Dr H. Fawzi

Mathematical Tripos Part II: Michaelmas Term 2023

Numerical Analysis – Lecture 10

Splitting for the 2D diffusion equation Recall that for the 2D diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial x^2}$$

using the five-point discretisation scheme for the Laplacian yields the following ODE

$$\frac{d\boldsymbol{u}}{dt} = \frac{1}{h^2}(A_x + A_y)\boldsymbol{u}$$

where the matrices A_x and A_y are expressed as $A_x = G \otimes I$ and $A_y = I \otimes G$, where $\otimes$ is the Kronecker product, and G is the $M \times M$ tridiagonal matrix

$$G = \begin{bmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{bmatrix} \in \mathbb{R}^{M\times M}.$$

It is straightforward to verify that A_x and A_y commute; namely $A_xA_y = A_yA_x = G \otimes G$ (this should not come as a suprise since the operators $\partial^2/\partial x^2$ and $\partial^2/\partial y^2$, which A_x/h^2 and A_y/h^2 approximate, are known to commute.) So we can write $\mathrm{e}^{k(A_x+A_y)/h^2} = \mathrm{e}^{kA_x/h^2}\mathrm{e}^{kA_y/h^2}$. This means that the solution of the semi-discretized diffusion equation in 2D, with zero boundary conditions, satisfies

$$\boldsymbol{u}^{n+1} = \mathrm{e}^{kA_x/h^2}\mathrm{e}^{kA_y/h^2}\boldsymbol{u}^n. \tag{2.17}$$

Split Crank-Nicolson: In the split Crank-Nicolson scheme, we approximate each exponential map in (2.17) by the rational function $r(z) = (1 + z/2)(1 - z/2)^{-1}$, which leads to

$$\boldsymbol{u}^{n+1} = (I + \tfrac{\mu}{2}A_x)(I - \tfrac{\mu}{2}A_x)^{-1}(I + \tfrac{\mu}{2}A_y)(I - \tfrac{\mu}{2}A_y)^{-1}\boldsymbol{u}^n. \tag{2.18}$$

Note that computing $\boldsymbol{u}^{n+1/2} = (I + \frac{\mu}{2}A_y)(I - \frac{\mu}{2}A_y)^{-1}\boldsymbol{u}^n$ can be done efficiently in $\mathcal{O}(M^2)$ time as A_y is block-diagonal, and the matrices G are tridiagonal (each tridiagonal solve requires $\mathcal{O}(M)$ time, and we have M of these). Computing $\boldsymbol{u}^{n+1} = (I + \frac{\mu}{2}A_x)(I - \frac{\mu}{2}A_x)^{-1}\boldsymbol{u}^{n+1/2}$ can also be done in $\mathcal{O}(M^2)$ time, since A_x is also block-diagonal provided we appropriately permute the rows and columns so that the grid ordering is by rows instead of columns. This means that the update step (2.18) of Split-Crank-Nicolson can be performed in time $\mathcal{O}(M^2)$ and only requires tridiagonal matrix solves (no FFT needed).

One can easily verify stability of the split Crank-Nicolson scheme. Indeed, we can write

$$\|r(\mu A_x)r(\mu A_y)\|_2 \le \|r(\mu A_x)\|_2\|r(\mu A_y)\|_2 \le 1$$

since, as seen in previous lectures, $\|r(\mu A_x)\|_2 = \|(I + \frac{\mu}{2}A_x)(I - \frac{\mu}{2}A_x)^{-1}\|_2 \le 1$ since A_x is symmetric and its eigenvalues are ≤ 0. (Same for $\|r(\mu A_y)\|_2$.)

To check the consistency of the scheme, we need to show that the difference

$$\boldsymbol{u}^{n+1} - r(\mu A_x)r(\mu A_y)\boldsymbol{u}^n$$

is $\mathcal{O}(k^2)$, when $\boldsymbol{u}^n$ and $\boldsymbol{u}^{n+1}$ hold the true solutions of the diffusion PDE at the corresponding time steps, i.e., $\boldsymbol{u}^{n+1} = \mathrm{e}^{k(\partial^2/\partial x^2+\partial^2/\partial y^2)}\boldsymbol{u}^n$. We can write $\mu A_y = kA_y/h^2 = k(\frac{\partial^2}{\partial y^2} + \mathcal{O}(h^2))$, and so $r(\mu A_y) = \mathrm{e}^{k\partial^2/\partial y^2} + \mathcal{O}(k^3 + kh^2)$. Similarly, $r(\mu A_x) = \mathrm{e}^{k\partial^2/\partial x^2} + \mathcal{O}(k^3 + kh^2)$. Hence we get $r(\mu A_x)r(\mu A_y) = \mathrm{e}^{k\partial^2/\partial x^2}\mathrm{e}^{k\partial^2/\partial y^2} + \mathcal{O}(k^3 + kh^2) = \mathrm{e}^{k(\partial^2/\partial x^2+\partial^2/\partial y^2)} + \mathcal{O}(k^3 + kh^2)$. This gives consistency since $h^2 = k/\mu = \mathcal{O}(k)$.

2D diffusion with variable diffusion coefficient In general, however, the matrices B and C in $A = B + C$ do not have to commute, as in the following example: The general diffusion equation with a diffusion coefficient $a(x, y) > 0$ is given by:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(a(x,y)\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(a(x,y)\frac{\partial u}{\partial y}\right), \tag{2.19}$$

together with initial conditions on $[0, 1]^2$ and Dirichlet boundary conditions along $\partial[0, 1]^2 \times [0, \infty)$. We replace each space derivative by *central differences* at midpoints,

$$\frac{\mathrm{d}g(\xi)}{\mathrm{d}\xi} \approx \frac{g(\xi + \frac{1}{2}h) - g(\xi - \frac{1}{2}h)}{h},$$

resulting in the ODE system

$$\begin{aligned} u'_{\ell,m} \;=\; \frac{1}{h^2}\Big[&a_{\ell-\frac{1}{2},m}u_{\ell-1,m} + a_{\ell+\frac{1}{2},m}u_{\ell+1,m} + a_{\ell,m-\frac{1}{2}}u_{\ell,m-1} + a_{\ell,m+\frac{1}{2}}u_{\ell,m+1} \\ &- \big(a_{\ell-\frac{1}{2},m} + a_{\ell+\frac{1}{2},m} + a_{\ell,m-\frac{1}{2}} + a_{\ell,m+\frac{1}{2}}\big)u_{\ell,m}\Big]. \end{aligned} \tag{2.20}$$

Assuming zero boundary conditions, we have a system $\boldsymbol{u}' = A\boldsymbol{u}$, and the matrix A can be split as $A = \frac{1}{h^2}(A_x + A_y)$. Here, A_x and A_y are again constructed from the contribution of discretizations in the x- and y-directions respectively, namely A_x includes all the $a_{\ell\pm\frac{1}{2},m}$ terms, and A_y consists of the remaining $a_{\ell,m\pm\frac{1}{2}}$ components. The resulting operators A_x and A_y do not necessarily commute, and so the splitting scheme

$$\boldsymbol{u}^{n+1} = \mathrm{e}^{kA_x/h^2}\mathrm{e}^{kA_y/h^2}\boldsymbol{u}^n$$

will carry an error of $\mathcal{O}(k^2)$, following Proposition 2.25.

Strang splitting: One can obtain better splitting approximations of $\mathrm{e}^{t(B+C)}$. For example it is not hard to prove that $\mathrm{e}^{\frac{1}{2}tB}\mathrm{e}^{tC}\mathrm{e}^{\frac{1}{2}tB}$ gives a $\mathcal{O}(t^3)$ approximation of $\mathrm{e}^{t(B+C)}$, i.e.,

$$\mathrm{e}^{t(B+C)} = \mathrm{e}^{\frac{1}{2}tB}\mathrm{e}^{tC}\mathrm{e}^{\frac{1}{2}tB} + \mathcal{O}(t^3). \tag{2.21}$$

Remark 2.31 (Splitting of inhomogeneous systems) Our exposition so far has been limited to the case of zero boundary conditions. In general, the linear ODE system is of the form

$$\boldsymbol{u}' = A\boldsymbol{u} + \boldsymbol{b}, \qquad \boldsymbol{u}(0) = \boldsymbol{u}^0, \tag{2.22}$$

where $\boldsymbol{b}$ originates in boundary conditions (and, possibly, in a forcing term $f(x, y)$ in the original PDE (2.19)). Note that our analysis should accommodate $\boldsymbol{b} = \boldsymbol{b}(t)$, since boundary conditions might vary in time! The *exact* solution of (2.22) is provided by the *variation of constants* formula

$$\boldsymbol{u}(t) = \mathrm{e}^{tA}\boldsymbol{u}(0) + \int_0^t \mathrm{e}^{(t-s)A}\boldsymbol{b}(s)\,\mathrm{d}s, \qquad t \ge 0,$$

therefore

$$\boldsymbol{u}(t_{n+1}) = \mathrm{e}^{kA}\boldsymbol{u}(t_n) + \int_{t_n}^{t_{n+1}} \mathrm{e}^{(t_{n+1}-s)A}\boldsymbol{b}(s)\,\mathrm{d}s\,.$$

The integral on the right-hand side can be evaluated using quadrature. For example, the trapezoidal rule $\int_0^k g(\tau)\,\mathrm{d}\tau = \frac{1}{2}k[g(0) + g(k)] + \mathcal{O}(k^3)$ gives

$$\boldsymbol{u}(t_{n+1}) \;\approx\; \mathrm{e}^{kA}\boldsymbol{u}(t_n) + \tfrac{1}{2}k[\mathrm{e}^{kA}\boldsymbol{b}(t_n) + \boldsymbol{b}(t_{n+1})],$$

with a local error of $\mathcal{O}(k^3)$. We can now replace exponentials with their splittings. For example, Strang's splitting (2.21), together with the rational function approximation $r(z) = (1 + z/2)/(1 - z/2)$ of the exponential map, results in

$$\boldsymbol{u}^{n+1} \;=\; r\big(\tfrac{1}{2}kB\big)\,r\big(kC\big)\,r\big(\tfrac{1}{2}kB\big)\big[\boldsymbol{u}^n + \tfrac{1}{2}k\boldsymbol{b}^n\big] + \tfrac{1}{2}k\boldsymbol{b}^{n+1}.$$

As before, everything reduces to (inexpensive) solution of tridiagonal systems.