Numerical Solutions for Partial Differential Equations

S. DELAHAIES

February 21, 2012

3.3 Stability

The stability of a numerical scheme is associated with propagation of numerical error. A finite difference scheme is stable if the error stays constant or decrease as the iterative process goes on. On the contrary, if the error grows with time, the scheme is said to be unstable. The stability of numerical schemes can be investigated by performing von Neumann stability analysis. Probably the most popular method, it has however strong restrictions : it only applies to linear, constant coefficiants PDEs, neglects the boundary conditions. The von Neumann stability method consists in:

- substituting the trial function
$$U_{j,n} = A\xi^n \mathrm{e}^{\mathrm{i}\omega j} \tag{1}$$
into the approximate difference scheme and find a characteristic equation for the amplification factor ξ.
- finding what restrictions on the parameters are required to have $|\xi| \leq 1$: the scheme is von Neumann stable if $|\xi| \leq 1$, and von Neumann unstable if $|\xi| > 1$. When the characteristic equation has multiple roots we require them to be distinct.

We apply this method to the FTCS scheme for the heat diffusion equation. The approximate difference equation is given by

$$U_{j,n+1} = rU_{j+1,n} + (1-2r)U_{j,n} + rU_{j-1,n}.$$

Substituting the trial solution $U_{j,n} = A\xi^n \mathrm{e}^{\mathrm{i}\omega j}$ into the above equation gives

$$A\xi^{n+1}\mathrm{e}^{\mathrm{i}\omega j} = rA\xi^n \mathrm{e}^{\mathrm{i}\omega j} + (1-2r)A\xi^n \mathrm{e}^{\mathrm{i}\omega j} + rA\xi^{n-1}\mathrm{e}^{\mathrm{i}\omega (j-1)},$$

dividing through by $A\xi^n \mathrm{e}^{\mathrm{i}\omega j}$ we obtain

$$\begin{aligned} \xi &= r\mathrm{e}^{\mathrm{i}\omega} + (1-2r) + r\mathrm{e}^{-\mathrm{i}\omega} \\ &= r2\cos\omega + 1 - 2r. \end{aligned}$$

Recall that $\cos\omega = 1 - 2\sin^2\frac{\omega}{2}$ therefore $\cos\omega - 1 = -2\sin^2\frac{\omega}{2}$ and we have

$$\xi = -4r\sin^2\frac{\omega}{2} + 1$$

Numerical stability requires $|\xi| \leq 1$, that is $-1 \leq \xi \leq 1$. Since $4r\sin^2\frac{\omega}{2} \geq 0$ we have $\xi \leq 1$. We then need

$$\xi = -4r\sin^2\frac{\omega}{2} + 1 \geq -1$$

which implies

$$-4r\sin^2\frac{\omega}{2} \leq -2$$

for all ω, that is $r \leq 1/2$.

3.4 Convergence

Definition 3.1 (Convergence)

Let $u(x^*, t^*)$ be the exact solution of a PDE at the point (x^*, t^*) and let $U_{t^*/\Delta t, x^*/\Delta x}$ be an approximate solution. The approximate solution is said to converge to the exact solution at (x^*, t^*) if

$$\lim_{\substack{\Delta t \to 0 \\ \Delta x \to 0}} |u(x^*, t^*) - U_{t^*/\Delta t, x^*/\Delta x}| = 0.$$

Theorem 3.2 (Lax equivalence theorem)

Given a properly posed initial value problem, boundary value problem, and a finite difference approximation that is consistent with the PDE, then stability is a necessary and sufficient condition for convergence.

3.5 θ-method

In the previous section we focused on a FTCS scheme for the heat diffusion equation. We can also consider the backward time central space (BTCS) scheme where we use

$$u_t\Big|_{j,n} \approx \frac{B_t U_{j,n}}{\Delta t} \quad , \quad u_{xx}\Big|_{j,n} \approx \frac{\delta_x^2 U_{j,n}}{\Delta x^2}.$$

The BTCS is then given by

$$\frac{U_{j,n} - U_{j,n-1}}{\Delta t} = \frac{U_{j+1,n} - 2U_{j,n} + U_{j-1,n}}{\Delta x^2}. \tag{2}$$

The θ-method consits in considering a weighted combination of the FTCS at time n, equation (25),and the BTCS schemes, equation (2), at time $n+1$, it gives

$$U_{j,n+1} = U_{j,n} + (1-\theta)r\delta_x^2 U_{j,n} + \theta r \delta_x^2 U_{j,n+1}, \tag{3}$$

where $\theta \in [0, 1]$. Typical values of θ lead to well known schemes:

- for $\theta = 0$ we recover the FTCS scheme,
- for $\theta = 1/2$ we have the trapezoidal or Crank-Nickolson scheme,
- for $\theta = 1$ we recover the BTCS scheme.

Finally we note that for $\theta = 0$ the θ-method is explicit, and for $\theta \in (0, 1]$ the θ-method is implicit.

We now investigate the consistency and stability of the θ-method. We start with the LTE. The θ-method is given by

$$\frac{B_t U_{j,n+1}}{\Delta t} = (1-\theta)\frac{\delta_x^2 U_{j,n}}{\Delta x^2} + \theta \frac{\delta_x^2 U_{j,n+1}}{\Delta x^2}.$$

We rearrange this expression to obtain the approximate difference operator

$$\mathcal{L}_\Delta U_{j,n} = \frac{B_t U_{j,n+1}}{\Delta t} - (1-\theta)\frac{\delta_x^2 U_{j,n}}{\Delta x^2} - \theta \frac{\delta_x^2 U_{j,n+1}}{\Delta x^2}.$$

To obtain the LTE we need to apply $\mathcal{L}_\Delta$ to the exact solution u:

$$\begin{aligned}\mathcal{L}_\Delta u = {} & \underbrace{\frac{u(x, t+\Delta t) - u(x,t)}{\Delta t}}_{A_1} - (1-\theta)\underbrace{\frac{u(x+\Delta x, t) - 2u(x,t) + u(x-\Delta x, t)}{\Delta x^2}}_{A_2} \\ & + \theta \underbrace{\frac{u(x+\Delta x, t+\Delta t) - 2u(x, t+\Delta t) + u(x-\Delta x, t+\Delta t)}{\Delta x^2}}_{A_3}.\end{aligned}$$

We use Taylor's theorem to expand u about (x,t), the terms A_1 and A_2 were calculated previously and we have

$$A_1 = u_t + \frac{\Delta t}{2!}u_{tt} + \frac{\Delta t^2}{3!}u_{ttt} + O(\Delta t^3),$$

and

$$A_2 = u_{xx} + \frac{\Delta x^2}{12}u_{4x} + O(\Delta x^4).$$

For A_3 we have

$$\begin{aligned}A_3 = {} & \frac{1}{\Delta x^2}\Bigg[u\Big|_{x,t+\Delta t} + \Delta x\, u_x\Big|_{x,t+\Delta t} + \frac{\Delta x^2}{2!}u_{xx}\Big|_{x,t+\Delta t} + \cdots + O(\Delta x^6) \\ & - 2u\Big|_{x,t} + u\Big|_{x,t+\Delta t} - \Delta x\, u_x\Big|_{x,t+\Delta t} + \frac{\Delta x^2}{2!}u_{xx}\Big|_{x,t+\Delta t} - \cdots + O(\Delta x^6)\Bigg] \\ = {} & u_{xx}\Big|_{x,t+\Delta t} + \frac{\Delta x^2}{12}u_{4x}\Big|_{x,t+\Delta t} + O(\Delta x^4) \\ = {} & u_{xx} + u_{xxt}\Delta t + u_{xxtt}\frac{\Delta t^2}{2!} + O(\Delta t^3) \\ & + \frac{\Delta x^2}{12}u_{4x} + \frac{\Delta x^2}{12}u_{4xt}\Delta t + \frac{\Delta x^2}{12}u_{4xtt}\frac{\Delta t^2}{2!} + O(\Delta t^3 \Delta x^2) + O(\Delta x^4)\end{aligned}$$

therefore we have

$$\begin{aligned}\mathcal{L}_\Delta u = {} & u_t + \frac{\Delta t}{2!}u_{tt} + \frac{\Delta t^2}{3!}u_{ttt} + O(\Delta t^3) + u_{xx} + \frac{\Delta x^2}{12}u_{4x} + O(\Delta x^4) \\ & + u_{xx} + u_{xxt}\Delta t + u_{xxtt}\frac{\Delta t^2}{2!} + O(\Delta t^3) + \frac{\Delta x^2}{12}u_{4x} + \frac{\Delta x^2}{12}u_{4xt}\Delta t \\ & + \frac{\Delta x^2}{12}u_{4xtt}\frac{\Delta t^2}{2!} + O(\Delta t^3 \Delta x^2) + O(\Delta x^4).\end{aligned}$$

We now use the fact that

$$u_t - (1-\theta)u_{xx} - \theta u_{xx} = u_t - u_{xx} = 0$$

$$u_{tt} - u_{xxxx} = 0$$

$$\dots$$

and we obtain

$$\mathcal{L}_\Delta u = \Delta t\left[\frac{1}{2}u_{tt} - \theta u_{tt}\right] + \Delta t^{\,2}\left[\frac{1}{3!}u_{ttt} - \frac{\theta}{2}u_{ttt}\right] - \Delta x\left[\frac{1-\theta}{12}u_{tt} + \frac{\theta}{12}u_{tt}\right]$$
$$+ \Delta t\Delta x^{\,2}\left[\frac{1}{12}u_{ttt}\right] + O(\Delta t^{\,3}, \Delta x^{\,4}, \Delta t^{\,2}\Delta x^{\,2})$$

which reduces to

$$\mathcal{L}_\Delta u = \left[\left(\frac{1}{2} - \theta\right)\Delta t - \frac{\Delta x^{\,2}}{12}\right]u_{tt} + \left(\frac{1}{26} - \frac{\theta}{2}\right)u_{ttt}\Delta t^{\,2} + O(\Delta t^{\,3}, \Delta x^{\,4}, \Delta t^{\,2}\Delta x^{\,2}).$$

We see that the θ-method is 1st order in time and 2nd order in space except for $\theta = 1/2$ where it is 2nd order in time and space. Moreover we see that

$$\lim_{\substack{\Delta t\to 0\\ \Delta x\to 0}} \mathcal{L}_\Delta u = 0,$$

therefore the θ-method is consistent with the heat diffusion equation.

To investigate the stability of the θ-method for the equation $u_t - u_{xx} = 0$ we apply the method outlined in 3.3. We consider an approximate solution $U_{j,n}$ of the form

$$U_{i,j} = A\xi^n e^{i\omega j}$$

and we substitute it in equation

$$A\xi^{n+1}e^{i\omega j} = A\xi^n e^{i\omega j} + r(1-\theta)\left(e^{i\omega(j-1)} - 2e^{i\omega j} + e^{i\omega(j+1)}\right)A\xi^n$$
$$+ r\theta\left(e^{i\omega(j-1)} - 2e^{i\omega j} + e^{i\omega(j+1)}\right)A\xi^{n+1}$$

dividing through by $A\xi^n e^{i\omega j}$ we obtain

$$\xi = 1 + r(1-\theta)\left(e^{-i\omega} - 2 + e^{i\omega}\right) + r\theta\left(e^{-i\omega} - 2 + e^{i\omega}\right)\xi.$$

Since $e^{-i\omega} - 2 + e^{i\omega} = 2\cos\omega - 2 = -4\sin^2(\omega/2)$ we get

$$\xi = 1 - 4r(1-\theta)\sin^2(\omega/2) - 4r\theta\sin^2(\omega/2)\xi,$$

then

$$\xi = \frac{1 - 4r(1-\theta)\sin^2(\omega/2)}{1 + 4r\theta\sin^2(\omega/2)}.$$

For stability we need $|\xi| \le 1$. Since $\theta \in [0,1]$ and $4r\sin^2(\omega/2) \ge 0$ we have

$$\xi = \frac{1 + 4r\theta\sin^2(\omega/2) - 4r\sin^2(\omega/2)}{1 + 4r\theta\sin^2(\omega/2)} \le 1.$$

We finally need

$$\frac{1-4r(1-\theta)\sin^2(\omega/2)}{1+4r\theta\sin^2(\omega/2)} \geq -1$$

$$\therefore \quad 1-4r(1-\theta)\sin^2(\omega/2) \geq -1-4r\theta\sin^2(\omega/2)$$

$$\therefore \quad 1 \geq 2r(1-2\theta)\sin^2(\omega/2),\ \forall\omega$$

$$\therefore \quad 1 \geq 2r(1-2\theta).$$

If $\theta \geq 1/2$ then we have $1-2\theta \leq 0$ and the previous inequality is always satisfied, if $\theta < 1/2$ then we require

$$r \leq \frac{1}{2(1-2\theta)}$$

3.6 Derivative boundary conditions

So far we considered Dirichlet boundary conditions, that is the values of the solution at the boundary were imposed by

$$u(0,t) = a(t)\ ,\ u(1,t) = b(t).$$

In many applications the boundary conditions are expressed as derivative (flux) boundary conditions

$$u_x(0,t) = c(t)\ u_x(0,t) = d(t),$$

or using mixed boundary conditions

$$\begin{aligned} u(0,t) + u_x(0,t) &= a(t) + c(t), \\ u(1,t) + u_x(1,t) &= b(t) + d(t). \end{aligned}$$

For the heat equation a derivative boundary condition $u_x(0,t) = 0$ means that there is no heat flux out the boundary, ie the boundary is insulating. Flux boundary conditions are known as Neumann boundary conditions.

We illustrate these Neumann boundary conditions with the heat diffusion equation $u_t = u_{xx}$ and the flux condition $u_x(0,t) = 0$. We consider a FTCS method.

- We choose a number N of spatial grid point and we choose a time step.
- We calculate $U_{j,0}$, $j = 0,\ldots,N$, from the initial condition.
- We calculate $U_{j,1}$, $j = 1,\ldots,N-1$, using the FTCS scheme.
- But how to we get $U_{0,1}$?

  Method 1: we use a one-sidded difference approximation for the derivative at $x = 0$

  $$\left.\frac{\partial u}{\partial x}\right|_{x=0} \approx \frac{U_{1,n} - U_{0,n}}{\Delta x}.$$

  Then if the Neumann condition is $u_x(0,t) = c(t)$ we have

  $$\frac{U_{1,n} - U_{0,n}}{\Delta x} = c(t_n),$$

that is $U_{1,n} = U_{0,n} + c(t_n)\Delta x$. In our case we obtain

$$\frac{U_{1,n} - U_{0,n}}{\Delta x} = 0,$$

that is $U_{1,n} = U_{0,n}$. This approximation is 1st order in space.

Method 2: we introduce some ghost points $\{U_{-1,n}\}$, and we use the FTCS scheme to calculate $U_{-1,n}$

$$U_{0,n} = U_{0,n} + r(U_{-1,n} - 2U_{0,n} + U_{1,n}).$$

We use the derivative boundary condition to derive a formula for $U_{1,n}$. We consider a central difference approximation, we have

$$\frac{U_{1,n} - U_{-1,n}}{2\Delta x} = c(t_n),$$

which gives $U_{1,n} = U_{-1,n} + 2c(t_n)\Delta x$. In our case this gives $U_{1,n} = U_{-1,n}$ and we have

$$U_{0,n} = U_{0,n} + r(2U_{1,n} - 2U_{0,n}).$$

Since we use a central difference approximation for u_x this approximation is 2nd order in space.

3.7 Multi-step schemes

So far we only considered single-step schemes, that is for which we only requires the values of U at the previous time step to calculate the values of U at the current time. Multi-step methods use more time steps to calculate the values of U at the current time, eg two-step schemes use the values $U_{j,n-1}$ and $U_{j,n}$ to obtain $U_{j,n+1}$.

3.7.1 Richardson's method

Richardson's method is a central time central space (CTCS) scheme. For the heat diffusion equation it gives

$$\frac{U_{j,n+1} - U_{j,n-1}}{2\Delta t} = \frac{U_{j+1,n} - 2U_{j,n} + U_{j-1,n}}{\Delta x^2}, \tag{4}$$

which can be written as

$$U_{j,n+1} = U_{j,n-1} + 2r(U_{j+1,n} - 2U_{j,n} + U_{j-1,n}),$$

where $r = \Delta t/\Delta x^2$. This method is an explicit two-step method. At the first iteration there is only one previous step available, we thus need to use a single-step method to calculate $U_{j,1}$. This scheme will be studied in the tutorials.

3.7.2 Du Fort-Frankel method

The Du Fort-Frankel method is similar to Richardson's method except that $U_{j,n}$ is replaced with the average of $U_{j,n+1}$ and $U_{j,n-1}$, then we have

$$U_{j,n+1} = U_{j,n-1} + 2r(U_{j+1,n} - U_{j,n+1} - U_{j,n-1} + U_{j-1,n}), \tag{5}$$

which can be rearrange as

$$U_{j,n+1} = \frac{1-2r}{1+2r}U_{j,n-1} + \frac{2r}{1+2r}(U_{j+1,n} + U_{j-1,n}). \tag{6}$$

We study the stability of the Du Fort-Frankel scheme, we apply equation (6) to a solution of the form $A\mathrm{e}^{\mathrm{i}\omega j}\xi^n$, we have

$$A\mathrm{e}^{\mathrm{i}\omega j}\xi^{n+1} = \frac{1-2r}{1+2r}A\mathrm{e}^{\mathrm{i}\omega j}\xi^{n-1} + \frac{2r}{1+2r}(\mathrm{e}^{\mathrm{i}\omega(j+1)} + \mathrm{e}^{\mathrm{i}\omega(j-1)})A\xi^n.$$

Divide the above expression by $A\mathrm{e}^{\mathrm{i}\omega j}\xi^{n-1}$, it gives

$$\xi^2 = \frac{1-2r}{1+2r} + \frac{2r}{1+2r}(\mathrm{e}^{\mathrm{i}\omega} + \mathrm{e}^{-\mathrm{i}\omega})\xi.$$

Using the relation $(\mathrm{e}^{\mathrm{i}\omega} + \mathrm{e}^{-\mathrm{i}\omega}) = 2\cos\omega$ we obtain

$$(1+2r)\xi^2 - 4r\xi\cos\omega - (1-2r) = 0.$$

Stability requires $|\xi| \leq 1$ and that the roots ξ are all distinct. The two roots of the above equation are given by

$$\xi_\pm = \frac{1}{1+2r}\left[2r\cos\omega \pm \sqrt{4r^2\cos^2\omega + 1 - 4r^2}\right],$$

and from the relation $4r^2\cos^2\omega - 4r^2 = -4r^2\sin^2\omega$ we obtain

$$\xi_\pm = \frac{1}{1+2r}\left[2r\cos\omega \pm \sqrt{1 - 4r^2\sin^2\omega}\right].$$

- case 1: $1 - 4r^2\sin^2\omega < 0$ ξ_- and ξ_+ are then complex, with $\xi_- = \overline{\xi_+}$, moreover

  $$|\xi_-|^2 = |\xi_+|^2 = \frac{4r^2\cos^2\omega + 4r^2\sin^2\omega + 1}{(1+2r)^2} = \frac{4r^2+1}{(1+2r)^2}$$

  and $0 < \frac{4r^2+1}{(1+2r)^2} < 1$, therefore $|\xi_+| \leq 1$ and $|\xi_+| \leq 1$.

- case 2: $1 - 4r^2\sin^2\omega > 0$

  $$\frac{1}{1+2r}\left[2r\cos\omega + \sqrt{1 - 4r^2\sin^2\omega}\right] \leq \frac{2r\cos\omega + 1}{1+2r} \leq 1$$

  therefore $\xi_+ \leq 1$, where we used the fact that $0 < 1 - 4r^2\sin^2\omega \leq 1$. Moreover

  $$\frac{1}{1+2r}\left[2r\cos\omega + \sqrt{1 - 4r^2\sin^2\omega}\right] \geq \frac{-2r}{1+2r} \geq -1$$

  therefore $\xi_+ \geq -1$, where we used the fact that $0 < 1 - 4r^2\sin^2\omega$ and $\cos\omega \geq -1$.
  We apply the same analysis for ξ_-, we have

  $$\frac{1}{1+2r}\left[2r\cos\omega - \sqrt{1 - 4r^2\sin^2\omega}\right] \leq \frac{2r}{1+2r} \leq 1$$

  therefore $\xi_+ \leq 1$. Morevoer

  $$\frac{1}{1+2r}\left[2r\cos\omega - \sqrt{1 - 4r^2\sin^2\omega}\right] \geq \frac{-2r-1}{1+2r} \geq -1$$

  therefore $\xi_+ \geq -1$.

The above analysis shows that the Du For-Frankel method is unconditionaly stable.