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COMPARISON OF SOLVERS FOR 2D SCHRÖDINGER PROBLEMS

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Abstract. This paper deals with the numerical solution of both linear and non-linear Schrödinger problems, which mathematically model many physical processes in a wide range of applications of interest. In particular, a comparison of different solvers and different approaches for these problems is developed throughout this work. Two finite difference schemes are analyzed: the classical Crank-Nicolson approach, and a high-order compact scheme. Solvers based on geometric multigrid, Fast Fourier Transform and Alternating Direction Implicit methods are compared. Finally, the efficiency of the considered solvers is tested for a linear Schrödinger problem, proving that the computational experiments are in good agreement with the theoretical predictions. In order to test the robustness of the MG solver two additional Schrödinger problems with a non-constant potential and nonlinear right-hand side are solved by the MG solver, since the efficiency of this solver depends on such data.

Key words. finite difference method, Schrödinger problem, multigrid method, Alternating Direction Implicit method, Fast Fourier Transform method.

1. Introduction

It is well-known that many mathematical problems of nonlinear optics, laser physics and quantum mechanics, for example, are described by Schrödinger problems. Therefore, the development of robust and efficient numerical algorithms for the solution of such problems still remains a very important challenge of computational mathematics. In particular, one of the most important aspects in the numerical solution of partial differential equations is the efficient solution of the corresponding large system of equations arising from their discretization.

Three different strategies are very popular for this purpose. The first strategy is based on operator splitting techniques. The main idea is to decompose the large system of linear equations arising after the discretization of a multidimensional problem to a sequence of simpler subproblems. Within this framework, here we only mention Alternating Direction Implicit (ADI), Locally One-Dimensional (LOD) and Implicit-Explicit (IMEX) methods (see [16, 20] for a good review on these methods). Secondly, we mention Fast Fourier Transform (FFT) techniques. The FFT algorithm was introduced in 1965 by Cooley and Tukey [12], for an overview of Fourier Transform methods we refer e.g. to [13]. In the case of PDEs with constant coefficients and uniform grids, these algorithms solve systems of linear equations with complexity close to optimal. Thus, we include solvers based on the FFT algorithm into the comparison of different solvers for 2D Schrödinger problems. The third class of solvers corresponds to multigrid (MG) methods. Since their development in the 70's, MG methods [5, 25] have been proved to be among the most efficient numerical algorithms for solving the large sparse systems of algebraic equations arising from the discretization of elliptic PDEs, achieving asymptotically

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optimal complexity. They are mainly based on the acceleration of the convergence of common iterative methods by using solutions obtained on coarser meshes as corrections. We note that MG solvers are not frequently used to solve Schrödinger type problems in industrial and academic applications.

Our aim in this paper is to investigate in detail the possibility of constructing robust and efficient MG solvers and compare these solvers with those based on ADI and FFT techniques. The biggest challenge is the development of robust MG solvers for multidimensional Schrödinger problems. There are not many papers devoted to this topic. We note, that similar challenges arise in application of MG solvers for the Helmholtz equation [14, 18].

The rest of the paper is organized as follows. In Section 2 the mathematical model is formulated and the main properties of the solution are given. The two-dimensional Schrödinger equation is approximated by the classical Crank-Nicolson method and by a high-order compact finite difference scheme in space. For the solution of the high-order scheme, an ADI type decomposition algorithm, from [15], is used. The stability and convergence analysis in the discrete L_2 norm of the high-order ADI scheme is done in Section 3, whereas the MG solver for Schrödinger problem is described and investigated in Section 4. Results of numerical experiments are presented in Section 5. Finally, in Section 6 some conclusions are formulated.

2. Problem Formulation

2.1. Mathematical model. For many applications in nonlinear optics, laser physics, quantum mechanics and plasma physics, for instance, the mathematical models of physical processes are described by nonlinear Schrödinger equations, see, e.g., [11, 16] and references therein. We consider the two-dimensional nonlinear Schrödinger equation in the domain $\Omega = (a_x, b_x) \times (a_y, b_y)$:

$$-i\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - q(x,y)u + f(u), \quad (x,y) \in \Omega, \ \ t \in (0,T], \tag{1}$$

with the following initial and boundary conditions

$$u(x,y,0) = u_0(x,y), \quad (x,y) \in \Omega \cup \partial\Omega, \tag{2}$$

$$u(x,y,t) = \mu(x,y,t), \quad (x,y) \in \partial\Omega, \ \ t \in (0,T]. \tag{3}$$

Here $u = u(x,y,t)$ is a complex-valued function, q is a given real-valued function, f, u_0 and μ are given complex-valued functions, and $\partial\Omega$ is the boundary of Ω.

It is well-known that the nonlinear Schrödinger equation (1) can have important conservation laws. Let us assume that $f(u) \equiv 0$. The following invariants of the solution of (1)–(3) are valid under the assumption of homogeneous boundary conditions $\mu \equiv 0$ [9, 27]:

$$Q = \int_\Omega |u(x,y,t)|^2 \, dxdy = \int_\Omega |u_0(x,y)|^2 \, dxdy, \tag{4}$$

$$E = \int_\Omega \left(\left|\frac{\partial u(t)}{\partial x}\right|^2 + \left|\frac{\partial u(t)}{\partial y}\right|^2 + q(x,y)|u(t)|^2 \right) dxdy$$

$$= \int_\Omega \left(\left|\frac{\partial u_0}{\partial x}\right|^2 + \left|\frac{\partial u_0}{\partial y}\right|^2 + q(x,y)|u_0|^2 \right) dxdy. \tag{5}$$