Comparison of different methods applied to the heat equation

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1 Problem

We consider the heat equation

Evolutionary Model Problem 1D: Heat Equation

Find u : $[0,T] \times [0,1] \to \mathbb{R}$ solution of

$$\frac{\partial u(t,x)}{\partial t} + \frac{\partial^2 u(t,x)}{\partial x^2} = 0, \quad (t,x) \in [0,T] \times [0,1] \tag{1}$$

$$u(t,0) = u(t,1) = 0, \quad \forall t > 0 \tag{2}$$

$$u(0,x) = u_0(x), \quad \forall 0 \le x \le 1 \tag{3}$$

with initial condition

$$u_0(x) = x(1-x) \tag{4}$$

We want to get numerical approximations to the solution applying the θ method with $\theta = 0$ (explicit method), $\theta = 1/2$ (Crank-Nicolson method) and $\theta = 1$ (implicit method). We choose as final time $T = 0.6$ and we consider a uniform mesh in the spatial variable x with mesh size Δx and in the temporal variable t with mesh size Δt.
Let us denote by Nx the number of nodes in x variable and by Nt the number of nodes in the t variable.
Let $(x_i)_0^{Nx}$ the regular discretization of the interval $[0,1]$ in Nx+1 points :

$$x_i = i.\Delta x, \quad \forall i \in [\![0, Nx]\!], \quad with \quad \Delta x = \frac{1}{Nx}$$

and $(t_n)_0^{Nt}$ the regular discretization of the interval $[0,T]$ in Nt+1 points :

$$t_n = n.\Delta t, \quad \forall n \in [\![0, Nt]\!], \quad with \quad \Delta t = \frac{T}{Nt}$$

Evolutionary Model Problem 1D: Heat Equation, formulation at the points of discretization

Find $u(t_n, x_i) \in \mathbb{R}$, $\forall n \in [\![0, Nt]\!]$, $\forall i \in [\![0, Nx]\!]$ such as

$$\frac{\partial u(t_n,x_i)}{\partial t} + \frac{\partial^2 u(t_n,x_i)}{\partial x^2} = 0, \quad \forall n \in]\!]0, Nt[\![, \quad \forall i \in]\!]0, Nx[\![\tag{5}$$

$$u(t_n,0) = u(t_n,1) = 0, \quad \forall n \in [\![0, Nt]\!] \tag{6}$$

$$u(0,x_i) = u_0(x_i), \quad \forall i \in [\![0, Nx]\!] \tag{7}$$

We now have to approach the partial derivative operators. For it we can use a scheme called θ-scheme.

2 The θ-scheme

Evolutionary Model Problem 1D: Heat Equation, θ-scheme

Find $u(t_n, x_i) \in \mathbb{R}$, $\forall n \in [\![0, Nt]\!]$, $\forall i \in [\![0, Nx]\!]$ such as

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} - [\ \theta \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{(\Delta x)^2} + (1-\theta)\frac{u_{i+1}^n - 2u_j^n + u_{i-1}^n}{(\Delta x)^2}\ ] = 0, \quad \forall n \in]\!]0, Nt[\![, \quad \forall i \in]\!]0, Nx[\![$$

$$u_0^n = u_{Nx}^n = 0, \quad \forall n \in [\![0, Nt]\!]$$
$$u_i^0 = x_i(1 - x_i), \quad \forall i \in [\![0, Nx]\!]$$

Remark :
The θ-schema is implicit for $\theta \neq 0$ and explicit for $\theta = 0$.

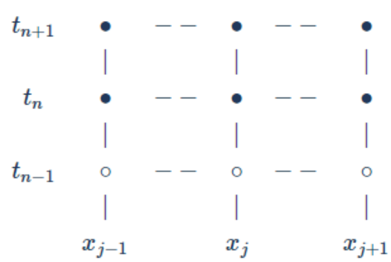

Figure 1: Stencil of the θ method

Now we have $\forall n \in]\!]0, Nt[\![$ *and* $\forall i \in]\!]0, Nx[\![$: $\frac{u_i^{n+1} - u_i^n}{\Delta t} - [\ \theta \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{(\Delta x)^2} + (1-\theta)\frac{u_{i+1}^n - 2u_j^n + u_{i-1}^n}{(\Delta x)^2}\ ] = 0$
So,

$$-\nu\theta u_{i+1}^{n+1} + (1 + 2\nu\theta)u_i^{n+1} - \nu\theta u_{i-1}^{n+1} = \nu(1-\theta)u_{i+1}^n + (1 - 2\nu(1-\theta))u_i^n + \nu(1-\theta)u_{i-1}^n, \quad with \quad \nu = \frac{\Delta t}{(\Delta x)^2}$$

and so the linear system is written :

$$AU_{n+1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -\nu\theta & 1+2\nu\theta & -\nu\theta & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & -\nu\theta & 1+2\nu\theta & -\nu\theta \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u_0^{n+1} \\ u_1^{n+1} \\ \vdots \\ \vdots \\ \vdots \\ u_{Nx-1}^{n+1} \\ u_{Nx}^{n+1} \end{pmatrix} =$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \nu(1-\theta) & 1-2\nu(1-\theta) & \nu(1-\theta) & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \nu(1-\theta) & 1-2\nu(1-\theta) & \nu(1-\theta) \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} u_0^n \\ u_1^n \\ \vdots \\ \vdots \\ \vdots \\ u_{Nx-1}^n \\ u_{Nx}^n \end{pmatrix} = BU_n$$

2.1 Consistency and order of the θ-scheme

To evaluate the order of the method we study the local truncation error of the schema defined by :

$$\epsilon_i^n = \frac{u(x_i,t_{n+1})-u(x_i,t_n)}{\Delta t} - \ [\ \theta\frac{u(x_{i+1},t_{n+1})-2u(x_i,t_{n+1})+u(x_{i-1},t_{n+1})}{(\Delta x)^2} + (1-\theta)\frac{u(x_{i+1},t_n)-2u(x_i,t_n)+u(x_{i-1},t_n)}{(\Delta x)^2}\ ]$$

According to the Taylor-Young formula, we have:

$$u(x_i,t_{n+1}) = u(x_i,t_n) + \Delta t\frac{\partial u}{\partial t}(x_i,t_n) + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2}(x_i,t_n) + O(\Delta t^3)$$

So,

$$\frac{u(x_i,t_{n+1})-u(x_i,t_n)}{\Delta t} = \frac{\partial u}{\partial t}(x_i,t_n) + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2}(x_i,t_n) + O(\Delta t^2)$$

And,

$$u(x_{i+1},t_n) = u(x_i,t_n) + \Delta x\frac{\partial u}{\partial x}(x_i,t_n) + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}(x_i,t_n) + \frac{\Delta x^3}{6}\frac{\partial^2 u}{\partial x^3}(x_i,t_n) + O(\Delta x^4)$$

$$u(x_{i-1},t_n) = u(x_i,t_n) - \Delta x\frac{\partial u}{\partial x}(x_i,t_n) + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}(x_i,t_n) - \frac{\Delta x^3}{6}\frac{\partial^2 u}{\partial x^3}(x_i,t_n) + O(\Delta x^4)$$

Therefore,

$$\theta(\frac{u(x_{i+1},t_n)-2u(x_i,t_n)+u(x_{i-1},t_n)}{(\Delta x)^2}\ ) = \ \theta\frac{\partial^2 u}{\partial x^2}(x_i,t_n) + O(\Delta x^2).$$

Then,

$$\begin{aligned}
u(x_{i+1},t_{n+1}) &= u(x_i,t_n) + \Delta x\frac{\partial u}{\partial x}(x_i,t_n) + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}(x_i,t_n) + \frac{\Delta x^3}{6}\frac{\partial^3 u}{\partial x^3}(x_i,t_n) + O(\Delta x^4)\\
&+ \Delta t\frac{\partial u}{\partial t}(x_i,t_n) + \Delta x\Delta t\frac{\partial^2 u}{\partial x\partial t}(x_i,t_n) + \frac{\Delta x^2\Delta t}{2}\frac{\partial^3 u}{\partial x^2\partial t}(x_i,t_n) + \frac{\Delta x^3\Delta t}{6}\frac{\partial^4 u}{\partial x^3\partial t}(x_i,t_n) + O(\Delta t\Delta x^4)\\
&+ \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2}(x_i,t_n) + \frac{\Delta t^2\Delta x}{2}\frac{\partial^3 u}{\partial t^2\partial x}(x_i,t_n) + \frac{\Delta t^2\Delta x^2}{2}\frac{\partial^4 u}{\partial t^2\partial x^2}(x_i,t_n) + \frac{\Delta t^2\Delta x^3}{6}\frac{\partial^5 u}{\partial t^2\partial x^3}(x_i,t_n) + O(\Delta t^2\Delta x^4)\\
&+ \frac{\Delta t^3}{6}\frac{\partial^3 u}{\partial t^3}(x_i,t_n) + \frac{\Delta t^3\Delta x}{6}\frac{\partial^4 u}{\partial t^3\partial x}(x_i,t_n) + \frac{\Delta t^3\Delta x^2}{12}\frac{\partial^5 u}{\partial t^3\partial x^2}(x_i,t_n) + \frac{\Delta t^3\Delta x^3}{36}\frac{\partial^6 u}{\partial t^3\partial x^3}(x_i,t_n) + O(\Delta t^3\Delta x^4)
\end{aligned}$$

And,

$$\begin{aligned}
u(x_{i-1},t_{n+1}) &= u(x_i,t_n) - \Delta x\frac{\partial u}{\partial x}(x_i,t_n) + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}(x_i,t_n) - \frac{\Delta x^3}{6}\frac{\partial^3 u}{\partial x^3}(x_i,t_n) + O(\Delta x^4)\\
&+ \Delta t\frac{\partial u}{\partial t}(x_i,t_n) - \Delta x\Delta t\frac{\partial^2 u}{\partial x\partial t}(x_i,t_n) + \frac{\Delta x^2\Delta t}{2}\frac{\partial^3 u}{\partial x^2\partial t}(x_i,t_n) - \frac{\Delta x^3\Delta t}{6}\frac{\partial^4 u}{\partial x^3\partial t}(x_i,t_n) + O(\Delta t\Delta x^4)\\
&+ \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2}(x_i,t_n) - \frac{\Delta t^2\Delta x}{2}\frac{\partial^3 u}{\partial t^2\partial x}(x_i,t_n) + \frac{\Delta t^2\Delta x^2}{2}\frac{\partial^4 u}{\partial t^2\partial x^2}(x_i,t_n) - \frac{\Delta t^2\Delta x^3}{6}\frac{\partial^5 u}{\partial t^2\partial x^3}(x_i,t_n) + O(\Delta t^2\Delta x^4)\\
&+ \frac{\Delta t^3}{6}\frac{\partial^3 u}{\partial t^3}(x_i,t_n) - \frac{\Delta t^3\Delta x}{6}\frac{\partial^4 u}{\partial t^3\partial x}(x_i,t_n) + \frac{\Delta t^3\Delta x^2}{12}\frac{\partial^5 u}{\partial t^3\partial x^2}(x_i,t_n) - \frac{\Delta t^3\Delta x^3}{36}\frac{\partial^6 u}{\partial t^3\partial x^3}(x_i,t_n) + O(\Delta t^3\Delta x^4)
\end{aligned}$$

And,

$$u(x_i,t_{n+1}) = u(x_i,t_n) + \Delta t\frac{\partial u}{\partial t}(x_i,t_n) + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2}(x_i,t_n) + \frac{\Delta t^3}{6}\frac{\partial^2 u}{\partial t^3}(x_i,t_n) + O(\Delta t^4)$$

Thus,

$$\begin{aligned}
\frac{u(x_{i+1},t_{n+1})-2u(x_i,t_{n+1})+u(x_{i-1},t_{n+1})}{(\Delta x)^2} &= \frac{\partial^2 u}{\partial x^2}(x_i,t_n) + \Delta t\frac{\partial^3 u}{\partial x^2\partial t}(x_i,t_n)\\
+ \Delta t^2\frac{\partial^4 u}{\partial x^2\partial t^2}(x_i,t_n) + \frac{\Delta t^3}{6}\frac{\partial^5 u}{\partial x^2\partial t^3}(x_i,t_n) &+ O(\Delta x^2) + O(\Delta t\Delta x^2) + O(\frac{\Delta t^4}{\Delta x^2}) + O(\Delta t^2\Delta x^2) + O(\Delta t^3\Delta x^2)\\
&= \frac{\partial^2 u}{\partial x^2}(x_i,t_n) + \Delta t\frac{\partial^3 u}{\partial x^2\partial t}(x_i,t_n) + O(\Delta t^2) + O(\Delta x^2)
\end{aligned}$$

Therefore,

$$\epsilon_i^n = \ \frac{\partial u}{\partial t}(x_i,t_n) + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2}(x_i,t_n) - \theta\frac{\partial^2 u}{\partial x^2}(x_i,t_n) - (1-\theta)(\frac{\partial^2 u}{\partial x^2}(x_i,t_n) + \Delta t\frac{\partial^3 u}{\partial x^2\partial t}(x_i,t_n)) + O(\Delta t^2) + O(\Delta x^2)$$

So,

$$\epsilon_i^n = \Delta t \; [\; \frac{1}{2}\frac{\partial^2 u}{\partial t^2}(x_i, t_n) - (1-\theta)\frac{\partial^3 u}{\partial x^2 \partial t}(x_i, t_n) \;] + O(\Delta t^2) + O(\Delta x^2)$$

Or,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad \Rightarrow \quad \frac{\partial^2 u}{\partial t^2} = \frac{\partial^3 u}{\partial x^2 \partial t}$$

Thus,

$$\epsilon_i^n = \Delta t \; (\theta - \frac{1}{2})\frac{\partial^3 u}{\partial x^2 \partial t}(x_i, t_n) \; + O(\Delta t^2) + O(\Delta x^2) \tag{8}$$

From where,

$$\begin{cases} \epsilon_i^n = O(\Delta t^2) + O(\Delta x^2), & \text{pour } \theta = \frac{1}{2} \\ \epsilon_i^n = O(\Delta t) + O(\Delta x^2), & \text{pour } \theta \neq \frac{1}{2} \end{cases}$$

Conclusion : The scheme is therefore consistent and of order 2 in time and space for $\theta = \frac{1}{2}$ and order 1 in time and 2 in space for $\theta \neq 0$.

2.2 Stability L^2 of the θ-scheme

Method of Von Neumann

- We consider a particular discrete solution in the form $u_i^n = A_n e^{ikx_i}$
- By injecting this solution into the scheme we find a formula for the amplification coefficient A.

Condition of stability of *Von Neumann* : the scheme is stable only if the amplification coefficient checks $|A| \leq 1$.
We have,

$$(1 + 2\nu\theta)u_i^{n+1} - \nu\theta(u_{i+1}^{n+1} + u_{i-1}^{n+1}) = (1 - 2\nu(1-\theta))u_i^n + \nu(1-\theta)(u_{i+1}^n + u_{i-1}^n)$$

We inject $u_i^n = A_n e^{ikx_i}$ in the scheme,

$$A_{n+1}e^{ikx_i}(1 + 2\nu\theta - 2\nu\theta\cos(k\Delta x)) = A_n e^{ikx_i}(1 - 2\nu(1-\theta) + 2\nu(1-\theta)\cos(k\Delta x))$$

So,

$$A_{n+1}(1 + 2\nu\theta(1 - \cos(k\Delta x)) = A_n(1 - 2\nu(1-\theta)(1 - \cos(k\Delta x))$$

Or, $\sin^2(x) = \frac{1-\cos(2x)}{2}$

$$\frac{A_{n+1}}{A_n} = \frac{1 - 4\nu(1-\theta)\sin^2(\frac{k\Delta x}{2})}{1 + 4\nu\theta\sin^2(\frac{k\Delta x}{2})}$$

For the scheme to be L^2-stable, the amplification factor $|\frac{A_{n+1}}{A_n}|$ must be less than 1 :

$$4\nu(1-\theta)\sin^2(\frac{k\Delta x}{2}) - 1 \leq 1 + 4\nu\theta\sin^2(\frac{k\Delta x}{2})$$

$$1 + 2\nu(2\theta - 1) \geq 0$$

If $\frac{1}{2} \leq \theta \leq 1$ we always have $1 + 2\nu(2\theta - 1) \geq 0$
If $0 \leq \theta < \frac{1}{2}$, it is necessary that

$$\nu \leq \frac{1}{2 - 4\theta}$$

2.3 Stability L^∞ of the θ-scheme

The scheme is L^∞-stable if :

$$\frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2(1-\theta)}$$

2.4 Convergence

The scheme is consistent and stable under certain conditions on θ and ν. According to Lax-Richtmyer's theorem, the scheme is convergent.

3 Separation of variables

We look for solutions of the form

$$u(t,x) = X(x).T(t)$$

where X and T are function which have to be determined. Substituting $u(t,x) = X(x).T(t)$ into the equation, we obtain :

$$X(x).T'(t) = X"(x).T(t)$$

from which, after dividing by $X(x).T(t)$, we get

$$\frac{T'(t)}{T(t)} = \frac{X"(x)}{X(x)}$$

The left side depends only on t whereas the right hand side depends only on x. Since they are equal, they must be equal to some constant $-\lambda$. Thus

$$T' + \lambda T = 0 \tag{9}$$

and

$$X" + \lambda X = 0 \tag{10}$$

The general solution of the first equation is given

$$T(t) = Ae^{-\lambda t} \quad \textit{for an arbitrary constant } A$$

The general solutions of the second equation are as follows.

1. $\lambda < 0$. Let $\lambda = -k^2 < 0$. Then the solution to (10) is

   $$X(x) = C_1 e^{kx} + C_2 e^{-kx}$$

   for integration constants C_1 and C_2 found from imposing BC's,

   $$X(0) = C_1 + C_2 = 0, \quad X(1) = C_1 e^k + C_2 e^{-k} = 0$$

   The first gives $C_1 = -C_2$, the second then gives $C_1(e^{2k} - 1) = 0$ and since $|k| > 0$ we have $A = B = u = 0$, which is the trivial solution. Thus we discard the case $\lambda < 0$.
2. $\lambda = 0$. Then $X(x) = C_1 x + C_2$ and the BCs imply $X(0) = C_2 = 0, X(1) = C_1 = 0$, so that $C_1 = C_2 = u = 0$. We discard this case also.
3. $\lambda > 0$. In this case,(2) is the simple harmonic equation whose solution is

   $$X(x) = C_1 cos(\sqrt{\lambda}x) + C_2 sin(\sqrt{\lambda}x)$$

The BCs imply $X(0) = C_1 = 0$ and $C_2 sin(\sqrt{\lambda}) = 0$. We don't want $C_2 = 0$, since that would give the trivial solution $u = 0$, so we must have

$$sin(\sqrt{\lambda}) = 0$$

Thus,

$$\sqrt{\lambda} = n\pi$$

Consequently,

$$\lambda_n = n^2\pi^2 \quad for \quad n = 1, 2, 3....$$

The problem (10) is called the eigenvalue problem, a nontrivial solution is called an eigenfunction associated with the eigenvalue λ. And the corresponding eigenfunction is given by

$$X_n(x) = \sin(n\pi x)$$

After substituting $\lambda_n = n^2\pi^2$ to (9), we get the family of solutions

$$T_n(t) = A_n e^{-n^2\pi^2 t}$$

Thus we have obtained the following sequence of solutions

$$u_n(t,x) = T_n(t)X_n(x) = A_n e^{-kn^2\pi^2 t} \sin(n\pi x)$$

We obtain more solutions by taking linear combinations of the u_n (recall the superposition principle)

$$u(t,x) = \sum_{i=1}^{N} u_n(t,x) = \sum_{i=1}^{N} A_n e^{-n^2\pi^2 t} \sin(n\pi x)$$

and then by passing to the limit $N \longrightarrow +\infty$

$$u(t,x) = \sum_{i=1}^{+\infty} A_n e^{-n^2\pi^2 t} \sin(n\pi x)$$

Finally, we consider the initial condition. At $t = 0$, we must have

$$u(0,x) = \sum_{i=1}^{+\infty} A_n \sin(n\pi x) = u_0(x) = f(x)$$

The coefficients, Bn can be computed as follows. Fix $m \in \mathbf{N}$. Multiplying the above equality by $\sin(m\pi x)$ and then integrating over $[0,1]$, we get

$$\int_0^1 f(x)\sin(m\pi x)\mathrm{d}x = \int_0^1 \sum_{i=1}^{+\infty} A_n \sin(n\pi x)\sin(m\pi x)\mathrm{d}x = \sum_{i=1}^{+\infty} \int_0^1 A_n \sin(n\pi x)\sin(m\pi x)\mathrm{d}x$$

Since

$$\int_0^1 A_n \sin(n\pi x)\sin(m\pi x)\mathrm{d}x = \begin{cases} 0 & if \quad n \neq m \\ \frac{1}{2} & if \quad n = m \end{cases}$$

We find that

$$A_n = 2\int_0^1 f(x)\sin(n\pi x)\mathrm{d}x$$

So,

$$A_n = 2\int_0^1 x(1-x)\sin(n\pi x)\mathrm{d}x = 2\left[\frac{1-2x}{n^2\pi^2}\cos(n\pi x) + \left(\frac{x^2-x}{n\pi} - \frac{2}{n^3\pi^3}\right)\cos(n\pi x)\right]_0^1$$

Thus,

$$A_n = \frac{4}{n^3\pi^3}\left(1-(-1)^n\right)$$

Thus, the solution of the PDE as,

$$u(t,x) = \frac{4}{\pi^3}\sum_{i=1}^{+\infty} \frac{(1-(-1)^n)}{n^3} e^{-n^2\pi^2 t}\sin(n\pi x) \tag{11}$$

4 Numerical solutions

4.1 Case where $\theta = 0$

For $\theta = 0$,

- The scheme is consistent and of order 1 in time and 2 in space.
- L^2-stable, if $\frac{\Delta t}{(\Delta x)^2} = \nu \leq \frac{1}{2}$
- L^∞-stable, if $\frac{\Delta t}{(\Delta x)^2} = \nu \leq \frac{1}{2}$

We represent the orders of the scheme : order 2 in space if $\nu = \frac{1}{2}$ and order 4 in space if $\nu = \frac{1}{6}$ (left) and CPU time required to compute the error (right).

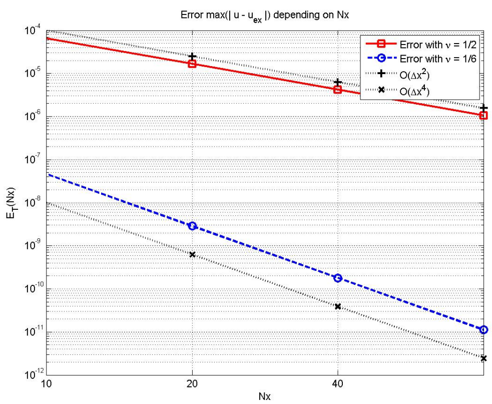

Figure 2: Orders for the explicit scheme, with $\nu = \frac{1}{2}$ and $\nu = \frac{1}{6}$

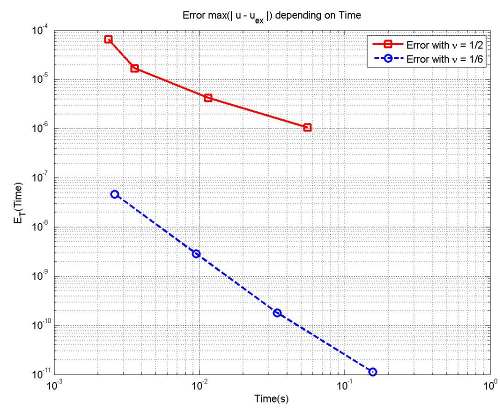

Figure 3: CPU time required to compute the error, with $\nu = \frac{1}{2}$ and $\nu = \frac{1}{6}$

Analysis of numerical results

- The scheme with $\nu = \frac{1}{2}$ is order 2 in space.
- The scheme is more accurate with $\nu = \frac{1}{6}$ than with $\nu = \frac{1}{2}$.
- The more we increase in precision, the more we increase the calculation time.
- The scheme with $\nu = \frac{1}{6}$ is order 4 in space (why?).

As can see in the figure 2 the scheme is order 4 in space with $\nu = \frac{1}{6}$, because the blue dotted ($O(\Delta x^4)$) curve and the orange curve have the same slope. Why ? ...
Let $\nu = \frac{1}{6}$ and $\theta = 0$, so

$$u_i^{n+1} = \frac{2}{3}u_i^n + \frac{1}{6}(u_{i+1}^n + u_{i-1}^n)$$

To evaluate the order of the method we study the local truncation error of the schema defined by :

$$\epsilon_i^n = u(x_i, t_{n+1}) - \frac{2}{3}u(x_i, t_n) - \frac{1}{6}(u(x_{i+1}, t_n) + u(x_{i-1}, t_n))$$

According to the Taylor-Young formula, we have:

$$u(x_i, t_{n+1}) = u(x_i, t_n) + \Delta t \frac{\partial u}{\partial t}(x_i, t_n) + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2}(x_i, t_n) + O(\Delta t^3)$$

And,

$$u(x_{i+1}, t_n) = u(x_i, t_n) + \Delta x \frac{\partial u}{\partial x}(x_i, t_n) + \frac{\Delta x^2}{2!}\frac{\partial^2 u}{\partial x^2}(x_i, t_n) + \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3}(x_i, t_n) + O(\Delta x^4)$$

$$u(x_{i-1}, t_n) = u(x_i, t_n) - \Delta x \frac{\partial u}{\partial x}(x_i, t_n) + \frac{\Delta x^2}{2!}\frac{\partial^2 u}{\partial x^2}(x_i, t_n) - \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3}(x_i, t_n) + O(\Delta x^4)$$

Therefore,

$$\epsilon_i^n = \frac{1}{3}u(x_i,t_n) + \Delta t\frac{\partial u}{\partial t}(x_i,t_n) + O(\Delta t^2) - \frac{1}{6}(2u(x_i,t_n) + \Delta x^2\frac{\partial^2 u}{\partial x^2}(x_i,t_n)) + O(\Delta x^4)$$

Thus,

$$\epsilon_i^n = \Delta t\frac{\partial u}{\partial t}(x_i,t_n) - \frac{1}{6}\Delta x^2\frac{\partial^2 u}{\partial x^2}(x_i,t_n) + O(\Delta x^4) + O(\Delta t^2)$$

Or we know that,

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

Hence,

$$\epsilon_i^n = \frac{\partial^2 u}{\partial x^2}(x_i,t_n)(\Delta t - \frac{1}{6}\Delta x^2) + O(\Delta x^4) + O(\Delta t^2)$$

Or, $\nu = \frac{1}{6} \quad \Rightarrow \quad \Delta t = \frac{1}{6}\Delta x^2$ So,

$$\epsilon_i^n = O(\Delta x^4) + O(\Delta t^2)$$

So the scheme is of order 4 in space and 2 in time, if $\nu = \frac{1}{6}$.
Instability, for $\theta = 0$ and $\nu = 0.535 > \frac{1}{2}$,

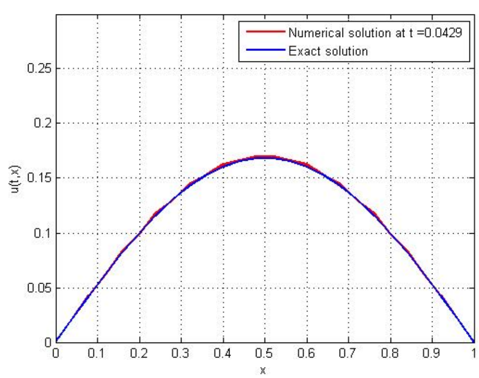

Figure 4: 1D heat equation with exact solution (in blue) at t = 0.043. Beginning of the phenomenon of instability

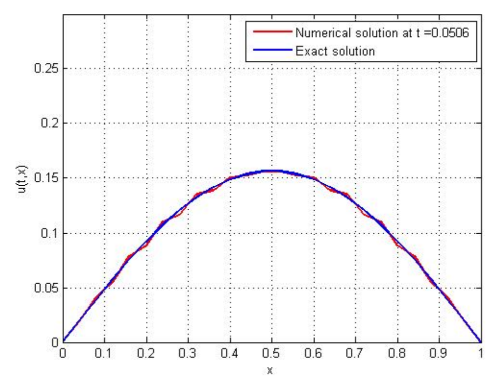

Figure 5: 1D heat equation with exact solution (in blue) at t = 0.051. Beginning of the phenomenon of instability

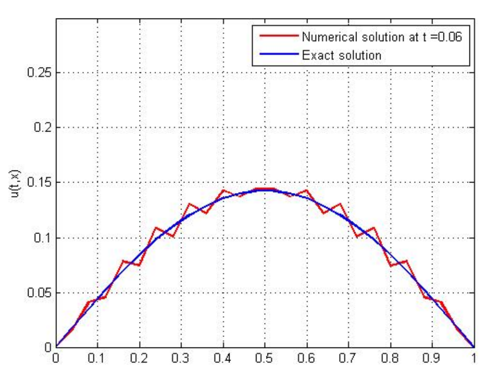

Figure 6: 1D heat equation with exact solution (in blue) at t = 0.060. Beginning of the phenomenon of instability

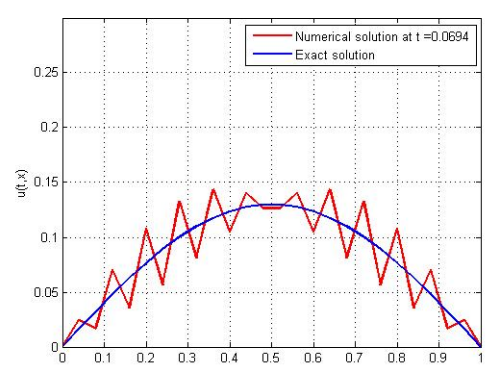

Figure 7: 1D heat equation with exact solution (in blue) at t = 0.069. Beginning of the phenomenon of instability

4.2 Case where $\theta = \frac{1}{2}$

For $\theta = \frac{1}{2}$,

- The scheme is consistent and of order 2 in space and 2 in time.
- L^2-stable
- L^∞-stable, if $\frac{\Delta t}{(\Delta x)^2} = \nu \leq 1$

We represent the orders of the scheme : order 2 in space (left) and CPU time required to compute the error (right).

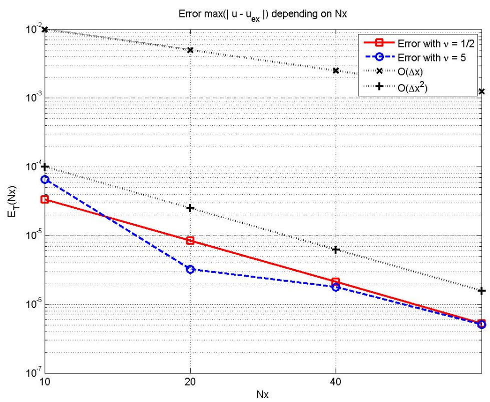

Figure 8: Orders for the Crank-Nicolson scheme in space, with $\nu = \frac{1}{2}$ and $\nu = 5$

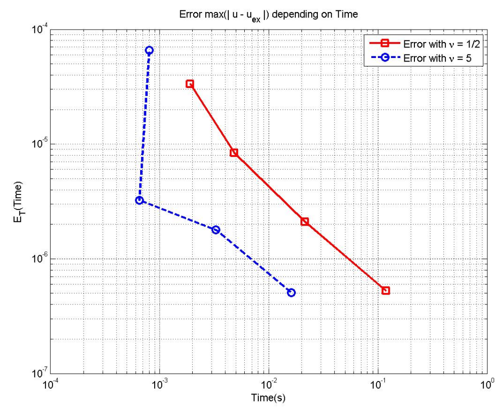

Figure 9: CPU time required to compute the error, with $\nu = \frac{1}{2}$ and $\nu = 5$

Nx	Nt	Crank-Nicolson, $\nu = \frac{1}{2}$	CPU	Nt	Crank-Nicolson, $\nu = 5$	CPU
10	120	3.35207766e-05	0.0015	12	6.59457365e-05	0.0011
20	480	8.41138182e-06	0.0051	48	3.24557177e-06	0.0009
40	1920	2.10464911e-06	0.0234	192	1.78278864e-06	0.0021
80	7680	5.26272705e-07	0.1128	768	5.06177310e-07	0.0114

Analysis of numerical results

- The figure 8 shows the Crank–Nicolson scheme, but here $\nu = 5$ is much larger. The numerical solution has oscillatory behaviour for small t.
- .For Nx larger than this the two graphs with $\nu = \frac{1}{2}$ and $\nu = 5$ are close together, illustrating the fact that the leading term in the truncation error in (8) is independent of ν.

4.3 Case where $\theta = 1$

For $\theta = 1$,

- The scheme is consistent and of order 2 in space and 1 in time.
- L^2-stable
- L^∞-stable, if $\frac{\Delta t}{(\Delta x)^2} = \nu \leq 1$

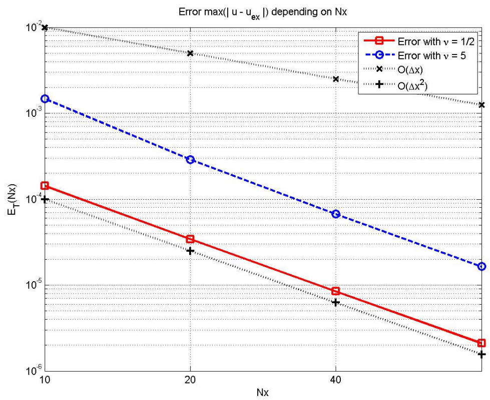

Figure 10: Orders for the implicit scheme, with $\nu = 5$ and $\nu = \frac{1}{2}$

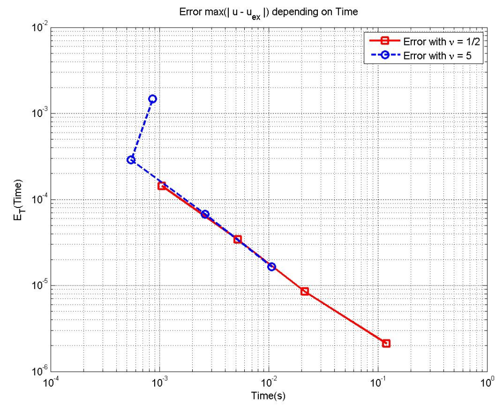

Figure 11: CPU time required to compute the error, with $\nu = \frac{1}{2}$ and $\nu = 5$

Nx	Nt	implicit scheme, $\nu = \frac{1}{2}$	CPU	Nt	implicit scheme, $\nu = 5$	CPU
10	120	1.42800859e-04	0.0011	12	1.47293997e-03	0.0012
20	480	3.41848185e-05	0.0044	48	2.88452161e-04	0.0006
40	1920	8.45221179e-06	0.0217	192	6.69774977e-05	0.0023
80	7680	2.10719036e-06	0.1232	768	1.64227881e-05	0.0119

Analysis of numerical results

- As we can see on both curves the scheme is order 2 in space for $\nu = \frac{1}{2}$ and $\nu = 5$.
- The scheme is more accurate with $\nu = \frac{1}{6}$ than with $\nu = 5$.

4.4 Comparison between the 3 cases

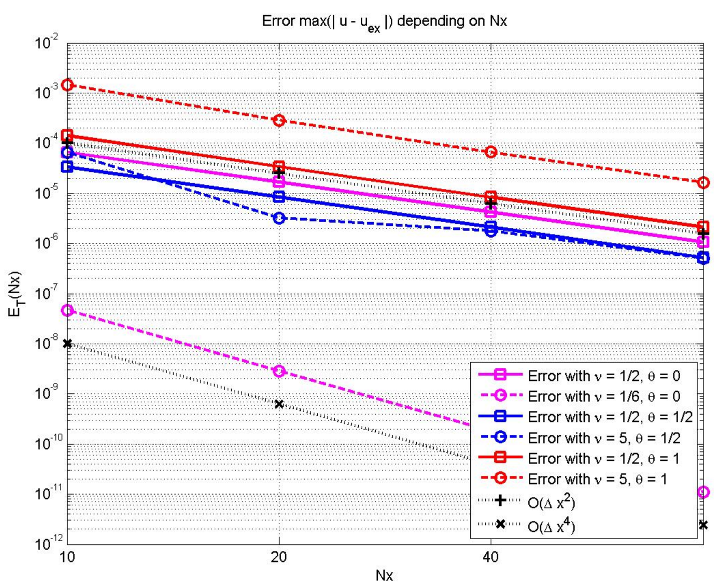

Figure 12: Orders for different scheme

These graphs do not give a true picture of the relative effectiveness of the various $\theta - methods$ because they do not take account of the work involved in each calculation. So in the graphs in Fig. 13 the same results are plotted against a measure of the computational effort involved in each calculation.

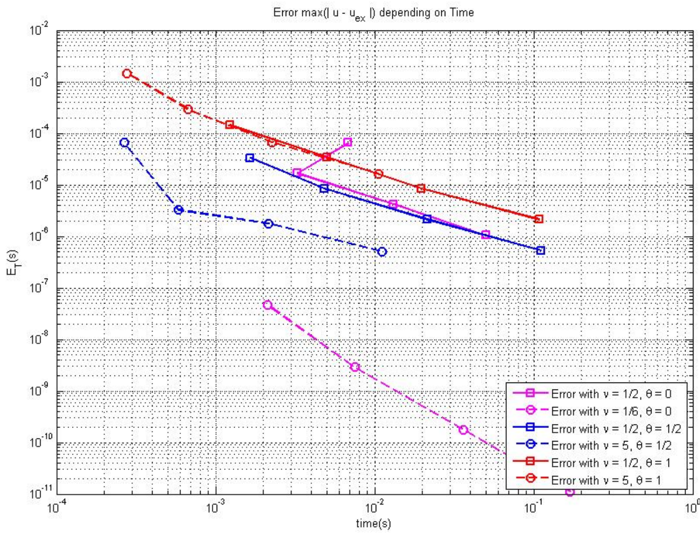

Figure 13: CPU time required to compute the error

5 Conclusion

- The explicit method require less effort than the implicit methods.
- These graphs show that, for this problem, the Crank–Nicolson method with $\nu = \frac{1}{2}$ is the most efficient of those tested.

- In the case $\theta = \frac{1}{2}$ and $\nu = 5 > 1$ the maximum principle does not hold, and we see that at the first time level the numerical solution becomes negative. This would normally be regarded as unacceptable.
- The exact solution of the problem will have only a single maximum for all t.
- These results correspond to a rather extreme case, and the unacceptable behaviour only persists for a few time steps, thereafter the solution becomes very smooth in each case.

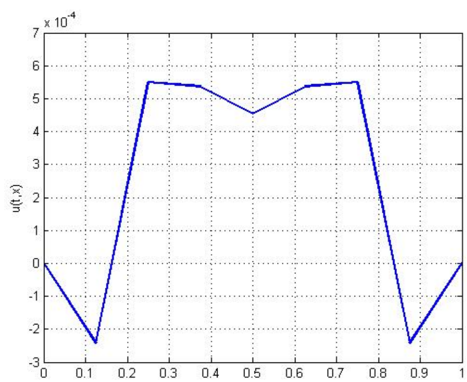

Figure 14: A maximum principle and convergence $\nu = 5 > 1$