Explicit method for the heat equation

In the simplest case, we impose the PDE of the problem at the interior grid points,

$$\frac{\partial u}{\partial t}(x_i, t_j) = \frac{\partial^2 u}{\partial x^2}(x_i, t_j) \tag{35}$$

and neglecting the truncation errors in (27) and (33) we consider the approximations

$$\begin{aligned}
\frac{\partial^2 u}{\partial x^2}(x_i, t_j) &\approx \partial^2_{x,h_x} u(x_i, t_j) \\
&= \frac{u(x_i + h_x, t_j) - 2u(x_i, t_j) + u(x_i - h_x, t_j)}{h_x^2} \\
&= \frac{u(x_{i+1}, t_j) - 2u(x_i, t_j) + u(x_{i-1}, t_j)}{h_x^2} \\
&= \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h_x^2}
\end{aligned}$$

and, in a similar fashion,

$$\begin{aligned}\frac{\partial u}{\partial t}(x_i, t_j) &\approx \partial^+_{t,h_t} u(x_i, t_j) \\ &= \frac{u(x_i, t_j + h_t) - u(x_i, t_j)}{h_t} \\ &= \frac{u(x_i, t_{j+1}) - u(x_i, t_j)}{h_t} \\ &= \frac{u_{i,j+1} - u_{i,j}}{h_t}\end{aligned}$$

and, instead of (35) we will impose

$$\frac{u_{i,j+1} - u_{i,j}}{h_t} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h_x^2}$$

which can be written as

$$u_{i,j+1} = u_{i,j} + \frac{h_t}{h_x^2}\left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right)$$

and defining $\lambda = \frac{h_t}{h_x^2}$ we get

$$u_{i,j+1} = \lambda u_{i+1,j} + (1-2\lambda)u_{i,j} + \lambda u_{i-1,j} \tag{36}$$

which means that the value $u_{i,j+1}$ can be determined once we know the values $u_{i+1,j}$, $u_{i,j}$ and $u_{i-1,j}$ as illustrated in next figure.

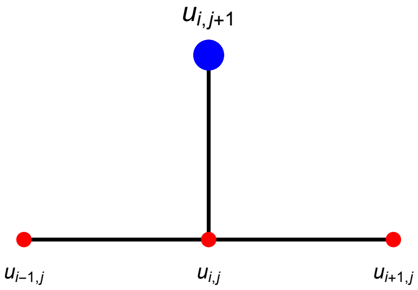

Figure: Stencil for the explicit method.

Since all the values $u_{i,0},\ i = 0, 1, ..., N_x$ are known by the initial conditions of problem, using (36) we can determine $u_{i,1},\ i = 1, ..., N_x - 1$. Note that $u_{0,1} = u_a(t_1)$ and $u_{N_x,1} = u_b(t_1)$ are known, by the boundary conditions of the problem. Therefore, the solution can be determined for all the grid points verifying $t = t_1$.

We can apply the same idea for determining $u_{i,2},\ i = 1, ..., N_x - 1$ in terms of $u_{i+1,1}$, $u_{i,1}$ and $u_{i-1,1}$ and $u_{0,2} = u_a(t_2)$ and $u_{N_x,2} = u_b(t_2)$ and repeating the procedure, until the level determined by $j = N_t - 1$ we determine the solution for all grid points.

This method is known as explicit method or forward-difference method because the solution at a certain level $t = t_j$ can be explicitly determined in terms of the values of the solution at the previous level.

Note that in the explicit method we consider the approximations of the partial derivatives (27) and (33) and thus, the error in the discretization of the PDE leads to a local truncation error of order $O(h_x^2) + O(h_t)$.

Thus, the explicit method is a method of first order in time and second order in space.

Next, we test the numerical method in a simple example for which the exact solution of the problem is $u(x,t) = \exp(-\pi^2 t)\sin(\pi x)$, defined in the region $\left\{(x,t) \in \mathbb{R}^2 : 0 \leq x \leq 1, 0 \leq t \leq 1\right\}$. In the first case we took $N_x = 20$ and $N_t = 800$, which implies that $\lambda = \frac{1}{2}$.

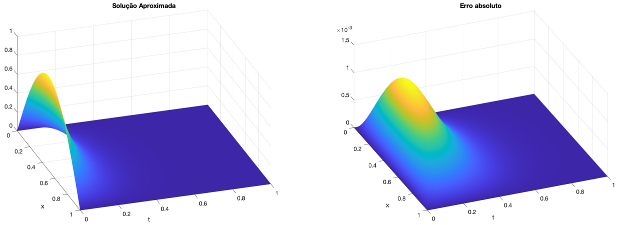

Figure: Approximate solution (left plot) and absolute error (right plot) obtained by the explicit method in the case $N_x = 20$ and $N_t = 800$ for which $\lambda = \frac{1}{2}$.

Next Figure shows the plot of the approximate solution for $N_x = 25$ and $N_t = 800$, which implies that $\lambda = \frac{25}{32} \approx 0.78$ and it is evident that in this case the approximate solution that was obtained has not any physical meaning.

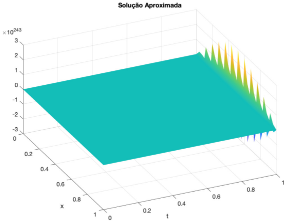

Figure: Approximate solution obtained by the explicit method in the case $N_x = 25$ and $N_t = 800$ for which $\lambda \approx 0.78$.

This example illustrates a problem of numerical instability of the explicit method for some choices N_x and N_t that we shall discuss next.

The stability of a numerical scheme ensures that the errors that accumulate in the successive time steps stay bounded. The usual way of evaluating the stability of a scheme is to perform Von Neumann stability analysis.

Essentially, we assume the initial solution to be a wave of the form $R_0 e^{\mathrm{i}kx}$, for a certain $R_0 \in \mathbb{R}$ and $k \in \mathbb{Z}$ and then study if the solution stays bounded in next time steps. So, we assume that

$$u_{i,0} = R_0 e^{\mathrm{i}kx_i}$$

and then study the next values of the form $u_{i,j} = R_j e^{\mathrm{i}kx_i}$ lead (or not) to a bounded sequence (R_j).

In the case of the explicit method,

$$\underbrace{u_{i,j+1}}_{R_{j+1}e^{\mathrm{i}kx_i}} = \lambda \underbrace{u_{i+1,j}}_{R_j e^{\mathrm{i}k(x_i+h_x)}} + (1-2\lambda) \underbrace{u_{i,j}}_{R_j e^{\mathrm{i}kx_i}} + \lambda \underbrace{u_{i-1,j}}_{R_j e^{\mathrm{i}k(x_i-h_x)}}$$

and dividing by $e^{\mathrm{i}kx_i}$ we get

$$\begin{aligned}
R_{j+1} &= \lambda R_j e^{\mathrm{i}kh_x} + (1-2\lambda)R_j + \lambda R_j e^{-\mathrm{i}kh_x} \\
&= R_j \left[1 + \lambda \left(e^{\mathrm{i}kh_x} - 2 + e^{-\mathrm{i}kh_x}\right)\right] \\
&= R_j \left[1 + \lambda \left(e^{\frac{\mathrm{i}kh_x}{2}} - e^{-\frac{\mathrm{i}kh_x}{2}}\right)^2\right] \\
&= R_j \left[1 + \lambda \left(2\mathrm{i}\sin\left(\frac{kh_x}{2}\right)\right)^2\right] \\
&= R_j \left[1 - 4\lambda \sin^2\left(\frac{kh_x}{2}\right)\right].
\end{aligned}$$

Therefore,

$$R_{j+1} = R_0 \left[1 - 4\lambda \sin^2\left(\frac{kh_x}{2}\right) \right]^{j+1}$$

and the sequence R_j is bounded if and only if $\left|1 - 4\lambda \sin^2\left(\frac{kh_x}{2}\right)\right| \leq 1$ and since $\lambda > 0$ we get

$$\left|1 - 4\lambda \sin^2\left(\frac{kh_x}{2}\right)\right| \leq 1 \Leftrightarrow 4\lambda \sin^2\left(\frac{kh_x}{2}\right) \leq 2 \Leftrightarrow \lambda \sin^2\left(\frac{kh_x}{2}\right) \leq \frac{1}{2}.$$

This last inequality shall hold for an arbitrary choice of k and then, in particular, the term $\sin^2\left(\frac{kh_x}{2}\right)$ can be equal to one. So, we get the stability condition $\lambda \leq \frac{1}{2}$.

Note that in the previous numerical example, the results plotted in Figure 10 were obtained for $\lambda = \frac{1}{2}$, which satisfies the stability condition, while the numerical results showing numerical instability in Figure 11 were obtained for $\lambda \approx 0.78 > \frac{1}{2}$ and the stability condition is not satisfied.

The stability condition of the explicit method is very restrictive in the sense that the step size in time must be very small compared to the step size in space. For instance, if we take $h_x = 0.001$, then the stability condition imply that we shall take $h_t \leq 5 \times 10^{-7}$.

We will consider other numerical schemes that avoid this constraint.

Implicit methods for the heat equation

In this section we will present a different finite difference scheme.

In this case, we will keep the second order finite difference for the approximation of the second order partial derivative in space but defined at the time instant t_{j+1},

$$
\begin{aligned}
\frac{\partial^2 u}{\partial x^2}(x_i, t_{j+1}) &\approx \partial^2_{x,h_x} u(x_i, t_{j+1}) \\
&= \frac{u(x_i + h_x, t_{j+1}) - 2u(x_i, t_{j+1}) + u(x_i - h_x, t_{j+1})}{h_x^2} \\
&= \frac{u(x_{i+1}, t_{j+1}) - 2u(x_i, t_{j+1}) + u(x_{i-1}, t_{j+1})}{h_x^2} \\
&= \frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{h_x^2}
\end{aligned}
$$

and we will use the backward finite difference in time (30),

$$\begin{aligned}\frac{\partial u}{\partial t}(x_i, t_{j+1}) &\approx \partial^+_{t,h_t} u(x_i, t_{j+1}) \\ &= \frac{u(x_i, t_j + h_t) - u(x_i, t_j)}{h_t} \\ &= \frac{u(x_i, t_{j+1}) - u(x_i, t_j)}{h_t} \\ &= \frac{u_{i,j+1} - u_{i,j}}{h_t}\end{aligned}$$

and we impose

$$\frac{u_{i,j+1} - u_{i,j}}{h_t} = \frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{h_x^2}$$

which implies

$$-\lambda u_{i+1,j+1} + (1+2\lambda)u_{i,j+1} - \lambda u_{i-1,j+1} = u_{i,j} \qquad (37)$$

which means that the values $u_{i+1,j+1}$, $u_{i,j+1}$ and $u_{i-1,j+1}$ are defined (implicitly) by equation (37), as illustrated in next figure and shall be determined by the solution of a linear system. This scheme is called implicit method.

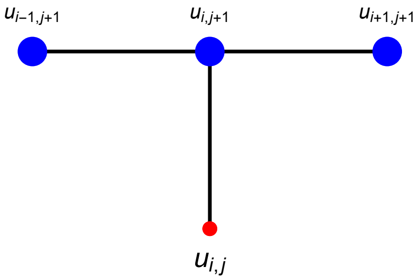

Figure: Stencil for the implicit method.

Taking into account that the values $u_{0,j+1}$ and $u_{N_x,j+1}$ are known by the boundary conditions of the problem we can write

$$\begin{bmatrix} 1+2\lambda & -\lambda & 0 & \dots & \dots & \dots & 0 \\ -\lambda & 1+2\lambda & -\lambda & 0 & \dots & \dots & 0 \\ 0 & -\lambda & 1+2\lambda & -\lambda & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & -\lambda & 1+2\lambda & -\lambda & 0 \\ 0 & \dots & \dots & 0 & -\lambda & 1+2\lambda & -\lambda \\ 0 & \dots & \dots & \dots & 0 & -\lambda & 1+2\lambda \end{bmatrix} \begin{bmatrix} u_{1,j+1} \\ u_{2,j+1} \\ u_{3,j+1} \\ \vdots \\ u_{N_x-3,j+1} \\ u_{N_x-2,j+1} \\ u_{N_x-1,j+1} \end{bmatrix} = \begin{bmatrix} u_{1,j} + \lambda u_{0,j+1} \\ u_{2,j} \\ u_{3,j} \\ \vdots \\ u_{N_x-3,j} \\ u_{N_x-2,j} \\ u_{N_x-1,j} + \lambda u_{N_x,j+1} \end{bmatrix}$$

Note that the matrix of the system is strictly diagonally dominant, because since $\lambda > 0$ we have $1 + 2\lambda > |\lambda| + |\lambda| = 2\lambda$, which implies invertibility of the matrix, by Gershgorin theorem. Moreover, it is a tridiagonal matrix and the system can be solved in a very efficient way by calculating a LU factorization of the matrix, and then solving two linear systems with triangular matrices.

The local truncation error is also of order $O(h_x^2) + O(h_t)$ which implies that the implicit method is also a method of first order in time and second order in space.

Concerning the stability of the scheme we perform Von Neumann stability analysis again. We consider $u_{i,j} = R_j e^{\mathrm{i}kx_i}$ and obtain

$$-\lambda \underbrace{u_{i+1,j+1}}_{R_{j+1}e^{\mathrm{i}k(x_i+h_x)}} +(1+2\lambda) \underbrace{u_{i,j+1}}_{R_{j+1}e^{\mathrm{i}kx_i}} -\lambda \underbrace{u_{i-1,j+1}}_{R_{j+1}e^{\mathrm{i}k(x_i-h_x)}} = \underbrace{u_{i,j}}_{R_j e^{\mathrm{i}kx_i}}$$

and dividing by $e^{\mathrm{i}kx_i}$ we obtain

$$-\lambda R_{j+1}e^{\mathrm{i}kh_x} + (1+2\lambda)R_{j+1} - \lambda R_{j+1}e^{-\mathrm{i}kh_x} = R_j,$$

then,

$$R_{j+1}\left[1 - \lambda\left(e^{\mathrm{i}kh_x} - 2 + e^{-\mathrm{i}kh_x}\right)\right] = R_j$$

and

$$R_{j+1} = \left(1 + 4\lambda\sin^2\left(\frac{kh_x}{2}\right)\right)^{-1} R_j.$$

In this case, we have

$$| \left(1 + 4\lambda \sin^2(kh_x)\right)^{-1} | \leq 1$$

and we conclude that the method is unconditionally stable, independently of the choices of h_x and h_t. This is an advantage of this method when compared with the explicit method.

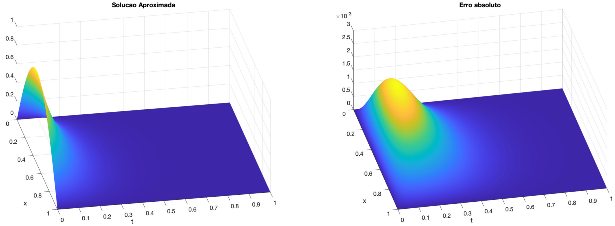

Figure: Approximate solution (left plot) and absolute error (right plot) obtained by the implicit method in the case $N_x = 25$ and $N_t = 800$ for which $\lambda \approx 0.78$. Note that this choice of parameters is prohibitive for the explicit method.

The implicit method, when compared with the explicit method, has the advantage of being unconditionally stable.

However it is just a first order method in time.

Next, we introduce another implicit method that not only is unconditionally stable but is also a second order method in time.

From Taylor expansion, assuming enough regularity of u, we get

$$u\left(x_i, t_{j+1}\right) = u\left(x_i, t_j + \frac{h_t}{2}\right) + \frac{h_t}{2}\frac{\partial u}{\partial t}\left(x_i, t_j + \frac{h_t}{2}\right) + \frac{1}{2}\left(\frac{h_t}{2}\right)^2\frac{\partial^2 u}{\partial t^2}\left(x_i, t_j + \frac{h_t}{2}\right) + O(h_t^3)$$

and

$$u\left(x_i, t_j\right) = u\left(x_i, t_j + \frac{h_t}{2}\right) - \frac{h_t}{2}\frac{\partial u}{\partial t}\left(x_i, t_j + \frac{h_t}{2}\right) + \frac{1}{2}\left(\frac{h_t}{2}\right)^2\frac{\partial^2 u}{\partial t^2}\left(x_i, t_j + \frac{h_t}{2}\right) + O(h_t^3),$$

from which we get

$$\frac{u\left(x_i, t_{j+1}\right) - u\left(x_i, t_j\right)}{h_t} = \frac{\partial u}{\partial t}\left(x_i, t_j + \frac{h_t}{2}\right) + O(h_t^2). \tag{38}$$

Also, from Taylor expansion, we obtain

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_j) = \frac{\partial^2 u}{\partial x^2}\left(x_i, t_j + \frac{h_t}{2}\right) - \frac{h_t}{2}\frac{\partial^3 u}{\partial x^2 \partial t}\left(x_i, t_j + \frac{h_t}{2}\right) + O(h_t^2)$$

and

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_{j+1}) = \frac{\partial^2 u}{\partial x^2}\left(x_i, t_j + \frac{h_t}{2}\right) + \frac{h_t}{2}\frac{\partial^3 u}{\partial x^2 \partial t}\left(x_i, t_j + \frac{h_t}{2}\right) + O(h_t^2).$$

Therefore,

$$\frac{\frac{\partial^2 u}{\partial x^2}(x_i, t_j) + \frac{\partial^2 u}{\partial x^2}(x_i, t_{j+1})}{2} = \frac{\partial^2 u}{\partial x^2}\left(x_i, t_j + \frac{h_t}{2}\right) + O(h_t^2). \quad (39)$$

Since we have

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_j) = \frac{u(x_{i+1}, t_j) - 2u(x_i, t_j) + u(x_{i-1}, t_j)}{h_x^2} + O(h_x^2)$$

and

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_{j+1}) = \frac{u(x_{i+1}, t_{j+1}) - 2u(x_i, t_{j+1}) + u(x_{i-1}, t_{j+1})}{h_x^2} + O(h_x^2),$$

from (38) and (39) we obtain

$$\begin{aligned}
&\frac{\partial u}{\partial t}\left(x_i, t_j + \frac{h_t}{2}\right) - \frac{\partial^2 u}{\partial x^2}\left(x_i, t_j + \frac{h_t}{2}\right) = \\
&\frac{u\left(x_i, t_{j+1}\right) - u\left(x_i, y_j\right)}{h_t} - \frac{u(x_{i+1}, t_j) - 2u(x_i, y_j) + u(x_{i-1}, t_j)}{2h_x^2} \\
&- \frac{u(x_{i+1}, t_{j+1}) - 2u(x_i, t_{j+1}) + u(x_{i-1}, t_{j+1})}{2h_x^2} + O(h_x^2) + O(h_t^2).
\end{aligned}$$

Thus, we obtain the second order scheme

$$\frac{u_{i,j+1} - u_{i,j}}{h_t} - \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{2h_x^2} - \frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{2h_x^2} = 0$$

that can be written as

$$-\frac{\lambda}{2}u_{i+1,j+1} + (1+\lambda)u_{i,j+1} - \frac{\lambda}{2}u_{i-1,j+1} = \frac{\lambda}{2}u_{i+1,j} + (1-\lambda)u_{i,j} + \frac{\lambda}{2}u_{i-1,j} \quad (40)$$

and the values $u_{i+1,j+1}$, $u_{i,j+1}$ and $u_{i-1,j+1}$ are obtained by solving a linear system involving the values $u_{i+1,j}$, $u_{i,j}$ and $u_{i-1,j}$, which are assumed to be already calculated.

$$
\begin{bmatrix}
1+\lambda & -\frac{\lambda}{2} & 0 & \dots & \dots & \dots & 0 \\
-\frac{\lambda}{2} & 1+\lambda & -\frac{\lambda}{2} & 0 & \dots & \dots & 0 \\
0 & -\frac{\lambda}{2} & 1+\lambda & -\frac{\lambda}{2} & 0 & \dots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \dots & 0 & -\frac{\lambda}{2} & 1+\lambda & -\frac{\lambda}{2} & 0 \\
0 & \dots & \dots & 0 & -\frac{\lambda}{2} & 1+\lambda & -\frac{\lambda}{2} \\
0 & \dots & \dots & \dots & 0 & -\frac{\lambda}{2} & 1+\lambda
\end{bmatrix}
\begin{bmatrix}
u_{1,j+1} \\ u_{2,j+1} \\ u_{3,j+1} \\ \vdots \\ u_{N_x-3,j+1} \\ u_{N_x-2,j+1} \\ u_{N_x-1,j+1}
\end{bmatrix}
=
$$

$$
\begin{bmatrix}
\frac{\lambda}{2} & 1-\lambda & \frac{\lambda}{2} & 0 & \dots & \dots & \dots & \dots & 0 \\
0 & \frac{\lambda}{2} & 1-\lambda & \frac{\lambda}{2} & 0 & \dots & \dots & \dots & 0 \\
0 & 0 & \frac{\lambda}{2} & 1-\lambda & \frac{\lambda}{2} & \dots & \dots & \dots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \dots & \dots & \vdots \\
0 & \dots & 0 & 0 & \frac{\lambda}{2} & 1-\lambda & \frac{\lambda}{2} & 0 & 0 \\
0 & \dots & \dots & \dots & 0 & \frac{\lambda}{2} & 1-\lambda & \frac{\lambda}{2} & 0 \\
0 & \dots & \dots & \dots & \dots & 0 & \frac{\lambda}{2} & 1-\lambda & \frac{\lambda}{2}
\end{bmatrix}
\begin{bmatrix}
u_{0,j} \\ u_{1,j} \\ u_{2,j} \\ \vdots \\ u_{N_x-2,j} \\ u_{N_x-1,j} \\ u_{N_x,j}
\end{bmatrix}
+
\begin{bmatrix}
\frac{\lambda}{2} u_{0,j+1} \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \frac{\lambda}{2} u_{N_x,j+1}
\end{bmatrix}.
$$

The stencil of the Crank-Nicolson method is

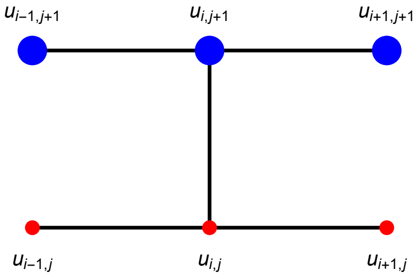

Figure: Stencil for the Crank-Nicolson method.

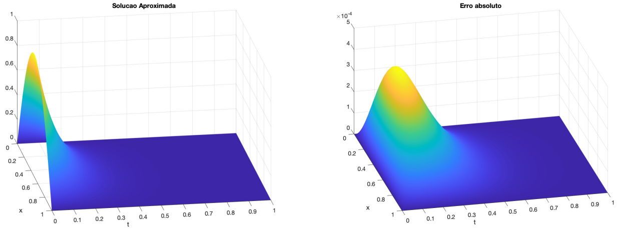

Figure: Approximate solution (left plot) and absolute error (right plot) obtained by the Crank-Nicolson method in the case $N_x = 25$ and $N_t = 800$.

For studying the stability of the scheme we perform Von Neumann stability analysis by considering $u_{i,j} = R_j e^{\mathrm{i}kx_i}$ and we obtain

$$-\frac{\lambda}{2}\underbrace{u_{i+1,j+1}}_{R_{j+1}e^{\mathrm{i}k(x_i+h_x)}}+(1+\lambda)\underbrace{u_{i,j+1}}_{R_{j+1}e^{\mathrm{i}kx_i}}-\frac{\lambda}{2}\underbrace{u_{i-1,j+1}}_{R_{j+1}e^{\mathrm{i}k(x_i-h_x)}}=\frac{\lambda}{2}\underbrace{u_{i+1,j}}_{R_j e^{\mathrm{i}k(x_i+h_x)}}+(1-\lambda)\underbrace{u_{i,j}}_{R_j e^{\mathrm{i}kx_i}}+\frac{\lambda}{2}\underbrace{u_{i-1,j}}_{R_j e^{\mathrm{i}k(x_i-h_x)}}$$

Dividing by $e^{\mathrm{i}kx_i}$ we get

$$R_{j+1}\left[1-\frac{\lambda}{2}\left(e^{\mathrm{i}kh_x}-2+e^{-\mathrm{i}kh_x}\right)\right]=R_j\left[1+\frac{\lambda}{2}\left(e^{\mathrm{i}kh_x}-2+e^{-\mathrm{i}kh_x}\right)\right]$$

that simplifies to

$$R_{j+1}\left[1+2\lambda\sin^2\left(\frac{kh_x}{2}\right)\right]=R_j\left[1-2\lambda\sin^2\left(\frac{kh_x}{2}\right)\right]$$

that is

$$R_{j+1}=\eta R_j,\ \text{where } \eta=\frac{1-2\lambda\sin^2\left(\frac{kh_x}{2}\right)}{1+2\lambda\sin^2\left(\frac{kh_x}{2}\right)}$$

and $|\eta|\leq 1$ and we conclude that the method is unconditionally stable, independently of the choices of h_x and h_t.