Fys4150
Project 5

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https://github.com/kaaja/fys4150

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Note to instructurs reagarding Github repository

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1.1 Derivation of schemes with truncation errors

All the schemes will be derived from Taylor series expansions, and the truncation error will be related to the remainder in the Taylor-series expansions. This remainded is the error we get when truncating the series by leaving out the remainder.

1.1.1 Forward Euler

For the time derivative, we expand $u(x, t + \Delta t)$ around t

$$u(x, t + \Delta t) = u(x, t) + u_t(x, t)\Delta t + \mathcal{O}(\Delta t^2) \tag{1a}$$

$$\rightarrow u_t(x, t) = \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} + \mathcal{O}(\Delta t) \tag{1b}$$

The space derivative, which is a 2nd derivative, we derive by combining two Taylor series'

$$u(x + \Delta x, t) = u(x, t) + u_x(x, t)\Delta x + \frac{u_{xx}(x, t)\Delta x^2}{2} + \frac{u_{xxx}(x, t)\Delta x^3}{6} + \mathcal{O}(\Delta x^4) \tag{2a}$$

$$u(x - \Delta x, t) = u(x, t) - u_x(x, t)\Delta x + \frac{u_{xx}(x, t)\Delta x^2}{2} - \frac{u_{xxx}(x, t)\Delta x^3}{6} + \mathcal{O}(\Delta x^4) \tag{2b}$$

Now we add (2a) and (2b) and solve for $u_{xx}(x,t)$

$$\begin{aligned}
\Big(u(x+\Delta x,t)+u(x-\Delta x,t)\Big) &= \Big(u(x,t)+u(x,t)\Big)\\
&+\Big(u_x(x,t)\Delta x+(-u_x(x,t)\Delta x)\Big)\\
&+\Big(\frac{u_{xx}(x,t)\Delta x^2}{2}+\frac{u_{xx}(x,t)\Delta x^2}{2}\Big) \qquad (3a)\\
&+\Big(\frac{u_{xxx}(x,t)\Delta x^3}{6}+(-\frac{u_{xxx}(x,t)\Delta x^3}{6})\Big)\\
&+\Big(\mathcal{O}(\Delta x^4)+\mathcal{O}(\Delta x^4)\Big)\\
&= 2u(x,t)+u_{xx}(x,t)\Delta x^2+\mathcal{O}(\Delta x^4) \qquad (3b)\\
\rightarrow u_{xx}(x,t) &= \frac{u(x-\Delta x,t)-2u(x,t)+u(x+\Delta x,t)}{\Delta x^2}+\mathcal{O}(\Delta x^2) \qquad (3c)
\end{aligned}$$

Combining (1b) and (3c) we get the Forward Euler scheme

$$u_t(x,t)=u_{xx}(x,t) \tag{4a}$$

$$\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t}+\mathcal{O}(\Delta t)=\frac{u(x-\Delta x,t)-2u(x,t)+u(x+\Delta x,t)}{\Delta x^2}+\mathcal{O}(\Delta x^2) \tag{4b}$$

From (4b) we see that the scheme has a truncation error that goes like $\mathcal{O}(\Delta t)$ in time and $\mathcal{O}(\Delta x^2)$ in space.

We will now analyze the stability of the Forward Euler scheme (4b) by applying Neuman stability analyzis. From the analytical solution of the problem, we know that the particular solutions are on the form $u=e^{-(k\pi)^2t}e^{ik\pi x}$, where k is an integer greater than one. We observe that the solutions are stable in t, meaning that the solutions do not blow up as t increaes. Based on the analytical particular solution, we make the numerical ansatz

$$u=a_k^n e^{ik\pi x_j} \tag{5}$$

For the numerical ansatz (5) to reproduce the characteristics of the analytical particular solution, with stability in t, we observe that $|a_k^n|<1$ in necessary. We now plug in the ansatz (5) into the (4b) and derive an equation for $|a_k^n|$:

$$\begin{aligned}
\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t} &= \frac{u(x-\Delta x,t)-2u(x,t)+u(x+\Delta x,t)}{\Delta x^2} \qquad (6a)\\
\frac{a_k^{n+1}e^{ik\pi(j+1)\Delta x}-a_k^n e^{ik\pi j\Delta x}}{\Delta t} &= \frac{a_k^n e^{ik\pi(j-1)\Delta x}-2a_k^n e^{ik\pi j\Delta x}+a_k^n e^{ik\pi(j+1)\Delta x}}{\Delta x^2} \qquad (6b)\\
a_k^n e^{ik\pi j\Delta x}\ \frac{a_k-1}{\Delta t} &= a_k^n e^{ik\pi j\Delta x}\ \frac{e^{-ik\pi\Delta x}-2+e^{ik\pi\Delta x}}{\Delta x^2} \qquad (6c)\\
\frac{a_k-1}{\Delta t} &= \frac{e^{-ik\pi\Delta x}-2+e^{ik\pi\Delta x}}{\Delta x^2} \qquad (6d)\\
a_k &= 1+\frac{\Delta t}{\Delta x^2}(e^{-ik\pi\Delta x}-2+e^{ik\pi\Delta x}) \qquad (6e)\\
&= 1+\frac{\Delta t}{\Delta x^2}\Big(2\cos(k\pi\Delta x)-2\Big) \qquad (6f)\\
&= 1+2\frac{\Delta t}{\Delta x^2}\Big(\cos(k\pi\Delta x)-1\Big) \qquad (6g)\\
&= 1+2\frac{\Delta t}{\Delta x^2}\Big(-2\sin^2(\frac{k\pi\Delta x}{2})\Big) \qquad (6h)\\
&= 1-4\frac{\Delta t}{\Delta x^2}\sin^2(\frac{k\pi\Delta x}{2}) \qquad (6i)\\
|a_k| &= |1-4\frac{\Delta t}{\Delta x^2}\sin^2(\frac{k\pi\Delta x}{2})| \qquad (6j)
\end{aligned}$$

From (6j) we get

$$|a_k| < 1 \text{ if } ||1 - 4\frac{\Delta t}{\Delta x^2}\sin^2(\frac{k\pi\Delta x}{2})|| < 1 \tag{7a}$$
$$\rightarrow |1 - 4\frac{\Delta t}{\Delta x^2}| < 1 \rightarrow |a_k| < 1 \text{ (Since } \sin^2(k\pi\Delta x/2)_{max} = 1) \tag{7b}$$
$$\rightarrow 1 - 4\frac{\Delta t}{\Delta x^2} > -1 \tag{7c}$$
$$\rightarrow \frac{\Delta t}{\Delta x^2} < \frac{1}{2} \tag{7d}$$

(7d) gives that the Forward Euler scheme is conditionally stable, and the condition that ensures stability.

1.2 Backward Euler

Here we will do the same as we did for Forward Euler above: Derive the scheme, including truncation errors, and analyze stability.

The only change compared to Forward Euler, is the time discretization, which now becomes

$$u(x, t - \Delta t) = u(x, t) + u_t(x, t)\Delta t - \mathcal{O}(\Delta t^2) \tag{8a}$$
$$\rightarrow u_t(x, t) = \frac{u(x, t) - u(x, t - \Delta t)}{\Delta t} + \mathcal{O}(\Delta t) \tag{8b}$$

The space discretization is the same as for Forward Euler, (3c). Combining the space discretization (3c) and (8b) gives

$$\frac{u(x, t) - u(x, t - \Delta t)}{\Delta t} + \mathcal{O}(\Delta t) = \frac{u(x - \Delta x, t) - 2u(x, t) + u(x + \Delta x, t)}{\Delta x^2} + \mathcal{O}(\Delta x^2) \tag{9a}$$

We note that the truncation errors have the same asymptoptic behavior as for the Forward Euler scheme.

Now lets check the stability of the Backward Euler scheme. We apply the same method as we did for Forward Euler, and insert the ansatz (5) into (9a) to get

$$\frac{u(x, t) - u(x, t - \Delta t)}{\Delta t} = \frac{u(x - \Delta x, t) - 2u(x, t) + u(x + \Delta x, t)}{\Delta x^2} \tag{10a}$$
$$\frac{a_k^n e^{ik\pi j\Delta x} - a_k^{n-1} e^{ik\pi j\Delta x}}{\Delta t} = \frac{a_k^n e^{ik\pi(j-1)\Delta x} - 2a_k^n e^{ik\pi j\Delta x} + a_k^n e^{ik\pi(1+j)\Delta x}}{\Delta x^2} \tag{10b}$$
$$a_k^n e^{ik\pi j\Delta x}\ \frac{1 - a_k^{-1}}{\Delta t} = a_k^n e^{ik\pi j\Delta x}\ \frac{e^{-ik\pi\Delta x} - 2 + e^{ik\pi\Delta x}}{\Delta x^2} \tag{10c}$$
$$\frac{1 - a_k^{-1}}{\Delta t} = \frac{e^{-ik\pi\Delta x} - 2 + e^{ik\pi\Delta x}}{\Delta x^2} \tag{10d}$$
$$a_k^{-1} = 1 - \frac{\Delta t}{\Delta x^2}(e^{-ik\pi\Delta x} - 2 + e^{ik\pi\Delta x}) \tag{10e}$$
$$a_k = \frac{1}{1 - \frac{\Delta t}{\Delta x^2}(e^{-ik\pi\Delta x} - 2 + e^{ik\pi\Delta x})} \tag{10f}$$
$$\stackrel{(6)}{=} \frac{1}{1 + 4\frac{\Delta t}{\Delta x^2}\sin^2(\frac{k\pi\Delta x}{2})} \tag{10g}$$
$$|a_k| = \left|\frac{1}{1 + 4\frac{\Delta t}{\Delta x^2}\sin^2(\frac{k\pi\Delta x}{2})}\right| < 1. \tag{10h}$$
$$\tag{10i}$$

From (10h) we see that, in contrast to the Forward Euler scheme, the Backward Euler scheme is unconditionally stable.

(9a) reveals another difference between the Backward Euler scheme and the Forward Euler scheme: (9a) is implicit in $u(x,t)$, meaning that we cannot solve (9a) directly for $u(x,t)$, as we did in the Forward Euler scheme. However, we can find $u(x,t)$ from (9a) by recognizing that (9a) can be rewritten as a linear system:

$$\frac{u(x,t)-u(x,t-\Delta t)}{\Delta t} = \frac{u(x-\Delta x,t)-2u(x,t)+u(x+\Delta x,t)}{\Delta x^2} \tag{11a}$$

$$\frac{u_i^n - u_i^{n-1}}{\Delta t} = \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2} \tag{11b}$$

$$\frac{\Delta x^2}{\Delta t}(u_i^n - u_i^{n-1}) = u_{i-1}^n - 2u_i^n + u_{i+1}^n \tag{11c}$$

$$-\Big(u_{i-1}^n - (2+\frac{\Delta x^2}{\Delta t})u_i^n + u_{i+1}^n\Big) = \frac{\Delta x^2}{\Delta t}u_i^{n-1} \tag{11d}$$

$$\Big(-u_{i-1}^n + (2+\frac{\Delta x^2}{\Delta t})u_i^n - u_{i+1}^n\Big) = \frac{\Delta x^2}{\Delta t}u_i^{n-1} \tag{11e}$$

$$\underbrace{\begin{bmatrix} 2+\frac{\Delta x^2}{\Delta t} & -1 & \cdots & 0 \\ -1 & 2+\frac{\Delta x^2}{\Delta t} & -1 & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & -1 & 2+\frac{\Delta x^2}{\Delta t} \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} u_1^n \\ u_2^n \\ \vdots \\ u_N^n \end{bmatrix}}_{\mathbf{U}} = \underbrace{\frac{\Delta x^2}{\Delta t}\begin{bmatrix} u_0^{n-1} \\ u_1^{n-1} \\ \vdots \\ u_N^{n-1} \end{bmatrix}}_{\tilde{\mathbf{b}}} \tag{11f}$$

We see from (11f) that solving Backward Euler corresponds to solving a linear system $AU = \tilde{b}$, where A is a trdiagonal matrix.

1.3 Crank-Nicolson

Here we Taylor expand $u(x+\Delta x, t+\Delta t)$ and $u(x-\Delta x, t+\Delta t)$ around $t' = t + \Delta t/2$ to get

$$\begin{aligned} u(x+\Delta x,t+\Delta t) &= u(x,t') + \frac{\partial u(x,t')}{\partial x}\Delta x + \frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{2} + \frac{\partial^2 u(x,t')}{2\partial x^2}\Delta x^2 + \frac{\partial^2 u(x,t')}{2\partial t^2}\frac{\Delta t^2}{4} \\ &\quad + \frac{\partial^2 u(x,t')}{\partial x \partial t}\frac{\Delta t}{2}\Delta x + \mathcal{O}(\Delta t^3) \end{aligned} \tag{12a}$$

$$\begin{aligned} u(x-\Delta x,t+\Delta t) &= u(x,t') - \frac{\partial u(x,t')}{\partial x}\Delta x + \frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{2} + \frac{\partial^2 u(x,t')}{2\partial x^2}\Delta x^2 + \frac{\partial^2 u(x,t')}{2\partial t^2}\frac{\Delta t^2}{4} \\ &\quad - \frac{\partial^2 u(x,t')}{\partial x \partial t}\frac{\Delta t}{2}\Delta x + \mathcal{O}(\Delta t^3) \end{aligned} \tag{12b}$$

$$\begin{aligned} u(x+\Delta x,t) &= u(x,t') + \frac{\partial u(x,t')}{\partial x}\Delta x - \frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{2} + \frac{\partial^2 u(x,t')}{2\partial x^2}\Delta x^2 + \frac{\partial^2 u(x,t')}{2\partial t^2}\frac{\Delta t^2}{4} \\ &\quad - \frac{\partial^2 u(x,t')}{\partial x \partial t}\frac{\Delta t}{2}\Delta x + \mathcal{O}(\Delta t^3) \end{aligned} \tag{12c}$$

$$\begin{aligned} u(x-\Delta x,t) &= u(x,t') - \frac{\partial u(x,t')}{\partial x}\Delta x - \frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{2} + \frac{\partial^2 u(x,t')}{2\partial x^2}\Delta x^2 + \frac{\partial^2 u(x,t')}{2\partial t^2}\frac{\Delta t^2}{4} \\ &\quad + \frac{\partial^2 u(x,t')}{\partial x \partial t}\frac{\Delta t}{2}\Delta x + \mathcal{O}(\Delta t^3) \end{aligned} \tag{12d}$$

$$u(x,t+\Delta t) = u(x,t') + \frac{\partial u(x,t')}{\partial t}\frac{\Delta_t}{2} + \frac{\partial^2 u(x,t')}{2\partial t^2}\Delta t^2 + \mathcal{O}(\Delta t^3) \tag{12e}$$

$$u(x,t) = u(x,t') - \frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{2} + \frac{\partial^2 u(x,t')}{2\partial t^2}\Delta t^2 + \mathcal{O}(\Delta t^3) \tag{12f}$$

The above formulae are taken from Hjorth-Jensen's slides [2].

Combining (12e) and (12f) gives the time derivative

$$\begin{aligned}
\Big(u(x,t+\Delta t)-u(x,t)\Big) &= \Big(u(x,t')-u(x,t')\Big)+\Big(\frac{\partial u(x,t')}{\partial t}\frac{\Delta_t}{2}-(-\frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{2})\Big) \\
&\quad +\Big(\frac{\partial^2 u(x,t')}{2\partial t^2}\Delta t^2-\frac{\partial^2 u(x,t')}{2\partial t^2}\Delta t^2\Big)+\Big(\mathcal{O}(\Delta t^3)-\mathcal{O}(\Delta t^3)\Big) \qquad (13a)\\
u(x,t+\Delta t)-u(x,t) &= \frac{\partial u(x,t')}{\partial t}\Delta t+\mathcal{O}(\Delta t^3) \qquad (13b)\\
\frac{\partial u(x,t')}{\partial t} &= \frac{u(x,t+\Delta t)-u(x,t)}{\Delta t}+\mathcal{O}(\Delta t^2) \qquad (13c)
\end{aligned}$$

Now for the spacial derivative. First we solve (12a) and (12b) for $u_{xx}(x,t')$

$$\begin{aligned}
u(x+\Delta x,t+\Delta t)+u(x-\Delta x,t+\Delta t) &= \Big(u(x,t')+u(x,t')\Big)+\Big(\frac{\partial u(x,t')}{\partial x}\Delta x-\frac{\partial u(x,t')}{\partial x}\Delta x\Big) \\
&\quad +\Big(\frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{2}+\frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{2}\Big)+\Big(\frac{\partial^2 u(x,t')}{2\partial x^2}\Delta x^2+\frac{\partial^2 u(x,t')}{2\partial x^2}\Delta x^2\Big) \\
&\quad +\Big(\frac{\partial^2 u(x,t')}{2\partial t^2}\frac{\Delta t^2}{4}+\frac{\partial^2 u(x,t')}{2\partial t^2}\frac{\Delta t^2}{4}\Big)+\Big(\frac{\partial^2 u(x,t')}{\partial x\partial t}\frac{\Delta t}{2}\Delta x-\frac{\partial^2 u(x,t')}{\partial x\partial t}\frac{\Delta t}{2}\Delta x\Big) \\
&\quad +\Big(\mathcal{O}(\Delta t^3)+\mathcal{O}(\Delta t^3)\Big)+\mathcal{O}(\Delta x^4) \qquad (14a)\\
&= 2u(x,t')+\frac{\partial u(x,t')}{\partial t}\Delta t+\frac{\partial^2 u(x,t')}{\partial x^2}\Delta x^2+\frac{\partial^2 u(x,t')}{2\partial t^2}\frac{\Delta t^2}{2}+\mathcal{O}(\Delta t^3)+\mathcal{O}(\Delta x^4) \qquad (14b)\\
&= 2u(x,t')+\frac{\partial u(x,t')}{\partial t}\Delta t+\frac{\partial^2 u(x,t')}{\partial x^2}\Delta x^2+\mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta x^4) \qquad (14c)\\
\frac{\partial^2 u(x,t')}{\partial x^2}\Delta x^2 &= u(x+\Delta x,t+\Delta t)+u(x-\Delta x,t+\Delta t)-2u(x,t') \\
&\quad +\frac{\partial u(x,t')}{\partial t}\Delta t+\mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta x^4) \qquad (14d)\\
\frac{\partial^2 u(x,t')}{\partial x^2} &= \frac{u(x-\Delta x,t+\Delta t)-2u(x,t')+u(x+\Delta x,t+\Delta t)}{\Delta x^2} \\
&\quad +\frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{\Delta x^2}+\mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta x^2) \qquad (14e)
\end{aligned}$$

Note that in (14e) we added $\mathcal{O}(\Delta x^4)$, since $\mathcal{O}(\Delta x^3)$ cancells out in the addition. Also note that the Δx^3-term was not originally included in (12a) and (12b), but these would have been of equal magnitude with opposite sign, so when adding the equaions we would have been left with $\mathcal{O}(\Delta x^4)$.

Doing the same as in (14e) for (12c) and (12d) we obtain

$$\begin{aligned}
\frac{\partial^2 u(x,t')}{\partial x^2} &= \frac{u(x-\Delta x,t)-2u(x,t')+u(x+\Delta x,t)}{\Delta x^2} \\
&\quad -\frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{\Delta x^2}+\mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta x^2) \qquad (15a)
\end{aligned}$$

Now we take the mean of (14e) and (15)

$$
\begin{aligned}
u_{xx}(x,t^{'}) &= \frac{1}{2}\Big(\frac{u(x-\Delta x,t+\Delta t)-2u(x,t')+u(x+\Delta x,t+\Delta t)}{\Delta x^2} + \frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{\Delta x^2} + \mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta x^2) \\
&+ \frac{u(x-\Delta x,t)-2u(x,t')+u(x+\Delta x,t)}{\Delta x^2} - \frac{\partial u(x,t')}{\partial t}\frac{\Delta t}{\Delta x^2} + \mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta x^2)\Big) \\
&= \frac{1}{2}\Big(\frac{u(x-\Delta x,t+\Delta t)-2u(x,t')+u(x+\Delta x,t+\Delta t)}{\Delta x^2} \\
&+ \frac{u(x-\Delta x,t)-2u(x,t')+u(x+\Delta x,t)}{\Delta x^2}\Big) + \mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta x^2) \\
&\overset{u(x,t^{'})=\frac{u(x,t)+u(x,t+\Delta t)}{2}}{=} \\
&\frac{1}{2}\Big(\frac{u(x-\Delta x,t+\Delta t)-u(x,t)+u(x,t+\Delta t)+u(x+\Delta x,t+\Delta t)}{\Delta x^2} \\
&+ \frac{u(x-\Delta x,t)-u(x,t)+u(x,t+\Delta t)+u(x+\Delta x,t)}{\Delta x^2}\Big) + \mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta x^2) \\
&= \frac{1}{2}\Big(\frac{u(x-\Delta x,t+\Delta t)-2u(x,t+\Delta t)+u(x+\Delta x,t+\Delta t)}{\Delta x^2} + \frac{u(x-\Delta x,t)-2u(x,t)+u(x+\Delta x,t)}{\Delta x^2}\Big) \\
&+ \mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta x^2)
\end{aligned}
\tag{16a}
$$

Now combining (13c) and (16a) we get the Crank-Nicolson scheme

$$
\begin{aligned}
\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t} + \mathcal{O}(\Delta t^2) = \frac{1}{2}\Big(&\frac{u(x-\Delta x,t+\Delta t)-2u(x,t+\Delta t)+u(x+\Delta x,t+\Delta t)}{\Delta x^2} \\
&+ \frac{u(x-\Delta x,t)-2u(x,t)+u(x+\Delta x,t)}{\Delta x^2}\Big) + \mathcal{O}(\Delta x^2),
\end{aligned}
\tag{17a}
$$

where we have put both $\mathcal{O}(\Delta t^2)$ into a common term.

(17) shows that the Crank-Nicolson scheme is 2nd order in both time and space, implying better convergence properties for the Crank-Nicolson scheme compared to the Backward Euler scheme and the Forward Euler scheme.

Using the same method as we used for the previous schemes, we now study the stability of the Crank-Nicolson scheme. We insert the ansatz (5) into the Crank-Nicolson scheme (17) and solve for $|a_k|$:

$$
\begin{aligned}
\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t} &= \frac{1}{2}\Big(\frac{u(x-\Delta x,t+\Delta t)-2u(x,t+\Delta t)+u(x+\Delta x,t+\Delta t)}{\Delta x^2} \\
&+ \frac{u(x-\Delta x,t)-2u(x,t)+u(x+\Delta x,t)}{\Delta x^2}\Big) \\
a_k^n e^{ik\pi j\Delta x}\ \frac{a_k-1}{\Delta t} &= \frac{a_k^n e^{ik\pi j\Delta x}}{2}\ \Big(\frac{a_k e^{-ik\pi\Delta x}-2a_k+a_k e^{ik\pi\Delta x}}{\Delta x^2} + \frac{e^{-ik\pi\Delta x}-2+e^{ik\pi\Delta x}}{\Delta x^2}\Big) \\
\frac{a_k-1}{\Delta t} &= \frac{1}{2}\Big(\frac{a_k e^{-ik\pi\Delta x}-2a_k+a_k e^{ik\pi\Delta x}}{\Delta x^2} + \frac{e^{-ik\pi\Delta x}-2+e^{ik\pi\Delta x}}{\Delta x^2}\Big) \\
&= \frac{1+a_k}{2\Delta x^2}(e^{-ik\pi\Delta x}-2+e^{ik\pi\Delta x}) \\
&\overset{(6)}{=} -4\frac{1+a_k}{2\Delta x^2}\sin^2(\frac{k\pi\Delta x}{2}) \\
a_k - 1 &= (1+a_k)(-\frac{2\Delta t}{\Delta x^2})\sin^2(\frac{k\pi\Delta x}{2}) \\
\Big(1+\frac{2\Delta t}{\Delta x^2}\sin^2(\frac{k\pi\Delta x}{2})\Big)a_k &= 1-\frac{2\Delta t}{\Delta x^2}\sin^2(\frac{k\pi\Delta x}{2})
\end{aligned}
\tag{18a}
$$

$$
a_k = \frac{1-\frac{2\Delta t}{\Delta x^2}\sin^2(\frac{k\pi\Delta x}{2})}{1+\frac{2\Delta t}{\Delta x^2}\sin^2(\frac{k\pi\Delta x}{2})} < 1 \tag{18b}
$$

(18b) shows that the Crank-Nicolson scheme is unconditionally stable.

Based on the analyzis of the different schemes, we expect the Crank-Nicolson scheme to be the best scheme with respect to convergence and stability.

1.4 θ-rule

All the schemes derived above can be derived from a more general scheme, called the θ-rule scheme. To see this, first notice that the Crank-Nicolson scheme (17) is the average of the Forward Euler scheme (4b) and the Backward Euler scheme (9a). We can think of the average, represented by the Crank-Nicolson scheme, as the special case of equals weights in a weighted average of the Backward Euler scheme and the Forward Euler scheme. Writing the weighted average of the Forward Euler and Backward Euler schemes with weights $0 \leq \theta \leq 1$, we get the θ-rule

$$\begin{aligned}
(1-\theta)\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t} + \theta\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t} &= \theta\frac{u(x-\Delta x,t+\Delta t)-2u(x,t+\Delta t)+u(x+\Delta x,t+\Delta t)}{\Delta x^2} \\
&+ (1-\theta)\frac{u(x-\Delta x,t)-2u(x,t)+u(x+\Delta x,t)}{\Delta x^2} \qquad (19a) \\
\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t} &= \theta\frac{u(x-\Delta x,t+\Delta t)-2u(x,t+\Delta t)+u(x+\Delta x,t+\Delta t)}{\Delta x^2} \\
&+ (1-\theta)\frac{u(x-\Delta x,t)-2u(x,t)+u(x+\Delta x,t)}{\Delta x^2} \qquad (19b)
\end{aligned}$$

From the θ-scheme (19b) we see that $\theta = 0,\ 1/2,\ 1$ corresponds to the Forward Euler, the Crank-Nicolson and the Backward Euler scheme respectively.

When implementing the 1D-schemes, we will use the θ-scheme. Using the θ-scheme, we need only write one scheme instead of three.

2 Bibliography

[1] Hjorth-Jensen, M.(2015) Computational physics. Lectures fall 2015. `https://github.com/CompPhysics/ComputationalPhysics/tree/master/doc/Lectures`

[2] `https://github.com/CompPhysics/ComputationalPhysics/tree/master/doc/pub/pde`