

The One-Dimensional Finite-Difference Time-Domain (FDTD) Algorithm Applied to the Schrödinger Equation

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1. INTRODUCTION

For anyone who has ever studied quantum mechanics, it is well-known that the Schrödinger equation can be very difficult to solve analytically. Occasionally, certain complex systems allow for approximate solutions through the use of the WKB method or perturbation theory, but the vast majority of physical systems that occur in nature are far too complicated to ever solve by hand. Therefore, it is desirable to enlist the aid of computers when searching for solutions to quantum systems.

One of the more common methods for numerically solving a time-dependent partial differential equation (PDE) is the finite-difference time-domain algorithm, or FDTD. The basic idea behind FDTD is to discretize the PDE in space and time and then approximate the derivatives by using finite differences. Essentially, the PDE is allowed to play itself out by gradually incrementing the time variable in discrete steps. The power behind FDTD is its simplicity of implementation and its ability to visualize the solutions as they act out in both space and time.

This paper derives the numerical update equations for the one-dimensional Schrödinger equation and then solves for the stability conditions on their use. Several examples are also given to demonstrate the FDTD in action.

2. UPDATE EQUATIONS

The one-dimensional time-dependent Schrödinger equation is given as

$$j\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t) , \quad (1)$$

where $\psi(x,t)$ is the wave function in space and time, $V(x)$ is the potential function, m is the particle mass, and \hbar is Plank's constant. Because complex-valued arithmetic can be numerically costly, it is helpful to first break up the wave function into real and imaginary components such that

$$\psi(x,t) = \psi_R(x,t) + j\psi_I(x,t) . \quad (2)$$

This step allows us to treat each component separately and perform only real-valued computations with each part. Plugging the real and imaginary components back into the Schrödinger equation thus produces two coupled partial differential equations of the form

$$\hbar \frac{\partial \psi_R(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_I(x,t)}{\partial x^2} + V(x)\psi_I(x,t) , \quad (3)$$

$$\hbar \frac{\partial \psi_I(x,t)}{\partial t} = +\frac{\hbar^2}{2m} \frac{\partial^2 \psi_R(x,t)}{\partial x^2} - V(x)\psi_R(x,t) . \quad (4)$$

The next step is to define a *mesh*, which is a discrete set of grid points that sample the wave function in space and time. If each spatial point is separated by a distance Δx and each temporal point by Δt , then the mesh points are given by

$$x_\ell = \ell \Delta x, \quad \text{and} \quad (5)$$

$$t_n = n \Delta t, \quad (6)$$

where $0 \leq n \leq N$ and $0 \leq \ell \leq L$. The wave function at a specific grid point can now be conveniently defined in terms of a *stencil*, which is a short-hand notation given by

$$\psi(x_\ell, t_n) = \psi^n(\ell). \quad (7)$$

With the wave function sampled on a discrete grid, the derivatives must now be approximated by using finite-differences. For convenience, it helps to define the imaginary part of the wave function to exist at half-step intervals from the real part. This allows us to use the central-difference method for the time derivatives, which is more accurate than a forward- or backward-difference method. The time derivative on the real-valued wave function is therefore given by

$$\frac{\partial \psi_R(x_\ell, t_{n+1/2})}{\partial t} \approx \frac{\psi_R^{n+1}(\ell) - \psi_R^n(\ell)}{\Delta t}. \quad (8)$$

Similarly, the time derivative on the imaginary-valued wave function is found to be

$$\frac{\partial \psi_I(x_\ell, t_n)}{\partial t} \approx \frac{\psi_I^{n+1/2}(\ell) - \psi_I^{n-1/2}(\ell)}{\Delta t}. \quad (9)$$

Applying a central-difference on the spatial derivative gives an approximation to the second-partial with the form

$$\frac{\partial^2 \psi_R(x_\ell, t_n)}{\partial x^2} \approx \frac{\psi_R^n(\ell+1) - 2\psi_R^n(\ell) + \psi_R^n(\ell-1)}{\Delta x^2}, \quad (10)$$

with a similar expression for the imaginary component at the $(n+1/2)$ time step. Plugging these approximations back into Equations 3 and 4 then gives

$$\begin{aligned} \frac{\hbar}{\Delta t} [\psi_R^{n+1}(\ell) - \psi_R^n(\ell)] &= -\frac{\hbar^2}{2m\Delta x^2} [\psi_I^{n+1/2}(\ell+1) - 2\psi_I^{n+1/2}(\ell) + \psi_I^{n+1/2}(\ell-1)] + V(\ell)\psi_I^{n+1/2}(\ell), \\ \frac{\hbar}{\Delta t} [\psi_I^{n+1/2}(\ell) - \psi_I^{n-1/2}(\ell)] &= +\frac{\hbar^2}{2m\Delta x^2} [\psi_R^n(\ell+1) - 2\psi_R^n(\ell) + \psi_R^n(\ell-1)] - V(\ell)\psi_R^n(\ell) \end{aligned}$$

Note how the real-valued derivative is centered at the time step $t = (n+1/2)\Delta t$, while the imaginary-valued derivative is centered at $t = n\Delta t$.

In practice, the function $\psi_R^{n+1}(\ell)$ is often called the *future state* of the real-valued wave function. Similarly, the function $\psi_I^{n+1/2}(\ell)$ is future state of the imaginary-valued wave function, while $\psi_R^n(\ell)$ and $\psi_I^{n-1/2}(\ell)$ are known as the *present states*. The goal of the FDTD algorithm is to solve for an unknown future state of the system in terms of the known present states. Thus, the final step is to solve for $\psi_I^{n+1/2}(\ell)$ and $\psi_R^{n+1}(\ell)$, which are found to be

$$\psi_I^{n+1/2}(\ell) = +c_1 [\psi_R^n(\ell+1) - 2\psi_R^n(\ell) + \psi_R^n(\ell-1)] - c_2 V(\ell)\psi_R^n(\ell) + \psi_I^{n-1/2}(\ell), \quad (11)$$

$$\psi_R^{n+1}(\ell) = -c_1 [\psi_I^{n+1/2}(\ell+1) - 2\psi_I^{n+1/2}(\ell) + \psi_I^{n+1/2}(\ell-1)] + c_2 V(\ell)\psi_I^{n+1/2}(\ell) + \psi_R^n(\ell), \quad (12)$$

where the constants c_1 and c_2 are given as

$$c_1 = \frac{\hbar \Delta t}{2m \Delta x^2}, \quad (13)$$

$$c_2 = \frac{\Delta t}{\hbar}. \quad (14)$$

Together, Equations 12 and 11 are called *update equations* because they give the future state of the wave function at a point ℓ in terms of nearby points in space and time. The FDTD algorithm iterates over half-step intervals in time by first solving for $\psi_I^{n+1/2}(\ell)$ and then $\psi_R^{n+1}(\ell)$ at every value of ℓ . The time step n increments with each iteration until finally terminating when $n = N$. The result is a simulated time-progression of the wave function along a discretized domain in space and time.

3. STABILITY

Suppose the potential function is a constant so that $V(\ell) = V_0$. Solutions to the Schrödinger equation then take on the form of free particles with wave functions given by

$$\psi(x, t) = A_1 e^{j(kx - \omega t)} + A_2 e^{j(kx + \omega t)} , \quad (15)$$

where k is the particle wavenumber and ω is the angular frequency. Without any loss of generality, consider the simple case of a free particle traveling to the right where $A_1 = 1$ and $A_2 = 0$. Thus, the real and imaginary components are simply

$$\begin{aligned} \psi_R(x, t) &= \cos(kx - \omega t) , \\ \psi_I(x, t) &= \sin(kx - \omega t) . \end{aligned}$$

In terms of the FDTD stencil, these can be written as

$$\psi_R^n(\ell) = \cos(k\ell\Delta x - \omega n\Delta t) , \quad (16)$$

$$\psi_I^n(\ell) = \sin(k\ell\Delta x - \omega n\Delta t) . \quad (17)$$

For convenience, let us now define $A = k\ell\Delta x - \omega n\Delta t$ so that

$$\psi_R^n(\ell) = \cos(A) , \quad (18)$$

$$\psi_I^n(\ell) = \sin(A) . \quad (19)$$

Furthermore, define the constants $B = k\Delta x$ and $C = \omega\Delta t$ so that

$$\psi_R^{n+1}(\ell) = \cos(A - C) , \quad (20)$$

$$\psi_I^{n+1/2}(\ell) = \sin(A - C/2) , \quad (21)$$

$$\psi_I^{n+1/2}(\ell + 1) = \sin(A + B - C/2) , \quad (22)$$

$$\psi_I^{n+1/2}(\ell - 1) = \sin(A - B - C/2) . \quad (23)$$

Next, plug Equations 18 - 23 back into Equation 12 to find

$$\cos(A - C) = -c_1 [\sin(A + B - C/2) - 2\sin(A - C/2) + \sin(A - B - C/2)] + c_2 V_0 \sin(A - C/2) + \cos(A) . \quad (24)$$

The importance of Equation 24 is that it places constraints on the available choices for c_1 and c_2 . If these constants are not properly defined, then Equation 24 can only be satisfied by allowing for imaginary components to A , B , or C . Consequently, a real component is introduced to the exponent of Equation 15, and the wave function increases without bound. When this happens, the simulation is said to be *unstable* and "blows up."

In order to maintain a stable simulation, it is necessary to choose the constants c_1 and c_2 such that Equation 24 is satisfied by only real values of A , B , and C . The simplest way to do this is by choosing a time step Δt that prevents the right-hand side from ever exceeding the natural bounds of the left-hand side. In other words, we must enforce the condition that

$$-1 \leq \cos(A - C) \leq 1 . \quad (25)$$

The upper bound of this expression occurs when $\cos(A - C) = 1$, or when $A = C$. Plugging into the right-hand side of Equation 24 and rearranging therefore gives

$$1 - \cos(A) \geq -c_1 [\sin(A + B - C/2) - 2\sin(A - C/2) + \sin(A - B - C/2)] + c_2 V_0 \sin(A - C/2) . \quad (26)$$

Next, we note that the extreme value on the left-hand side of this expression occurs when $\cos(A) = -1$. Under this condition, several simplifications can be made to the right-hand side, and the final result is found to be

$$2 \geq -c_1 [2\cos(B) - 2] + c_2 V_0 . \quad (27)$$

Once again, we note that the extreme value of the right-hand side occurs when $\cos(B) = -1$, which gives

$$2 \geq 4c_1 + c_2 V_0 , \quad (28)$$

or equivalently

$$2 \geq \frac{2\hbar\Delta t}{m\Delta x^2} + \frac{\Delta t V_0}{\hbar} . \quad (29)$$

Finally, solve for Δt to find

$$\Delta t \leq \frac{\hbar}{\frac{\hbar^2}{m\Delta x^2} + \frac{V_0}{2}} . \quad (30)$$

The upper bound on Δt is called the *critical time step*, Δt_c , and represents the maximum allowable time increment that will maintain a stable simulation. Any value of Δt greater than Δt_c will introduce unbounded components into the simulation. If the potential function is not a constant value over all x , then stability is ensured by simply replacing V_0 with the maximum potential over the simulation interval.

4. EXAMPLE: QUANTUM TUNNELING

One of the more interesting predictions of quantum mechanics is that a particle can penetrate through a potential barrier even if the potential is greater than the kinetic energy of the particle. This phenomenon, called *tunneling*, is easily demonstrated through the FDTD algorithm. To begin, we define an initial value for the wave packet to represent a free particle traveling to the right (see Equation 15) and then localize it in space by multiplying with a Gaussian envelope. The mean kinetic energy of the particle is then related to the wavenumber by the expression

$$KE = \frac{\hbar^2 k^2}{2m} . \quad (31)$$

For a potential barrier of thickness T , the potential function is simply defined as $V(x) = V_0$, where $-T/2 \leq x \leq T/2$, and V_0 is some potential energy that is only slightly greater than KE .

Figure 1 shows a simulated demonstration of just such a system. A wave packet with mean kinetic energy of $KE = 500$ eV is sent towards a potential barrier with $V_0 = 600$ eV. The grid step size is fixed at $dx = 0.01$ Å, and the barrier thickness is set to $T = 0.25$ Å, or 25 grid points. The simulation domain consists of $L = 3000$ grid points, and the simulation was run for $N = 12,000$ time steps. The figure shows four snapshots of the simulation as it progressed in time. As the particle collides with the potential barrier, some of the wave function is able to penetrate through while the rest is reflected. Thus, there is a finite probability for the particle to be found on the right side of the barrier.

REFERENCES

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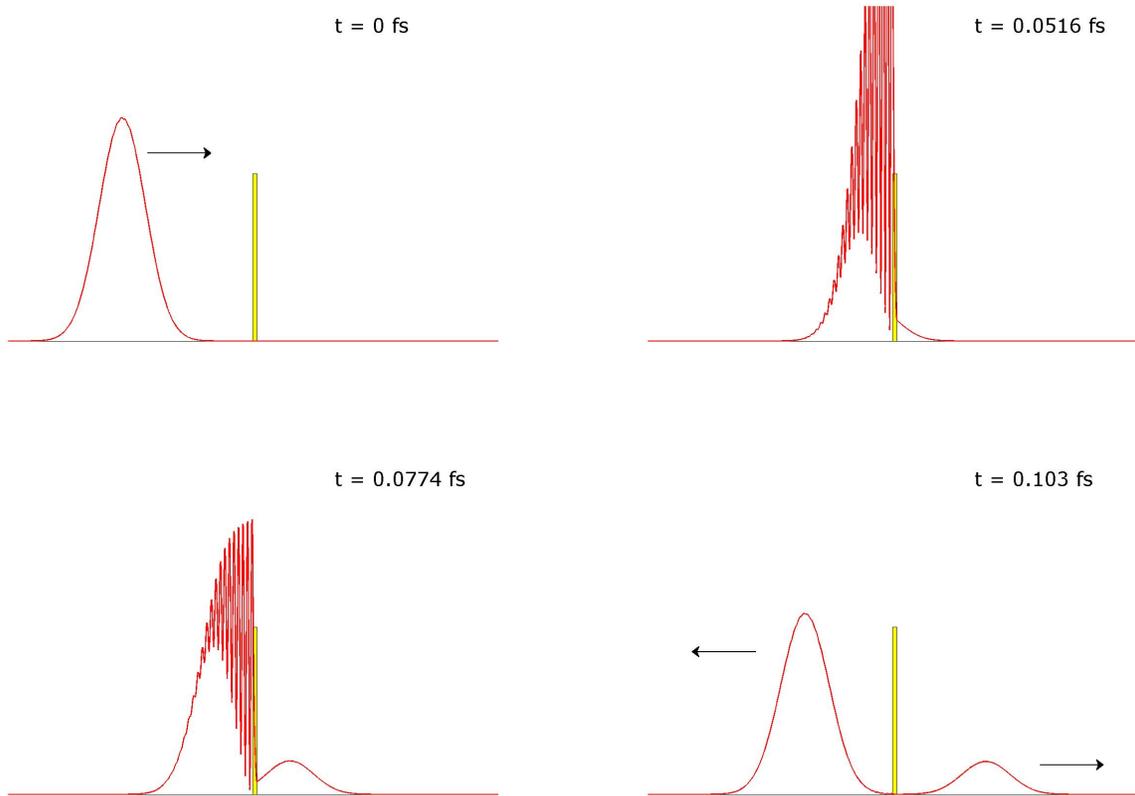


Figure 1. Snapshots of a wave packet as it collides with a potential barrier. The particle has a kinetic energy of 500 eV and the potential barrier is 600 eV. The thickness of the barrier is 0.25 \AA (25 grid points), and some of the probability penetrates to the other side.