Numerical simulation of Schrödinger equation on a time dependent curvilinear grid

Diploma work (15 HP) in scientific computing

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Abstract

The first main focus in the present project is to derive a well-posed model for Shrödinger equation on a time-dependent curvilinear grid. The second main focus is to derive a suitable numerical solution using a high-order finite difference method (HOFDM). The boundary closures of the HOFDM are based on the summation-by-parts (SBP) framework, thereby guaranteeing linear stability. The boundary conditions are imposed using a penalty technique, leading to an ODE system. We will employ the traditional way of time-integration using the fourth order Runge-Kutta. The numerical model will be validated against analytic solutions.

1 Motivation

A robust and well-proven high-order finite difference methodology that ensures the strict stability of time-dependent partial differential equations (PDEs) is the SBP-SAT method. The SBP-SAT method combines semi-discrete operators that satisfy a summation-by-parts (SBP) formula [3], with physical boundary conditions implemented using the simultaneous approximation term (SAT) method [2].

The main focus in the present study is to construct a high-order accurate SBP-SAT approximation of the Shrödinger equation in 2-D (here in non-dimensional form),

$$iu_t = u_{xx} + u_{yy} + u\,F\ .$$

on a time-dependent curvilinear grid. Here F is a know forcing function (potential).

The main mathematical and numerical difficulties of this model comes from the boundary treatment and the mapping onto a time dependent curvilinear grid. Another numerical difficulty comes from the fact that this model leads to stiff semi-discrete models, after deriving a stable semi-discrete SBP-SAT model. For details concerning the spatial discretisation including SBP operators for second derivatives with variable coefficients see [1, 5]. In this project the focus is not on optimal time-integrators. We will employ a the fourth order accurate Runge-Kutta method. (A potentially more efficient time-integration technique for this stiff ODE system could be achieved by employing a novel SBP-SAT technique to discretise the time-derivative [4]. This could be done in a continuation of this work, for example a diploma work). The accuracy and stability properties will be investigated mathematically using the energy method and later verified against analytical solutions.

2 Project plan and time frame

- Start by a literature study to learn about the Shrödinger equation equation model to understand the underlying physics and applications (1 weeks).
- Analyze well-posedness using the energy method for a continuous 1-D model on a dynamic domain (1 weeks).
- Analyze well-posedness using the energy method for the continuous 2-D model on a dynamic curvilinear domain (2 weeks).
- Derive a stable semi-discrete SBP-SAT approximation of well-posed problems above (2 weeks).
- Verify the stability and accuracy against analytic solution solutions (1 weeks).
- Complete the report (2 weeks).

References

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