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A parallel algorithm for solving the 3d Schrödinger equation

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ABSTRACT

We describe a parallel algorithm for solving the time-independent 3d Schrödinger equation using the finite difference time domain (FDTD) method. We introduce an optimized parallelization scheme that reduces communication overhead between computational nodes. We demonstrate that the compute time, t, scales inversely with the number of computational nodes as $t \propto (N_{\text{nodes}})^{-0.95 \pm 0.04}$. This makes it possible to solve the 3d Schrödinger equation on extremely large spatial lattices using a small computing cluster. In addition, we present a new method for precisely determining the energy eigenvalues and wavefunctions of quantum states based on a symmetry constraint on the FDTD initial condition. Finally, we discuss the usage of multi-resolution techniques in order to speed up convergence on extremely large lattices.

1. Introduction

Solving the 3d Schrödinger equation given an arbitrary potential $V(\vec{r})$ is of great practical use in modern quantum physics; however, there are only a handful of potentials for which analytic solution is possible. In addition, any potential that does not have a high degree of symmetry, e.g. radial symmetry, requires solution in full 3d, making standard "point-and-shoot" methods [1] for solving one-dimensional partial differential equations of little use. In this paper we discuss a parallel algorithm for solving the 3d Schrödinger equation given an arbitrary potential $V(\vec{r})$ using the finite difference time domain (FDTD) method.

The FDTD method has a long history of application to computational electromagnetics [2–5]. In the area of computational electromagnetics parallel versions of the algorithms have been developed and tested [6–12]. In this paper, we discuss the application of parallelized FDTD to the 3d Schrödinger equation. The standard FDTD method has been applied to the 3d Schrödinger equation by several authors in the past [23–29]. Here we show how to efficiently parallelize the algorithm. We describe our parallel algorithm for finding ground and excited state wavefunctions and observables such as energy eigenvalues, and root-mean-squared radii. Additionally, we introduce a way to use symmetry constraints for determining excited state wavefunctions/energies and introduce a multi-resolution technique that dramatically decreases compute time on large lattices. This paper is accompanied by an open-source release of a code that implements the algorithm detailed in this paper. The code uses the Message Passing Interface (MPI) protocol for message passing between computational nodes.

We note that another popular method for numerical solution of the 3d Schrödinger equation is the Diffusion Monte Carlo (DMC) technique, see [13–17] and references therein. The starting point for this method is the same as the FDTD method applied here, namely transformation of the Schrödinger equation to imaginary time. However, in the DMC algorithm the resulting "dynamical" equations are transformed into an integral Green's function form and then the resulting integral equation is computed using stochastic sampling. The method is highly inefficient unless importance sampling [18,19] is used.

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DMC is efficiently parallelized and there are several codes which implement parallelized DMC [20–22]. The method is similar in many ways to the one presented herein; however, the method we use does not suffer from the fermion sign problem which forces DMC to use the so-called "fixed-node approximation" [14]. In addition, although the DMC algorithm can, in principle, be applied to extract properties of the excited states of the system most applications to date only calculate the ground state wavefunction and its associated expectation values. The FDTD method described herein can extract both ground and excited state wavefunctions.

The organization of the paper is as follows. In Sections. 2 and 3 we briefly review the basics of the FDTD method applied to the 3d Schrödinger equation and derive the equations necessary to evolve the quantum mechanical wavefunction. In Section 4 we discuss the possibility of imposing a symmetry constraint on the FDTD initial condition in order to pick out different quantum mechanical states. In Section 5 we describe our strategy for parallelizing the FDTD evolution equations and the measurement of observables. In Section 6 we introduce an efficient method of using lower-resolution FDTD wavefunctions as initial conditions for higher-resolution FDTD runs that greatly speeds up determination of high-accuracy wavefunctions and their associated observables. In Section 7 we give results for a few potentials including benchmarks showing how the code scales as the number of computational nodes is increased. Finally, in Section 8 we conclude and give an outlook for future work.

2. Setup and theory

In this section we introduce the theory necessary to understand the FDTD approach for solving the time-independent Schrödinger equation. Here we will briefly review the basic idea of the FDTD method and in the next section we will describe how to obtain the discretized "equations of motion".

We are interested in solving the time-independent Schrödinger equation with a static potential $V(\vec{r},t) = V(\vec{r})$ and a particle of mass m

$$E_n\psi_n(\vec{r}) = \widehat{H}\psi_n(\vec{r}), \tag{2.1}$$

where ψ_n is a quantum–mechanical wavefunction that solves this equation, E_n is the energy eigenvalue corresponding to ψ_n, and $\widehat{H} = -\hbar^2\nabla^2/2m + V(\vec{r})$ is the Hamiltonian operator. In order to solve this time-independent (static) problem it is efficacious to consider the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \widehat{H}\Psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\Psi(\vec{r},t). \tag{2.2}$$

A solution to (2.2) can be expanded in terms of the basis functions of the time-independent problem, i.e.

$$\Psi(\vec{r},t) = \sum_{n=0}^{\infty} a_n\psi_n(\vec{r})e^{-iE_nt}, \tag{2.3}$$

where $\{a_n\}$ are expansion coefficients which are fixed by initial conditions ($n = 0$ represents the ground state, $n = 1$ the first excited state, etc.) and E_n is the energy associated with each state.[1]

By performing a Wick rotation to imaginary time, $\tau = it$, and setting $\hbar = 1$ and $m = 1$ in order to simplify the notation, we can rewrite Eq. (2.2) as

$$\frac{\partial}{\partial\tau}\Psi(\vec{r},\tau) = \frac{1}{2}\nabla^2\Psi(\vec{r},\tau) - V(\vec{r})\Psi(\vec{r},\tau), \tag{2.4}$$

which has a general solution of the form

$$\Psi(\vec{r},\tau) = \sum_{n=0}^{\infty} a_n\psi_n(\vec{r})e^{-E_n\tau}. \tag{2.5}$$

Since $E_0 < E_1 < E_2 < \cdots$, for large imaginary time τ the wavefunction $\Psi(\vec{r},\tau)$ will be dominated by the ground state wavefunction $a_0\psi_0(\vec{r})e^{-E_0\tau}$. In the limit τ goes to infinity we have

$$\lim_{\tau\to\infty}\Psi(\vec{r},\tau) \approx a_0\psi_0(\vec{r})e^{-E_0\tau}. \tag{2.6}$$

Therefore, if one evolves Eq. (2.4) to large imaginary times one will obtain a good approximation to the ground state wavefunction.[2]

This allows one to determine the ground state energy by numerically solving Eq. (2.4) for large imaginary time, and then use this wavefunction to find the energy expectation value E_0:

[1] The index n is understood to represent the full set of quantum numbers of a given state of energy E_n. In the degenerate case ψ_n is an admixture of the different degenerate states.

[2] In this context a large imaginary time is defined relative to the energy splitting between the ground state and the first excited state, e.g. $e^{(E_0-E_1)\tau} \ll 1$; therefore, one must evolve to imaginary times much larger than $1/(E_1 - E_0)$.