Lecture 22: Operator Splitting – Fractional Step Methods

If we have a parabolic-like equation and discretise the spatial derivatives, we have a set of differential equations of the form

$$\mathbf{u}_t = L\mathbf{u}, \qquad \text{where } L \text{ is an operator, perhaps a matrix.} \tag{22.1}$$

Using a Taylor series, we have

$$\frac{\mathbf{u}^{j+1} - \mathbf{u}^j}{k} = \mathbf{u}_t + \tfrac{1}{2}k\mathbf{u}_{tt} + \ldots \tag{22.2}$$

Assuming the operator L is time-independent, then using the Lax-Wendroff idea, we can write $\mathbf{u}_{tt} = L\mathbf{u}_t = L(L\mathbf{u}) \equiv L^2\mathbf{u}$ and then

$$\mathbf{u}^{j+1} = \mathbf{u}^j + kL\mathbf{u}^j + \tfrac{1}{2}k^2L^2\mathbf{u}^j + \ldots = (I + kL + \tfrac{1}{2}k^2L^2 + \ldots)\mathbf{u}^j. \tag{22.3}$$

Here I denotes the identity operator – we can think of it as "1". Defining the exponential operator $\exp(kL) \equiv (I + kL + \frac{1}{2}k^2L^2 + \frac{1}{6}k^3L^3 \ldots)$, then the exact solution of (22.2) can be written

$$\mathbf{u}^{j+1} = \exp(kL)\mathbf{u}^j. \tag{22.4}$$

But we will only be concerned with the $O(k^2)$ terms below.

Often we will be dealing with equations with qualitatively different terms (e.g. advection, diffusion, nonlinear forcing) which, drawing on our previous experience, we may wish to deal with individually in different manners. For example, perhaps one part we feel should be dealt with explicitly using Lax-Wendroff, and another implicitly using multigrid. Can we treat the two parts differently without sacrificing the overall accuracy of the scheme? This is the idea behind **Operator Splitting**. Recall lecture 7 on the ADI method, where for the 2D diffusion equation we alternately treated the Laplacian explicitly in the x-direction and implicitly in the y-direction and then vice versa. Can we do the same thing in general?

Suppose we have two processes which we represent by spatial discretisations L and M

$$\mathbf{u}_t = L\mathbf{u} + M\mathbf{u} \tag{22.5}$$

which has the solution

$$\mathbf{u}^{j+1} = \mathbf{u}^j + k(L+M)\mathbf{u}^j + \tfrac{1}{2}k^2(L+M)^2\mathbf{u}^j + \ldots \tag{22.6}$$

Note this is a schematic representation – the operators could involve iteration or implicit methods, but ultimately we represent the operation in this manner. Suppose we alternate solving $u_t = Lu$ and $u_t = Mu$ by our favourite methods solving

$$\begin{aligned} \widehat{\mathbf{u}} &= (I + kL + \tfrac{1}{2}k^2L^2)\mathbf{u}^j, \qquad \text{and then} \\ \mathbf{u}^{j+1} &= (I + kM + \tfrac{1}{2}k^2M^2)\widehat{\mathbf{u}} \end{aligned} \tag{22.7}$$

We then have

$$\begin{aligned}\mathbf{u}^{j+1} &= (I + kM + \tfrac{1}{2}k^2M^2)(I + kL + \tfrac{1}{2}k^2L^2)\mathbf{u}^j \\ &= \mathbf{u}^j + k(L+M)\mathbf{u}^j + \tfrac{1}{2}k^2(M^2 + L^2 + 2ML)\mathbf{u}^j.\end{aligned} \tag{22.8}$$

Is this the same as (22.6)? Only if $ML = LM$ so that the two operators commute. This will not usually be the case, so that the simple splitting method has an error of $O(k)$, even if L and M are implemented in an $O(k^2)$ manner.

With a little more work, we can achieve 2nd order accuracy. We could, for example, now go back to $\mathbf{u}^j$ and do an L step and then an M step upon it. Averaging the two resulting estimates for $\mathbf{u}^{j+1}$, we will have the correct $O(k^2)$ term, $\frac{1}{2}(L^2+M^2+LM+ML)$. More subtly, and more efficiently, we could adopt the time-symmetric scheme of taking a half-step with L, a full step with M and then a half-step with L, a process known as Strang splitting. Thus

$$\begin{aligned}\widehat{\mathbf{u}} &= (I + \tfrac{1}{2}kL + \tfrac{1}{2}(\tfrac{1}{2}k)^2L^2)\mathbf{u}^j \\ \mathbf{u}^* &= (I + kM + \tfrac{1}{2}k^2M^2)\widehat{\mathbf{u}} \qquad . \\ \mathbf{u}^{j+1} &= (I + \tfrac{1}{2}kL + \tfrac{1}{2}(\tfrac{1}{2}k)^2L^2)\widehat{\mathbf{u}}^*\end{aligned} \tag{22.9}$$

The final estimate is $\mathbf{u}^{j+1} = P\mathbf{u}^j$ where, neglecting terms of $O(k^3)$,

$$\begin{aligned}P &= (I + \tfrac{1}{2}kL + \tfrac{1}{8}k^2L^2)(I + kM + \tfrac{1}{2}k^2M^2)(I + \tfrac{1}{2}kL + \tfrac{1}{8}k^2L^2) \\ &= I + k(\tfrac{1}{2}L + M + \tfrac{1}{2}L) + k^2\left(\tfrac{1}{8}L^2 + \tfrac{1}{2}M^2 + \tfrac{1}{8}L^2 + \tfrac{1}{2}LM + \tfrac{1}{2}ML + \tfrac{1}{4}L^2\right) \\ &= I + k(L+M) + \tfrac{1}{2}k^2(L^2 + M^2 + LM + ML),\end{aligned} \tag{22.10}$$

which agrees with the estimate (22.6). The method (22.9) uses two calls to the "L"-routine and one to the "M" routine. Other things being equal, we would choose M to be the more time-expensive routine.

But wait! We're not just doing one step, we're taking several. Our 1st time step ends with a half-step in L, and the second begins with a half step in L – we could combine those and take a full step with L. As a check we note that taking two half-steps involves

$$(I + \tfrac{1}{2}kL + \tfrac{1}{8}k^2L^2)^2 = I + kL + (\tfrac{2}{8} + \tfrac{1}{4})k^2L^2 = I + kL + \tfrac{1}{2}k^2L^2, \tag{22.11}$$

which is the same as one complete k-step. To put it another way, we have shown that operating alternately with L and M is the same as $(L+M)$. Clearly the operator $\frac{1}{2}L$ commutes with itself. Thus we can preserve $O(k^2)$ accuracy by beginning with a half-step with L, then alternating full-steps with M and then L, ending with a half-step in L.