Optimized and Quasi-optimal Schwarz Waveform Relaxation for the One Dimensional Schrödinger Equation

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Summary. We design and study Schwarz Waveform relaxation algorithms for the linear Schrödinger equation with a potential in one dimension. We show that the overlapping algorithm with Dirichlet exchanges of informations on the boundary is slowly convergent, and we introduce two new classes of algorithms: the optimized Robin algorithm and the quasi-optimal algorithm. Numerical results illustrate the great improvement of these methods over the classical algorithm.

1 Introduction

We investigate the design of domain decomposition algorithms for the linear Schrödinger equation with a real potential V, in one space dimension:

$$\begin{cases} i\partial_t u(t,x) + \partial_x^2 u(t,x) + V(x)u(t,x) = 0,\ t \geq 0,\ x \in \mathbb{R}, \\ u(0,x) = u_0(x). \end{cases} \tag{1}$$

This equation is an important model in quantum mechanics, in electromagnetic wave propagation, and in optics (Fresnel equation). To our knowledge, there is no study prior to the present work on domain decomposition methods for the Schrödinger equation.

We first introduce the classical algorithm, with overlapping subdomains, exchanging Dirichlet data on the boundaries. Its slow convergence emphasizes the need for new algorithms.

The key point of these new algorithms is to notice that the convergence in two iterations is obtained when using transparent boundary operators as transmission operators between the subdomains, even in the non-overlapping case. However, these operators are not available for a general potential. Thus, we introduce a quasi-optimal algorithm using the transparent operators corresponding to the value of the potential on the boundary. We also study the

possibility of using simpler transmission conditions on the boundary, of complex Robin type.

We then introduce a discretization of the Robin algorithm and a discretization of the quasi-optimal algorithm.

We finally illustrate the results through numerical simulations, for various types of potentials, like constant, barrier, or parabolic. We show how slow the convergence is with Dirichlet Schwarz Waveform Relaxation (SWR), and how the optimized SWR greatly improves the convergence. We also show, that the best results by far are obtained by the discrete quasi-optimal algorithm.

Remark 1. For a more detailed study, we refer the reader to [6].

2 Classical Schwarz Waveform Relaxation

Let $\mathcal{L} := i\partial_t + \partial_x^2 + V(x)$. We decompose the spatial domain $\Omega = \mathbb{R}$ into two overlapping subdomains $\Omega_1 = (-\infty, L)$ and $\Omega_2 = (0, \infty)$, with $L > 0$. The overlapping Schwarz waveform relaxation algorithm consists in solving iteratively subproblems on $\Omega_1 \times (0,T)$ and $\Omega_2 \times (0,T)$, using as a boundary condition at the interfaces $x = 0$ and $x = L$ the values obtained from the previous iteration. The algorithm is thus for iteration index $k = 1, 2, \ldots$ given by

$$\begin{cases} \mathcal{L}u_1^k = f \text{ in } \Omega_1 \times (0,T), \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1, \\ u_1^k(L,\cdot) = u_2^{k-1}(L,\cdot), \end{cases} \qquad \begin{cases} \mathcal{L}u_2^k = f \text{ in } \Omega_2 \times (0,T), \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2, \\ u_2^k(0,\cdot) = u_1^{k-1}(0,\cdot). \end{cases} \tag{2}$$

Using the Fourier transform in time, we easily compute the convergence factor of the classical algorithm in the case where the potential V is constant:

$$\Theta(\tau, L) = exp\left[-\left(\frac{-\tau + V + \sqrt{1 + (\tau - V)^2}}{2} \right)^{1/2} L \right], \tag{3}$$

where τ is the time frequency.

The convergence factor in (3) tends to 1 when the overlap L tends to 0, as all overlapping Schwarz methods do. But it also tends to 1 when τ tends to infinity, which differs from what happens for wave equations [5] or parabolic equations [3]. This deterioration of the convergence factor for high frequencies suggests a poor performance of the classical algorithm for the Schrödinger equation. This is confirmed by the numerical results. In figure 1, we present the exact solution and the approximate solution computed with the classical algorithm at various times for the free Schrödinger equation ($V = 0$). The results are displayed after 200 iterations of the algorithm. We take two subdomains $\Omega_1 = (-5, 4\Delta x)$ and $\Omega_2 = (0, 5)$, and the step sizes are $\Delta t = 0.00125$, $\Delta x = 0.0125$.

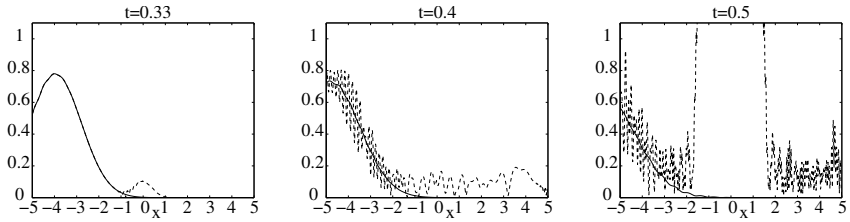

Fig. 1. Exact solution (solid) and approximate solution computed with the classical algorithm at iteration 200 (dashed). **(a)** $t = 0.33$, **(b)** $t = 0.4$, **(c)** $t = 0.5$

Although the algorithm works well for times up to $t = 0.3$, it then deteriorates so that the approximate solution becomes extremely oscillating and does not approximate the exact solution at all. Since this bad behavior happens after 200 iterations, this clearly demonstrates that one should avoid the classical algorithm when computing the Schrödinger equation. This also motivates the need for new algorithms, which we investigate in the next sections.

3 Optimal Schwarz Waveform Relaxation Algorithm

When V is constant, it is possible to compute the optimal algorithm. Let $\mathcal{S}_1$ and $\mathcal{S}_2$ be linear operators acting only in time. We introduce the algorithm

$$\begin{cases} \mathcal{L}u_1^k = f \text{ in } \Omega_1 \times (0,T), \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1, \\ (\partial_x + \mathcal{S}_1)u_1^k(L,\cdot) \\ \qquad = (\partial_x + \mathcal{S}_1)u_2^{k-1}(L,\cdot), \end{cases} \quad \begin{cases} \mathcal{L}u_2^k = f \text{ in } \Omega_2 \times (0,T), \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2, \\ (\partial_x + \mathcal{S}_2)u_2^k(0,\cdot) \\ \qquad = (\partial_x + \mathcal{S}_2)u_1^{k-1}(0,\cdot). \end{cases} \tag{4}$$

We define the symbol σ_j of $\mathcal{S}_j(\partial_t)$ by $\sigma_j(\tau) = \mathcal{S}_j(i\tau)$. Using Fourier transform in time, we can prove that the algorithm (4) converges to the solution u of (1) in two iterations independently of the size of the overlap $L \geq 0$, if and only if the operators $\mathcal{S}_1$ and $\mathcal{S}_2$ have the corresponding symbols

$$\sigma_1 = (\tau - V)^{1/2}, \quad \sigma_2 = -(\tau - V)^{1/2} \tag{5}$$

with

$$(\tau - V)^{1/2} = \begin{cases} \sqrt{\tau - V} \text{ if } \tau \geq V, \\ -i\sqrt{-\tau + V} \text{ if } \tau < V. \end{cases} \tag{6}$$

For variable potentials, the optimal operators are in general not at hand. We present here and will compare two approximations of those. The first one is to use a "frozen coefficients" variant of these operators. The second one is to replace them by a constant, obtaining "Robin type" transmission conditions, and to optimize them by minimizing the convergence factor in the constant case.

4 The Quasi-optimal Algorithm

We use as transmission operators the optimal operators for the constant potential equal to the value of V on the interface. The quasi-optimal algorithm is thus for iteration index $k = 1, 2, \ldots$ given by

$$\begin{cases} \mathcal{L}u_1^k = f \text{ in } \Omega_1 \times (0,T), \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1, \\ (\partial_x + \sqrt{-i\partial_t - V(L)})u_1^k(L,\cdot) = \\ (\partial_x + \sqrt{-i\partial_t - V(L)})u_2^{k-1}(L,\cdot), \end{cases} \quad \begin{cases} \mathcal{L}u_2^k = f \text{ in } \Omega_2 \times (0,T), \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2, \\ (\partial_x - \sqrt{-i\partial_t - V(0)})u_2^k(0,\cdot) = \\ (\partial_x - \sqrt{-i\partial_t - V(0)})u_1^{k-1}(0,\cdot) \end{cases} \tag{7}$$

where $\sqrt{-i\partial_t - V(x)}$ is the operator acting only in time with symbol given by (6). Though being not differential, this operator is still easy to use numerically [2].

We call the algorithm (7) quasi-optimal, since it is optimal for a constant potential. Even for a non constant potential V, we are able to prove its convergence when there is no overlap, *i.e.* $L = 0$, and when $T = +\infty$ in the following spaces:

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

The proof is based on energy estimates and follows an idea from [7], which has widely been used since (see [4, 8] for steady problems, [5] for evolution equations). Here, the additional difficulty is to deal with the nonlocal operator $\sqrt{-i\partial_t - V(0)}$.

5 The Algorithm with Robin Transmission Conditions

A simple alternative to the previous approach is to use Robin transmission conditions, *i.e.* to replace the optimal operators $\mathcal{S}_j$ by $\mathcal{S}_1 = -\mathcal{S}_2 = -ipI$ where p is a real number, which gives the algorithm

$$\begin{cases} \mathcal{L}u_1^k = f \text{ in } \Omega_1 \times (0,T), \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1, \\ (\partial_x - ip)u_1^k(L,\cdot) \\ \qquad = (\partial_x - ip)u_2^{k-1}(L,\cdot), \end{cases} \quad \begin{cases} \mathcal{L}u_2^k = f \text{ in } \Omega_2 \times (0,T), \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2, \\ (\partial_x + ip)u_2^k(0,\cdot) \\ \qquad = (\partial_x + ip)u_1^{k-1}(0,\cdot). \end{cases} \tag{8}$$

Remark 2. This algorithm is not the usual Robin algorithm as the constant ip used here is complex, whereas the usual Robin algorithm uses a real constant.

Relying on energy estimates, we are able to prove the convergence even for a non constant potential V when there is no overlap, *i.e.* $L = 0$, and for any $p > 0$ in the following spaces:

$$L^\infty(0,T;L^2(\Omega_1)) \times L^\infty(0,T;L^2(\Omega_2)).$$

Of course, the convergence taking place for any $p > 0$, we will optimize the convergence rate with respect to $p > 0$ in order to accelerate the convergence.

6 Construction of the Discrete Algorithms

For the Robin algorithm, we use a finite volume discretization. In the interior, it produces the Crank-Nicolson scheme, widely used in the linear and nonlinear computations for the Schrödinger equation, whereas the Robin transmission conditions are naturally taken into account. This idea was first introduced in [5] for the wave equation in one dimension.

For the discretization of the quasi-optimal algorithm, we also use the Crank-Nicolson scheme on the interior. Here, the main task is to discretize the nonlocal transmission condition. We thus have to discretize the operator $\sqrt{-i\partial_t + V}$. We use the discrete transparent boundary condition designed by Arnold and Ehrhardt precisely for the Crank-Nicolson scheme [2]. It is a discrete convolution:

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

where the convolution kernel $S(m)$ is given by a recurrence formula (see [2]).

Remark 3. Other choices of discrete transparent boundary conditions (for example the one designed in [1]) could be used to discretize the quasi-optimal algorithm.

7 Numerical Results

The physical domain is $(a,b) = (-5,+5)$. It is divided in two subdomains of equal size. Our algorithms are implemented the Gauss-Seidel way, *i.e.* we compute u_1 with g_L, then deduce g_0 by u_1 and give it to the right domain for the computation of u_2. Thus iteration $\#k$ in this section corresponds to the computation of u_1^{2k-1}, u_2^{2k} in the theoretical setting.

7.1 The Free Schrödinger Equation

In the case of the free Schrödinger equation, the quasi-optimal algorithm coincides with the optimal one and converges in two iterations as expected by the theory. It is thus the best algorithm, but we would still like to see how the Robin algorithm behaves and to compare it with the classical algorithm. We consider in Figure 2 an overlap of 2%. The error is the L^2 norm of the error on the boundary of Ω_2. We clearly see the great improvement.

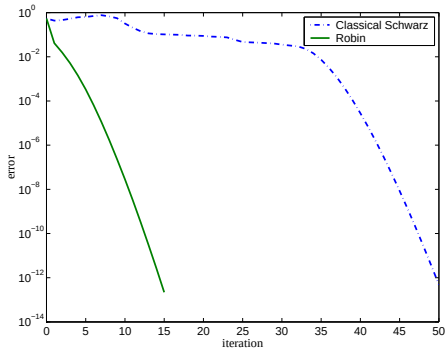

Fig. 2. Convergence history: comparison of the Dirichlet and optimized Robin Schwarz algorithm. $\delta = 2\%$.

7.2 Non Constant Potentials

We consider the interval $(-5, 5)$, with a final time $T = 1$, discretized with $\Delta x = 0.05$ and $\Delta t = 0.005$. The size of the overlap is $4\Delta x$. The potential is a barrier equal to 20 times the characteristic function of the interval $(-1, 1)$. In figure 3, we draw the convergence history for Dirichlet and Robin algorithms. In this case again, the Robin condition behaves much better than the Dirichlet condition.

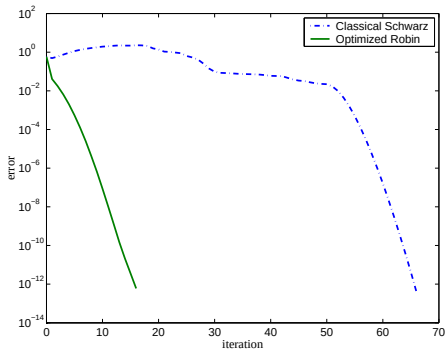

Fig. 3. Convergence history: comparison of the Dirichlet and optimized Robin Schwarz algorithm for a potential barrier. The overlap is equal to 4%.

The quasi-optimal algorithm is by far the most efficient. In all cases, even when the potential is not constant, the precision 10^{-12} is reached in at most five iterations with or without overlap. As an example, we show in Figure 4 the convergence history with an overlap of 8 grid points, for a parabolic potential, for various mesh sizes. The convergence does not depend on the mesh size.

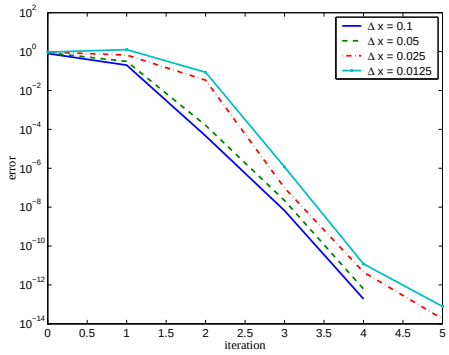

Fig. 4. Convergence history for the quasi-optimal Schwarz algorithm in presence of a parabolic potential

Finally, we present the exact solution and the approximate solution computed with the three algorithms at time $t = 0.9$ for a parabolic potential. The results are displayed after only three iterations of the algorithm. We take two subdomains $\Omega_1 = (-5, 4\Delta x)$ and $\Omega_2 = (0, 5)$, and the step sizes are $\Delta t = 0.0025$ and $\Delta x = 0.025$. As expected, the classical algorithm produces a highly oscillating solution. The Robin algorithm behaves far better and clearly approximates the exact solution. Finally, the quasi-optimal algorithm is the best as we can not distinguish between the exact and the approximate solution.

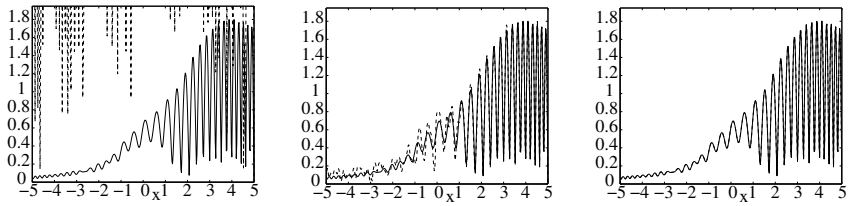

Fig. 5. Exact solution (solid) and approximate solution computed with the three algorithms after 3 iterations (dashed) at time $t = 0.9$. **(a)** Classical algorithm, **(b)** Robin algorithm, **(c)** quasi-optimal algorithm

Remark 4. The Robin algorithm is very sensitive to the value of $p > 0$. In our numerical experiments, we take the optimal value of p obtained for a constant potential V which is given by an explicit formula.

Remark 5. As predicted by the theory, our numerical results indicate that the Robin algorithm and the quasi-optimal algorithm both converge even without overlap unlike the classical algorithm.

8 Conclusion

We have presented here a general approach to design optimized and quasi-optimal domain decomposition algorithms for the linear Schrödinger equation with a potential in one dimension. It allows the use of any discretization, any time and space steps in the subdomains. These algorithms greatly improve the performances of the classical Schwarz relaxation algorithm. We intend to extend our analysis to the two-dimensional case in a close future.

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