§ 8.2 Finite differences for the heat equation

For \( \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \), the FTCS scheme works as

\[
\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{(\Delta x)^2}
\]

Let \( s = \frac{\Delta x^2}{(\Delta t)^2} \). \( u_j^{n+1} = (1-2s)u_j^n + s(u_{j+1}^n + u_{j-1}^n) \)

which is an explicit numerical scheme.

\( s = 1 \) leads to a wild numerical solution, while \( s = \frac{1}{2} \) results in a somewhat reasonable approximation, which is related to the stability of numerical schemes.

Consider a particular solution of the difference equation,

\( u_j^n = x_j T_n \rightarrow x_j T_{n+1} = s(x_{j+1}T_n + x_{j-1}T_n) + (1-2s)x_j T_n \)

\[
\frac{T_{n+1}}{T_n} = \frac{3(x_{j+1} + x_{j-1}) + (1-2s)x_j}{2}
\]

where \( \frac{3}{2} \) is independent of \( j \) and \( n \).

\( T_{n+1} = \frac{3}{2} T_n \) and \( T_n = \frac{3}{2} T_0 \)

The scheme is stable if \( |\frac{3}{2}| \leq 1 \), since it would lead to solutions that grow exponentially in time otherwise.

Plugging a discretized Fourier mode \( x_j = e^{ik_jx} \) into

\[
s \left( e^{ik_{j+1}x} + e^{ik_{j-1}x} \right) + (1-2s) x_j e^{ik_jx} = \frac{3}{2}
\]

we obtain

\[
\frac{3}{2} = s \left( e^{ik_{j+1}x} + e^{ik_{j-1}x} + (1-2s) e^{ik_jx} \right)
\]

\[
\frac{3}{2} = 2s \omega x + 1 - 2s
\]

\( |\frac{3}{2}| \leq 1 \rightarrow 0 \leq 2s (1-\omega x) \leq 2 \)

If \( \omega x = 1 \) \( s \leq \frac{1}{2} \),

which is the stability condition for the FTCS scheme.

* Boundary Conditions

| Dirichlet BC: \( u(0,t) = g(t) \) \( u(l,t) = h(t) \) |

| \( u_0^n = g(t_0n) \) \( u_N^n = h(t_0n) \) |
Neumann BC: \( u_x(0,t) = g(t), \quad u_x(l,t) = h(t) \)

The values of the solution on the boundary points of the grid are not immediately available, so one has to use a finite difference approximation for the conditions in order to march forward in time.

Backward or forward differences introduce \( O(\Delta x) \) error, which would kill the \( O(\Delta x) \) error for the spatial discretization.

Introducing "ghost points" \( u^n_0 \) and \( u^n_{J+1} \) in addition to the grid points \( u^n_1, u^n_2, \ldots, u^n_J \), we have the following centered difference approximation for the Neumann conditions

\[
\begin{align*}
g(\text{neu}) & = g^n = \frac{u^n_1 - u^n_0}{2\Delta x}, \\
h(\text{neu}) & = \frac{u^n_{J+1} - u^n_J}{2\Delta x}
\end{align*}
\]

From the above identities we can compute the values \( u^n_i \) and \( u^n_{J+1} \) at the ghost points at time level \( n \), which will be used to compute \( u^{n+1}_i \) and \( u^{n+1}_{J+1} \).

* The implicit BTCS scheme

\[
\frac{u^{n+1}_i - u^n_i}{\Delta t} = \frac{u^{n+1}_{i+1} - 2u^{n+1}_i + u^{n+1}_{i-1}}{(\Delta x)^2}
\]

\[
S = \frac{\Delta t}{(\Delta x)^2}, \quad -S u^{n+1}_{i-1} + (1 + 2S) u^{n+1}_i - S u^{n+1}_{i+1} = u^n_i
\]

For a fixed \( n \), the last equation forms a linear system for \( u^{n+1}_1, u^{n+1}_2, \ldots, u^{n+1}_J \), which is an implicit scheme with the follow stencil

\[
\begin{pmatrix}
\frac{S}{1+2S} & \cdots & \frac{S}{1+2S} \\
\vdots & \ddots & \vdots \\
\frac{S}{1+2S} & \cdots & \frac{S}{1+2S}
\end{pmatrix}
\]

In the presence of Dirichlet BC, we have

\[
\begin{pmatrix}
1+2S & -S & 0 & \cdots & 0 \\
-S & 1+2S & -S & 0 & \vdots \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & \cdots & -S & 1+2S & -S \\
0 & \cdots & -S & -S & 1+2S
\end{pmatrix}
\begin{pmatrix}
U^{n+1}_1 \\
U^{n+1}_2 \\
\vdots \\
U^{n+1}_{J-2} \\
U^{n+1}_{J-1}
\end{pmatrix}
= \begin{pmatrix}
U^n_1 + 5u^n_0 \\
U^{n+1}_2 \\
\vdots \\
U^{n+1}_{J-2} \\
U^{n+1}_{J-1} + 5u^{n+1}_J
\end{pmatrix}
\]

\[
\begin{pmatrix}
U^{n+1}_1 \\
U^{n+1}_2 \\
\vdots \\
U^{n+1}_{J-2} \\
U^{n+1}_{J-1}
\end{pmatrix}
= \begin{pmatrix}
U^n_1 + 5u^n_0 \\
U^{n+1}_2 \\
\vdots \\
U^{n+1}_{J-2} \\
U^{n+1}_{J-1} + 5u^{n+1}_J
\end{pmatrix}
\]
Now let's check the stability of this scheme.
Assuming \( u^*_j = e^{ik\alpha x} \), we have
\[
-\frac{\Delta t}{\Delta x^2} e^{-ik\alpha x} \frac{\partial^2 u^*}{\partial x^2} + (1+2s) \frac{\partial u^*_j}{\partial x} - s e^{ik\alpha x} \frac{\partial u^*_j}{\partial x} = 1
\]
Factoring \( \frac{\partial}{\partial x} \) on the left hand side, and solving for it gives
\[
\frac{\partial}{\partial x} = \frac{1}{1+2s(1-cosk\alpha x)}
\]
Since \( 1-cosk\alpha x > 0 \), \( |\frac{\partial}{\partial x}| \leq 1 \).
Thus, the BTCS scheme is (unconditionally) stable.

We can choose \( s \) arbitrarily, or \( \Delta t \). However, the accuracy of the scheme is bounded by \( O(\Delta t) + O(\Delta x^2) \).
Typically, \( \Delta t = \Delta x^2 \)

* The \( \theta \)-scheme (\( 0 \leq \theta \leq 1 \))
\[
\frac{u_j^{n+1} - u_j^n}{\Delta t} = (1-\theta) \left( \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} \right) + \theta \left( \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2} \right)
\]

\( \theta = 0 \), the FTCS scheme
\( \theta = 1 \), the BTCS scheme
\( \theta = \frac{1}{2} \), the Crank-Nicholson scheme

\[
-\frac{\Delta t}{\Delta x^2} u_{j+1}^{n+1} + (1+2s) u_j^{n+1} - \frac{\Delta t}{\Delta x^2} u_{j-1}^{n+1} = \frac{\Delta t}{\Delta x^2} \left( u_{j+1}^n - 2u_j^n + u_{j-1}^n \right) + \theta \left( u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1} \right)
\]

We analyze the stability by substituting \( u_j^n = e^{ik\alpha x} \)
\[
\frac{\Delta}{\Delta x} = (1-\theta) s (e^{ik\alpha x} + e^{-ik\alpha x} - 2) + \theta s (e^{ik\alpha x} + e^{-ik\alpha x} - 2)
\]
\[
\frac{\Delta}{\Delta x} = \frac{1-2(1-\theta)s(1-wk\alpha x)}{1+2\theta s(1-wk\alpha x)}
\]

\( 1 \leq 1 \rightarrow -1 - 2\theta s(1-wk\alpha x) \leq 2(1-\theta)s(1-wk\alpha x) \leq 1+2\theta s(1-wk\alpha x) \)

After combining like terms, we get
\[
-2 \leq s(4\theta - 2)(1-wk\alpha x)
\]
for the left inequality. (The right one holds for all \( s \).)
The worst case is \( \cos \theta \approx -1 \), resulting in
\[-2 \leq 2s (4\theta - 2) \]
This inequality is true (always) for \( \theta \geq \frac{1}{2} \)
Hence the \( \theta \)-scheme is unconditionally stable for \( \frac{1}{2} \leq \theta \leq 1 \)
For \( 0 \leq \theta \leq \frac{1}{2} \),
\[
  s = \frac{1}{2 - 4\theta}
\]
For \( \theta = 0 \), i.e., the FTCS scheme, \( s = \frac{1}{2} \).
Numerically, the Crank–Nicholson scheme is more accurate than FTCS & BTCS scheme since the accuracy of that is \( O(\Delta t^2) + O(\Delta x^4) \). On the other hand, there is no free lunch. We have to solve a linear system at each time step.