Model Equations

In general, when we develop a numerical scheme to approximate a PDE, we anticipate that our scheme will not allow us to solve the PDE exactly: rather, it will produce a solution that contains some error. In particular, the local truncation error of a given method is merely a measure of how well the true solution of the difference equation satisfies our numerical method. An interesting question to ask, then, is the following:

> Is there a PDE to which our numerical approximation Q_i^n is actually the exact solution?

This question may be difficult to answer, but we should believe that the following is somewhat easier:

> Can we at least find an equation that is better satisfied by Q_i^n than the original PDE we were attempting to solve?

If we can find such an equation, we can often learn a great deal about the numerical method used to generate it, since it is usually much easier to study the solutions of PDEs than those of finite difference formulas.

In fact, using a Taylor series expansion, we can find a PDE which satisfies the difference equation exactly, but it will have infinitely many terms. The idea is to truncate this series at some point, yielding a PDE that is simple enough to study while simultaneously giving a good indication of the behavior of Q_i^n. One interesting fact is that, if the method is accurate to order s, the new equation (which we call the **model equation**) is generally a modification of the original PDE with new terms of order s.

Example Consider the the first order upwind method for the one dimensional advection equation $\phi_t + u\phi_x = 0$ in the case $u > 0$.

$$\frac{Q_i^{n+1} - Q_i^n}{\Delta t} + u\frac{Q_i^n - Q_{i-1}^n}{\Delta x} = 0$$

$$Q_i^{n+1} = Q_i^n - u\frac{\Delta t}{\Delta x}\left(Q_i^n - Q_{i-1}^n\right) \tag{1}$$

We can insert a function $v(x,t)$ into the numerical method (much in the same way we insert the true solution $q(x,t)$ when determining the local truncation error) in order to find a differential equation that is satisied by v. Note that v is a function that agrees with Q_i^n exactly at the grid points, and thus $v(x,t)$ satisfies (1) exactly:

$$v(x, t + \Delta t) = v(x,t) - u\frac{\Delta t}{\Delta x}\left[v(x,t) - v(x - \Delta x, t)\right].$$

Now, if we Taylor expand about (x,t) and simplify, we get

$$\left(v_t + \frac{1}{2}\Delta t\ v_{tt} + \frac{1}{6}(\Delta t)^2 v_{ttt} + \cdots\right) + u\left(v_x - \frac{1}{2}\Delta x\ v_{xx} + \frac{1}{6}(\Delta x)^2 v_{xxx} + \cdots\right) = 0.$$

This can be rewritten as

$$v_t + uv_x = \frac{1}{2}\left(u\Delta x\ v_{xx} - \Delta t\ v_{tt}\right) - \frac{1}{6}\left[u(\Delta x)^2 v_{xxx} + (\Delta t)^2 v_{ttt}\right] + \cdots .$$

This resulting equation is precisely the PDE that v satisfies. If we assume $\Delta t/\Delta x$ is fixed, then the terms on the right hand side are $O(\Delta t)$, $O(\Delta t^2)$, etc., so for small Δt we can truncate the series to obtain a PDE that is well satisfied by the Q_i^n. In particular, if we drop *all* the terms on the right, we recover the original advection equation. Since this is equivalent to dropping terms of $O(\Delta t)$, we expect that Q_i^n satisfies this equation to $O(\Delta t)$, which we know to be correct since this upwind method is first order accurate.

If, instead, we *keep* the $O(\Delta t)$ terms, we get:

$$v_t + uv_x = \frac{1}{2}\left(u\Delta x\ v_{xx} - \Delta t\ v_{tt}\right). \tag{2}$$

This involves second derivatives in both x and t, but we can derive a slightly different model equation with the same accuracy by differentiating (2) with respect to t to obtain

$$v_{tt} = -uv_{xt} + \frac{1}{2}\left(u\Delta x\ v_{xxt} - \Delta t\ v_{ttt}\right)$$

and with respect to x to obtain

$$v_{tx} = -uv_{xx} + \frac{1}{2}\left(u\Delta x\ v_{xxx} - \Delta t\ v_{ttx}\right).$$

Combining these equations (by reording the partials) gives us

$$v_{tt} = u^2\ v_{xx} + O(\Delta t).$$

Combining this equation with (2) gives

$$v_t + uv_x = \frac{1}{2}(u\Delta x\ v_{xx} - u^2\Delta t\ v_{xx}) + O(\Delta t^2).$$

Since we have already dropped $O(\Delta t^2)$ terms, we may do so here to obtain

$$v_t + uv_x = \frac{1}{2}u\Delta x(1-\nu)v_{xx}$$

where $\nu = u\Delta t/\Delta x$ is the *Courant number*.

We have now transformed our model equation into a more familiar advection-diffusion equation, and the grid function Q_i^n can be viewed as giving a second order accurate approximation to the true solution of this equation. The fact that the model equation for the upwind method is an advection-diffusion equation explains a great deal about how the numerical solution behaves. Solutions to the advection-diffusion equation translate at the proper speed u, but become smeared out over time.

If we examine the diffusion coefficient in our equation, we note that it vanishes in the special case $u\Delta t = \Delta x$. In this case, the exact solution to the advection equation is recovered by the upwind method. Also, we note that the diffusion coefficient is positive only if $0 < u\Delta t/\Delta x < 1$. This is precisely the stability limit of the upwind method! If it is violated, the diffusion coefficient in the model equation is negative, giving an ill-posed *backward heat equation*.

Dissipation v. Dispersion

As we have already seen, dissipation is essentially a kind of energy loss. Adding dissipation to the advection equation essentially says that the change in ϕ over time results *mostly* from the bulk motion of the fluid flow, but not entirely. Dissipation has the net effect of making a wave form decay over time (things get smeared out) and can thus be useful in damping spurious oscillations. Formally we say that a one-step scheme has **dissipation** of order $2r$ if there exists a positive constant c independent of Δt and Δx, such that

$$|g(\Delta x\xi)| \leq 1 - c(\sin \frac{1}{2}\Delta x\xi)^{2r}.$$

If dissipation causes a wave to decay over time, dispersion is a phenomena that leads to the gradual separation of a waveform into a trail of oscilations. We recall (via a few judicious applications of the Fourier inversion formula) that we can write the solution of the one-way wave equation as

$$u(t,x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega x} e^{-i\omega a t} \hat{u}_0(\omega) d\omega.$$

From this, we can conclude that the Fourier transform of the solution satisfies

$$\hat{u}(t + \Delta t, \omega) = e^{-i\omega a \Delta t} \hat{u}(t, \omega).$$

Recall too that, when we consider a one-step finite difference scheme, we have seen that

$$\hat{v}^{n+1} = g(\Delta x\xi)\hat{v}^n.$$

By comparing these two equations, we see that we can expect that $g(\Delta x\xi)$ will be a good approximation to $e^{-i\omega a\Delta x}$. In particular, we can write:

$$g(\Delta x\xi) = |g(\Delta x\xi)| e^{-i\xi\alpha(\Delta x\xi)\Delta t}.$$

The quantity $\alpha(\Delta x\xi)$ is called the *phase speed* and is the speed at which waves of frequency ξ are propogated by the finite difference scheme. If $\alpha(\Delta x\xi)$ were equal to a for all ξ, then waves would propogate with the correct speed. However, in practice, this is almost never the case. This is the precise definition of **dispersion**: the finite different scheme propogates waves of different frequencies with different speeds. To precisely quantify the error generated by dispersion, it is oftentimes useful to examine the *phase error* of a finite difference scheme, which is given by $a - \alpha(\Delta x\xi)$.

Kinematic Description of Rigid Body Orientation

If we simulate a rigid body in space, we need only track it's position $\mathbf{x}$ and its orientation $\mathbf{R}$. $\mathbf{R}$ describes the current rotation of the rigid body, relative to some initial (or rest) state. In 2-D, the orientation of a rigid body is completely described by an angle θ, and

$$\mathbf{R} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}. \tag{3}$$

In 3-D, the orientation of a rigid body is described by the 3-vector θ whose elements describe the rotation in the x-, y- and z-axis respectively, and $\mathbf{R}$ is a 3×3 matrix. Note, for example, that $\mathbf{R}$ is a rotation matrix and therefore orthogonal, so $\mathbf{R}^T\mathbf{R} = \mathbf{R}\mathbf{R}^T = \delta$ (where δ here represents the identity matrix — $\mathbf{I}$ is used to notate the inertia tensor). Indeed,

$$\begin{aligned} (\mathbf{R}\mathbf{R}^T)' &= \delta' \\ \mathbf{R}'\mathbf{R}^T + \mathbf{R}\mathbf{R}'^T &= 0 \\ &\Rightarrow \mathbf{R}'\mathbf{R}^T + (\mathbf{R}'\mathbf{R}^T)^T = 0 \end{aligned}$$

so $\mathbf{R}'\mathbf{R}^T$ is a skew-symmetric matrix. In fact,

$$\mathbf{R}'\mathbf{R}^T = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} = \omega^\star \tag{4}$$

Where $\omega^\star$ is a matrix with the property that $\omega^\star\vec{u} = \omega \times \vec{u}$ for any vector $\vec{u}$. The physical intuition behind ω is that it describes the rotation about the axis $\omega/\|\omega\|$ at an angular velocity $\|\omega\|$ (in radians). From this derivation we can see (since $\mathbf{R}$ is orthogonal) that we have an ODE that describes how the orientation is evolved forward in time (assuming that ω is known – this would typically come from an "$F = ma$"-type formulation):

$$\mathbf{R}' = \omega^\star\mathbf{R}. \tag{5}$$