

1. Let

$$\left. \begin{aligned} U_{lmn}^j &= f^j \exp[i(l\xi + m\eta + n\tau)] \\ U_{lmn}^{*j} &= f_*^{*j} \exp[i(l\xi + m\eta + n\tau)] \\ U_{*lmn}^{*j} &= f_*^{*j} \exp[i(l\xi + m\eta + n\tau)] \end{aligned} \right\} \quad \text{so that} \quad \begin{cases} \delta_x^2 \rightarrow -4 \sin^2 \frac{1}{2} \xi \\ \delta_y^2 \rightarrow -4 \sin^2 \frac{1}{2} \eta \\ \delta_z^2 \rightarrow -4 \sin^2 \frac{1}{2} \tau \end{cases}$$

We write $a = 2r \sin^2 \frac{1}{2} \xi$, $b = 2r \sin^2 \frac{1}{2} \eta$ and $c = 2r \sin^2 \frac{1}{2} \tau$. The equations become

$$\begin{aligned} (1+a)f^{*j+1} &= (1-a-2b-2c)f^j \\ (1+b)f_*^{*j+1} &= (1-a-b-2c)f^j - af^{*j+1} \\ (1+c)f^{j+1} &= (1-a-b-c)f^j - af^{*j+1} - bf_*^{*j+1} \end{aligned} .$$

Eliminating f^* and f_* , we find after some algebra, $f^{j+1} = \lambda f^j$, where

$$\lambda = \frac{1-a-b-c+ab+bc+ca+abc}{(1+a)(1+b)(1+c)} .$$

Now the denominator expands to $1+a+b+c+ab+bc+ca+abc$, and since a , b and c are positive, this has greater modulus than the numerator. Thus $|\lambda| \leq 1$ and the method is **unconditionally stable**.

2. The θ -method discussed in lectures (equation 9.8) can be written

$$\begin{aligned} \frac{1}{s^2} \delta_t^2 U_n^j &= \theta \delta_x^2 U_n^{j+1} + (1-2\theta) \delta_x^2 U_n^j + \theta \delta_x^2 U_n^{j-1} \\ &= \delta_x^2 U_n^j + \theta \delta_t^2 (\delta_x^2 U_n^j) \\ \text{or } \delta_t^2 U_n^j &= s^2 \delta_x^2 (1 + \theta \delta_t^2) U_n^j , \end{aligned}$$

as required. Now for any $f(x, t)$,

$$\begin{aligned} \delta_t^2 u &= k^2 u_{tt} + \frac{1}{12} k^4 u_{tttt} + O(k^6) \\ \delta_x^2 f &= h^2 f_{xx} + \frac{1}{12} h^4 f_{xxxx} + O(h^6) . \end{aligned}$$

So writing $f = (1 + \theta \delta_t^2)u = u + \theta k^2 u_{tt} + O(k^4)$, the truncation error, R_n^j , is given by

$$\begin{aligned} R_n^j &= \frac{1}{k^2} [\delta_t^2 u - s^2 \delta_x^2 (1 + \theta \delta_t^2) u] - (u_{tt} - u_{xx}) \\ &= u_{tt} + \frac{1}{12} k^2 u_{tttt} - (u + \theta k^2 u_{tt})_{xx} - \frac{1}{12} h^2 (u + \theta k^2 u_{tt})_{xxxx} - (u_{tt} - u_{xx}) + O(k^4, h^4) \\ &= \frac{1}{12} k^2 u_{tttt} - \theta k^2 u_{ttxx} - \frac{1}{12} h^2 u_{xxxx} + O(k^4, h^4, k^2 h^2) . \end{aligned}$$

Now since $u_{tt} = u_{xx}$, we know $u_{tttt} = u_{ttxx} = u_{xxxx}$. Thus the truncation error is

$$R_n^j = k^2 u_{tttt} \left[\frac{1}{12} - \theta - \frac{1}{12s^2} \right] + O(h^4, k^4) .$$

Thus the scheme is usually second order, but if we choose $\theta = (s^2 - 1)/(12s^2)$ then it is fourth order. However, this would be a very bad idea. From lectures (equation 9.10), we saw the stability constraint for $\theta \geq 0$ was $\theta \geq (s^2 - 1)/(4s^2)$, and thus the scheme with the smallest truncation error would be unstable.

3. Let $U_n^j = (\lambda)^j \exp(in\xi)$ and $q = kV/h$. For comparison, the exact solution has a growth factor $\lambda = \exp(-iq\xi)$. The box scheme becomes

$$\begin{aligned} (\lambda - 1)(1 + e^{i\xi}) + q(\lambda + 1)(e^{i\xi} - 1) &= 0 \\ \text{or } \frac{\lambda - 1}{\lambda + 1} &= -q \left(\frac{e^{i\xi} - 1}{e^{i\xi} + 1} \right) = -q \left(\frac{e^{i\xi/2} - e^{-i\xi/2}}{e^{i\xi/2} + e^{-i\xi/2}} \right) = -qi \tan \frac{1}{2}\xi . \end{aligned}$$

So regrouping, we have

$$\lambda = \frac{1 - iq \tan \frac{1}{2}\xi}{1 + iq \tan \frac{1}{2}\xi} \quad \text{and} \quad |\lambda|^2 = \frac{1 + q^2 \tan^2 \frac{1}{2}\xi}{1 + q^2 \tan^2 \frac{1}{2}\xi} = 1 .$$

Thus the scheme is stable and conservative. The argument of λ is

$$\text{Arg}[\lambda] = \text{Arg}[1 - iq \tan \frac{1}{2}\xi] - \text{Arg}[1 + iq \tan \frac{1}{2}\xi] = -2 \tan^{-1}[q \tan \frac{1}{2}\xi] .$$

When $\xi \ll 1$, $\text{Arg}[\lambda] \simeq -2q \frac{1}{2}\xi = -q\xi + O(\xi^3)$, which agrees with the exact solution. The low harmonics are modelled well. When $q = 1$, clearly $\text{Arg}[\lambda] = -\xi$ exactly. Since $|\lambda|$ and $\text{Arg}[\lambda]$ are correct, it follows that λ is exactly correct, and the scheme is perfect. This is because the characteristics pass through the grid points when $q = 1$.

4. $\underline{u}_t + A\underline{u}_x = 0$, with $f = Au$, with A constant. We eliminate the values at half-timesteps from the two-step Lax-Wendroff scheme, to obtain

$$\begin{aligned} \underline{U}_n^{j+1} - \underline{U}_n^j &= -sA [\underline{U}_{n+1/2}^{j+1/2} - \underline{U}_{n-1/2}^{j+1/2}] \\ &= -sA \left[\frac{1}{2}(\underline{U}_{n+1}^j - \underline{U}_{n-1}^j) - \frac{1}{2}sA(\underline{U}_{n+1}^j - 2\underline{U}_n^j + \underline{U}_{n-1}^j) \right] . \end{aligned}$$

Let $\underline{U}_n^j = (\lambda)^j \exp(in\xi)\underline{V}$, where \underline{V} is some vector. Then the scheme becomes

$$\begin{aligned} (\lambda - 1)\underline{V} &= -\frac{1}{2}sA(2i \sin \xi)\underline{V} + \frac{1}{2}s^2A^2(-4 \sin^2 \frac{1}{2}\xi)\underline{V} \\ \text{or } 0 &= [2s^2A^2 \sin^2 \frac{1}{2}\xi + isA \sin \xi + (\lambda - 1)I] \underline{V} \end{aligned} \quad (*)$$

If A is a $p \times p$ matrix with p linearly independent eigenvectors, then each of these eigenvectors is also an eigenvector of the $p \times p$ matrix $(I - isA \sin \xi - 2s^2A^2 \sin^2 \frac{1}{2}\xi)$, and so each of these is a solution of (*) for suitable λ . Suppose $A\underline{V} = \mu\underline{V}$. Then

$$2s^2\mu^2 \sin^2 \frac{1}{2}\xi + is\mu \sin \xi + (\lambda - 1) = 0 .$$

If the eigenvalue μ is real, then

$$\begin{aligned}\lambda &= 1 - 2s^2\mu^2 \sin^2 \frac{1}{2}\xi - i(\mu s \sin \xi) \\ |\lambda|^2 &= (1 - 2s^2\mu^2 \sin^2 \frac{1}{2}\xi)^2 + \mu^2 s^2 \sin^2 \xi \\ &= 1 - 4s^2\mu^2 \sin^2 \frac{1}{2}\xi + 4s^4\mu^4 \sin^4 \frac{1}{2}\xi + 4\mu^2 s^2 \sin^2 \frac{1}{2}\xi \cos^2 \frac{1}{2}\xi \\ &= 1 + 4\mu^2 s^2 (\mu^2 s^2 - 1) \sin^4 \frac{1}{2}\xi .\end{aligned}$$

For stability, we need $\mu^2 s^2 \leq 1$ for every eigenvalue μ , or $s \max |\mu| \leq 1$.

If there exists a complex eigenvalue $\mu = a + ib$, where $b > 0$ (if $b < 0$ we use instead the complex conjugate of μ which must also be an eigenvalue), then considering small values of ξ ,

$$\lambda = 1 - i\mu s \xi + O(\xi^2) = (1 + s\xi b) - ias\xi + O(\xi^2) .$$

Then

$$|\lambda|^2 = 1 + 2s\xi b + O(\xi)^2 > 1 \quad \text{as } b > 0 .$$

Thus if μ is complex the scheme is unstable. This is to be expected. From lectures (equation 10.2) $\underline{u}_t + A\underline{u}_x = 0$ has p characteristic directions if and only if the eigenvalues of A are all real. If some of the eigenvalues are complex, then the problem is partially elliptic, and time-stepping from initial values is likely to be physically unstable.

5. Using a double Taylor series,

$$\begin{aligned}u_{m+1,n+1} &= [u + hu_x + hu_y + \frac{1}{2}h^2[u_{xx} + 2u_{xy} + u_{yy}] + \frac{1}{6}h^3[u_{xxx} + 3u_{xxy} + 3u_{xyy} + u_{yyy}] \\ &\quad + \frac{1}{24}h^4(u_{xxxx} + 4u_{xxxy} + 6u_{xxyy} + 4u_{xyyy} + u_{yyyy}) + O(h^5)]_{mn} + O(h^5).\end{aligned}$$

Similar expressions can be found for u at $(m-1, n-1)$, $(m+1, n-1)$ and $(m-1, n+1)$. Adding these expressions up, noting that all odd derivatives cancel by symmetry,

$$\begin{aligned}u_{m+1,n+1} + u_{m+1,n-1} + u_{m-1,n+1} + u_{m-1,n-1} &= [4u + 2h^2(u_{xx} + u_{yy}) \\ &\quad + \frac{1}{6}h^4(u_{xxxx} + 6u_{xxyy} + u_{yyyy}) + O(h^6)]_{mn} .\end{aligned}$$

Thus we obtain the diagonal 5-point scheme,

$$\begin{aligned}(u_{xx} + u_{yy})_{mn} &= \frac{1}{2h^2} [u_{m+1,n+1} + u_{m+1,n-1} + u_{m-1,n+1} + u_{m-1,n-1} - 4u_{mn}] \\ &\quad - \frac{1}{12}h^2 [u_{xxxx} + 6u_{xxyy} + u_{yyyy}]_{mn} + O(h^4) .\end{aligned}$$

We compare the usual five point scheme,

$$\begin{aligned}(u_{xx} + u_{yy})_{mn} &= \frac{1}{h^2} [u_{m+1,n} + u_{m-1,n} + u_{m,n+1} + u_{m,n-1} - 4u_{mn}] \\ &\quad - \frac{1}{12}h^2 [u_{xxxx} + u_{yyyy}]_{mn} + O(h^4) .\end{aligned}$$

Because of the u_{xxyy} term, no linear combination of these two schemes removes the $O(h^2)$ term precisely. However, if we are solving the Poisson equation $\nabla^2 u = f$, we know that $\nabla^2(\nabla^2 u) = \nabla^2 f$, which is known. If we take a times the first equation and add b times the second, where $a + b = 1$, we will get an approximation for $\nabla^2 u$ with a truncation error

$$R_{mn} = \frac{1}{12}h^2 [6au_{xxyy} + (a+b)(u_{xx} + u_{yy})] + O(h^4) .$$

If we choose $6a = 2$, so that $a = \frac{1}{3}$ and $b = \frac{2}{3}$, then

$$R_{mn} = \frac{1}{12}h^2 \nabla^2(\nabla^2 u) + O(h^4) .$$

Thus $\nabla^2 u = f$ is accurately modelled by

$$\begin{aligned} \frac{1}{6h^2} \begin{Bmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{Bmatrix} u &= f + \frac{1}{12}h^2 \nabla^2 f + O(h^4) \\ &= \frac{1}{12} \begin{Bmatrix} 0 & 1 & 0 \\ 1 & 8 & 1 \\ 0 & 1 & 0 \end{Bmatrix} f + O(h^4) . \end{aligned}$$

6. Using Taylor series,

$$\begin{aligned} g(A) &= u(A) = u_{MN} + \theta h(u_x)_{MN} + \frac{1}{2}\theta^2 h^2(u_{xx})_{MN} + O(h^3) \\ u_{M-1N} &= u_{MN} - h(u_x)_{MN} + \frac{1}{2}h^2(u_{xx})_{MN} + O(h^3) . \end{aligned}$$

Adding the first equation to θ times the second,

$$g(A) + \theta u_{M-1N} = (1 + \theta)u_{MN} + \frac{1}{2}h^2\theta(1 + \theta)(u_{xx})_{MN} + O(h^3) .$$

Similarly,

$$g(B) + \phi u_{MN-1} = (1 + \phi)u_{MN} + \frac{1}{2}h^2\phi(1 + \phi)(u_{yy})_{MN} + O(h^3) .$$

So at (M, N) ,

$$h^2(u_{xx} + u_{yy})_{MN} = \frac{2g(A)}{\theta(1 + \theta)} + \frac{2g(B)}{\phi(1 + \phi)} - \frac{2u_{M-1N}}{1 + \theta} + \frac{2u_{MN-1}}{1 + \phi} - 2\left(\frac{1}{\theta} + \frac{1}{\phi}\right)u_{MN} + O(h^3) .$$

The truncation of this scheme is $O(h)$ at the boundary, essentially because the differences we have used are not centred.