Absorbing boundary conditions and domain decomposition methods for nonlinear Schrödinger equations

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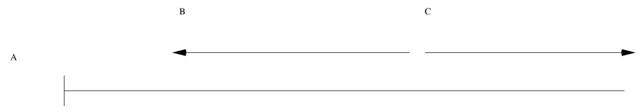
Absorbing Boundary Conditions for nonlinear Schrödinger equations

ABC for linear variable coefficients equations (Engquist-Majda)

1D wave equation : $\partial_t^2 - \partial_x^2 = -(\partial_x + \partial_t)(\partial_x - \partial_t)$.

We annihilate the reflected wave : $(\partial_x - \partial_t)u = 0$.



$$\partial_t^2 - \partial_x^2 + \alpha(t,x) + \beta(t,x)\partial_t + \gamma(t,x)\partial_x$$
$$= -(\partial_x - a(x,t,D_t))(\partial_x - b(x,t,D_t)) + S^{-\infty}$$

where $a(x,t,D_t)$ and $b(x,t,D_t)$ are pseudodifferential operators

Transparent boundary condition : $(\partial_x - b(x,t,D_t))u = 0$

ABC for linear variable coefficients equations (Engquist-Majda)

$a(x,t,\tau) = \sum_{j\geq 0} a_{1-j}(x,t,\tau)$ and $b(x,t,\tau) = \sum_{j\geq 0} b_{1-j}(x,t,\tau)$

$$\begin{cases} b_1 = i\tau \text{ and } a_1 = -i\tau, \\ b_0 = \dfrac{\gamma-\beta}{2} \text{ and } a_0 = \dfrac{\beta+\gamma}{2}, \\ b_{-1} = \dfrac{-\alpha + (\beta^2-\gamma^2)/4 + (\partial_x - \partial_t)(\gamma-\beta)/2}{2i\tau} = -a_{-1}. \end{cases}$$

The k-th order absorbing boundary condition is

$$\left(\partial_x - \sum_{j=0}^{k} b_{1-j}(0,t,D_t)\right) u|_{x=0} = 0.$$

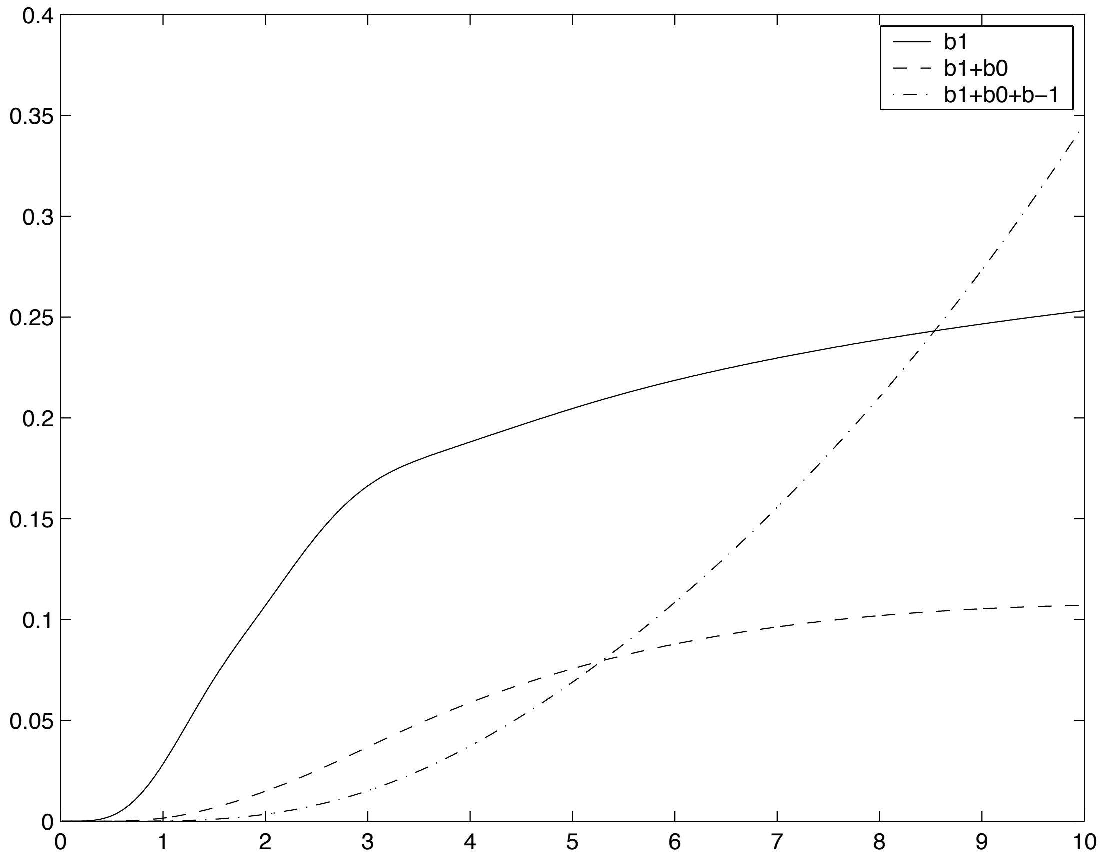


FIG. 1 – $\partial_t^2 u - \partial_x^2 u + \partial_t u = 0$. Relative error in L^2 in function of time. abc —— order 0, $- -$ order 1 and $\cdot - \cdot$ order 2

Short-time behaviour of ABC

High frequency asymptotic expansions

Numerical frequencies $= [\pi/T, \pi/\Delta t]$

$T \ll 1 \Rightarrow$ only high frequencies

Thus, ABC always good for small times

Goal : We would like to recover the properties of the Engquist-Majda method in the nonlinear case

Potential strategy

Gauge change strategy

Linearization strategy

Numerical results

Potential strategy

$$(i\partial_t + \partial_x^2)u + |u|^2 u = 0$$

$$V(t,x) = |u(t,x)|^2$$

$$(i\partial_t + \partial_x^2)u + Vu = 0$$

We can see this as a linear equation with a potential term and apply the Engquist-Majda method

$\Rightarrow$ We obtain BC involving V

ABC of order 0 : $\partial_x u + \sqrt{-i\partial_t}u = 0$

Potential strategy

$$(i\partial_t + \partial_x^2)u + |u|^2 u = 0$$

ABC order 1 : $\partial_x u + \sqrt{-i\partial_t}u = 0$

ABC order 2 : $\partial_x u + \sqrt{-i\partial_t}u + |u|^2/2\sqrt{-i\partial_t}^{-1}u = 0$

ABC order 3 :
$$\partial_x u + \sqrt{-i\partial_t}u + |u|^2/2\sqrt{-i\partial_t}^{-1}u + i\partial_x(|u|^2)/4\partial_t^{-1}u = 0$$

$\sqrt{-i\partial_t}$ and $\sqrt{-i\partial_t}^{-1}$ are approximated using quadrature formulas

Other models : reaction-diffusion, semi-linear wave equation

Gauge change strategy

$$(i\partial_t + \partial_x^2)u + |u|^2 u = 0$$

$$v(x,t) = e^{-i\mathcal{B}(t,x)}u(x,t), \text{ where } \mathcal{B}(t,x) = \int_0^t |u|^2(\tau,x)d\tau,$$

$$i\partial_t v + \partial_x^2 v + (2i\partial_x\mathcal{B})\partial_x v + (i\partial_x^2\mathcal{B} - (\partial_x\mathcal{B})^2)v = 0$$

Linear equation for v with coefficients $2i\partial_x\mathcal{B}$ and $i\partial_x^2\mathcal{B} - (\partial_x\mathcal{B})^2$

We may apply the Engquist-Majda method

$\Rightarrow$ We obtain BC involving $\mathcal{B}$

ABC of order 0 : $\partial_{\mathbf{n}}u + e^{-i\frac{\pi}{4}}e^{i\mathcal{B}}\partial_t^{1/2}(e^{-i\mathcal{B}}u) = 0$

Gauge change strategy

$$(i\partial_t + \partial_x^2)u + |u|^2 u = 0$$

$$\mathcal{B}(t,x) = \int_0^t |u|^2(\tau,x)d\tau$$

ABC order 1 : $\partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}} e^{i\mathcal{B}} \partial_t^{1/2}(e^{-i\mathcal{B}}u) = 0$

ABC order 3 :

$$\partial_{\mathbf{n}} u + e^{-i\frac{\pi}{4}} e^{i\mathcal{B}} \partial_t^{1/2}(e^{-i\mathcal{B}}u) - i\frac{\partial_{\mathbf{n}}(|u|^2)}{4} e^{i\mathcal{B}} \int_0^t (e^{-i\mathcal{B}}u)d\tau = 0$$

Potential and Gauge change strategy coincide at high frequencies, but different for low frequencies

Linearization strategy

$$(i\partial_t + \partial_x^2)u + u\partial_x u = 0$$

Linearize around u : $(i\partial_t + \partial_x^2)v + u\partial_x v + \partial_x u v = 0$

This is a linear equation for v with coefficients $u(t,x)$ and $\partial_x u(t,x)$

We may apply the Engquist-Majda method

$\Rightarrow$ We obtain BC for v involving u and $\partial_x u$

We have then to 'unlinearize'

For example, $(\partial_x + \sqrt{-i\partial_t})v + uv/2 = 0$

is unlinearized to give the first order ABC :

$$(\partial_x + \sqrt{-i\partial_t})u + u^2/4 = 0$$

Linearization strategy

$$(i\partial_t + \partial_x^2)u + u\partial_x u = 0$$

ABC order 0 : $\partial_x u + \sqrt{-i\partial_t}u = 0$

ABC order 1 : $\partial_x u + \sqrt{-i\partial_t}u + u^2/4 = 0$

ABC order 2 : $\partial_x u + \sqrt{-i\partial_t}u + u^2/8 - \sqrt{-i\partial_t}^{-1}(u\partial_x u/4) = 0$

Problem of the linearization strategy :

It is not always clear how to 'unlinearize'

Other model : semi-linear wave equation

Numerical results

$(i\partial_t + \partial_x^2)u + |u|^2 u = 0$: **relative error**

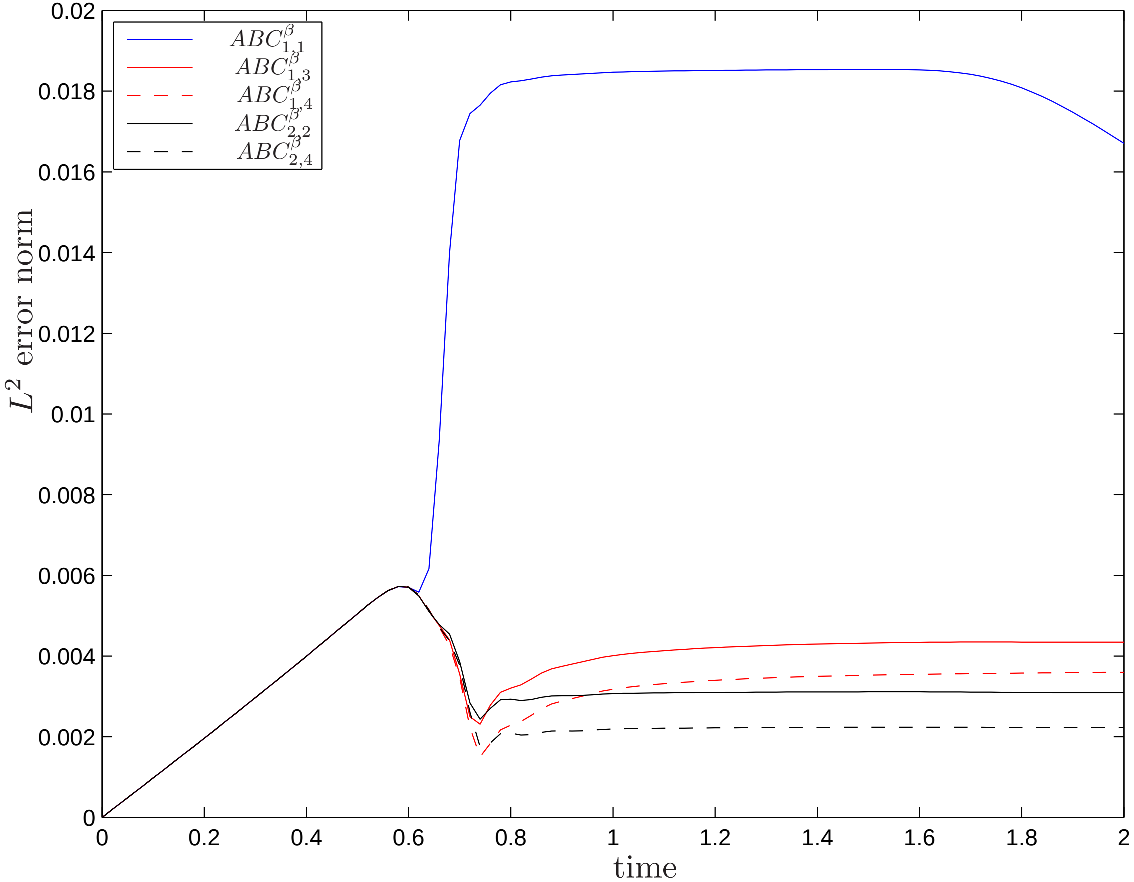


FIG. 2 – Comparison of potential and gauge change strategy

$(i\partial_t + \partial_x^2)u + u\partial_x u = 0$: **relative error**

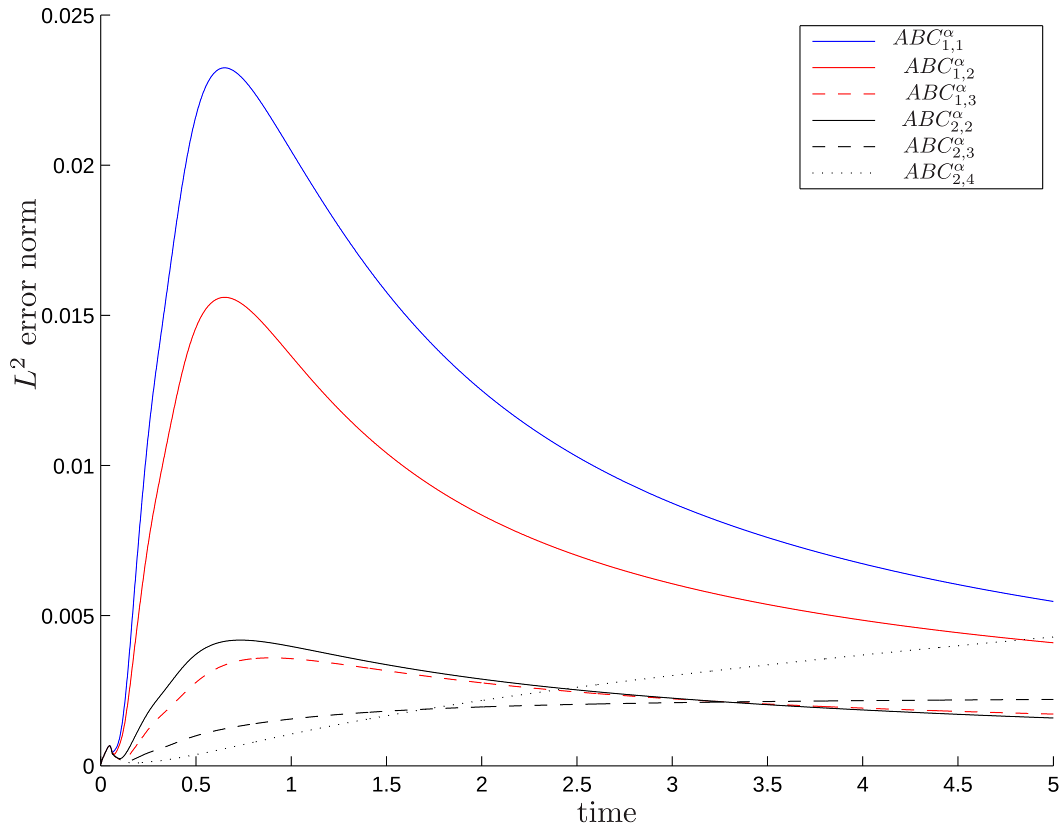


FIG. 3 – Comparision of potential and linearization strategy

Optimality of the ABC

$$\begin{cases} (i\partial_t + \partial_x^2)u + u\partial_x u = 0 \text{ in }]0,T[\times]0,2[\\ \partial_x u - \sqrt{-i\partial_t}u - \alpha\, u^2 = 0 \text{ at } x = 0 \\ \partial_x u + \sqrt{-i\partial_t}u + \alpha\, u^2 = 0 \text{ at } x = 2 \end{cases}$$

order zero : $\alpha = 0$, order 1 with potential strategy : $\alpha = 1/2$, and order 1 with linearization strategy : $\alpha = 1/4$

$\alpha = 0$	$\alpha = \frac{1}{8}$	$\alpha = \frac{1}{4}$	$\alpha = \frac{1}{2}$	$\alpha = 1$	$\alpha = 2$	$\alpha = 5$	$\alpha = -\frac{1}{4}$
0.0231	0.0136	0.0042	0.0155	0.0551	0.1390	0.3463	0.0601

TAB. 1 – Maximum of the relative error for $0 \le t \le 10$ and for various choices of α.

Conclusions and perspectives

- We have extended the method of B. Engquist and A. Majda to nonlinear problems in three ways : the potential strategy, the gauge change strategy and the linearization strategy

- Improve the method for long-time computations

- Extend the results to higher dimensions, curved boundaries and systems

Domain Decomposition Methods for linear Schrödinger equations

The Schrödinger equation

$$\begin{cases} i\partial_t u(t,x) + \partial_x^2 u(t,x) + V(x)u(t,x) = 0 \\ u(0,x) = u_0(x) \end{cases}$$

Quantum mechanics, electromagnetic wave propagation,

optic (Fresnel equation)

Goal : Design efficient Schwarz Waveform Relaxation algorithms

for the Schrödinger equation

Schwarz Waveform Relaxation algorithm

= global in time domain decomposition method

Classical Schwarz Waveform Relaxation

Optimal Schwarz Waveform Relaxation Algorithm

The Quasi-Optimal Algorithm

The Robin Algorithm

Numerical schemes

Numerical results

Classical Schwarz Waveform Relaxation

$$\begin{cases} (i\partial_t + \partial_x^2 + V)u_1^k = 0 \text{ in } \Omega_1 \times (0,T) \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1 \\ u_1^k(L,\cdot) = u_2^{k-1}(L,\cdot) \text{ in } (0,T) \end{cases} \qquad \begin{cases} (i\partial_t + \partial_x^2 + V)u_2^k = 0 \text{ in } \Omega_2 \times (0,T) \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2 \\ u_2^k(0,\cdot) = u_1^{k-1}(0,\cdot) \text{ in } (0,T) \end{cases}$$

Convergence factor :

$$\Theta(\tau, L) = e^{-(\tau - V)^{1/2} L}$$

$\Theta(\tau, 0) = 1$: no convergence without overlap !

Optimal Schwarz Waveform Relaxation Algorithm

$$\begin{cases} (i\partial_t + \partial_x^2 + V)u_1^k = 0 \text{ in } \Omega_1 \times (0,T) \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1 \\ (\partial_x + \mathcal{S}_1)u_1^k(L,\cdot) \\ = (\partial_x + \mathcal{S}_1)u_2^{k-1}(L,\cdot) \text{ in } (0,T) \end{cases} \quad \begin{cases} (i\partial_t + \partial_x^2 + V)u_2^k = 0 \text{ in } \Omega_2 \times (0,T) \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2 \\ (\partial_x + \mathcal{S}_2)u_2^k(0,\cdot) \\ = (\partial_x + \mathcal{S}_2)u_1^{k-1}(0,\cdot) \text{ in } (0,T) \end{cases}$$

Convergence in 2 iterations if and only if

$$\sigma_1 = (\tau - V)^{1/2}, \quad \sigma_2 = -(\tau - V)^{1/2}$$

$$(\tau - V)^{1/2} = \begin{cases} \sqrt{\tau - V} \text{ if } \tau \geq V \\ -i\sqrt{-\tau + V} \text{ if } \tau < V \end{cases}$$

For non constant V : optimal operators not at hand

The Quasi-Optimal Algorithm

$$\begin{cases} (i\partial_t + \partial_x^2 + V)u_1^k = 0 \text{ in } \Omega_1 \times (0,T) \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1 \\ (\partial_x + \sqrt{-i\partial_t - V(L)})u_1^k(L,\cdot) \\ = (\partial_x + \sqrt{-i\partial_t - V(L)})u_2^{k-1}(L,\cdot) \end{cases} \quad \begin{cases} (i\partial_t + \partial_x^2 + V)u_2^k = 0 \text{ in } \Omega_2 \times (0,T) \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2 \\ (\partial_x - \sqrt{-i\partial_t - V(0)})u_2^k(0,\cdot) \\ = (\partial_x - \sqrt{-i\partial_t - V(0)})u_1^{k-1}(0,\cdot) \end{cases}$$

$$(\tau - V(x))^{1/2} = \begin{cases} \sqrt{\tau - V(x)} \text{ if } \tau \geq V(x) \\ -i\sqrt{-\tau + V(x)} \text{ if } \tau < V(x) \end{cases}$$

The algorithm converges in

$$(H^{1/4}(0,T,L^2(\Omega_1)) \cap H^{-1/4}(0,T,H^1(\Omega_1))) \\ \times (H^{1/4}(0,T,L^2(\Omega_2)) \cap H^{-1/4}(0,T,H^1(\Omega_2)))$$

The Complex Robin Algorithm

Zero order approximation of the Optimal Algorithm :

$$\begin{cases} (i\partial_t + \partial_x^2 + V)u_1^k = 0 \text{ in } \Omega_1 \times (0,T) \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1 \\ (\partial_x - ip)u_1^k(L,\cdot) \\ = (\partial_x - ip)u_2^{k-1}(L,\cdot) \text{ in } (0,T) \end{cases} \quad \begin{cases} (i\partial_t + \partial_x^2 + V)u_2^k = 0 \text{ in } \Omega_2 \times (0,T) \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2 \\ (\partial_x + ip)u_2^k(0,\cdot) \\ = (\partial_x + ip)u_1^{k-1}(0,\cdot) \text{ in } (0,T) \end{cases}$$

$$\rho(\tau,p,L) = \frac{ip + (\tau - V)^{1/2}}{ip - (\tau - V)^{1/2}} \, e^{-(\tau - V)^{1/2} L}$$

Convergence for any $p > 0$ even without overlap

Optimization with respect to $p > 0$ to improve the convergence

Numerical schemes

Finite volumes discretization

Interior = Crank Nicolson scheme

Quasi-Optimal algorithm : discretize $\sqrt{-i\partial_t + V}$

Approximation of Arnold and Ehrhardt

$$\sqrt{-i\partial_t + V}U(0,n) \simeq \sum_{m=0}^{n} S(n-m)U(0,m)$$

where $S(m)$ is given by a recurrence formula

Other possible approximations : Antoine and Besse, ...

Numerical results

Optimal p for the Robin algorithm

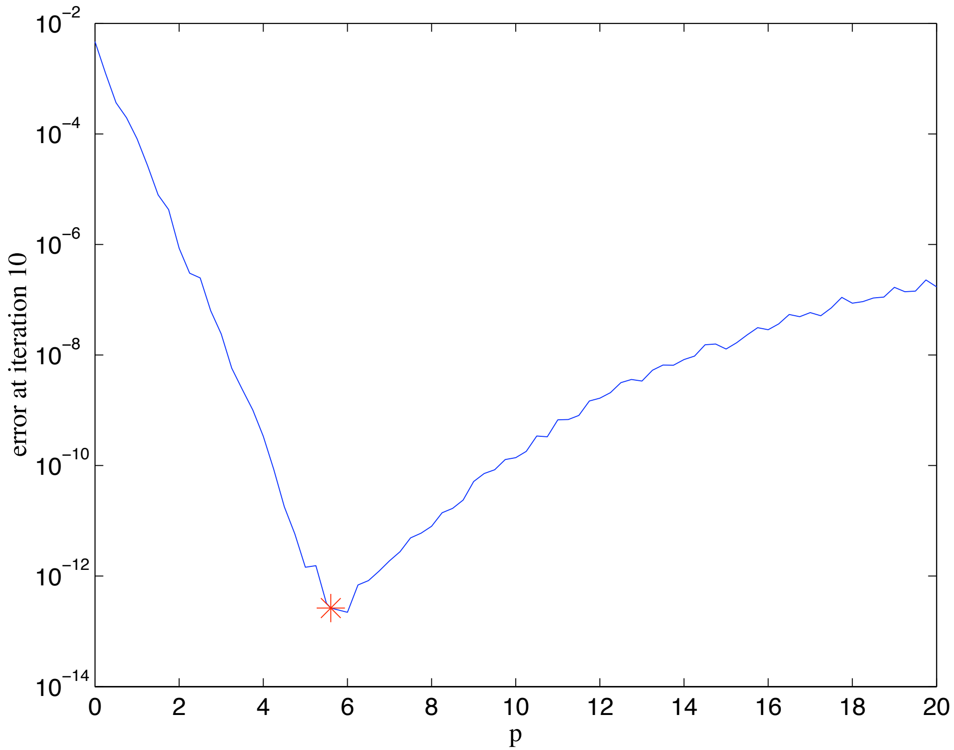


FIG. 4 – Variation of the quadratic error in time and space in Ω_1 as a function of p. The overlap is equal to 1%. The star corresponds to the theoretical optimal value p_T. Free Schrödinger equation

Comparison Classical/Robin algorithms

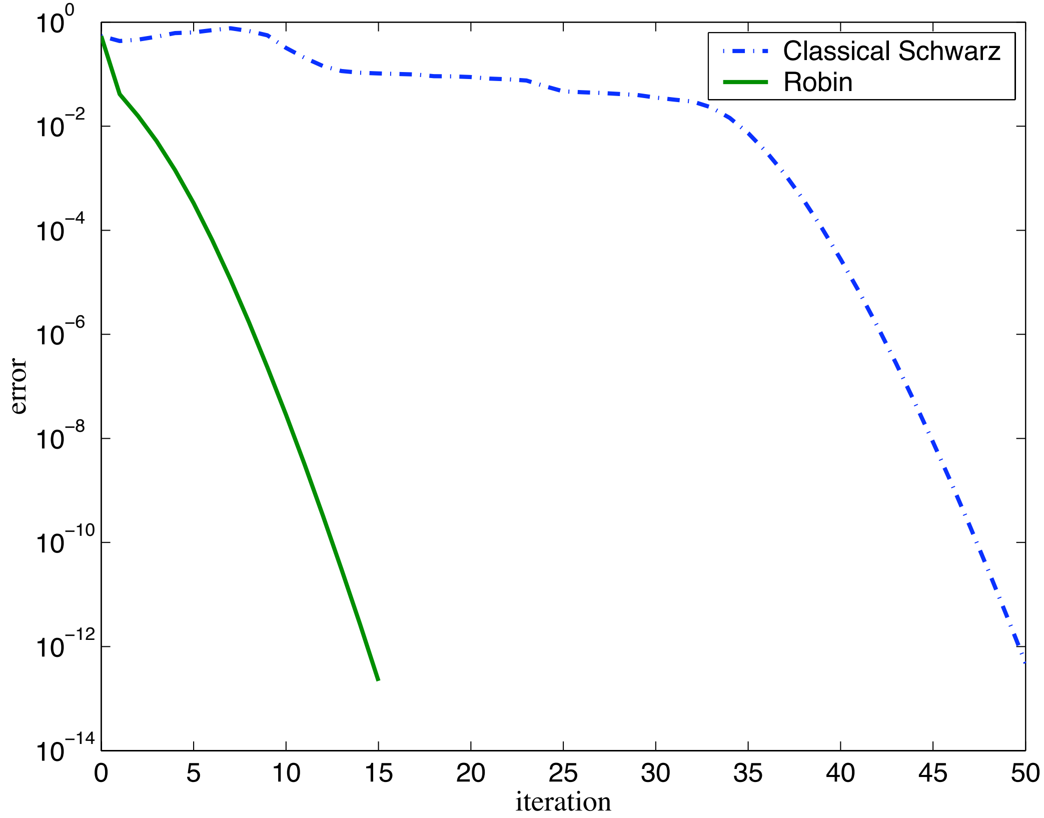


FIG. 5 – Convergence history : comparison of the Classical and Optimized Robin Schwarz algorithm. Free Schrödinger equation. $\delta = 2\%$

Robin algorithm without overlap

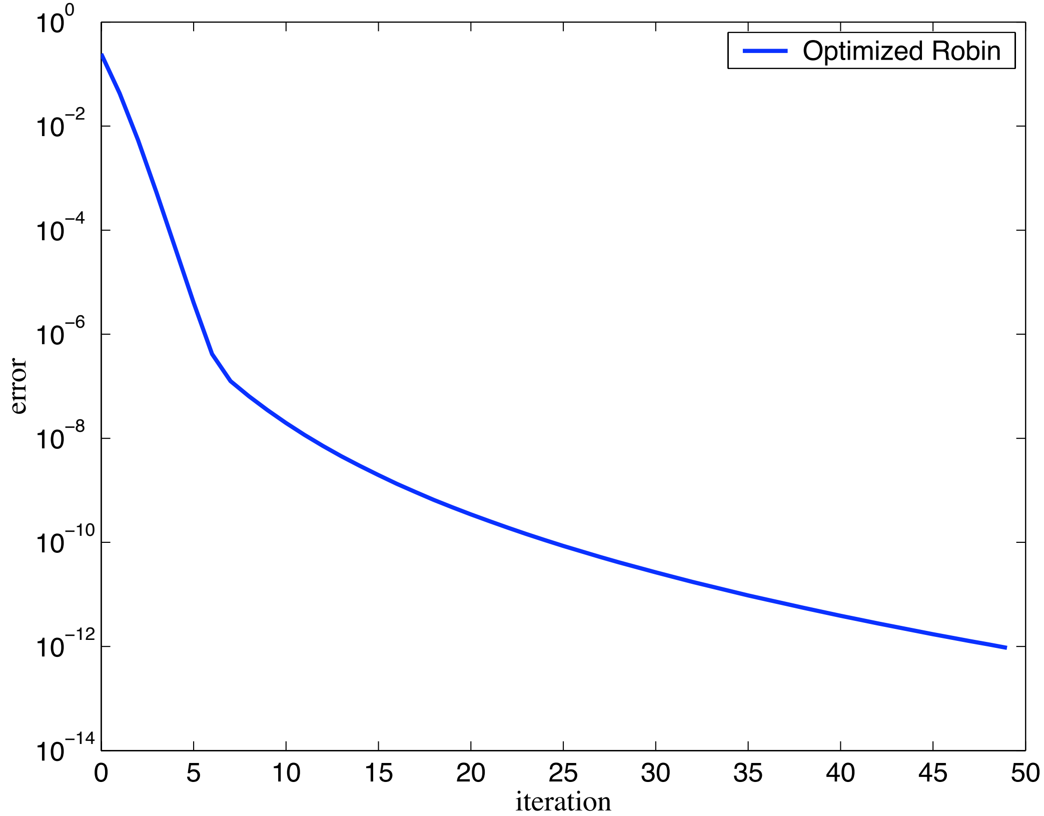


FIG. 6 – Convergence history for the Optimized Robin Schwarz algorithm in the non overlapping case. Free Schrödinger equation

Comparison Classical/Robin algorithms

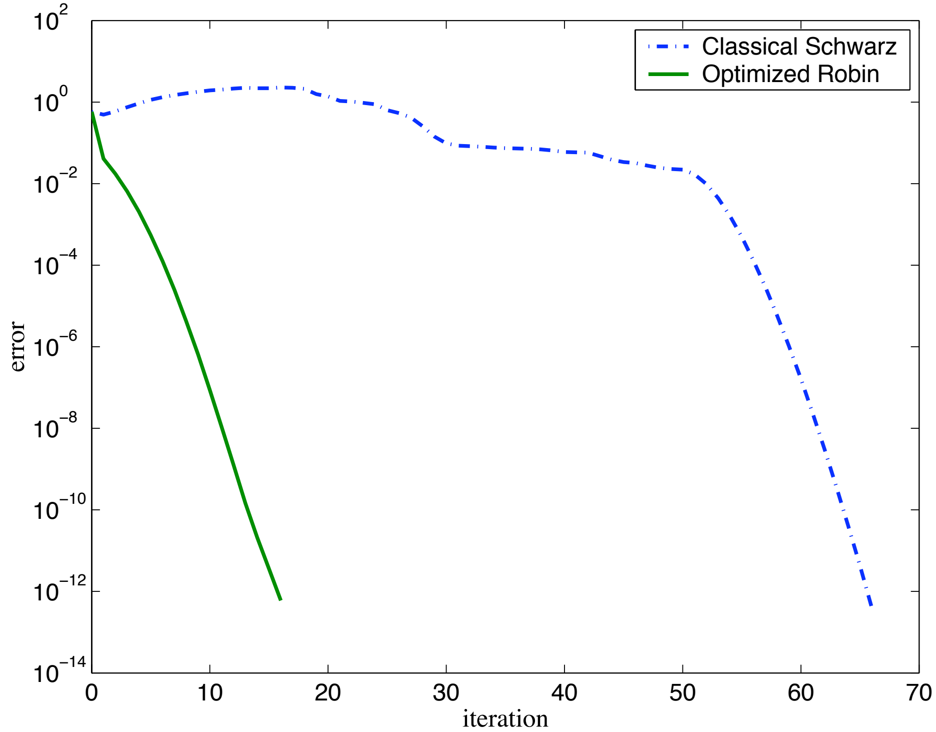


FIG. 7 – Convergence history : comparison of the Classical and Optimized Robin Schwarz algorithm for a potential barrier. The overlap is equal to 4%

The Quasi-Optimal algorithm

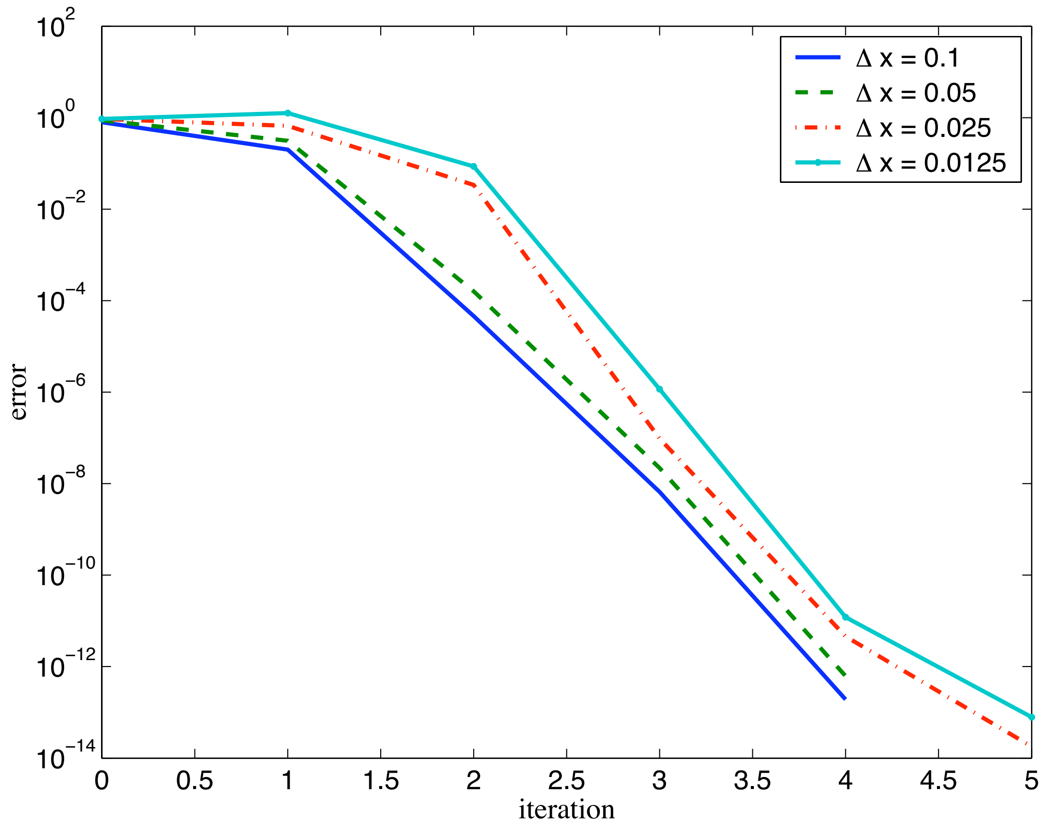


FIG. 8 – Convergence history for the Quasi-Optimal Schwarz algorithm in presence of a parabolic potential

Conclusions and perspectives

- The Classical algorithm converges extremely slowly for the Schrödinger equation with or without a potential

- We have designed two alternative algorithms : a Complex Optimized Robin algorithm and a Quasi-Optimal algorithm

- These algorithms greatly improve the performances of the classical Schwarz relaxation algorithm

- Extend the results to higher dimensions, nonlinear problems

- Use ABC to improve the transmission conditions