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Explicit Computation of Robin Parameters in Optimized Schwarz Waveform Relaxation Methods for Schrödinger Equations Based on Pseudodifferential Operators

Xavier Antoine[1,1] and Emmanuel Lorin[2,3]

[1] *Institut Elie Cartan de Lorraine, Université de Lorraine, Sphinx Inria team, Inria Nancy-Grand Est, F-54506 Vandoeuvre-lès-Nancy Cedex, France.*
[2] *School of Mathematics and Statistics, Carleton University, Ottawa, Canada, K1S 5B6.*
[3] *Centre de Recherches Mathématiques, Université de Montréal, Montréal, Canada, H3T 1J4.*

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Abstract. The Optimized Schwarz Waveform Relaxation algorithm, a domain decomposition method based on Robin transmission condition, is becoming a popular computational method for solving evolution partial differential equations in parallel. Along with well-posedness, it offers a good balance between convergence rate, efficient computational complexity and simplicity of the implementation. The fundamental question is the selection of the Robin parameter to optimize the convergence of the algorithm. In this paper, we propose an approach to explicitly estimate the Robin parameter which is based on the approximation of the transmission operators at the subdomain interfaces, for the linear/nonlinear Schrödinger equation. Some illustrating numerical experiments are proposed for the one- and two-dimensional problems.

AMS subject classifications: 65M55, 65M60, 65M06, 35S10

Key words: Optimized Schwarz Waveform Relaxation, domain decomposition method, Schrödinger equation, dynamics, stationary states, Robin boundary condition, pseudodifferential operators, fast convergence.

1 Introduction

Domain decomposition method (DDM) is a general strategy for solving high-dimensional PDEs. Among DDMs, the Schwarz Waveform Relaxation (SWR) method is a popular al-

[1]Corresponding author. *Email addresses:* `xavier.antoine@univ-lorraine.fr` (X. Antoine), `elorin@math.carleton.ca` (E. Lorin)

gorithm for the parallel numerical computation of evolution equations [15–21], in particular wave-like equations. SWR methods are characterized by the choice of the Transmission Conditions (TC) at the subdomain interfaces: Classical SWR is based on Dirichlet TC, Robin SWR uses Robin TC, Optimal SWR is related to transparent TC, and quasi-optimal SWR is based on accurate absorbing TC. Optimized SWR usually refers to Robin SWR, where the Robin parameters are optimized to ensure the fastest convergence possible of the algorithm. The latter then offers a good balance between fast convergence rate and efficient IBVP solver. In this paper, we are specifically interested in Optimized SWR methods. We now briefly describe the Schwarz Waveform Relaxation algorithms and set the problem of the selection of an optimized choice of the Robin parameter in the transmission conditions. Consider a d-dimensional evolution partial differential equation $P\phi = f$ in the spatial domain $\Omega \subseteq \mathbb{R}^d$, and time domain (t_1,t_2), where $t_2 > t_1 \geqslant 0$. The initial data is denoted by ϕ_0. We first split Ω into two open subdomains $\Omega_\varepsilon^\pm$ with smooth boundary, with or without overlap ($\Omega_\varepsilon^+ \cap \Omega_\varepsilon^- \neq \emptyset$ or $\Omega_\varepsilon^+ \cap \Omega_\varepsilon^- = \emptyset$), where $\varepsilon > 0$ denotes the overlap parameter. The SWR algorithm consists in iteratively solving IBVPs in $\Omega_\varepsilon^\pm \times (t_1,t_2)$, using transmission conditions at the subdomain interfaces $\Gamma_\varepsilon^\pm := \partial\Omega_\varepsilon^\pm \cap \Omega_\varepsilon^\mp$, where the imposed conditions are established using the preceding Schwarz iteration data in the adjacent subdomain. The Robin-Schwarz Waveform Relaxation algorithm can be seen as an approximate version of Optimal SWR algorithm [7], where the transparent transmission operator is approximated by a Robin transmission operator as follows, see also [1,23]: for $k \geqslant 1$, and denoting $\phi^\pm$ the solution in $\Omega_\varepsilon^\pm$ we define

$$\begin{cases} P\phi^{\pm,(k)} = f, & \text{in } \Omega_\varepsilon^\pm \times (t_1,t_2), \\ \phi^{\pm,(k)}(\cdot,0) = \phi_0^\pm, & \text{in } \Omega_\varepsilon^\pm, \\ \mathcal{T}_\pm \phi^{\pm,(k)} = \mathcal{T}_\pm \phi^{\mp,(k-1)}, & \text{on } \Gamma_\varepsilon^\pm \times (t_1,t_2), \end{cases} \tag{1.1}$$

with a given initial guess $\phi^{\pm,(0)}$, and $\mathcal{T}^\pm = \partial_{\boldsymbol{n}^\pm} \pm \mathtt{i}\lambda^\pm_{\Gamma_\varepsilon}$ with $\lambda^\pm_{\Gamma_\varepsilon^\pm} \in \mathbb{R}^*$ or $\mathtt{i}\mathbb{R}^*$, and outward normal vector $\boldsymbol{n}^\pm$ to $\Gamma_\varepsilon^\pm$.

Our strategy to select the Robin parameter relies on existing results on the convergence rate of SWR methods. As it is well-known [6,7,16], for quantum wave equations the fastest convergence rate of SWR methods is obtained with transparent transmission conditions leading to the so-called Optimal SWR method. The latter is however usually very inefficient due to their computational complexity [7]. In order to select the Robin parameter, we then first i) approximate the symbol of the transparent transmission operator in the asymptotic regime, ii) reconstruct the corresponding operator at the interface. Although, the general idea is in principle applicable to a large class of PDE, we will focus in this paper on the Schrödinger equation i) in real-time and ii) imaginary-time within the Normalized Gradient Flow method (NGF) for computing the Schrödinger Hamiltonian point spectrum [6,7,12]. In the first work on OSWR with two-subdomains for the one-dimensional Schrödinger equation [22], the authors assume that the transmission conditions are of Robin-type, and then optimize the constant to get the fastest convergence by minimizing the contraction factor in a fixed point algorithm related to the Robin-SWR