5 The Explicit Method for the 1-D Diffusion Equation

Let us consider the problem for $u(x,\,t)$:

$$\left.\begin{array}{lll} \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} \quad (\text{or } \; u_t = u_{xx}\;), & & \in \;\; 0 < x < 1, \;\; t > 0 \\[2ex] \text{with} \quad u(0,\,t) = 0, & u(1,\,t) = 0\;, & u(x,\,0) = f(x) \end{array}\right\}, \tag{5.1}$$

where the variable t denotes time and x is the spatial coordinate; note too the suffix notation used to denote partial derivatives *i.e.* $\partial u/\partial t \equiv u_t$ and $\partial^2 u/\partial x^2 \equiv u_{xx}$.

In general (more complicated PDEs), it is impossible to determine the solution of the boundary-value problem exactly in closed form. Thus we aim to describe a simple and general numerical technique to solve the problem using the finite difference method (FDM). The construction of a finite difference scheme consists of two steps :

1. The computational domain is approximated by a finite set of **grid** points, on a **mesh**.
2. The derivatives in the differential equation (and, possibly also in the boundary condition(s)) are approximated by difference weights on the mesh.

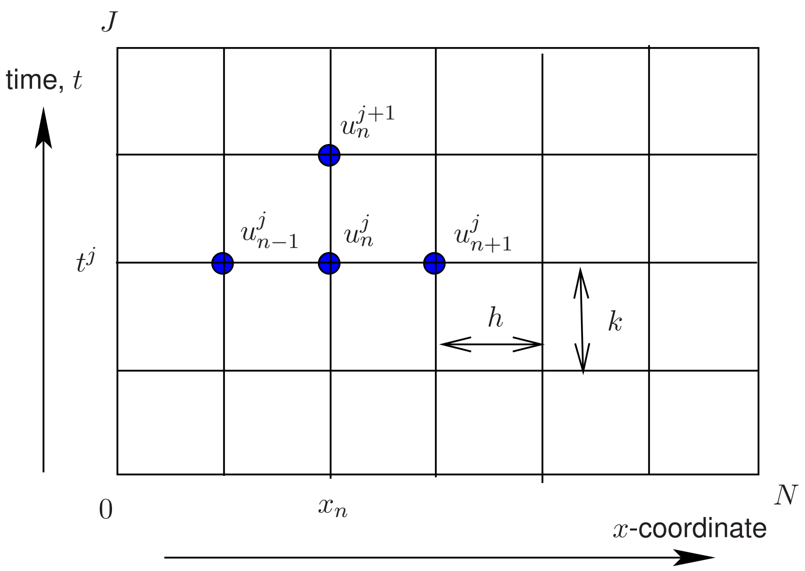

Figure 5.1: Discretised diffusion equation *mesh*.

We define a regular, rectangular grid $(x_n,\,t^j)$ for $0 \le n \le N$, $0 \le j \le J$ of lengths $(h,\,k)$, so that $Nh = 1,\; x_n = nh,\; t^j = jk$. We shall seek an approximation U_n^j to the exact solution evaluated on the grid points, $u_n^j \equiv u(nh,\,jk)$. The boundary conditions require $u_0^j = 0$, $u_N^j = 0$ and $u_n^0 = f_n \equiv f(x_n)$. Recalling the results from §3, we have

$$\frac{u_n^{j+1} - u_n^j}{k} = \frac{\partial u_n^j}{\partial t} + \tfrac{1}{2}k\frac{\partial^2 u_n^j}{\partial t^2} + O(k^2)\;,$$

and

$$\frac{u_{n+1}^j - 2u_n^j + u_{n-1}^j}{h^2} = \frac{\partial^2 u_n^j}{\partial x^2} + \tfrac{1}{12}h^2\frac{\partial^4 u_n^j}{\partial x^4} + O(h^4)\;.$$

Using the above in the equation $u_t = u_{xx}$, we have

$$\frac{u_n^{j+1} - u_n^j}{k} = \frac{u_{n+1}^j - 2u_n^j + u_{n-1}^j}{h^2} + R_n^j \, , \tag{5.2}$$

where the **Truncation Error**, R_n^j is

$$R_n^j = \tfrac{1}{12}h^2 \frac{\partial^4 u_n^j}{\partial x^4} - \tfrac{1}{2}k \frac{\partial^2 u_n^j}{\partial t^2} + O(k^2, h^4) \, . \tag{5.3}$$

The simplest explicit method neglects terms of $O(k,\, h^2)$. If we write

$$r = k/h^2 \, ,$$

neglect R_n^j and replace u by U in (5.2), we obtain the scheme

$$U_n^{j+1} = rU_{n+1}^j + (1-2r)U_n^j + rU_{n-1}^j \, , \tag{5.4}$$

with the boundary conditions

$$U_0^j = 0 \, , \qquad U_n^j = 0 \;\text{ and }\; U_n^0 = f_n \equiv f(x_n) \, .$$

With a little thought, we see that these boundary conditions and repeated use of (5.4) enable us to calculate U_n^j everywhere. We must now consider how accurate the approximation is. We next perform a simple " *Maximum Principle Analysis*" to show that under some conditions U_n^j can be made as close as we choose to the real solution u_n^j, for all n and j.

5.1 Maximum Principle Analysis (MPA)

In general, suppose a PDE

$$Lu = f,$$

where L is some differential operator, is approximated on a suitable grid $(nh,\, jk)$, at which points u and f take the values u_n^j and f_n^j, by the FDM

$$MU_n^j = f_n^j,$$

where M is a difference operator. The **solution error**, z_n^j and the **truncation error**, R_n^j, are defined by

$$z_n^j \equiv u_n^j - U_n^j \, , \;\text{ and }\; R_n^j \equiv (Lu)_n^j - MU_n^j \, . \tag{5.5}$$

Returning to our specific equation, subtracting (5.4) from (5.2), and using (5.5), we obtain

$$z_n^{j+1} = rz_{n+1}^j + (1-2r)z_n^j + rz_{n-1}^j + kR_n^j \;\text{ and }\; z_0^j = z_N^j = z_n^0 = 0 \, . \tag{5.6}$$

Now

$$|z_n^{j+1}| \leq |r|\;|z_{n+1}^j| + |(1-2r)|\;|z_n^j| + |r|\;|z_{n-1}^j| + |kR_n^j|.$$

Since $R_n^j = O(k, h^2)$, over the finite interval $0 < t < T \equiv Jk$ we can find a positive constant A such that $|R_n^j| \leq A(|k| + h^2)$. We shall also define the norm

$$||z^j|| \equiv \max_{n=0\ldots N} |z_n^j| \, ,$$

which is the maximum error over all the points at a fixed time-level j. Then $|z_n^j| \leq ||z^j||$ for all n, and so we have

$$|z_n^{j+1}| \leq \Big(|r| + |1-2r| + |r|\Big)||z^j|| + A(k^2 + |k|h^2)$$

As this is true for all values of n, it is true for that value which maximises its LHS, and so

$$||z^{j+1}|| \leq \Big(|r| + |1-2r| + |r|\Big)||z^j|| + A(k^2 + |k|h^2)$$

We now **assume** that $0 < r \leq \frac{1}{2}$, so that the quantities inside modulus signs are positive. Then the maximum possible error at the time-level $(j+1)$ is related to the maximum at time j by

$$||z^{j+1}|| \leq ||z^j|| + A(k^2 + |k|h^2)$$

Now the initial error, $||z^0||$, is zero because we know the solution exactly at $t = 0$. Applying the above repeatedly therefore implies

$$||z^1|| \leq |k|A(|k| + h^2)\ , \qquad ||z^2|| \leq 2|k|A(|k| + h^2) \text{ and } ||z^j|| \leq j|k|A(|k| + h^2)\ .$$

We have therefore shown that provided $0 < r \leq \frac{1}{2}$, the maximum possible error at time $t^j \equiv jk$ is $O(k,\, h^2)t^j$, which can be made as small as we choose by choosing small enough step-lengths, k and h. Note that $r < 0$ would correspond to $k < 0$, which involves stepping *backwards in time*, which we saw in §4 leads to an ill-posed problem for this *Parabolic* equation. We have proved nothing yet about the case $r > \frac{1}{2}$, but we will find that for such values of r the FDM (5.2) is numerically unstable.

6 Explicit Method for the General Non-linear Parabolic Problem in 1-D

Last time we proved that the simple explicit method for $u_t = u_{xx}$ would work provided $r < 1/2$ where $r = k/h^2$. Experiments with the program AdvDiff.m, show that if $r > 1/2$, the method breaks down seriously as small errors get amplified out of proportion. The program also considered the effect of an advecting velocity V, solving $u_t + Vu_x = au_{xx}$. It was found that even if $r < 1/2$, the method could be unstable. We can understand that by solving the scheme exactly, using separation of variables. Suppose at time $t = 0$ there is a small error proportional to εe^{inph}, namely a *Fourier series* component and where $\varepsilon \ll 1$. Here p represents a spatial wavenumber of the Fourier wave (or mode) and h the discretisation step size. Neglecting all subsequent truncation errors R_n^j, then from (5.6), the error z_n^j obeys the equation

$$z_n^{j+1} = rz_{n+1}^j + (1-2r)z_n^j + rz_{n-1}^j, \qquad z_n^0 = \varepsilon e^{inph}. \tag{6.1}$$

We can find **separable** solutions to this equation with $z_n^j = \varepsilon \xi^j \exp(inph)$ provided

$$\xi = re^{iph} + (1-2r) + re^{-iph} = 1 - 2r(1-\cos(ph)) = 1 - 4r\sin^2(\frac{ph}{2}). \tag{6.2}$$

If this error is not to grow, then we require $|\xi| \le 1$. Now clearly $\xi < 1$, but we need to ensure that $\xi > -1$. The worst case is when $ph = \pi$, and then we must require $1 - 4r \ge -1$ or $r \le 1/2$. If this constraint is violated, we expect the errors to grow. Note that the worst case $ph = \pi$ corresponds to a perturbation $\exp(inph)$ which alternates between $+1$ and -1 on neighbouring grid points. This is quite a common instability of finite difference methods. This is an example of the **Fourier** or **Von Neumann stability** method. Note the Fourier method ignores boundary conditions insofar as to how they might affect the numerical stability* – nevertheless it is a powerful yet simple procedure to determine the numerical stability of the approximations using FDs.

Consider a more general nonlinear equation,

$$\frac{\partial u}{\partial t} = \frac{\partial^2(u^p)}{\partial x^2} \quad \text{or equivalently} \quad u_t = (u^p)_{xx}, \tag{6.3}$$

where p is some value (for example $p = 3$, say). Applying the finite difference discretisation to this gives

$$u_n^{j+1} = u_n^j + r\left[(u_{n-1}^j)^p - 2(u_n^j)^p + (u_{n+1}^j)^p\right].$$

From a stability perspective, it is easy to see that for a **linear** PDE of the form $u_t = \beta u_{xx}$ with β some constant value, the stability criterion satisfies

$$\beta r \le \frac{1}{2} \quad \text{instead of} \quad r \le \frac{1}{2}.$$

The **effective** diffusion coefficient of (6.3) is pu^{p-1} if we rewrite this as follows

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(pu^{p-1}\frac{\partial u}{\partial x}\right) \equiv (pu^{p-1}u_x)_x.$$

*the matrix method is a more general approach, which allows effects of boundary conditions to be also incorporated into a detailed numerical stability analysis.

This then suggests possible stability of the numerical method provided

$$pu^{p-1}r \leq \frac{1}{2}. \tag{6.4}$$

This simple intuitive analysis suggests that stability of nonlinear parabolic PDEs, not only depends of the finite difference discretisation but also generally upon the solution being obtained, which clearly will be varying as the t-variable (time say) progresses. Thus the numerical scheme may well be stable for some values of t and not for others! In practice, one monitors the stability criterion (6.4) and alters the $k = \Delta t$ size to remain below the stability constraint requirement.

Let us try to generalise the Maximum Principle Analysis (MPA) to this more general type of parabolic PDEs.

Consider the problem defined for an arbitrary function Φ,

$$u_t = \Phi(x,\ t,\ u,\ u_x,\ u_{xx}) \in 0 < x < 1 = Nh, \qquad 0 < t < T = Jk. \tag{6.5}$$

For physical sense, we will assume that the effective diffusivity is positive and bounded, so that

$$A \geq \frac{\partial \Phi}{\partial u_{xx}} \geq\ a > 0 \tag{6.6}$$

for some constants A and a. A simple, centred, explicit method replaces

$$\left.\begin{array}{lll} u_x & \text{by} & \dfrac{1}{2h}\triangle U_n^j \equiv \dfrac{U_{n+1}^j - U_{n-1}^j}{2h}, \\[2ex] u_{xx} & \text{by} & \dfrac{1}{h^2}\delta^2 U_n^j \equiv \dfrac{U_{n+1}^j + U_{n-1}^j - 2U_n^j}{h^2} \end{array}\right\} \ +\ O(h^2), \tag{6.7}$$

so that

$$U_n^{j+1} = U_n^j + k\Phi\left[nh,\ jk,\ U_n^j,\ \frac{\triangle U_n^j}{2h}, \frac{\delta^2 U_n^j}{h^2}\right] + O(k^2 + kh^2). \tag{6.8}$$

As before, we define the local error $z_n^j = u_n^j - U_n^j$. Now u obeys the same equation as U with a truncation error $R_n^j = O(k,\ h^2)$ added in. Furthermore,

$$\begin{aligned} \Phi\left[nh,\ jk,\ u_n^j,\ \frac{\triangle u_n^j}{2h}, \frac{\delta^2 u_n^j}{h^2}\right] &- \Phi\left[nh,\ jk,\ U_n^j,\ \frac{\triangle U_n^j}{2h}, \frac{\delta^2 U_n^j}{h^2}\right], \\ &= \frac{\partial \Phi}{\partial u} z_n^j + \frac{\partial \Phi}{\partial u_x}\frac{\triangle z_n^j}{2h} + \frac{\partial \Phi}{\partial u_{xx}}\frac{\delta^2 z_n^j}{h^2} + O((z)^2). \end{aligned} \tag{6.9}$$

Subtracting (6.8) from the equation involving u and using the above, gives

$$z_n^{j+1} = r\left[\frac{\partial \Phi}{\partial u_{xx}} - \frac{h}{2}\frac{\partial \Phi}{\partial u_x}\right] z_{n-1}^j + r\left[\frac{\partial \Phi}{\partial u_{xx}} + \frac{h}{2}\frac{\partial \Phi}{\partial u_x}\right] z_{n+1}^j + \left[1 + k\frac{\partial \Phi}{\partial u} - 2r\frac{\partial \Phi}{\partial u_{xx}}\right] z_n^j + kR_n^j \tag{6.10}$$

Now the Maximum Principle argument requires the three coefficients in square brackets to be positive (see the arguments of §5, Eqn. (5.6) thereafter). Suppose therefore that

$$A \geq \frac{\partial \Phi}{\partial u_{xx}} \geq\ a > 0, \qquad \left|\frac{\partial \Phi}{\partial u_x}\right| \leq\ b\,, \qquad C \geq \frac{\partial \Phi}{\partial u} \geq\ c\,, \tag{6.11}$$

where $b > 0$, c and C are constants. Then

$$\frac{\partial \Phi}{\partial u_{xx}} \pm \tfrac{1}{2}h\frac{\partial \Phi}{\partial u_x} \geq\ a - \tfrac{1}{2}hb \ \text{ and } \ 1 + k\frac{\partial \Phi}{\partial u} - 2r\frac{\partial \Phi}{\partial u_{xx}} \geq\ 1 + kc - 2rA. \tag{6.12}$$

For the MPA, we therefore require

$$a - \tfrac{1}{2}hb \geq\ 0 \ \text{ and } \ 1 + kc - 2rA \geq\ 0. \tag{6.13}$$

If (6.13) holds then we can show in the notation of §5.1 that (6.10) implies

$$\left|z_n^{j+1}\right| \leq\ \left(1 + k\frac{\partial \Phi}{\partial u}\right) \max_n \left[\left|z_n^j\right|\right] + kR_n^j \leq\ (1 + kC)\left|\left|z^j\right|\right| + D(k^2 + |k|h^2)$$

for some constant $D > 0$, and so

$$\left|\left|z^{j+1}\right|\right| \leq\ (1 + kC)\left|\left|z^j\right|\right| + D(k^2 + |k|h^2)$$

Now the initial error $||z^0|| = 0$. Consequently

$$\begin{aligned} \left|\left|z^j\right|\right| &\leq\ \left[1 + (1 + kC) + (1 + kC)^2 + \ldots + (1 + kC)^{j-1}\right]\ D(k^2 + |k|h^2) \\ &\leq e^{CT}\ jD(k^2 + |k|h^2) \leq Te^{CT}D(|k|{+}h^2). \end{aligned} \tag{6.14}$$

Since†,

$$(1 + Ck)^n \leq \left(1 + \frac{CT}{n}\right)^n < e^{CT},$$

it follows that

$$\left|\left|z^j\right|\right| \leq\ \frac{e^{Cjk} - 1}{C}D(k + h^2) \qquad \text{for} \quad 1 \leq\ j \leq\ J \tag{6.15}$$

By choosing k and h small enough for fixed $T = Jk$ we can ensure that the errors are as small as we choose. Note that the exponential growth in the error term is due to the PDE itself possessing exponentially growing solutions. Compare with the equation $u_t = \nu u_{xx}$. We conclude that the explicit method will work for the nonlinear equation (6.5) provided (6.13) holds. These conditions are **sufficient** but may be overcautious.

As an example, consider Burgers' equation

$$u_t + uu_x = \nu u_{xx} \qquad \text{so that} \qquad \Phi = \nu u_{xx} - uu_x \tag{6.16}$$

where ν is constant. Then

$$A = a = \nu, \qquad b = \max_{x,t}\left[|u|\right], \qquad c = \min_{x,t}\left[-u_x\right],\ C = \max_{x,t}\left[-u_x\right]\ . \tag{6.17}$$

So the explicit method for this equation is stable if

$$\begin{aligned} \nu - \tfrac{1}{2}h\max\left[|u|\right] \geq\ 0 \qquad &\text{or} \qquad |u| \leq\ 2\nu/h \\ \text{and} \quad 1 + k\min\left[-u_x\right] - 2r\nu \geq\ 0 \quad &\text{or} \quad -u_x \geq\ (2r\nu - 1)/k \end{aligned} \tag{6.18}$$

The first of these conditions is a restriction on the size of the spatial step-length h for large values of the advective velocity u. In the absence of diffusion ($\nu = 0$) the centred scheme given by (6.8) is always unstable (see later). The second condition is a generalisation of the '$r < 1/2$' relation with which we are familiar. We note that if $2r\nu > 1$, no value of k will guarantee a stable scheme, and as $k \to 0$ the stability condition is violated.

† $k \equiv T/n$, with T a total time (say); moreover as a reminder $e^x = 1 + x + x^2/2 + x^3/3! + \ldots$

7 Implicit Scheme for the 1-D Diffusion equation

As we discussed last time, the explicit scheme (5.4) has effective characteristics with gradients $dx/dt = \pm h/k$. Arguably, this gradient should approach infinity if it is to model the physics, which might explain why the explicit scheme requires $k = O(h^2)$ for stability. Mathematically, the solution at time level $j+1$ should depend on all the values at time level j. Today we consider **implicit** methods for this problem, which do have this property. Let us choose a parameter θ and approximate $u_t = u_{xx}$ by

$$U_n^{j+1} - U_n^j = r\left[\theta\delta^2 U_n^{j+1} + (1-\theta)\delta^2 U_n^j\right]. \tag{7.1}$$

Note that the RHS now involves the unknown variables U_n^{j+1}. To find them we will have to solve a set of simultaneous linear equations (unless $\theta = 0$). Before considering how to do this numerically, we observe that for this linear problem, both the PDE and our Finite Difference approximation may be solved exactly by the method of separation of variables.

We seek solutions of the form $U_n^j = X_n T^j$. Substituting into (7.1) and separating the terms depending on j and n leads to

$$\frac{T^{j+1} - T^j}{r\left[\theta T^{j+1} + (1-\theta)T^j\right]} = \frac{X_{n+1} - 2X_n + X_{n-1}}{X_n} = \sigma, \quad \text{say.} \tag{7.2}$$

As the LHS varies with j but not n, and the RHS the other way round, σ must be a constant. X_n therefore obeys the second order difference equation

$$X_{n+1} - (\sigma+2)X_n + X_{n-1} = 0, \tag{7.3}$$

which has solutions of Fourier form $X_n = e^{\pm in\xi}$ provided $\sigma + 2 = 2\cos\xi$. In general ξ is arbitrary, but if we impose the boundary conditions $X_0 = 0 = X_n$, then we can show that

$$\xi = \frac{m\pi}{N} = m\pi h \qquad \text{for} \quad m = 1, 2\dots \quad \text{and} \quad \sigma = -4\sin^2\left(\frac{m\pi h}{2}\right) = \sigma_m, \tag{7.4}$$

say. Then X_n is given by

$$X_n = A\sin(nm\pi h). \tag{7.5}$$

For each such permissible value $\sigma = \sigma_m$, T^j can be found from (7.2).

$$T^{j+1} = \lambda_m T^j, \qquad \text{so that} \quad T^j = C(\lambda_m)^j \qquad \text{where} \quad \lambda_m = \left[\frac{1 + \sigma_m r(1-\theta)}{1 - \sigma_m r\theta}\right]. \tag{7.6}$$

Now we have

$$\lambda_m = \frac{1 - 4r(1-\theta)\sin^2\frac{1}{2}\xi}{1 + 4r\theta\sin^2\frac{1}{2}\xi} = 1 - \frac{4r\sin^2\frac{1}{2}\xi}{1 + 4r\theta\sin^2\frac{1}{2}\xi}. \tag{7.7}$$

The stability requirement is that $|\lambda_m| \le 1$ for all m. Clearly $\lambda_m \le 1$, while $\lambda_m \ge -1$ if

$$1 + 4r\theta\sin^2\tfrac{1}{2}\xi \;\ge\; 2r\sin^2\tfrac{1}{2}\xi, \tag{7.8}$$

or

$$(1-2\theta)2r\sin^2\tfrac{1}{2}\xi \;\le\; 1. \tag{7.9}$$

If $\theta \geq \frac{1}{2}$, therefore, the FDM (7.1) is **unconditionally stable**. If on the other hand

$$0 \;\leq\; \theta < \tfrac{1}{2},$$

stability for all m and h can be guaranteed only if

$$r \;\leq\; \frac{1}{2(1-2\theta)}. \tag{7.10}$$

Note that when $\theta = 0$ we recover the relation $r \;\leq\; \frac{1}{2}$ and (7.1) is then **conditionally stable.**

We can obtain the general solution by taking an arbitrary linear sum,

$$U_n^j = \sum_{m=1}^{\infty} B_m \sin(nm\pi h)(\lambda_m)^j, \tag{7.11}$$

where the coefficients B_m can be found from the Fourier expansion of the initial condition $u_0(x)$ of (7.1). We can now compare (7.11) with the exact solution evaluated at the grid points

$$U_n^j \equiv u(nh,\, jk) = \sum_{m=1}^{\infty} B_m \sin(nm\pi h)(e^{-m^2\pi^2 k})^j \tag{7.12}$$

The accuracy of the F.D. approximation may thus be determined by comparing λ_m and $\exp(-m^2\pi^2 k)$.

We see that it is the high modes, the large values of m for which $m \sim N$ and $\xi \sim \pi$ which are most likely to be unstable. This is typical behaviour for FDMs; instabilities tend to manifest themselves on the scale of the grid. The low modes, for which $m = O(1)$, and ξ is small are modelled well. For them we may approximate $\sin\beta \approx \beta - \frac{1}{6}\beta^3$ to give

$$\begin{aligned}
\lambda_m &\approx 1 - \frac{r(\xi - \frac{1}{24}\xi^3 + O(\xi^5))^2}{1 + r\theta\xi^2 + O(r\xi^4)}, \\
&= 1 - r\xi^2(1 - \tfrac{1}{12}\xi^2)(1 - r\theta\xi^2) + O(r^3\xi^6). \\
&= 1 - m^2\pi^2 k + \left(\theta + \frac{1}{12r}\right) m^4\pi^4 k^2 + O(m^6 k^3) \\
\text{while} \quad e^{-m^2\pi^2 k} &= 1 - m^2\pi^2 k + \tfrac{1}{2} m^4\pi^4 k^2 + O(m^6 k^3).
\end{aligned} \tag{7.13}$$

The agreement between λ_m and $\exp(-m^2\pi^2 k)$ is quite good, while the greatest accuracy is achieved if

$$\theta = \frac{1}{2} - \frac{1}{12r} \qquad \text{or} \qquad r(1-2\theta) = \frac{1}{6}.$$

We see from (7.9) that such a scheme would be stable. It is the generalisation of Milne's method ($\theta = 0,\; r = \frac{1}{6}$). If r is large, then the Crank-Nicolson scheme ($\theta = \frac{1}{2}$) is close to optimal.

Most importantly, using implicit methods we can produce stable schemes with $k \sim h$, and hence large values of $r = k/h^2$. Compared with the explicit schemes, we may choose relatively large time-steps.

7.1 The Crank-Nicolson method and (nearly) Tridiagonal systems

If we choose an unconditionally stable scheme with $\theta > 1/2$, then we may choose the time-step as large as we like, and our only concern is the accuracy of our approximation of the derivatives. A popular (and sensible) choice is the **Crank-Nicolson** scheme, $\theta = 1/2$. This scheme is centred about the time-level $(j + 1/2)$, and so is second-order accurate in both space and time, $R_n^j = O(k^2, h^2)$. The price we pay for an implicit scheme is that each time-step we have to solve some simultaneous linear equations. However, as the system is tri-diagonal this is not so hard. If we represent a list of all the U-values at time j by a vector U^j , then the system we need to solve is

$$AU^{j+1} = BU^j, \quad \text{where} \quad U^j = (U_1^j, U_2^j, \ldots, U_N^j)^T$$

for suitable matrices A and B. In this problem, A and B are tridiagonal, which permits efficient solution. The Crank-Nicolson ($\theta = 1/2$) method for the equation $u_t = u_{xx}$ has

$$\mathcal{A} = \begin{pmatrix} 1+r & -r/2 & 0 & \ddots & 0 \\ -r/2 & 1+r & -r/2 & \ddots & \ddots \\ 0 & -r/2 & 1+r & -r/2 & 0 \\ \ddots & \ddots & \ddots & \ddots & -r/2 \\ 0 & \ddots & 0 & -r/2 & 1+r \end{pmatrix},$$

To solve $Ax = b$, where A is an $M \times M$ matrix. usually requires $O(M^3)$ operations. Here, however, the sparseness and structure of A renders the process much more efficient. Using Gaussian elimination, subtracting $(-r/2)/(1+r)$ times the first row from the second transforms A_{21} to zero and alters A_{22} and b_2. Then subtracting a suitable multiple of the 2nd row from the 3rd and continuing, leaves us with

$$\mathcal{A} = \begin{pmatrix} 1+r & -r/2 & 0 & \ddots & 0 \\ 0 & a_2 & -r/2 & \ddots & \ddots \\ 0 & 0 & 1+r & a_3 & 0 \\ \ddots & \ddots & \ddots & \ddots & -r/2 \\ 0 & \ddots & 0 & 0 & a_n \end{pmatrix} x = b^*,$$

where a_i and b^* are known values. The last equation is now trivial, $a_n x_n = b_n^*$, while the penultimate term $a_{n-1}x_{n-1} = b_{n-1}^* + (r/2)x_n$ which we now know, giving us x_{n-1}. Systematically back-substituting determines all the x_i unknowns.

The algorithm, also known as the **Thomas algorithm**, is a simplified form of Gaussian elimination that can be used to solve tridiagonal systems of equations. For such systems, the solution can be obtained in $O(M)$ operations instead of $O(M^3)$ required by Gaussian elimination. See the routine tridiag.m.

7.2 Aside – Separation of variables solution to Diffusion eqn.

We consider a slight modification of (7.1), namely:

$$\begin{aligned} u_t = u_{xx} \in 0 < x < 1,\ t > 0, \\ \text{with}\ \ u(0,t) = u(1,t) = 0, \quad u(x,0) = u_0(x). \end{aligned} \tag{7.14}$$

The PDE has separable solutions of the form $u(x,t) = X(x)T(t)$ provided

$$XT' = X''T \qquad \text{or} \qquad \frac{T'}{T} = \frac{X''}{X} = -\omega^2, \qquad \text{say.}$$

As T'/T is a function of t only, while X''/X is a function of x only, both functions must be a constant, which we take to be negative. Then the functions $X(x)$ and $T(t)$ take the forms

$$X = A\cos\omega x + B\sin\omega x, \ \text{ and } \ T = Ce^{-\omega^2 t}.$$

If we require X to obey the boundary conditions in (7.3), namely $X(0) = X(1) = 0$, we obtain non-zero solutions only if $A = 0$ and $\omega = m\pi$, for some integer m, so that

$$u = B_m \sin m\pi x\, e^{-m^2\pi^2 t},$$

for some constant B_m. As (7.14) is a linear problem, we may combine solutions to obtain a more general solution in the form

$$u(x,\,t) = \sum_{m=1}^{\infty} B_m \sin m\pi x\, e^{-m^2\pi^2 t}. \tag{7.15}$$

The initial condition will be satisfied if

$$u(x,\,0) = \sum_{m=1}^{\infty} B_m \sin m\pi x = u_0(x). \tag{7.16}$$

Thus all we need do to obtain the solution of (7.14) is to expand the initial condition $u = u_0(x)$ in a Fourier series, and substitute the appropriate values of the constants B_m into (7.15).

8 Implicit Method for Nonlinearities

How should we adapt our implicit methods for nonlinear PDEs? While it would be possible to solve nonlinear equations each time-step, that is not usually necessary, or advisable. Instead, we can seek linear approximations whose errors are the same order as our original truncation. For example, consider

$$\frac{\partial u}{\partial t} = \mathcal{D}\frac{\partial^2 u}{\partial x^2} + f(u)$$

for some function $f(u)$.

As an example, the Fisher-Kolmogorov-Petrovsky-Piskunov (Fisher-KPP) equation with

$$f(u) = ru\left(1 - \frac{u}{K}\right)$$

is one of the simplest examples of a nonlinear reaction-diffusion equation. Fisher proposed this as a model of diffusion of species in a 1-D habitat; $\mathcal{D}$ is the diffusion constant, r is the growth rate of the species, and K is the carrying capacity. A dimensionless version takes the form

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u(1-u).$$

Model forms of the equation arise in diverse physical, chemical and biological phenomena. In flame propagation

$$f(u) = \frac{\beta^2}{2}u(1-u)e^{-\beta(1-u)}, \text{ with } \beta \text{ known as the Zeldovich number.}$$

Similar forms arise in nuclear reactors and neutron population modelling, chemical reaction and Brownian-motion type problems.

The simplest thing to do would be to treat the nonlinear term $f(u)$ explicitly. Alternatively, if using a Crank-Nicolson formulation, we might expect best accuracy if we centre $f(u)$ about $j+\frac{1}{2}$, writing

$$U_n^{j+1} - U_n^j = \frac{r}{2}\left(\delta^2 U_n^j + \delta^2 U_n^{j+1}\right) + \frac{k}{2}\left(f(U_n^j) + f(U_n^{j+1})\right). \tag{8.1}$$

If $f(u)$ is differentiable, we could then approximate the nonlinear unknown term by

$$f(U_n^{j+1}) = f(U_n^j) + f'(U_n^j)\left(U_n^{j+1} - U_n^j\right) + O\left(|U_n^{j+1} - U_n^j|^2\right). \tag{8.2}$$

Combining Eqns. 8.1 and 8.2, U_n^{j+1} now appears linearly on the RHS. We can then modify the matrices $\mathcal{A}$ and $\mathcal{B}$ developed earlier:

$$\mathcal{A}\, U^{j+1} = \mathcal{B}\, U^j + c^j$$

accordingly. Note that in general, the stability of the method depends on the eigenvalues of $\mathcal{A}^{-1}\mathcal{B}$, which may change if we alter $\mathcal{A}$ and $\mathcal{B}$.