Pentadiagonal alternating-direction-implicit finite-difference time-domain method for two-dimensional Schrödinger equation

Tay, Wei Choon; Tan, Eng Leong

2014

Tay, W. C., & Tan, E. L. (2014). Pentadiagonal alternating-direction-implicit finite-difference time-domain method for two-dimensional Schrödinger equation. *Computer Physics Communications*, 185(7), 1886–1892.

<https://hdl.handle.net/10356/79681>

<https://doi.org/10.1016/j.cpc.2014.03.014>

© 2014 Elsevier. This is the author created version of a work that has been peer reviewed and accepted for publication by *Computer Physics Communications*, Elsevier. It incorporates referee's comments but changes resulting from the publishing process, such as copyediting, structural formatting, may not be reflected in this document. The published version is available at: [<http://dx.doi.org/10.1016/j.cpc.2014.03.014>].

Downloaded on 26 Apr 2023 20:22:56 SGT

Pentadiagonal Alternating-Direction-Implicit Finite-Difference Time-Domain Method for Two-Dimensional Schrödinger Equation

Wei Choon Tay*, Eng Leong Tan

School of EEE, Nanyang Technological University, Singapore 639798

Abstract

In this paper, we have proposed a pentadiagonal alternating-direction-implicit (Penta-ADI) finite-difference time-domain (FDTD) method for the two-dimensional Schrödinger equation. Through the separation of complex wave function into real and imaginary parts, a pentadiagonal system of equations for the ADI method is obtained, which results in our Penta-ADI method. The Penta-ADI method is further simplified into pentadiagonal fundamental ADI (Penta-FADI) method, which has matrix-operator-free right-hand-sides (RHS), leading to the simplest and most concise update equations. As the Penta-FADI method involves five stencils in the left-hand-sides (LHS) of the pentadiagonal update equations, special treatments that are required for the implementation of the Dirichlet's boundary conditions will be discussed. Using the Penta-FADI method, a significantly higher efficiency gain can be achieved over the conventional Tri-ADI method, which involves a tridiagonal system of equations.

Keywords: Schrödinger equation, Alternating-Direction-Implicit (ADI), Finite-Difference Time-Domain (FDTD) methods, Pentadiagonal, Tridiagonal.

1. Introduction

The time-dependent Schrödinger equation forms the basis of quantum mechanics [1, 2, 3] in modern physics. The equation in two-dimensional is given as

$$-i\frac{\partial\Psi(x,y,t)}{\partial t} = \frac{\partial^2\Psi(x,y,t)}{\partial x^2} + \frac{\partial^2\Psi(x,y,t)}{\partial y^2} + \omega(x,y)\Psi(x,y,t) \quad (1)$$

with certain initial and boundary condition and $\omega(x,y)$ is the electrostatic potential function.

Various methods have been proposed to solve Schrödinger equation. In [4], the meshless local Petrov-Galerkin (MLPG) method based on local weak form and moving least squares (MLS) approximation has been proposed to solve Schrödinger equation. The meshless local boundary integral equation (LBIE) method developed in [5] for numerical solution of Schrödinger equation is based on LBIE with MLS approximation. The compact boundary value method introduced in [6] to solve Schrödinger equation involves a combination of compact finite difference approximation of fourth-order and fourth-order boundary value method. In [7], the time-space pseudo-spectral method based on Chebyshev-Gauss-Lobatto quadrature points is developed for numerical solution of Schrödinger equation. One of the famous techniques to solve Schrödinger equation is known to be the Finite-Difference Time-Domain (FDTD) method [8, 9]. Based on the FDTD method, various numerical schemes have been proposed, such as the explicit finite-difference method [10, 11, 12], Crank-Nicolson method [13], split-step method [14, 15] and Alternating-Direction-Implicit (ADI) method [16, 17, 18]. The ADI methods in [16] are based on Peaceman and Rachford second-order ADI method and Mitchell

*Tel.: +65 98320575 Fax.: +65 67933318

Email address: tayw0034@e.ntu.edu.sg (Wei Choon Tay)

and Fairweather fourth-order ADI method for solving two-dimensional time dependent diffusion equation with non-local boundary conditions. The Noye and Hayman fourth-order ADI method developed in [17] is used to solve two-dimensional time dependent diffusion equation with an integral condition. In [18], second-order and fourth-order Crank-Nicolson ADI scheme as well as linearized ADI scheme are introduced to solve Schrödinger equation.

For fast and simple implementation, one can consider using the explicit method. However, this comes with a drawback of stability constraint [19, 20, 21] restricted by the minimum cell size of the domain. This limitation can be overcome through the implementation of tridiagonal ADI (Tri-ADI) method [16, 17, 18], which involves a tridiagonal system of equations. Nevertheless, the conventional Tri-ADI method involves direct computations of the complex wave function, resulting in lower efficiency as the computations of complex variables are rather taxing and time consuming. Furthermore, all the implicit methods so far still contain operators on the right-hand-sides (RHS), which call for considerable arithmetic operations.

To improve the overall efficiency, we propose a pentadiagonal ADI (Penta-ADI) method for the Schrödinger equation. Through the separation of complex wave function into real and imaginary parts, a pentadiagonal system of equations for the ADI method is obtained, which results in our Penta-ADI method. Using this algorithm, the overall efficiency improves as no complex variables and operations are required. To further simplify the algorithm, the concept of fundamental ADI (FADI) method [22, 23] is borrowed and extended from the electromagnetics. This algorithm has its RHS free of matrix operators, resulting in the simplest and most concise update equations. Note that for FADI method in electromagnetics [24, 25], it is not directly applicable here because it involves tridiagonal system of equations. In our case here for Schrödinger equation, it involves pentadiagonal system of equations, which shall be called as pentadiagonal FADI (Penta-FADI) method. As the Penta-FADI method involves five stencils in the left-hand-sides (LHS) of the pentadiagonal update equations, special treatments that are required for the implementation of Dirichlet's boundary conditions will be discussed. Using the Penta-FADI method, a high efficiency gain of up to 33 times can be achieved over the conventional Tri-ADI method.

2. Tridiagonal Alternating-Direction-Implicit Method (Tri-ADI)

We first introduce a set of notations that will be used throughout this paper. In order to apply FDTD method to the Schrödinger equations, a computational domain is established with grid spacing of Δx and Δy and time step Δt . Therefore, $\Psi_R(x, y, t)$ can be redefined as $\Psi_R(i\Delta x, j\Delta y, n\Delta t)$ for a particular time step n with grid point (i, j) , where i, j and n are integers. For simplicity, the notation $\Psi_{i,j}^n$ is used to denote $\Psi_R(i\Delta x, j\Delta y, n\Delta t)$ for the FDTD method.

An unconditionally stable ADI method has been introduced by Peaceman-Rachford [26] to circumvent the stability constraint imposed in the explicit method. Based on this ADI method, we can discretize (1) into the following two sub-steps:

$$\left(1 - \frac{\Delta t}{2}A\right)\Psi^{n+\frac{1}{2}} = \left(1 + \frac{\Delta t}{2}B\right)\Psi^n \quad (2a)$$

$$\left(1 - \frac{\Delta t}{2}B\right)\Psi^{n+1} = \left(1 + \frac{\Delta t}{2}A\right)\Psi^{n+\frac{1}{2}} \quad (2b)$$

where

$$A = \mathbf{i} \frac{\partial^2}{\partial x^2} + \mathbf{i} \frac{\omega_{i,j}}{2} \quad \text{and} \quad B = \mathbf{i} \frac{\partial^2}{\partial y^2} + \mathbf{i} \frac{\omega_{i,j}}{2}.$$

By discretizing using central approximation for (2), we can obtain

$$\begin{aligned} -\mathbf{i}a_{2x}\left(\Psi|_{i-1,j}^{n+\frac{1}{2}} + \Psi|_{i-1,j}^{n+\frac{1}{2}}\right) + \left(1 + \mathbf{i}a_{1x} - \mathbf{i}b_{i,j}\right)\Psi|_{i,j}^{n+\frac{1}{2}} \\ = \mathbf{i}a_{2y}\left(\Psi|_{i,j-1}^n + \Psi|_{i,j-1}^n\right) + \left(1 - \mathbf{i}a_{1y} + \mathbf{i}b_{i,j}\right)\Psi|_{i,j}^n \end{aligned} \quad (3a)$$

$$\begin{aligned} -\mathbf{i}a_{2y}\left(\Psi|_{i,j-1}^{n+1} + \Psi|_{i,j-1}^{n+1}\right) + \left(1 + \mathbf{i}a_{1y} - \mathbf{i}b_{i,j}\right)\Psi|_{i,j}^{n+1} \\ = \mathbf{i}a_{2x}\left(\Psi|_{i-1,j}^{n+\frac{1}{2}} + \Psi|_{i-1,j}^{n+\frac{1}{2}}\right) + \left(1 - \mathbf{i}a_{1x} + \mathbf{i}b_{i,j}\right)\Psi|_{i,j}^{n+\frac{1}{2}} \end{aligned} \quad (3b)$$

where $a_{\zeta\xi} = \frac{\Delta t}{\zeta\Delta\xi^2}$, $b_{i,j} = \frac{\Delta t\omega_{i,j}}{4}$, $\xi = x, y$ and ζ is an integer.

It can be seen that the LHS of (3a) and (3b) constitute the tridiagonal system of equations which shall be known as the Tri-ADI method. However, due to the nature of the complex wave function Ψ which involves real and imaginary parts, the computation of this algorithm is rather taxing and time consuming. In addition, the operators on the RHS of the equations further diminish the efficiency of this algorithm.

3. Pentadiagonal Alternating-Direction-Implicit Method (Penta-ADI)

To overcome the deficiency of the complex wave function Ψ in the Tri-ADI method, we first separate the complex wave function into real and imaginary parts

$$\Psi|_{i,j} = \Psi_R|_{i,j} + \mathbf{i}\Psi_I|_{i,j}. \quad (4)$$

Upon doing so, we can now convert (2) into a compact matrix form as

$$\left(\mathbf{I} - \frac{\Delta t}{2}\mathbf{A}\right)\Psi^{n+\frac{1}{2}} = \left(\mathbf{I} + \frac{\Delta t}{2}\mathbf{B}\right)\Psi^n \quad (5a)$$

$$\left(\mathbf{I} - \frac{\Delta t}{2}\mathbf{B}\right)\Psi^{n+1} = \left(\mathbf{I} + \frac{\Delta t}{2}\mathbf{A}\right)\Psi^{n+\frac{1}{2}} \quad (5b)$$

where

$$\Psi = \begin{bmatrix} \Psi_R \\ \Psi_I \end{bmatrix}, \quad \mathbf{A} = \begin{bmatrix} 0 & -H_x \\ H_x & 0 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 0 & -H_y \\ H_y & 0 \end{bmatrix} \quad \text{and} \quad H_\xi = \frac{\partial^2}{\partial \xi^2} + \frac{\omega_{i,j}}{2}.$$

By discretizing (5a), we get

$$\begin{aligned} \Psi_R|_{i,j}^{n+\frac{1}{2}} + a_{2x}\left(\Psi_I|_{i+1,j}^{n+\frac{1}{2}} + \Psi_I|_{i-1,j}^{n+\frac{1}{2}}\right) - (a_{1x} - b_{i,j})\Psi_I|_{i,j}^{n+\frac{1}{2}} \\ = \Psi_R|_{i,j}^n - a_{2y}\left(\Psi_I|_{i,j+1}^n + \Psi_I|_{i,j-1}^n\right) + (a_{1y} - b_{i,j})\Psi_I|_{i,j}^n \end{aligned} \quad (6a)$$

$$\begin{aligned} \Psi_I|_{i,j}^{n+\frac{1}{2}} - a_{2x}\left(\Psi_R|_{i+1,j}^{n+\frac{1}{2}} + \Psi_R|_{i-1,j}^{n+\frac{1}{2}}\right) + (a_{1x} - b_{i,j})\Psi_R|_{i,j}^{n+\frac{1}{2}} \\ = \Psi_I|_{i,j}^n + a_{2y}\left(\Psi_R|_{i,j+1}^n + \Psi_R|_{i,j-1}^n\right) - (a_{1y} - b_{i,j})\Psi_R|_{i,j}^n. \end{aligned} \quad (6b)$$

By substituting (6b) into (6a), we can obtain the implicit pentadiagonal update equation for the first

sub-step from n to $n + \frac{1}{2}$:

$$\begin{aligned}
& \left[1+2a_{2x}^2 + (a_{1x} - b_{i,j})^2\right] \Psi_R|_{i,j}^{n+\frac{1}{2}} - a_{2x} \left[2a_{1x} - b_{i-1,j} - b_{i,j}\right] \Psi_R|_{i-1,j}^{n+\frac{1}{2}} \\
& - a_{2x} \left[2a_{1x} - b_{i,j} - b_{i+1,j}\right] \Psi_R|_{i+1,j}^{n+\frac{1}{2}} + a_{2x}^2 \left(\Psi_R|_{i+2,j}^{n+\frac{1}{2}} + \Psi_R|_{i-2,j}^{n+\frac{1}{2}}\right) \\
& = \left[1 - (a_{1x} - b_{i,j})(a_{1y} - b_{i,j})\right] \Psi_R|_{i,j}^n \\
& - a_{2x}a_{2y} \left(\Psi_R|_{i+1,j+1}^n + \Psi_R|_{i-1,j+1}^n + \Psi_R|_{i-1,j-1}^n + \Psi_R|_{i+1,j-1}^n\right) \\
& + a_{2y}(a_{1x} - b_{i,j}) \left(\Psi_R|_{i,j+1}^n + \Psi_R|_{i,j-1}^n\right) + a_{2x}(a_{1y} - b_{i+1,j}) \Psi_R|_{i+1,j}^n + a_{2x}(a_{1y} - b_{i-1,j}) \Psi_R|_{i-1,j}^n \\
& + (a_{1x} + a_{1y} - 2b_{i,j}) \Psi_I|_{i,j}^n - a_{2x} \left(\Psi_I|_{i+1,j}^n + \Psi_I|_{i-1,j}^n\right) - a_{2y} \left(\Psi_I|_{i,j+1}^n + \Psi_I|_{i,j-1}^n\right). \tag{7}
\end{aligned}$$

$\Psi_I^{n+\frac{1}{2}}$ can then be updated explicitly through (6b) as

$$\begin{aligned}
\Psi_I|_{i,j}^{n+\frac{1}{2}} &= \Psi_I|_{i,j}^n + a_{2y} \left(\Psi_R|_{i,j+1}^n + \Psi_R|_{i,j-1}^n\right) - (a_{1y} - b_{i,j}) \Psi_R|_{i,j}^n \\
& + a_{2x} \left(\Psi_R|_{i+1,j}^{n+\frac{1}{2}} + \Psi_R|_{i-1,j}^{n+\frac{1}{2}}\right) - (a_{1x} - b_{i,j}) \Psi_R|_{i,j}^{n+\frac{1}{2}}. \tag{8}
\end{aligned}$$

Similarly, we can obtain the implicit pentadiagonal update equation for the second sub-step from $n + \frac{1}{2}$ to $n + 1$:

$$\begin{aligned}
& \left[1+2a_{2y}^2 + (a_{1y} - b_{i,j})^2\right] \Psi_R|_{i,j}^{n+1} - a_{2y} \left[2a_{1y} - b_{i,j-1} - b_{i,j}\right] \Psi_R|_{i,j-1}^{n+1} \\
& - a_{2y} \left[2a_{1y} - b_{i,j} - b_{i,j+1}\right] \Psi_R|_{i,j+1}^{n+1} + a_{2y}^2 \left(\Psi_R|_{i,j+2}^{n+1} + \Psi_R|_{i,j-2}^{n+1}\right) \\
& = \left[1 - (a_{1y} - b_{i,j})(a_{1x} - b_{i,j})\right] \Psi_R|_{i,j}^{n+\frac{1}{2}} \\
& - a_{2x}a_{2y} \left(\Psi_R|_{i+1,j+1}^{n+\frac{1}{2}} + \Psi_R|_{i-1,j+1}^{n+\frac{1}{2}} + \Psi_R|_{i-1,j-1}^{n+\frac{1}{2}} + \Psi_R|_{i+1,j-1}^{n+\frac{1}{2}}\right) \\
& + a_{2x}(a_{1y} - b_{i,j}) \left(\Psi_R|_{i+1,j}^{n+\frac{1}{2}} + \Psi_R|_{i-1,j}^{n+\frac{1}{2}}\right) + a_{2y}(a_{1x} - b_{i,j+1}) \Psi_R|_{i,j+1}^{n+\frac{1}{2}} + a_{2y}(a_{1x} - b_{i,j-1}) \Psi_R|_{i,j-1}^{n+\frac{1}{2}} \\
& + (a_{1x} + a_{1y} - 2b_{i,j}) \Psi_I|_{i,j}^{n+\frac{1}{2}} - a_{2y} \left(\Psi_I|_{i,j+1}^{n+\frac{1}{2}} + \Psi_I|_{i,j-1}^{n+\frac{1}{2}}\right) - a_{2x} \left(\Psi_I|_{i+1,j}^{n+\frac{1}{2}} + \Psi_I|_{i-1,j}^{n+\frac{1}{2}}\right). \tag{9}
\end{aligned}$$

Ψ_I^{n+1} can then be updated explicitly through

$$\begin{aligned}
\Psi_I|_{i,j}^{n+1} &= \Psi_I|_{i,j}^{n+\frac{1}{2}} + a_{2x} \left(\Psi_R|_{i+1,j}^{n+\frac{1}{2}} + \Psi_R|_{i-1,j}^{n+\frac{1}{2}}\right) - (a_{1x} - b_{i,j}) \Psi_R|_{i,j}^{n+\frac{1}{2}} \\
& + a_{2y} \left(\Psi_R|_{i,j+1}^{n+1} + \Psi_R|_{i,j-1}^{n+1}\right) - (a_{1y} - b_{i,j}) \Psi_R|_{i,j}^{n+1}. \tag{10}
\end{aligned}$$

Applying separation of the complex wave function in (4), we obtain a pentadiagonal system of equations in the LHS of (7) and (9), which results in our Penta-ADI method. Note that for two-dimensional system, the order of computational complexity for solving pentadiagonal system of equations is $O(n^2)$. As this algorithm does not involve complex variables, the computation is much simpler and less time consuming. The efficiency gain will be further demonstrated in Section 6.

4. Fundamental ADI (FADI) Method

To further simplify the complexity of the RHS update equations in (5), we now introduce an auxilliary matrix operator $\tilde{\mathbf{V}}$ and rewrite (5) as

$$\tilde{\mathbf{V}}^n = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{B} \right) \Psi^n \quad (11a)$$

$$\left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{A} \right) \Psi^{n+\frac{1}{2}} = \tilde{\mathbf{V}}^n \quad (11b)$$

$$\tilde{\mathbf{V}}^{n+\frac{1}{2}} = \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{A} \right) \Psi^{n+\frac{1}{2}} \quad (11c)$$

$$\left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{B} \right) \Psi^{n+1} = \tilde{\mathbf{V}}^{n+\frac{1}{2}} \quad (11d)$$

where

$$\tilde{\mathbf{V}} = [\tilde{V}_R \quad \tilde{V}_I]^T.$$

First, we alter (11d) by one time step backward to get

$$\tilde{\mathbf{V}}^{n-\frac{1}{2}} = \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{B} \right) \Psi^n. \quad (12)$$

Further manipulation of (11a), we can obtain

$$\begin{aligned} \tilde{\mathbf{V}}^n &= \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{B} \right) \Psi^n \\ &= 2\Psi^n - \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{B} \right) \Psi^n \\ &= 2\Psi^n - \tilde{\mathbf{V}}^{n-\frac{1}{2}}. \end{aligned} \quad (13)$$

Similiarly, through (11b), we are able to reduce (11c) into

$$\begin{aligned} \tilde{\mathbf{V}}^{n+\frac{1}{2}} &= \left(\mathbf{I} + \frac{\Delta t}{2} \mathbf{A} \right) \Psi^{n+\frac{1}{2}} \\ &= 2\Psi^{n+\frac{1}{2}} - \left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{A} \right) \Psi^{n+\frac{1}{2}} \\ &= 2\Psi^{n+\frac{1}{2}} - \tilde{\mathbf{V}}^{n+\frac{1}{2}}. \end{aligned} \quad (14)$$

Combining (13) and (14), we have simplified the algorithm in (11) to

$$\tilde{\mathbf{V}}^n = 2\Psi^n - \tilde{\mathbf{V}}^{n-\frac{1}{2}} \quad (15a)$$

$$\left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{A} \right) \Psi^{n+\frac{1}{2}} = \tilde{\mathbf{V}}^n \quad (15b)$$

$$\tilde{\mathbf{V}}^{n+\frac{1}{2}} = 2\Psi^{n+\frac{1}{2}} - \tilde{\mathbf{V}}^n \quad (15c)$$

$$\left(\mathbf{I} - \frac{\Delta t}{2} \mathbf{B} \right) \Psi^{n+1} = \tilde{\mathbf{V}}^{n+\frac{1}{2}}. \quad (15d)$$

By simple re-definition of field variables

$$\mathbf{V}^{n-\frac{1}{2}} = \frac{1}{2} \tilde{\mathbf{V}}^{n-\frac{1}{2}}, \quad \mathbf{V}^n = \frac{1}{2} \tilde{\mathbf{V}}^n, \quad \mathbf{V}^{n+\frac{1}{2}} = \frac{1}{2} \tilde{\mathbf{V}}^{n+\frac{1}{2}},$$

we obtain the final update procedures as

$$\mathbf{V}^n = \Psi^n - \mathbf{V}^{n-\frac{1}{2}} \quad (16a)$$

$$\left(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{A}\right)\Psi^{n+\frac{1}{2}} = \mathbf{V}^n \quad (16b)$$

$$\mathbf{V}^{n+\frac{1}{2}} = \Psi^{n+\frac{1}{2}} - \mathbf{V}^n \quad (16c)$$

$$\left(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{B}\right)\Psi^{n+1} = \mathbf{V}^{n+\frac{1}{2}} \quad (16d)$$

with initialization

$$\mathbf{V}^{-\frac{1}{2}} = \left(\frac{1}{2}\mathbf{I} - \frac{\Delta t}{4}\mathbf{B}\right)\Psi^0. \quad (17)$$

where the temporary auxiliary variables

$$\mathbf{V} = [V_R \quad V_I]^T.$$

The algorithm (16) has now been reduced into the simplest form with no matrix operators $\mathbf{A}$ or $\mathbf{B}$ in the RHS. This results in the most concise update equation in the RHS, leading to programming ease and improved computational efficiency. The word fundamental in this paper is used to aptly describe the ADI method in the most fundamental (basic) form that cannot be reduced further in the RHS. Such concept of fundamental scheme is borrowed and extended from the electromagnetics [22, 23]. Note that for FADI method in electromagnetics [24, 25], it is not directly applicable here because it involves tridiagonal system of equations. In our case here for Schrödinger equation, it involves pentadiagonal system of equations, which shall be called as Penta-FADI method.

To obtain the implicit pentadiagonal update equations, we apply central approximation to (16b) and upon some manipulations, we have

$$\frac{1}{2}\Psi_R|_{i,j}^{n+\frac{1}{2}} + a_{4x}\left(\Psi_I|_{i+1,j}^{n+\frac{1}{2}} + \Psi_I|_{i-1,j}^{n+\frac{1}{2}}\right) - \frac{a_{1x} - b_{i,j}}{2}\Psi_I|_{i,j}^{n+\frac{1}{2}} = V_R|_{i,j}^n \quad (18a)$$

$$\frac{1}{2}\Psi_I|_{i,j}^{n+\frac{1}{2}} - a_{4x}\left(\Psi_R|_{i+1,j}^{n+\frac{1}{2}} + \Psi_R|_{i-1,j}^{n+\frac{1}{2}}\right) + \frac{a_{1x} - b_{i,j}}{2}\Psi_R|_{i,j}^{n+\frac{1}{2}} = V_I|_{i,j}^n. \quad (18b)$$

By substituting (18b) into (18a), we can obtain the update equations of (16a)-(16b) for the first sub-step from n to $n + \frac{1}{2}$:

$$V_R|_{i,j}^n = \Psi_R|_{i,j}^n - V_R|_{i,j}^{n-\frac{1}{2}} \quad (19)$$

$$V_I|_{i,j}^n = \Psi_I|_{i,j}^n - V_I|_{i,j}^{n-\frac{1}{2}} \quad (20)$$

$$\begin{aligned} & \frac{1}{2}\left[1 + 2a_{2x}^2 + (a_{1x} - b_{i,j})^2\right]\Psi_R|_{i,j}^{n+\frac{1}{2}} - a_{4x}\left[2a_{1x} - b_{i-1,j} - b_{i,j}\right]\Psi_R|_{i-1,j}^{n+\frac{1}{2}} \\ & - a_{4x}\left[2a_{1x} - b_{i,j} - b_{i+1,j}\right]\Psi_R|_{i+1,j}^{n+\frac{1}{2}} + \frac{a_{2x}^2}{2}\left(\Psi_R|_{i+2,j}^{n+\frac{1}{2}} + \Psi_R|_{i-2,j}^{n+\frac{1}{2}}\right) \\ & = V_R|_{i,j}^n - a_{2x}\left(V_I|_{i+1,j}^n + V_I|_{i-1,j}^n\right) + (a_{1x} - b_{i,j})V_I|_{i,j}^n. \end{aligned} \quad (21)$$

$\Psi_I^{n+\frac{1}{2}}$ can then be updated explicitly through (18b) as

$$\Psi_I|_{i,j}^{n+\frac{1}{2}} = 2V_I|_{i,j}^n + a_{2x}\left(\Psi_R|_{i+1,j}^{n+\frac{1}{2}} + \Psi_R|_{i-1,j}^{n+\frac{1}{2}}\right) - (a_{1x} - b_{i,j})\Psi_R|_{i,j}^{n+\frac{1}{2}}. \quad (22)$$

Similarly, we can obtain the update equations of (16c)-(16d) for the second sub-step from $n + \frac{1}{2}$ to $n + 1$:

$$V_R|_{i,j}^{n+\frac{1}{2}} = \Psi_R|_{i,j}^{n+\frac{1}{2}} - V_R|_{i,j}^n \quad (23)$$

$$V_I|_{i,j}^{n+\frac{1}{2}} = \Psi_I|_{i,j}^{n+\frac{1}{2}} - V_I|_{i,j}^n \quad (24)$$

$$\begin{aligned} & \frac{1}{2} \left[1 + 2a_{2y}^2 + (a_{1y} - b_{i,j})^2 \right] \Psi_R|_{i,j}^{n+1} - a_{4y} \left[2a_{1y} - b_{i,j-1} - b_{i,j} \right] \Psi_R|_{i,j-1}^{n+1} \\ & - a_{4y} \left[2a_{1y} - b_{i,j} - b_{i,j+1} \right] \Psi_R|_{i,j+1}^{n+1} + \frac{a_{2y}^2}{2} \left(\Psi_R|_{i,j+2}^{n+1} + \Psi_R|_{i,j-2}^{n+1} \right) \\ & = V_R|_{i,j}^{n+\frac{1}{2}} - a_{2y} \left(V_I|_{i,j+1}^{n+\frac{1}{2}} + V_I|_{i,j-1}^{n+\frac{1}{2}} \right) + (a_{1y} - b_{i,j}) V_I|_{i,j}^{n+\frac{1}{2}}. \end{aligned} \quad (25)$$

Ψ_I^{n+1} can then be updated explicitly through

$$\Psi_I|_{i,j}^{n+1} = 2V_I|_{i,j}^{n+\frac{1}{2}} + a_{2y} \left(\Psi_R|_{i,j+1}^{n+1} + \Psi_R|_{i,j-1}^{n+1} \right) - (a_{1y} - b_{i,j}) \Psi_R|_{i,j}^{n+1}. \quad (26)$$

For non-zero initial $\Psi_R|_{i,j}^0$ and $\Psi_I|_{i,j}^0$, we need to apply the initialization as follows:

$$V_R|_{i,j}^{-\frac{1}{2}} = \frac{1}{2} \Psi_R|_{i,j}^0 + a_{4y} \left(\Psi_I|_{i,j+1}^0 + \Psi_I|_{i,j-1}^0 \right) - \frac{a_{1y} - b_{i,j}}{2} \Psi_I|_{i,j}^0 \quad (27)$$

$$V_I|_{i,j}^{-\frac{1}{2}} = \frac{1}{2} \Psi_I|_{i,j}^0 - a_{4y} \left(\Psi_R|_{i,j+1}^0 + \Psi_R|_{i,j-1}^0 \right) + \frac{a_{1y} - b_{i,j}}{2} \Psi_R|_{i,j}^0. \quad (28)$$

Comparing (6)-(10) with (18)-(26), it can be seen that the update equations for the latter has decreased significantly in the number of floating point arithmetic operations and memory indexing. This is due to the matrix-operator-free RHS for the FADI algorithm in (16) which is in the simplest and most concise form. Note that although not shown here, using this technique, we are also able to reduce the conventional Tri-ADI method in (2) into the fundamental form.

5. Boundary Conditions

We have previously mentioned that separating the complex wave function Ψ into real and imaginary parts in (4) will lead to a pentadiagonal system of equations. Problems arise at the boundaries where the wave function Ψ is located out of the simulated domain. For instance, we consider a computation domain of 11×11 shown in Figure 1. The grid points ('•') inside the computation domain are updated using the pentadiagonal systems of equations while the grid points ('o') on the boundaries are updated explicitly by the implementation of Dirichlet's boundary conditions. We will now look at the update equations for the circled grid points in the first sub step from n to $n + \frac{1}{2}$ by forming a pentadiagonal matrix system depicted as

$$\begin{bmatrix} \alpha_1 & \gamma_1 & \delta_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \beta_2 & \alpha_2 & \gamma_2 & \delta_2 & 0 & 0 & 0 & 0 & 0 \\ \epsilon_3 & \beta_3 & \alpha_3 & \gamma_3 & \delta_3 & 0 & 0 & 0 & 0 \\ 0 & \epsilon_4 & \beta_4 & \alpha_4 & \gamma_4 & \delta_4 & 0 & 0 & 0 \\ 0 & 0 & \epsilon_5 & \beta_5 & \alpha_5 & \gamma_5 & \delta_5 & 0 & 0 \\ 0 & 0 & 0 & \epsilon_6 & \beta_6 & \alpha_6 & \gamma_6 & \delta_6 & 0 \\ 0 & 0 & 0 & 0 & \epsilon_7 & \beta_7 & \alpha_7 & \gamma_7 & \delta_7 \\ 0 & 0 & 0 & 0 & 0 & \epsilon_8 & \beta_8 & \alpha_8 & \gamma_8 \\ 0 & 0 & 0 & 0 & 0 & 0 & \epsilon_9 & \beta_9 & \alpha_9 \end{bmatrix} \begin{bmatrix} \Psi_R|_{1,1}^{n+\frac{1}{2}} \\ \Psi_R|_{2,1}^{n+\frac{1}{2}} \\ \Psi_R|_{3,1}^{n+\frac{1}{2}} \\ \Psi_R|_{4,1}^{n+\frac{1}{2}} \\ \Psi_R|_{5,1}^{n+\frac{1}{2}} \\ \Psi_R|_{6,1}^{n+\frac{1}{2}} \\ \Psi_R|_{7,1}^{n+\frac{1}{2}} \\ \Psi_R|_{8,1}^{n+\frac{1}{2}} \\ \Psi_R|_{9,1}^{n+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} \Gamma_1 + a_{4x}(a_{1x} - b_{1,1})\Psi_R|_{0,1}^{n+\frac{1}{2}} - a_{4x}\Psi_I|_{0,1}^{n+\frac{1}{2}} \\ \Gamma_2 - \epsilon_2\Psi_R|_{0,1}^{n+\frac{1}{2}} \\ \Gamma_3 \\ \Gamma_4 \\ \Gamma_5 \\ \Gamma_6 \\ \Gamma_7 \\ \Gamma_8 - \delta_8\Psi_R|_{10,1}^{n+\frac{1}{2}} \\ \Gamma_9 + a_{4x}(a_{1x} - b_{10,1})\Psi_R|_{10,1}^{n+\frac{1}{2}} - a_{4x}\Psi_I|_{10,1}^{n+\frac{1}{2}} \end{bmatrix} \quad (29)$$

Figure 1: Computation domain of 11 x 11 grids.

where ϵ , β , α , γ and δ are coefficients of pentadiagonal matrix while Γ consists of RHS terms in the update equations.

Note that (21) is only applicable from $\Psi_R|_{3,1}^{n+\frac{1}{2}}$ to $\Psi_R|_{7,1}^{n+\frac{1}{2}}$. Special boundary treatments are required for the rest of the update equations. The update equation for $\Psi_R|_{1,1}^{n+\frac{1}{2}}$ is obtained by substituting (18b) into $\Psi_I|_{1,1}^{n+\frac{1}{2}}$ and $\Psi_I|_{2,1}^{n+\frac{1}{2}}$ of (18a). $\Psi_I|_{0,1}^{n+\frac{1}{2}}$ and $\Psi_R|_{0,1}^{n+\frac{1}{2}}$ are then transferred to the RHS of the update equation seen in (29). The second update equation for $\Psi_R|_{2,1}^{n+\frac{1}{2}}$ is the same as (21), but requires $\Psi_R|_{0,1}^{n+\frac{1}{2}}$ to be transferred over to the RHS of the update equation. Similar procedures can be repeated in $\Psi_R|_{8,1}^{n+\frac{1}{2}}$ and $\Psi_R|_{9,1}^{n+\frac{1}{2}}$ to obtain their respective update equations. For clarity, the update equations for $\Psi_R|_{1,1}^{n+\frac{1}{2}}$ and $\Psi_R|_{2,1}^{n+\frac{1}{2}}$ are presented as follows:

$$\begin{aligned} & \frac{1}{2} \left[1 + a_{2x}^2 + (a_{1x} - b_{1,1})^2 \right] \Psi_R|_{1,1}^{n+\frac{1}{2}} - a_{4x} \left[2a_{1x} - b_{1,1} - b_{2,1} \right] \Psi_R|_{2,1}^{n+\frac{1}{2}} + \frac{a_{2x}^2}{2} \Psi_R|_{3,1}^{n+\frac{1}{2}} \\ & = V_R|_{1,1}^n - a_{2x} V_I|_{2,1}^n + (a_{1x} - b_{1,1}) V_I|_{1,1}^n + a_{4x} (a_{1x} - b_{1,1}) \Psi_R|_{0,1}^{n+\frac{1}{2}} - a_{4x} \Psi_I|_{0,1}^{n+\frac{1}{2}} \end{aligned} \quad (30a)$$

$$\begin{aligned} & \frac{1}{2} \left[1 + 2a_{2x}^2 + (a_{1x} - b_{2,1})^2 \right] \Psi_R|_{2,1}^{n+\frac{1}{2}} - a_{4x} \left[2a_{1x} - b_{1,1} - b_{2,1} \right] \Psi_R|_{1,1}^{n+\frac{1}{2}} \\ & - a_{4x} \left[2a_{1x} - b_{2,1} - b_{3,1} \right] \Psi_R|_{3,1}^{n+\frac{1}{2}} + \frac{a_{2x}^2}{2} \Psi_R|_{4,1}^{n+\frac{1}{2}} \\ & = V_R|_{2,1}^n - a_{2x} \left(V_I|_{3,1}^n + V_I|_{1,1}^n \right) + (a_{1x} - b_{2,1}) V_I|_{2,1}^n - \frac{a_{2x}^2}{2} \Psi_R|_{0,1}^{n+\frac{1}{2}}. \end{aligned} \quad (30b)$$

6. Numerical Experiments

In this section, we compare the numerical errors of Penta-FADI method with two examples where the exact solutions are known. Next, we will investigate the efficiency of Penta-ADI and Penta-FADI method compared to the conventional Tri-ADI method.

Figure 2: Waveform at observation point (31,51) for example 1.

6.1. Example 1

The exact solution of a transient gaussian distribution is given as [27]

$$\Psi_{\text{exact}}(x, y, t) = \frac{\mathbf{i}}{\mathbf{i} - 4t} e^{-\mathbf{i}((x^2+y^2+\mathbf{i}k_0x+\mathbf{i}k_0^2t)/(\mathbf{i}-4t))} \quad (31)$$

which has a zero potential function

$$\omega(x, y) = 0. \quad (32)$$

We are able to obtain the initial conditions by setting $t = 0$ s in (31):

$$\Psi_R(x, y, 0) = \Psi_{R_{\text{exact}}}(x, y, 0) \quad (33)$$

$$\Psi_I(x, y, 0) = \Psi_{I_{\text{exact}}}(x, y, 0) \quad (34)$$

and the boundary conditions

$$\Psi_R(a, b, t) = \Psi_{R_{\text{exact}}}(a, b, t) \quad (35)$$

$$\Psi_I(a, b, t) = \Psi_{I_{\text{exact}}}(a, b, t) \quad (36)$$

where $a = 0$ or 5 , $b = 0$ or 5 and $0 < t \leq T$.

The computation domain is given as $0 \leq x \leq 5$, $0 \leq y \leq 5$, $T = 1$ s, $\Delta x = \Delta y = 0.05$ m and $\Delta t = 6.25 \times 10^{-4}$ s. The Gaussian wave starts from the center of the domain $x = y = 2.5$ m with a wave number of $k_0 = 2.5$. The maximum relative error of Penta-FADI method is computed as

$$\text{Error} = \frac{\max_{\forall i, \forall j} \sqrt{|\Psi_{\text{exact}}|_{i,j} - \Psi_{\text{Penta-FADI}}|_{i,j}|^2}}{\max_{\forall i, \forall j} \sqrt{|\Psi_{\text{exact}}|_{i,j}|^2}}. \quad (37)$$

Figure 2 shows the waveform obtained from $|\Psi|$ with different Δt at observation point (31,51). It is worth noting that all three curves of the Penta-FADI methods are very close to the exact solution. This proves that a good accuracy can be obtained through the Penta-FADI method.

Table 1: Maximum relative error for Penta-FADI method at different times for example 1 with $\Delta x = \Delta y = 0.05\text{m}$ and $\Delta t = 6.25 \times 10^{-4}\text{s}$.

t	Maximum Relative Error					
	Penta-FADI (with Δt)		Penta-FADI (with $20\Delta t$)		Penta-FADI (with $40\Delta t$)	
	real	imag	real	imag	real	imag
0.1	2.8×10^{-3}	3.2×10^{-3}	6.2×10^{-3}	6.9×10^{-3}	1.6×10^{-2}	1.8×10^{-2}
0.3	6.5×10^{-3}	1.5×10^{-2}	1.5×10^{-2}	3.5×10^{-2}	4.5×10^{-2}	9.6×10^{-2}
0.5	1.1×10^{-2}	1.3×10^{-2}	2.3×10^{-2}	2.2×10^{-2}	6.6×10^{-2}	6.1×10^{-2}
0.7	1.4×10^{-2}	1.4×10^{-2}	3.0×10^{-2}	3.6×10^{-2}	8.6×10^{-2}	8.1×10^{-2}
1.0	3.3×10^{-2}	4.4×10^{-2}	6.3×10^{-2}	9.1×10^{-2}	1.5×10^{-1}	2.7×10^{-1}

Table 2: Maximum relative error for Penta-FADI method at time $T = 1\text{s}$ for example 1 with different Δx and Δy where $\Delta t = 6.25 \times 10^{-4}\text{s}$.

$\Delta x = \Delta y$	Maximum Relative Error		
	Penta-FADI (with Δt)	Penta-FADI (with $20\Delta t$)	Penta-FADI (with $40\Delta t$)
	absolute	absolute	absolute
0.05	4.1×10^{-2}	8.3×10^{-2}	2.3×10^{-1}
0.025	1.0×10^{-2}	5.0×10^{-2}	1.9×10^{-1}
0.0125	2.6×10^{-3}	4.2×10^{-2}	1.8×10^{-1}

Table 1 reports the maximum relative error for Penta-FADI method in both real and imaginary parts of the wave function Ψ for Δt , $20\Delta t$ and $40\Delta t$. It can be seen that as Δt increases, the error for the Penta-FADI method increases. This is inevitable as the increase in Δt will incur a greater error but this may still be tolerable for some applications.

We further investigate the accuracy of Penta-FADI method by reducing the spatial steps Δx and Δy . Table 2 shows the maximum relative error for Penta-FADI method at time $T = 1\text{s}$ at finer Δx and Δy . From the Table, we can deduce that finer spatial step will result in smaller error.

6.2. Example 2

The exact solution of this example [11]

$$\Psi_A(x, y, t) = x^2 y^2 e^{it} \quad (38)$$

comes with a potential function

$$\omega(x, y) = 1 - \frac{2}{x^2} - \frac{2}{y^2} \quad (39)$$

where the initial and boundary conditions are similar to (33)-(36).

The computation domain is given as $0 \leq x \leq 1$, $0 \leq y \leq 1$, $T = 1\text{s}$, $\Delta x = \Delta y = 0.1\text{m}$ and $\Delta t = 1.0 \times 10^{-3}\text{s}$. Figures 3(a) and (b) show the waveforms for real and imaginary parts of Ψ at observation point (4,4). It can be seen that all three curves of Penta-FADI method are very close to the exact solution. This again shows the results of Penta-FADI method as accurate approximations of Schrödinger equations.

Table 3 reports the maximum relative error for Penta-FADI method in both real and imaginary parts of the wave function Ψ for Δt , $50\Delta t$ and $100\Delta t$. Similar to the analysis above, we can observe that as the Δt increases, the error also increases. This shows a trade-off between accuracy and efficiency.

6.3. Efficiency

In order to validate the efficiency gain of our proposed Penta-FADI method over the conventional Tri-ADI method, we simulate the numerical experiment of example 2 using C++ codes with Intel(R) Xeon(R) 2.40 GHz CPU. The computation domain size ranges from 1000×1000 to 5000×5000 grids, with $\Delta t =$

Figure 3: Waveform of (a) $\Psi_R|_{4,4}$ and (b) $\Psi_I|_{4,4}$.

Table 3: Maximum relative error for Penta-FADI method at different times for example 2 with $\Delta x = \Delta y = 0.1\text{m}$ and $\Delta t = 1.0 \times 10^{-3}\text{s}$.

t	Maximum Relative Error					
	Penta-FADI (with Δt)		Penta-FADI (with $50\Delta t$)		Penta-FADI (with $100\Delta t$)	
	real	imag	real	imag	real	imag
0.1	1.9×10^{-7}	1.1×10^{-6}	4.1×10^{-4}	1.9×10^{-3}	2.1×10^{-3}	1.1×10^{-2}
0.3	1.7×10^{-7}	2.9×10^{-7}	5.2×10^{-4}	9.2×10^{-4}	1.6×10^{-3}	2.5×10^{-3}
0.5	1.7×10^{-7}	3.8×10^{-7}	5.3×10^{-4}	4.1×10^{-4}	1.9×10^{-3}	3.8×10^{-3}
0.7	2.7×10^{-7}	2.2×10^{-7}	4.7×10^{-4}	5.7×10^{-4}	2.6×10^{-3}	1.9×10^{-3}
1.0	2.1×10^{-7}	2.3×10^{-7}	4.3×10^{-4}	2.7×10^{-4}	2.3×10^{-3}	2.4×10^{-3}

$4.0 \times 10^{-3}\text{s}$ over 250 time steps. The CPU run time of Penta-ADI, Penta-FADI and Tri-ADI methods are obtained and the efficiency gains are tabulated.

Table 4 shows the efficiency gains among various methods over a range of computation domains. The efficiency gain of Penta-ADI over Tri-ADI method is over 22 times. This can be explained by the complex wave function Ψ in Tri-ADI method, where the direct computation of complex variables is rather complicated, leading to longer CPU times. By further comparing Penta-FADI with Tri-ADI method, the efficiency gain is over 30 times. This justifies the overall reduction of flops count and memory indexing of Penta-FADI method (as mentioned in Section 4). This is because it has matrix-operator-free RHS, resulting in most concise update equations with the minimum number of arithmetic operations.

7. Conclusion

We have presented a Penta-ADI method for the two-dimensional Schrödinger equations. Through the separation of complex wave function into real and imaginary parts, a pentadiagonal system of equations for the ADI method is obtained, which results in our Penta-ADI method. The Penta-ADI method has been further simplified into the Penta-FADI method with matrix-operator-free RHS, leading to the simplest and most concise update equations. As the Penta-FADI method involves five stencils in the LHS of the pentadiagonal update equations, special treatments that are required for the implementation of Dirichlet's boundary conditions has been discussed. Using the Penta-FADI method, a high efficiency gain of up to 33 times can be achieved over the Tri-ADI method, which involves a tridiagonal system of equations.

Table 4: Efficiency gains of Penta-FADI over Tri-ADI method for various computation domains ($\Delta t = 4.0 \times 10^{-3}$ s, 250 time steps)

Domain Size	Efficiency Gain	
	Penta-ADI v.s. Tri-ADI	Penta-FADI v.s. Tri-ADI
1000×1000	24.63	33.27
2000×2000	24.14	33.61
3000×3000	23.74	32.07
4000×4000	22.41	30.16
5000×5000	23.23	30.65

References

- [1] S. Brandt, H. D. Dahmen, The picture book of quantum mechanics (Springer, New York, 2012) p. 46.
- [2] D. J. Griffiths, Introduction to quantum mechanics (Prentice-Hall, New Jersey, 2005) p. 1.
- [3] D. M. Sullivan, D. S. Citrin, J. Appl. Phys. 97 (2005) 104305.
- [4] M. Dehghan, D. Mirzaei, Eng. Anal. with Boundary Elem. 32 (2008) 747.
- [5] M. Dehghan, D. Mirzaei, Int. J. Numer. Methods Eng. 76 (2008) 501.
- [6] A. Mohebbi, M. Dehghan, J. Comput. Appl. Math. 225 (2009) 124.
- [7] M. Dehghan, A. Taleei, Numer. Methods Partial Differ. Equations 26 (2010) 979.
- [8] T.E. Simos, P.S. Williams, Computers and Chemistry 23 (1999) 513.
- [9] M. Dehghan, Math. Comput. Simulation 71 (2006) 16.
- [10] I. W. Sudiarta, D. J. W. Geldart, J. Phys. A: Math. Theor. 40 (2007) 1885.
- [11] M. Subaşı, Numer. Methods Partial Differential Equations 18 (2002) 752.
- [12] A. Soriano, E.A. Navarro, J.A. Portí, V. Such, J. Appl. Phys. 95 (2004) 8011.
- [13] Q.S. Chang, Erhui Jia, W. Sun, J. Comput. Phys. 148 (1999) 397.
- [14] H.Q. Wang, Appl. Math. Comput. 170 (2005) 17.
- [15] M. Dehghan, A. Taleei, Comput. Phys. Commun. 181 (2010) 43.
- [16] M. Dehghan, Int. J. Comput. Math. 72 (1999) 349.
- [17] M. Dehghan, Comput. Math. Appl. 43 (2002) 1477.
- [18] Y. Xu, L. Zhang, Comput. Phys. Commun. 183 (2012) 1082.
- [19] D. M. Sullivan, Electromagnetic simulation using the FDTD method (IEEE Press, New Jersey, 2013) p. 153.
- [20] M. Dehghan, Nonlinear Anal., TMA 48 (2002) 637.
- [21] W. Dai, G. Li, R. Nassar, S. Su, Numer. Methods Partial Differential Equations 21 (2005) 1140.
- [22] E. L. Tan, IEEE Trans. Antennas Propagat. 17 (2007) 7.
- [23] E. L. Tan, IEEE Trans. Antennas Propagat. 56 (2008) 170.
- [24] K. S. Yee, IEEE Trans. Antennas Propagat. 14 (1966) 302.
- [25] A. Taflov, S. C. Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain Method (Artech House, Boston, 2005) p. 182.
- [26] D. W. Peaceman, H. H. Rachford, Jr., J. Soc. Ind. Appl. Math. 3 (1955) 28.
- [27] M. Dehghan, A. Shokri, Comput. Math. Appl. 54 (2007) 136.