Applied Mathematics and Computation 336 (2018) 403–417

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Multilevel preconditioning technique for Schwarz waveform relaxation domain decomposition method for real- and imaginary-time nonlinear Schrödinger equation

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ARTICLE INFO

Keywords:
Domain decomposition method
Schwarz waveform relaxation algorithm
Multilevel preconditioning
Nonlinear Schrödinger equation
Dynamics
Stationary states

ABSTRACT

This paper is dedicated to the derivation of multilevel Schwarz Waveform Relaxation (SWR) Domain Decomposition Methods (DDM) in real- and imaginary-time for the Non-Linear Schrödinger Equation (NLSE). In imaginary-time, it is shown that the multilevel SWR-DDM accelerates the convergence compared to the one-level SWR-DDM, resulting in an important reduction of the computational time and memory storage. In real-time, the method requires in addition the storage of the solution in overlapping zones at any time, but on coarser discretization levels. The method is numerically validated on the Classical SWR and Robin-based SWR methods, but can however be applied to any SWR-DDM approach.

1. Introduction

This paper is devoted to the derivation of a multilevel Schwarz Waveform Relaxation (SWR) method for computing both in real- and imaginary-time the solution to the NonLinear Schrödinger Equation (NLSE) that models many physics problems, including nonlinear optics and Bose–Einstein condensates [1–7]. The proposed method is also applicable to the Linear Schrödinger Equation (LSE) in real- and imaginary-time, in particular for solving intense and short laser-molecule interaction including ionization processes. In this framework real-space numerical methods are largely used, see [8–11], and DDM method is then the center of main interests. Domain decomposition SWR methods for solving wave equations have a long history from the classical SWR method with overlapping zones, to optimal version without overlap (see e.g. [8,12–20] as well as http://www.ddm.org, for a complete review and references about this method). Basically in SWR methods, the transmission conditions at the subdomain interfaces are derived from the solution to the corresponding wave equation, usually using Dirichlet boundary conditions (Classical SWR), Robin boundary conditions (optimized SWR), transparent or high-order Absorbing Boundary Conditions (ABCs) including Dirichlet-to-Neumann (DtN) transmitting conditions (Optimal SWR), or Perfectly Matched Layers [8,21,22]. We also refer to [21,23–25] for some reviews on truncation techniques for quantum wave equations in infinite domains. SWR methods can be *a priori* applied to any type of wave equation [15,26,27].

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[1] X. Antoine thanks the support of the french ANR, France grants “Bond” (ANR-13-BS01-0009-01) and ANR-12-MONU-0007-02 BECASIM (Modèles Numériques call). E. Lorin thanks NSERC for the financial support via the Discovery Grant program.

https://doi.org/10.1016/j.amc.2018.04.075
0096-3003/

In this paper, we focus on multilevel SWR for the NLSE. More specifically, we consider the cubic time-dependent (real-time) NLSE set on $\mathbb{R}^d$, with $d \geq 1$,

$$\begin{cases} \mathrm{i}\partial_t \phi = -\triangle\phi + V(\mathbf{x})\phi + \kappa|\phi|^2\phi, \ \mathbf{x} \in \mathbb{R}^d, \ t > 0, \\ \phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), \ \mathbf{x} \in \mathbb{R}^d. \end{cases} \tag{1}$$

The real-valued space-dependent smooth potential V is positive for attractive interactions, and negative for repulsive interactions. The nonlinearity strength κ is a real-valued constant which is positive for a focusing nonlinearity and negative for a defocusing nonlinearity. The function ϕ_0 is a given initial data. In the sequel of the paper, $\mathcal{P}(|\phi|)$ denotes the nonlinear operator

$$\mathcal{P}(|\phi|)\phi = (\mathrm{i}\partial_t + \triangle - V(\mathbf{x}) - \kappa|\phi|^2)\phi. \tag{2}$$

Compared to the real-time dynamics, the imaginary-time formulation [1–5] is used to compute the stationary solutions to the NLSE. The corresponding method is referred to as Normalized Gradient Flow (NGF) formulation [1,3–5] in the Mathematics literature and imaginary-time method in the Physics literature. This is a very common and easy-to-implement method for computing the point spectrum of operators with bounded or semi-bounded spectra. It is particularly suitable for nonlinear operators, and it only requires (imaginary-)time-dependent computations. The current paper is an extension of [12,28], where was derived and mathematically analyzed the convergence and the rate of convergence of 1-level SWR methods for solving the NLSE in imaginary time, in one and two dimensions. In this paper, we focus on multilevel *preconditioning* techniques, for accelerating the overall convergence of the SWR algorithm. In the imaginary-time framework (stationary state computation), we refer to as *preconditioning* the storage and use of a converged solution at a lower (coarser) level for i) initializing the NGF algorithm (Cauchy data selection) and for ii) deriving the transmission conditions in the overlapping zone interfaces at an upper (finer) level. In real-time (computation of the dynamics), *preconditioning* also includes the storage of the converged solution in the overlapping zones, *at any time*, for accurately deriving the transmission conditions. We numerically show that the convergence of the SWR method is improved in both cases. Although, the acceleration of the convergence is moderate in imaginary-time, it is however shown that the computational cost per Schwarz iteration, that is the NGF convergence, is strongly accelerated compared to unpreconditioned SWR methods.

The paper is organized as follows. In Sections 2.1 and 2.2, we recall some results about SWR methods in real- and imaginary-time. In Section 2.2, we provide some elements about the Normalized Gradient Flow (NGF) method for solving the stationary NLSE. Section 2.3 gives some notations about the multilevel approximation. In Section 3, we describe the two-level SWR method in imaginary-time, and next in real-time. A discussion on the computational complexity is also addressed. Section 4 is devoted to some numerical experiments, where two types of results are presented: (i) convergence rates for Schwarz algorithms, and (ii) NGF convergence time in imaginary-time. We finally conclude in Section 5.

2. SWR methods in real- and imaginary-time; notations

2.1. SWR algorithms in real-time

We recall the basics of SWR algorithms for two subdomains for the sake of conciseness. We introduce two open sets $\Omega_\epsilon^{\pm}$ such that $\mathbb{R}^d = \Omega_\epsilon^+ \cup \Omega_\epsilon^-$, with overlapping region $\Omega_\epsilon^+ \cap \Omega_\epsilon^-$, where ϵ is a (small) non-negative parameter. In 1-d ($d = 1$), the domains of interest read: $\Omega_\epsilon^+ = \big(-\infty, \epsilon/2\big)$, $\Omega_\epsilon^- = \big(-\epsilon/2, \infty\big)$ and $\mathbb{R} = \Omega_\epsilon^+ \cup \Omega_\epsilon^-$. with $\Omega_\epsilon^+ \cap \Omega_\epsilon^- = \big(-\epsilon/2, \epsilon/2\big)$. We denote by $\phi^{\pm}$ the solution to the time-dependent NLSE in $\Omega_\epsilon^{\pm}$. Solving the NLSE by a Schwarz waveform domain decomposition [8] requires some transmission conditions at the subdomain interfaces. More specifically, for any Schwarz iteration $k \geq 1$, the equation in $\Omega_\epsilon^{\pm}$ reads, for a given $T > 0$,

$$\begin{cases} (\mathrm{i}\partial_t + \triangle - V - \kappa|\phi^{\pm,(k)}|^2)\phi^{\pm,(k)} = 0, \ \text{ on } \Omega_\epsilon^{\pm} \times (0, T), \\ \mathcal{B}^{\pm}\phi^{\pm,(k)} = \mathcal{B}^{\pm}\phi^{\mp,(k-1)}, \ \text{ on } \Gamma_\epsilon^{\pm} \times (0, T), \\ \phi^{\pm,(k)}(\cdot, 0) = \phi_0(\cdot) \ \text{ on } \Omega_\epsilon^{\pm}, \end{cases} \tag{3}$$

where $\Gamma_\epsilon^{\pm} = \partial\Omega_\epsilon^{\pm}$. The notation $\phi^{\pm,(k)}$ stands for the solution $\phi^{\pm}$ in $\Omega_\epsilon^{\pm} \times (0, T)$ at Schwarz iteration k. Initially, $\phi^{\pm,(0)}$ are two given functions defined in $\Omega_\epsilon^{\pm}$. We denote by $\mathcal{B}^{\pm}$ an operator characterizing the type of SWR algorithm. In the CSWR case, $\mathcal{B}^{\pm}$ is the identity operator and $\mathcal{B}^{\pm} = \partial_{\mathbf{n}^{\pm}} + \gamma \mathrm{Id}$ ($\gamma \in \mathbb{R}_+^*$) for the Robin-like SWR method. For the optimal SWR algorithm, $\mathcal{B}^{\pm}$ can be a local or a nonlocal approximation of the DtN operator (see [8,22]). The convergence criterion for the Schwarz DDM is given by

$$\Big\| \ \|\phi^{+,(k)}_{|\Gamma_\epsilon^+} - \phi^{-,(k)}_{|\Gamma_\epsilon^-}\|_{\infty,\Gamma_\epsilon} \Big\|_{L^2(0,T)} \leq \delta^{\mathrm{Sc}}. \tag{4}$$

typically with $\delta^{\mathrm{Sc}} = 10^{-14}$ (“Sc” is added for Schwarz). The convergence occurs at an iteration denoted by k^{cvg} and the converged global solution in real time, is given by $\phi^{\mathrm{cvg}} := \phi^{(k^{\mathrm{cvg}})}$.