi(\cdot, 0) = \psi_0, \quad \partial_t\psi(\cdot, 0) = \psi_{t,0} & \text{on } \Omega, \\ \partial_n\psi(x, t) + \frac{1}{c}\partial_t\psi(x, t) = 0 & \text{on } \partial\Omega \times [0, T]. \end{cases}$$

- Finite difference centered **second-order** scheme for main equation:

$$\frac{\psi_j^{n+1} - 2\psi_j^n + \psi_j^{n-1}}{\Delta t^2} = c^2 \frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2}$$

- CFL : $c\Delta t \leq \Delta x$
 - $\psi_j^n \rightsquigarrow \psi(n\Delta t, j\Delta x)$

- Initialization:

- $\psi_j^0 = \psi_0(j\Delta x)$
 - $\psi_i^1 = \psi_i^0 + \Delta_t \psi_{t,0}(j\Delta x)$

- ABCs discretization:

$$\left\{ \begin{array}{l} \frac{1}{2\Delta x} \left(3\psi_0^{n+1} - 4\psi_1^{n+1} + \psi_2^{n+1} \right) = -\frac{1}{2c\Delta t} \left(\psi_0^{n+1} - \psi_0^{n-1} \right) \\ \frac{1}{2\Delta x} \left(\psi_{J-2}^{n+1} - 4\psi_{J-1}^{n+1} + 3\psi_J^{n+1} \right) = -\frac{1}{2c\Delta t} \left(\psi_J^{n+1} - \psi_J^{n-1} \right) \end{array} \right.$$

Wave equation: ABCs simulation result

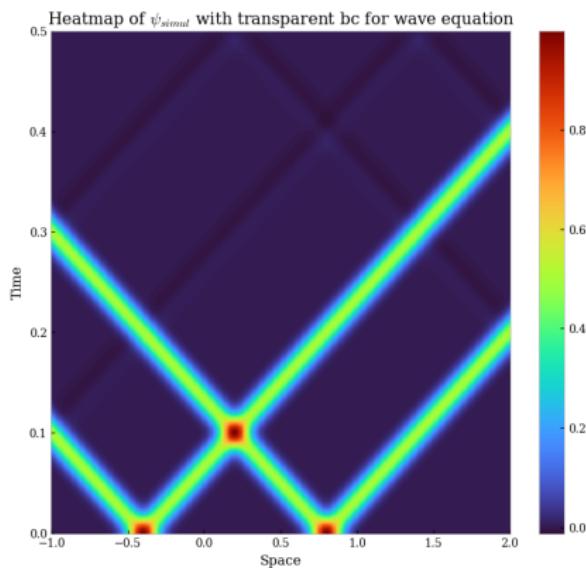


Figure: ABCs boundary condition

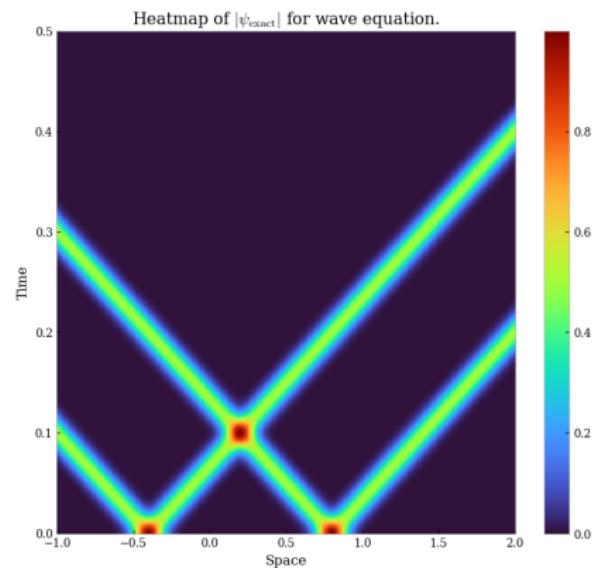


Figure: Exact solution

Simulation parameters:

$T = 0.5$, $\#T_{\text{mesh}} = 1000$, $\Omega = [-1, 2]$, $\#X_{\text{mesh}} = 500$, and $c = 6$.

Wave equation: ABCs error study

We introduce an **error function**

$$\forall t, \quad e_r(t) = \frac{\max_x (|\psi_{\text{sim}}(x, t) - \psi_{\text{ex}}(x, t)|)}{\max_{x, t'} (|\psi_{\text{ex}}(x, t')|)}$$

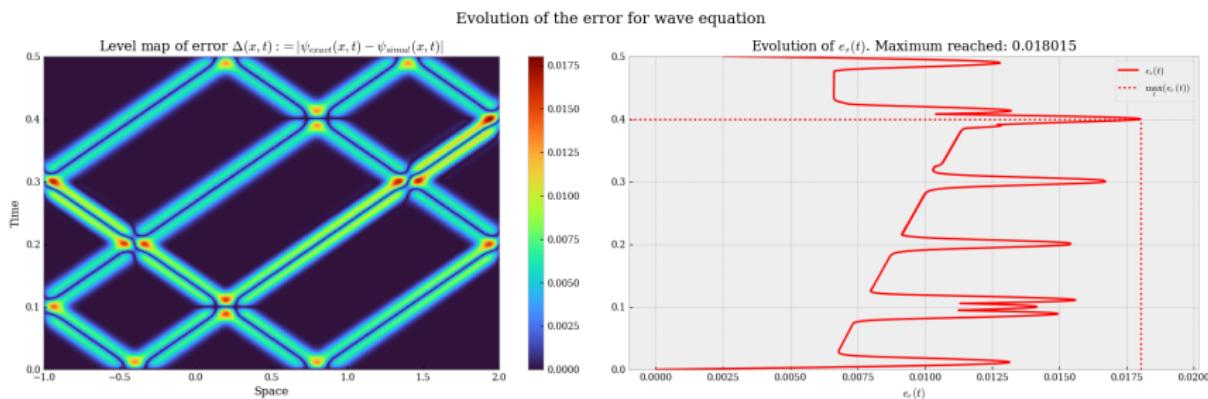


Figure: Evolution of e_r .

- ↳ Amplitude of the reflections obtained with the use of ABCs is observed to be 100 times smaller than the original amplitude of the wave.

Initial value problem for Schrödinger equation (1D)

System of equation: Initial Value Problem (IVP)

$$\begin{cases} \partial_t \psi - i \partial_{xx} \psi = 0, & \text{on } \mathbb{R} \times \mathbb{R}^+, \\ \psi(\cdot, 0) = \psi_0, & \text{on } \mathbb{R}, \end{cases}$$

Exact solution:

The unique solution to previous Schrödinger Initial Value Problem with initial condition in the Schwartz class is

$$\forall t \geq 0, \forall x \in \mathbb{R}, \quad \psi(x, t) = e^{-i\frac{\pi}{4}} \frac{1}{\sqrt{4\pi t}} (\psi_0 * \mathcal{G}_{-i/4t})(x),$$

where \mathcal{G} is the Gaussian kernel defined as $\mathcal{G}_a(x) = e^{-ax^2}$.

Note: we don't necessarily have the exact solution.

Schrödinger equation: ABCs idea

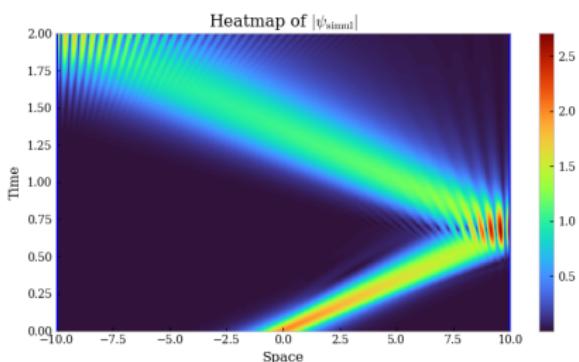


Figure: The reflections we have
(simulation with Neumann's conditions)

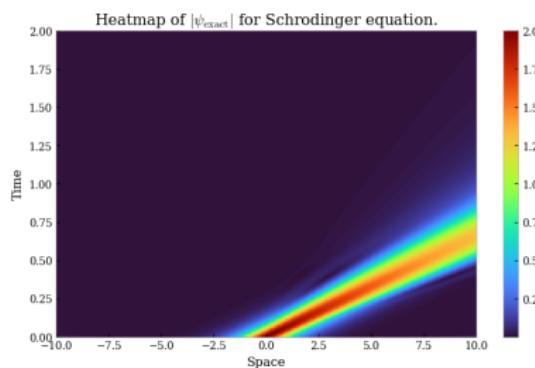


Figure: The result we want (the wave being *absorbed* by the boundary)

How to get a scheme that absorbs the energy going out of the frame?

Conditions derived from the system of equations using the Laplace transform at the boundaries to simulate the behaviour.

Schrödinger equation: ABCs mathematical formulation for simulation

Complete simulated system: Initial Boundary Value Problem (*IBVP* : *IVP* + *ABCs*)

$$\begin{cases} \partial_t \psi - i \partial_{xx} \psi = 0, & \text{on } \Omega \times (0, T), \\ \psi(\cdot, 0) = \psi_0, & \text{on } \Omega, \\ \partial_n \psi(x, t) + e^{-i \frac{\pi}{4}} \partial_t^{1/2} \psi(x, t) = 0, & \text{on } \partial\Omega \times [0, T]. \end{cases}$$

- Initialization: $\psi_0(x) = 2\operatorname{sech}(\sqrt{2}x)e^{i\frac{15}{2}x}$ ($\in \mathcal{S}(\mathbb{R})$).
 - Crank-Nicolson scheme:

$$\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = \frac{c}{2(\Delta x)^2} \left[\left(\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1} \right) + \left(\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n \right) \right].$$

- ↳ Unconditionally stable;
 - ↳ Centered, second order.

- Caputo derivative discretization:

$$\partial_t^{\frac{1}{2}} \psi(t^n) \approx \sqrt{\frac{2}{\Delta t}} \sum_{k=0}^n \beta_k \psi^{n-k} \text{ where } \beta_k = (-1)^k \alpha_k.$$

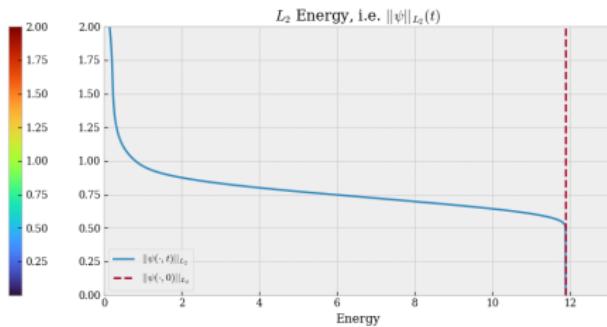
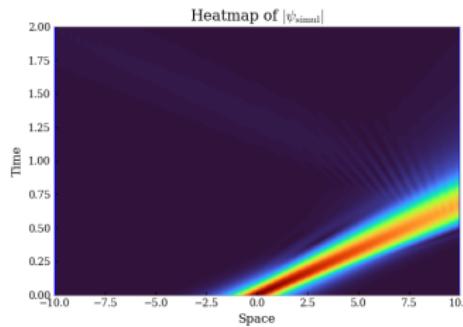
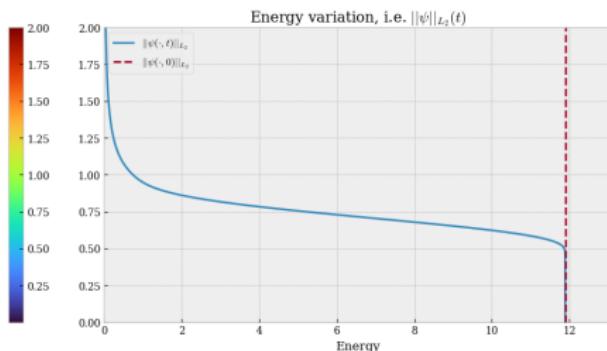
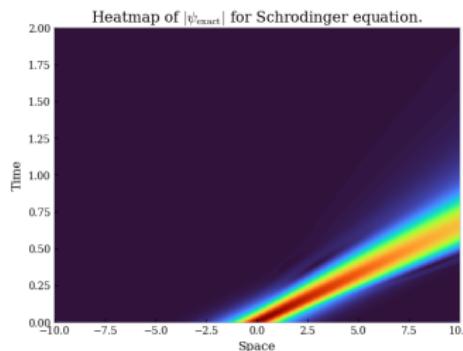
Proposed solutions

Schrödinger equation: Simulation results using ABC

Exact (top) vs ABC (bottom)

Simulation parameters:

$T = 0.2$, $\#T_{\text{mesh}} = 501$, $\Omega = [-10, 10]$ and $\#X_{\text{mesh}} = 501$.



Schrödinger equation: ABCs error study

Compare to exact solution

We use the same **error function** e_r .

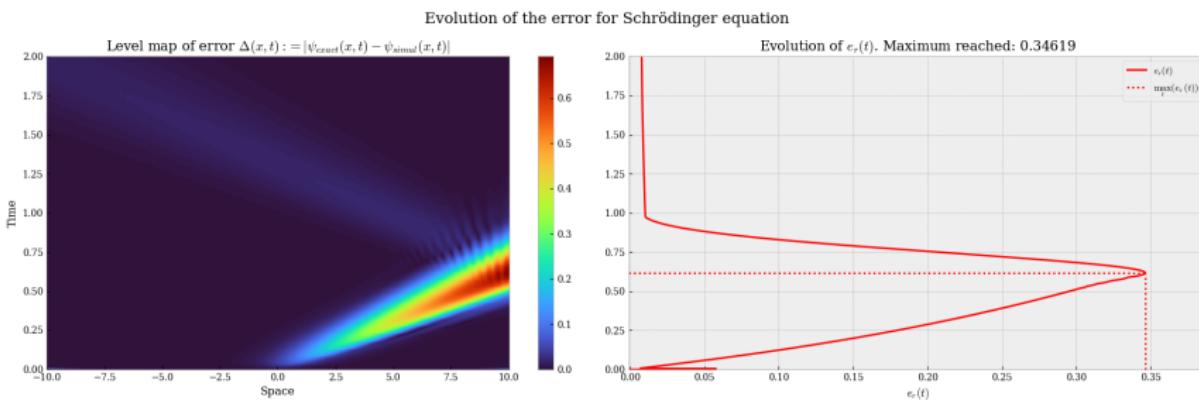


Figure: Evolution of e_r .

- The predominant error is induced by the main simulation scheme and not the boundary conditions.
 - It therefore becomes necessary to isolate the reflections

Proposed solutions

Schrödinger equation: ABCs error study

Isolating reflections 1/2

Key idea:

- The same simulation as initial one will be run on a larger domain Θ , providing a result ϕ .
- Reflections are isolated in the function $\psi - \phi|_{\Omega}$

For instance, if ψ is computed on $[-10, 10]$ with 501 space points, then ϕ would be computed on $[-30, 30]$ with $501 \times 3 - 2 = 1501$ space points.

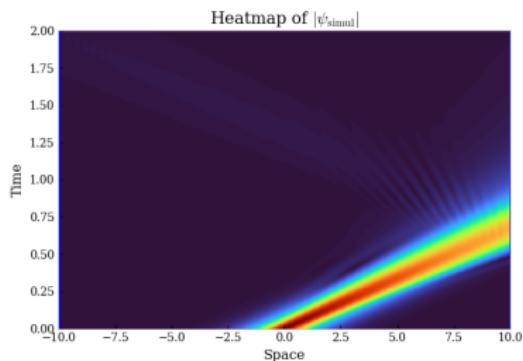


Figure: $\Omega = [-10, 10]$, $\#X_{\text{mesh}} = 501$

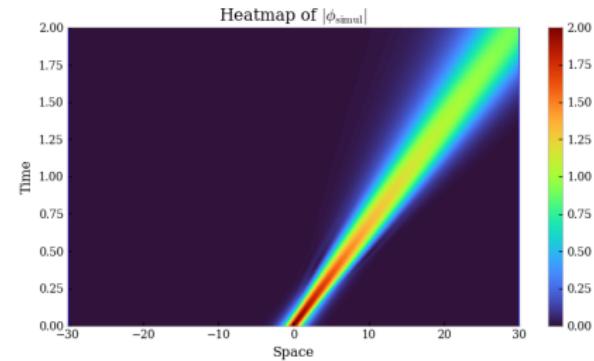


Figure: $\Theta = [-30, 30]$, $\#X_{\text{mesh}} = 1501$

Schrödinger equation: ABCs error study

Isolating reflections 2/2

We introduce a **new error function**

$$\forall t, \quad e_{r,i}(t) = \frac{\max_{x \in \Omega} (|\psi(x, t) - \phi|_{\Omega}(x, t)|)}{\max_{t', x \in \Omega} (|\psi(x, t')|)}$$

Isolating reflections for Schrödinger equation

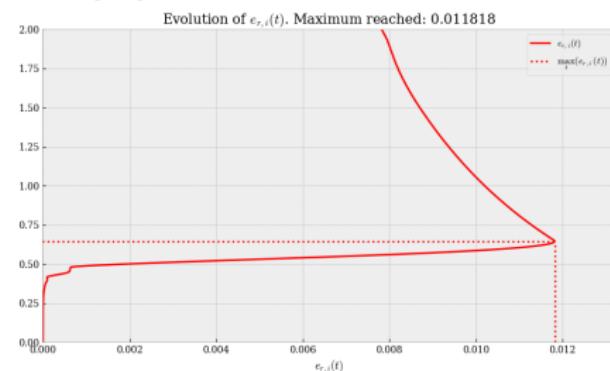
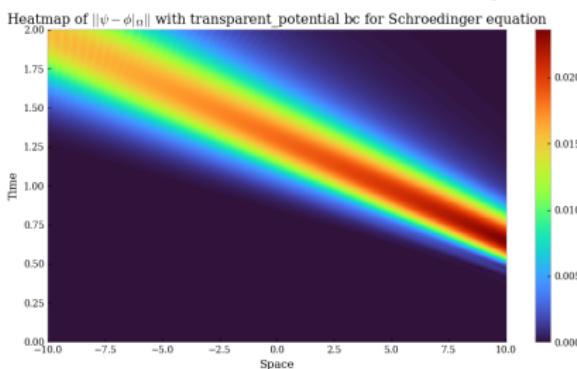
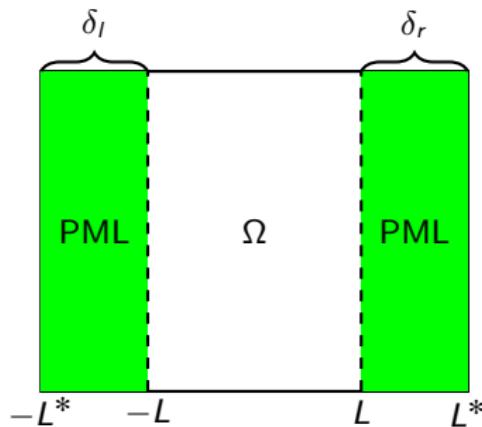


Figure: Evolution of $e_{r,i}$.

↳ As expected: error incurred by ABCs for the Schrödinger equation is similar to that for the wave equation.

PMLs general idea



Key idea: Add absorbing layers on each side:

- Extend the domain $\Omega = [-L, L]$:
 - ↳ $\Omega_{\text{PML}} = [-L^*, L^*]$
 - Add an absorbing function $Z(x)$ to the PMLs:
 - ↳ $Z \equiv 1$ on the physical domain Ω
 - ↳ Z chosen s.t. ψ decays fast enough in the layers

- Easier to implement
 - Practical in cases where ABCs are difficult or impossible to use

Mathematical formulation

- Z function chosen as

$$Z(x) = \begin{cases} 1 & \text{if } |x| \leq L \\ 1 + e^{\frac{i\pi}{4}} \sigma_0 (|x| - L)^2 & \text{if } L < |x| \leq L^* \end{cases}$$

↳ σ_0 parameter to be adjusted

- New Schrödinger equation

$$\begin{cases} \partial_t \psi - \frac{i}{2} \frac{\partial_x}{Z(x)} \left(\frac{\partial_x}{Z(x)} \right) \psi = 0 & (x, t) \in \Omega_T \\ \psi(x, 0) = \psi_0(x) & x \in \Omega \end{cases}$$

- Initial conditions same as for ABCs

$$\psi_0(x) = 2 \operatorname{sech}(\sqrt{2}x) e^{i \frac{15}{2} x}$$

- Dirichlet BC

Implementation

- New Crank-Nicolson scheme:

$$\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = \frac{c}{4(\Delta x)^2 Z(x)^2} \left[(\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}) + (\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n) \right]$$

- ↳ Easy to implement!
- ↳ Only need to care about Z in the layers
- **Problem:** We aspire to keep a fixed complexity
- ↳ Trade-off between scheme accuracy in Ω and layer width

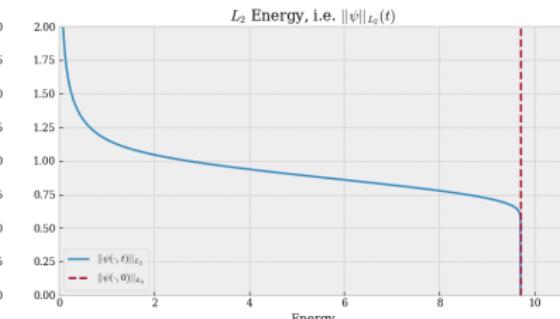
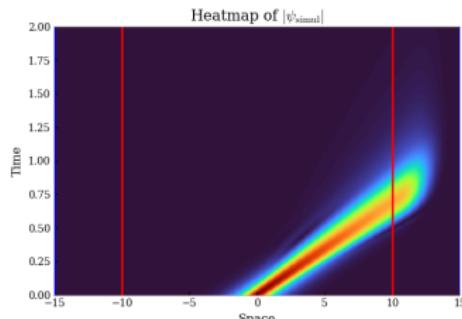
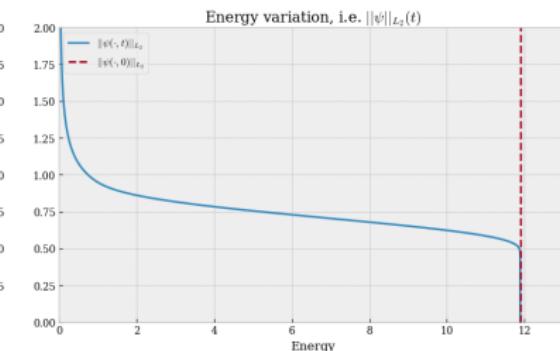
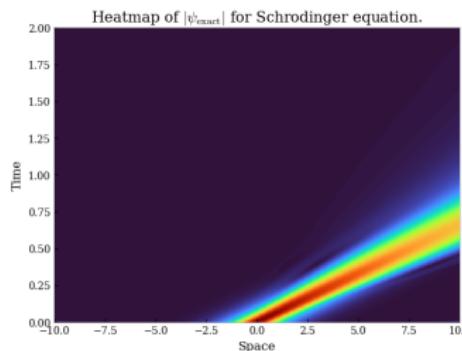
Proposed solutions

Schrödinger equation: Simulation results using PML

Exact (top) vs PML (bottom)

Initial simulation parameters:

$$T = 2, \#T_{\text{mesh}} = 501, \Omega = [-10, 10], \Omega_{\text{PML}} = [-15, 15] \text{ and } \#X_{\text{mesh}} = 501.$$



Schrödinger equation: PMLs error study

Compare to exact solution (1/2)

Error function: e_r is only considered on Ω , i.e. the area of physical interest.

Evolution of the error for Schrödinger equation

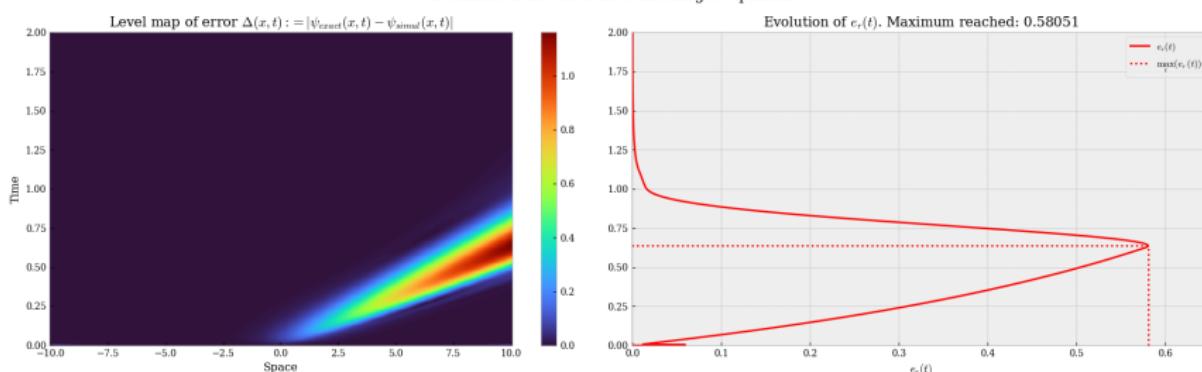


Figure: $\Omega_{\text{PML}} = [-15, 15]$

- Error made by the scheme is again of a higher order than the reflections.
- The cost of using PML manifests as a reduction in the number of space discretization points in the domain of interest.
- Initially 501 points in Ω , with such PML: 250. Consequence : $\max e_r = 0.34$ increase at 0.58.

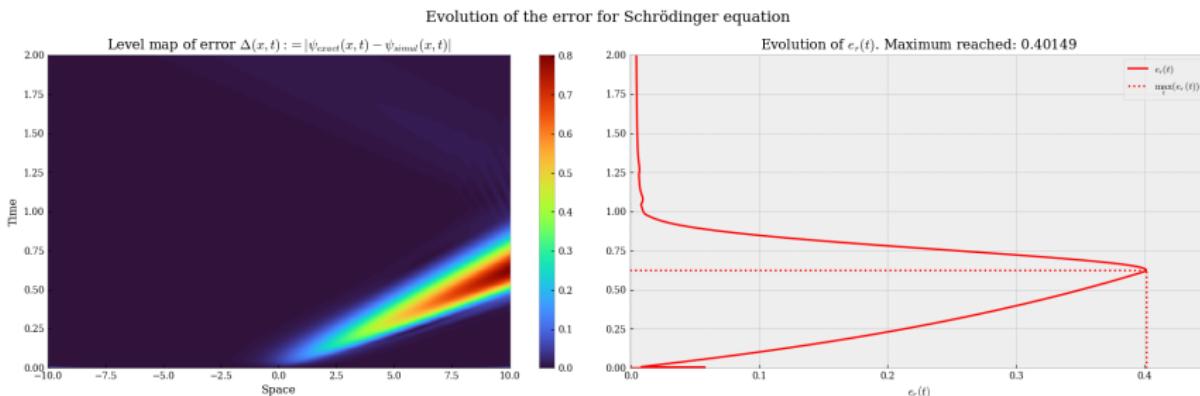
Proposed solutions

Schrödinger equation: PMLs error study

Compare to exact solution (2/2)

Solution:

- Increase number of simulation points (increase therefore complexity).
- Reduce PML size.

Figure: $\Omega_{\text{PML}} = [-10, 13]$

- Reflections order is higher than for $\Omega_{\text{PML}} = [-15, 15]$, i.e. we got some reflections.
- Initially 501 points in Ω , with such PML: 435. Consequence : $\max e_r = 0.34$ increase at 0.40.

Proposed solutions

Schrödinger equation: PMLs error study

Isolating reflections

Error function: we use $e_{r,i}$ only on Ω .

Isolating reflections for Schrödinger equation inner

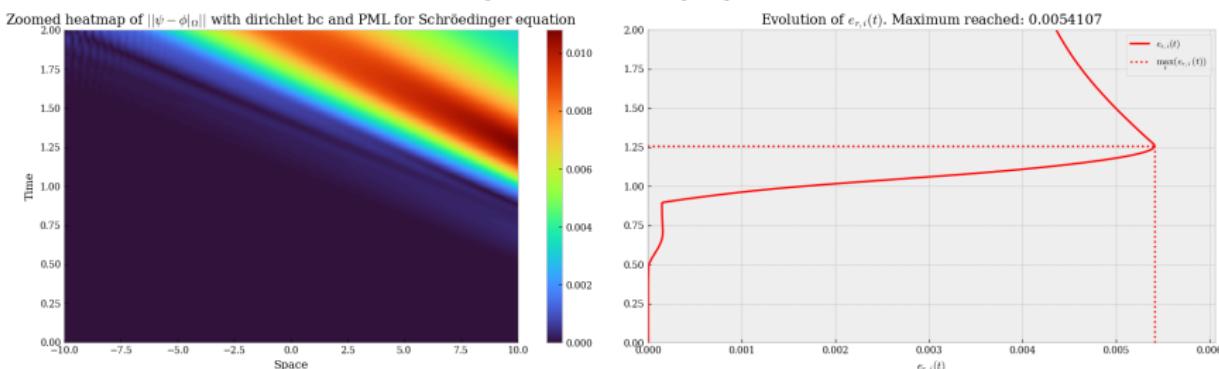


Figure: Evolution of $e_{r,i}$ for $\Omega_{\text{PML}} = [-10, 13]$.

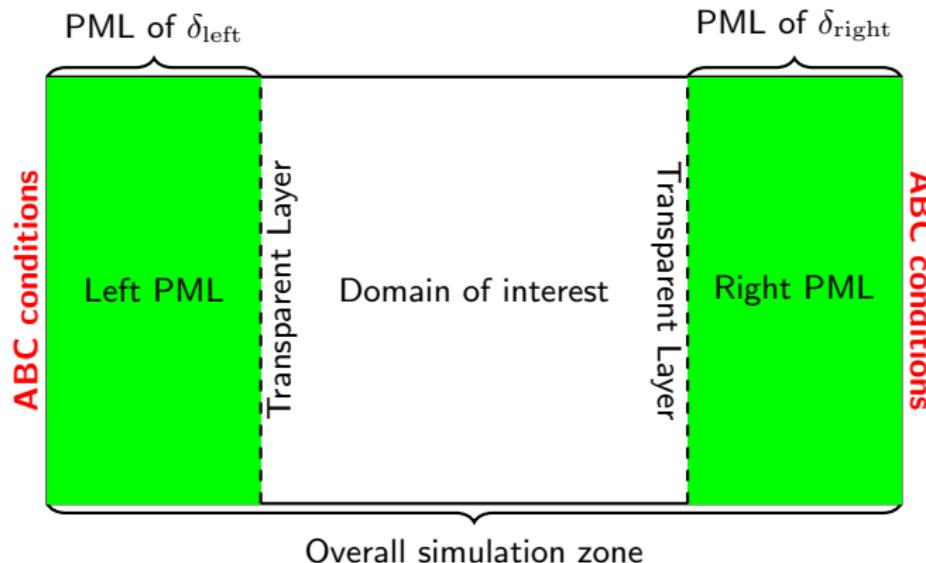
- Error incurred by PMLs in solving the Schrödinger equation is significantly lower compared to that for ABCs, decreasing from 1% to 0.5%.
- For $\Omega_{\text{PML}} = [-15, 15]$ we have an isolated error of 0.01% (plot in appendix).
- ↳ **Trade-off** for PML method between the accuracy of the main equation simulation and the amplitude of reflections.

ABCs and PMLs, challenges and presentation

Key idea: Improve the **PML trade-off** by adding ABCs.

- Let's imagine we have a constraint on the complexity of calculations (1) and on the main simulation precision (i.e. before reaching the boundary)(2).
 - (1) implies $\#X_{\text{mesh}}$ fixed and (1) + (2) implies a maximum size for Ω_{PML} .

Solution: merge ABCs to PMLs.



Schrödinger equation: ABCs and PMLs error study

Isolating reflections

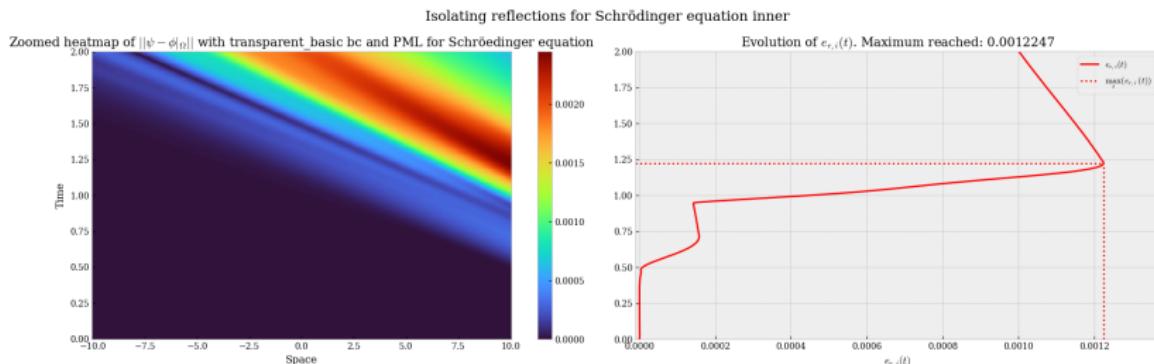


Figure: Suppose the constraints impose $\Omega_{\text{PML}} = [-10, 13]$ and $\# T_{\text{mesh}} = 501$.

Summary of error :

| | ABC | PML $[-15, 15]$ | PML $[-10, 13]$ | ABC & PML $[-10, 13]$ |
|-----------------|-----|-----------------|-----------------|-----------------------|
| $\max(e_r)$ | 34% | 58% | 40% | 40% |
| $\max(e_{r,i})$ | 1% | 0.01% | 0.5% | 0.1% |

- The study of this trade-off could be very interesting but will require considerable computing power.

Conclusion about the results

ABC:

- + Does not change the accuracy of the simulation before the wave encounter the boundary.
- Hard generalization, problem dependencies.
- Hard implementation, difficulty of application to various equations.

PML:

- + More efficient than ABC.
- + Easy to implement, generalizable to all EDP simulations.
- Affects simulation accuracy (at fixed complexity).
- The use of this method reveals a trade-off between complexity and precision.

ABC & PML:

- + Greatly improves the trade-off.
- Requires implementation of ABCs.

Outcomes of our study

Results reproduction

- Wave and Schrödinger equations
- ↳ Reflection isolation
- ↳ Error study

Code

- Modular sources
- Showcase through Jupyter Notebook

Openings

- Beyond on theory
- TBC + PML.
- ↳ PML : more parameters

Report

- Theoretical & simulations
- ↳ Many explanation & examples
- Appendix
- ↳ Self supporting
- ↳ Proof for stability
- ↳ Analytical solutions, energy conservation

Academical feedback

Communication

- Structure thinking
- ↳ Between us
- ↳ For this presentation
- Justify statements
- ↳ Much reading & coding
- ↳ Accessible
- ↳ Pleasant

Team work

- First of that size
- Roles were natural

Distribution of tasks

- Equivalent workload
- Aspect of interest to us
- ↳ Happy to have chosen MS.

Difficulties

- Course + other projects
- Regularity

Acknowledgment

Thank you for listening !

- [ALT17] X. Antoine, E. Lorin, and Q. Tang. "A Friendly Review of Absorbing Boundary Conditions and Perfectly Matched Layers for Classical and Relativistic Quantum Waves Equations". In: (Oct. 2017). DOI: [10.1080/00268976.2017.1290834](https://doi.org/10.1080/00268976.2017.1290834).

Schrödinger with potential

- Governing equation : $\partial_t \psi - i\partial_{xx} \psi = i\nabla \psi$, on $\Omega \times (0, T)$
 - ABC (order 4) :

$$\partial_n \psi + e^{-i\frac{\pi}{4}} e^{i\nu} \partial_t^{1/2} \left(e^{-i\nu} \psi \right) + i \text{sg}(\partial_n V) \frac{\sqrt{|\partial_n V|}}{2} e^{i\nu} I_t \left(\frac{\sqrt{|\partial_n V|}}{2} e^{-i\nu} \psi \right) = 0.$$

- sg : sign function;
 - $\partial_t^{1/2}$: Caputo derivative operator
 - $I_t = \int_0^t$, integral over $(0, T)$
 - $\mathcal{V} = I_t V$

- Caputo derivative discretization: $\partial_t^{1/2} \psi(t^n) \approx \sqrt{\frac{2}{\Delta t}} \sum_{k=0}^n \beta_k \psi^{n-k}$

- $\beta_k = (-1)^k \alpha_k$

$$\bullet \quad \alpha_k = \begin{cases} 1 & \text{if } k = 0 \text{ or } 1, \\ \gamma_k + \gamma_{k-1} & \text{else,} \end{cases}$$

$$\bullet \quad \gamma_k = \begin{cases} 1 & \text{if } k = 0, \\ 0 & \text{if } k = 2p + 1, \\ \prod_{i=1}^p \frac{2j-1}{2i} = \frac{2p-1}{2p} \gamma_{2(p-1)} & \text{if } k = 2p. \end{cases}$$

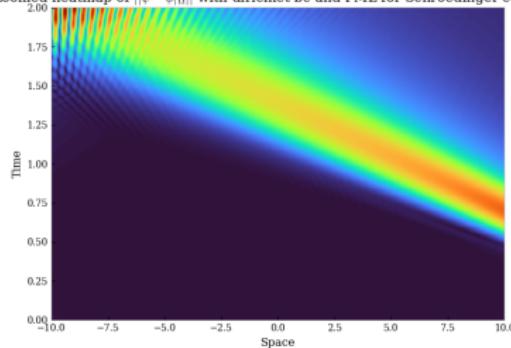
Schrödinger equation: Isolating reflection for $\Omega_{\text{PML}} = [-15, 15]$

Indeed the simulation was realized for $\Omega_{\text{PML}} = [-10, 15]$ (implies no PML on the left boundary).

Meanwhile we can deduce at $t = 0.75$ that for $\Omega_{\text{PML}} = [-15, 15]$ we get
 $\max e_{r,i} = 0.01\%$.

Isolating reflections for Schrödinger equation inner

Zoomed heatmap of $||\psi - \phi_{|0\rangle}||$ with dirichlet bc and PML for Schrödinger equation



Evolution of $e_{r,i}(t)$. Maximum reached: 0.00019542

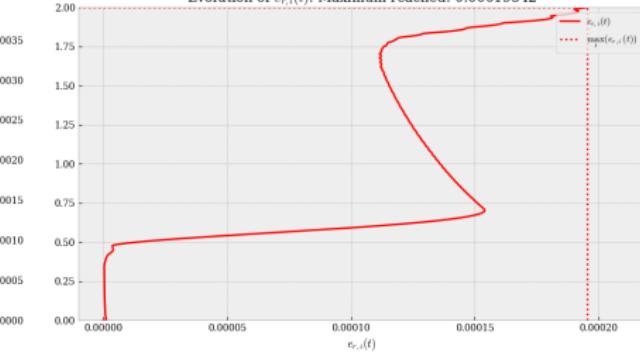


Figure: $\Omega_{\text{PML}} = [-10, 15]$, the simulation took about an hour.

Optimization of σ_0

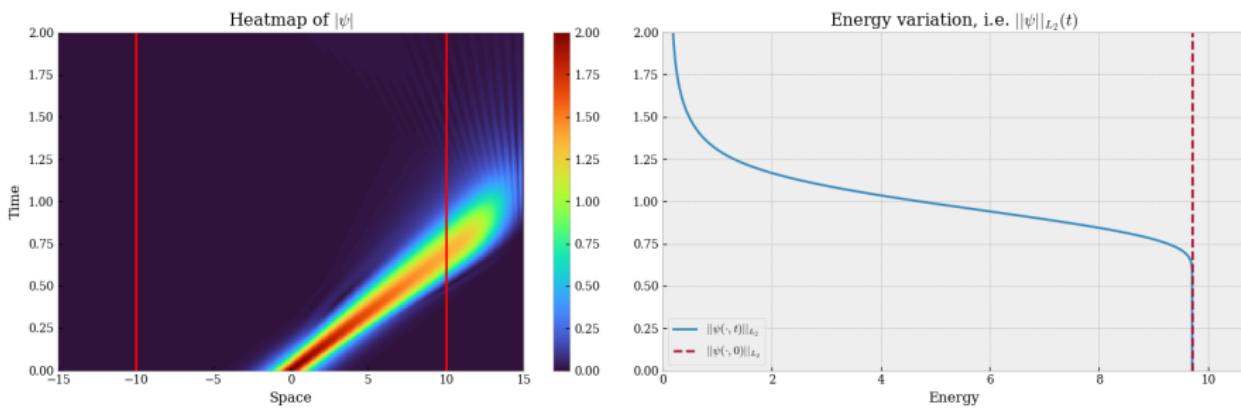


Figure: $\sigma_0 = 0.05$

