§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

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

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

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 ~~separated~~ solution of the difference equation,

$u_j^n = X_j T_n \rightarrow X_j T_{n+1} = s(X_{j+1} T_n + X_{j-1} T_n) + (1-2s) X_j T_n$

$$\rightarrow \frac{T_{n+1}}{T_n} = \frac{s(X_{j+1} + X_{j-1}) + (1-2s) X_j}{X_j} = \xi$$

where ξ is independent of j and n.

$T_{n+1} = \xi T_n$ and $T_n = \xi^n T_0$

The scheme is stable if $|\xi| \leq 1$, since it would lead to solutions ~~that~~ grow exponentially in time otherwise.

Plugging a discretized Fourier mode $X_j = e^{ikj\Delta x}$ into

$$\frac{s(X_{j+1} + X_{j-1}) + (1-2s) X_j}{X_j} = \xi$$

we obtain
$$\xi = \frac{s(e^{ik(j+1)\Delta x} + e^{ik(j-1)\Delta x}) + (1-2s)\, e^{ikj\Delta x}}{e^{ikj\Delta x}}$$

$$= 2s \cos k\Delta x + 1 - 2s$$

$|\xi| \leq 1 \rightarrow 0 \leq 2s(1-\cos k\Delta x) \leq 2$

If $\cos k\Delta x \approx -1$ $\quad s \leq \frac{1}{2}$,

which is the stability condition for the FTCS scheme.

* Boundary conditions

① Dirichlet BC: $u(0,t) = g(t)$ $\quad u(l,t) = h(t)$

$u_0^n = g(t_n)$ $\quad u_N^n = h(t_n)$

Neumann BC: $u_x(0,t) = g(t)$, $u_x(l,t) = h(t)$

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 match forward in time.

Backward or forward differences introduce $O(\Delta x)$ error, which would kill the $O(\Delta x^2)$ error for the spatial discretization.

Introducing "ghost points" u_{-1}^n and u_{J+1}^n in addition to the grid points $u_0^n, u_1^n, \cdots, u_J^n$, we have the following centered difference approximation for the Neumann conditions

$$g(n\Delta t) = g^n = \frac{u_1^n - u_{-1}^n}{2\Delta t}, \qquad h(n\Delta t) = \frac{u_{J+1}^n - u_{J-1}^n}{2\Delta t}$$

From the above identities we can compute the values u_{-1}^n and u_{J+1}^n at the ghost points at time level n, which will be used to compute u_0^{n+1} and u_J^{n+1}.

* The implicit BTCS scheme

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

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

For a fixed n, the last equation forms a linear system for $u_1^{n+1}, u_2^{n+1}, \cdots, u_J^{n+1}$, which is an implicit scheme with the follow stencil

$$\begin{array}{ccc} \frac{s}{1+2s}\ \bullet & * & \bullet\ \frac{s}{1+2s} \\ & \bullet\ \frac{1}{1+2s} & \end{array}$$

In the presence of Dirichlet BC we have

$$\begin{pmatrix} 1+2s & -s & 0 & \cdots & 0 \\ -s & 1+2s & -s & 0 & \cdots \\ & \ddots & \ddots & \ddots & \\ & & -s & 1+2s & -s \\ & & 0 & -s & 1+2s \end{pmatrix} \begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ u_{J-2}^{n+1} \\ u_{J-1}^{n+1} \end{pmatrix} = \begin{pmatrix} u_1^n + s u_0^{n+1} \\ u_2^n \\ \vdots \\ u_{J-2}^n \\ u_{J-1}^n + s u_J^{n+1} \end{pmatrix}$$

Now let's check the stability of this scheme

Assuming $u_j^n = \xi^n e^{ikj\Delta x}$, we have

$$-\xi e^{-ik\Delta x}\xi + (1+2s)\xi - s e^{ik\Delta x}\xi = 1$$

Factoring ξ on the left hand side, and solving for it gives

$$\xi = \frac{1}{1+2S(1-\cos k\Delta x)}$$

Since $1-\cos k\Delta x \geq 0$ $\quad |\xi| \leq 1$

Thus, the BTCS scheme is (uncontionally) stable.

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

Typically, $\Delta t = 5 \sim 10\,(\Delta x)^2$

* The θ- scheme $\quad (0 \leq \theta \leq 1)$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = (1-\theta)\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} + \theta\,\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2}$$

$\theta = 0$, the FTCS scheme

$\theta = 1$, the BTCS scheme

$\theta = \frac{1}{2}$, the Crank - Nicholson scheme

$$-\frac{S}{2}u_{j+1}^{n+1} + (1+S)u_j^{n+1} - \frac{S}{2}u_{j+1}^{n+1} = \frac{S}{2}u_{j+1}^n + (1-S)u_j^n + \frac{S}{2}u_{j-1}^n$$

$+\frac{S}{2(1+S)}$ $\quad \cdot \quad * \quad \cdot \quad$ $+\frac{S}{2(1+S)}$

$\frac{S}{2(1+S)}$ $\quad \cdot \quad \underset{\frac{1-S}{1+S}}{\cdot} \quad \cdot \quad$ $\frac{S}{2(1+S)}$

We analyze the stability by substituting $u_j^n = \xi^n e^{ikj\Delta x}$

$$\xi - 1 = (1-\theta)S\,(e^{ik\Delta x} + e^{-ik\Delta x} - 2) + \theta S\,(e^{ik\Delta x} + e^{-ik\Delta x} - 2)\,\xi$$

$$\xi = \frac{1 - 2(1-\theta)S(1-\cos kx)}{1 + 2\theta S(1-\cos kx)}$$

$$|\xi| \leq 1 \;\rightarrow\; -1 - 2\theta S(1-\cos kx) \leq 1 - 2(1-\theta)S(1-\cos kx) \leq 1 + 2\theta S(1-\cos kx)$$

After combing like terms, we get

$$-2 \leq S(4\theta - 2)(1-\cos kx)$$

for the left inequality (The right one valids for all s)

The worst case is $\cos k\Delta x \approx -1$ resulting in

$$-2 \leq 2s(4\theta - 2)$$

This inequality is true (always) for $\theta \geq \frac{1}{2}$

Hence the θ- scheme is unconditionally stable for $\frac{1}{2} \leq \theta \leq 1$

For $0 \leq \theta < \frac{1}{2}$

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

For $\theta = 0$, i.e., the FTCS scheme, $s \leq \frac{1}{2}$

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