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Introduction

Numerical modeling has become an essential component of most research in physical oceanography. Once the domain of specialists, interpretation of model results has become part of the routine scientific practice. The highly schematic models of the 1970s and 1980s with their highly idealized geometry, coarse resolution and crudely parameterized small-scale processes could give only rough qualitative insights into applicability of theory. With the computing power available to nearly every scientist today, numerical models are expected to compare in detail with observation.

Field experiments are now designed with the intention of providing models with initial conditions, boundary conditions and verification data. Non-specialists, who, even five years ago, would not have given much thought to the implications of modeling results, now routinely ask themselves, “What do the models tell us?” Increasingly, this is the way oceanography is done.

Ocean modeling is closely related in method and spirit to atmospheric modeling, but atmospheric modeling was developed earlier, driven by the need for operational weather prediction. The basic methodology for weather forecasting was first set out by Richardson in a remarkable book (Richardson, 1965), first published in 1922. In that book, all of the steps for constructing a numerical weather forecast were set out in detail. A sample calculation was performed for two points in Europe, but the forecast turned out to be markedly different from the state of the atmosphere observed at the forecast time.

No automatic computing machinery was available to Richardson. He put considerable effort into the design of computing forms which would make the tabulation of data and intermediate results as convenient as possible. Actual calculations were performed with a slide rule and with log tables. In the preface to his book, dated October, 1921, he wrote:

> Perhaps some day in the dim future it will be possible to advance the computations faster than the weather advances and at a cost less than the saving to mankind due to the information gained. But that is a dream.

The next chapter follows in the spirit of Richardson's work. We examine schemes that appear reasonable but give entirely unreasonable results. We know now that the striking departure of Richardson's first forecast from reality was due to the failure of the calculation to satisfy a basic criterion for computational stability. Careful as Richardson was, he did not realize that his computing scheme, though evidently intuitively reasonable, was inherently unstable.

2

Some basic results from numerical analysis

2.1 Simple discretizations of a linear advection equation

We will use the simple one-dimensional advection equation with unit advection speed,

$$u_t + u_x = 0, \tag{2.1}$$

to study some of the fundamental consequences of discretization of partial differential equations. The exact solution to (2.1) can be found by examining curves in the $x - t$ plane of the form $t = x + x_0$. Along such curves,

$$\frac{\mathrm{d}u}{\mathrm{d}x} = u_t \frac{\mathrm{d}t}{\mathrm{d}x} + u_x = u_t + u_x.$$

So (2.1) states that along these curves u is constant. These curves are known as the *characteristics* of (2.1). We can use the characteristics to solve the initial value problem for (2.1). Consider the point $(\hat{x}, \hat{t})$ in the $x - t$ plane. The characteristic passing through $(\hat{x}, \hat{t})$ is

$$t = x + (\hat{t} - \hat{x}).$$

If we extrapolate this line back to the x-axis, we find, at $t = 0$, $x = -(\hat{t} - \hat{x})$. If we are given the initial condition $u(x, 0) = F(x)$, we have

$$u(\hat{x}, \hat{t}) = F(\hat{x} - \hat{t}) \quad \text{for any } \hat{x} \text{ and } \hat{t}.$$

One way of visualizing the foregoing is to note that, given the graph of the initial condition, the solution to (2.1) at time t can be constructed by translating the graph t units to the right.

For our first examples of different choices of discretization, we consider (2.1) with the periodic boundary condition $u(0, t) = u(2\pi, t)$. We choose

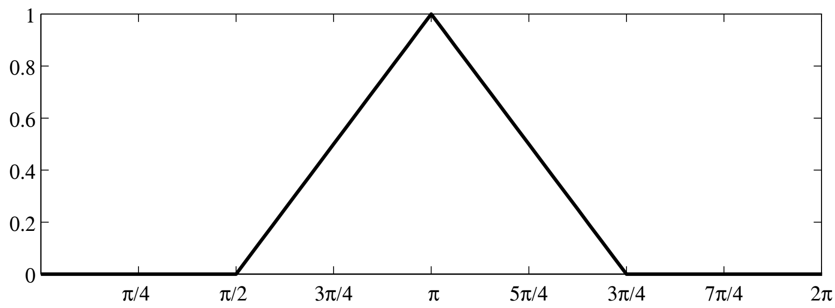

Fig. 2.1 Initial condition for advection equation (2.1).

a piecewise linear initial condition:

$$u(x,0) = \begin{cases} 0, & 0 \leq x \leq \pi/2, \\ (x-\pi/2)/(\pi/2), & \pi/2 < x \leq \pi, \\ (3\pi/2 - x)/(\pi/2), & \pi < x \leq 3\pi/2, \\ 0, & 3\pi/2 < x < 2\pi. \end{cases}$$

A graph of this function is shown in Figure 2.1 At time intervals of 2π, the solution should be identical to the initial condition. This is sometimes called the "one-dimensional color problem." One of the most obvious simple things to do is to approximate (2.1) in the interior by

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right), \tag{2.2}$$

where subscripts represent spatial grid position and superscripts represent time step. Periodic boundary conditions are applied to (2.2) at the boundary points. There are many ways to discretize (2.1), and others may seem more obvious, especially to the reader with a bit of experience in numerical solution of partial differential equations. Two things should be noted here about this particular choice. First, the spatial derivative of the solution at the point x_j is approximated by a difference between u_{j+1} and u_{j-1}. This is known as a centered difference scheme. Formal expansion of u in Taylor series about u_j easily shows the centered scheme to be more accurate than either of the so-called one-sided schemes, in which the derivative is approximated by $u_j - u_{j-1}$ or $u_{j+1} - u_j$. Second, (2.2) can be viewed as a method for finding an approximate solution to a system of coupled ordinary differential equations given by $\dot{u}_j = -(u_{j+1} - u_{j-1})/(2\Delta x)$. Methods of this form are sometimes placed in the general classification of "Method of Lines." The term comes from the fact that approximate solutions of the partial differential equation are computed on a family of lines in the $x-t$ plane. In this case, these lines are vertical, if we take x as the horizontal axis and t as the vertical axis.

The scheme (2.2) can be rearranged to form

$$u_j^{n+1} = u_j^n - \frac{\lambda}{2}(u_{j+1}^n - u_{j-1}^n), \tag{2.3}$$

where $\lambda = \Delta t/\Delta x$. If we choose 32 gridpoints and $\lambda = 0.5$, watch what happens at $t = 2\pi$; see Figure 2.2.

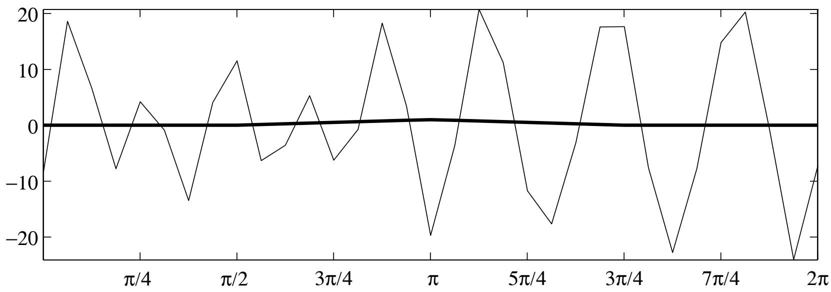

Fig. 2.2 Result of simple scheme for the advection equation (2.1). The heavy line depicts the true solution. The fine line depicts the computed approximate solution.

This result would certainly not lead us to put much faith in this scheme. The amplitude of the computed solution is an order of magnitude too great, and cursory inspection shows that it does not bear the slightest resemblance to the true solution. It turns out that fiddling with λ doesn't help.

Next try

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -\left(\frac{u_j^n - u_{j-1}^n}{\Delta x}\right), \tag{2.4}$$

which can be written as

$$u_j^{n+1} = u_j^n - \lambda(u_j^n - u_{j-1}^n). \tag{2.5}$$

This is an example of a family of methods known as "upwind schemes," because the solution at a given point depends only on the initial condition at the point itself and points upwind relative to the advection velocity. The result for the same Δx and λ used in the above example is shown in Figure 2.3.

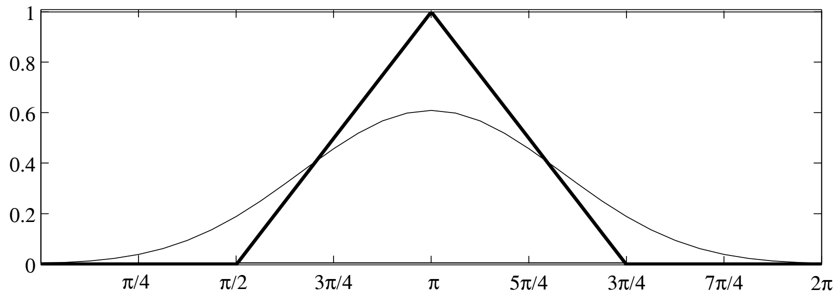

Fig. 2.3 Result of calculation with upwind scheme. Legend as in Fig. 2.2.

In this case, the amplitude is of the correct order of magnitude, and the approximate solution bears a clear resemblance to the true solution, but the spatial resolution is poor, i.e., the corners are rounded off. What happens if we increase the spatial resolution to 128 gridpoints, i.e., $\lambda = 2$? The result is shown in Figure 2.4. This is even worse than the result

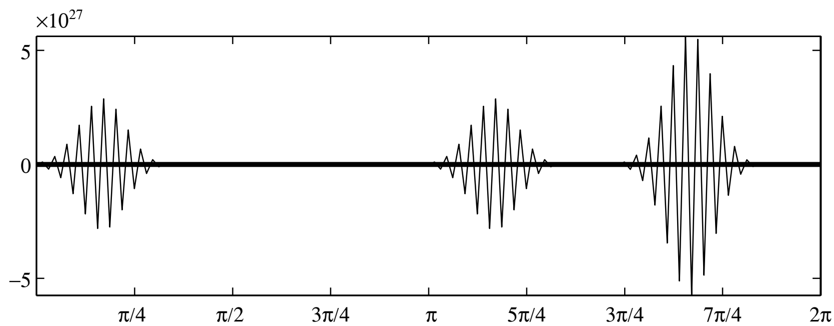

Fig. 2.4 Result of calculation with upwind scheme, $\lambda = 2$. Legend as before.

shown in Figure 2.2. The amplitude is 27 orders of magnitude too great, which is an unsatisfactory result by any standard. One might suspect that further continuation of this calculation could result in an overflow.

If we now return to the old value, i.e., $\lambda = 0.5$, by changing Δt appropriately, we see in Figure 2.5 that we have the better-resolved solution that we were seeking.

Next, let us investigate whether we can fix the centered scheme by trying

$$u_j^{n+1} = \frac{1}{2}(u_{j+1}^n + u_{j-1}^n) - \frac{\lambda}{2}(u_{j+1}^n - u_{j-1}^n). \tag{2.6}$$

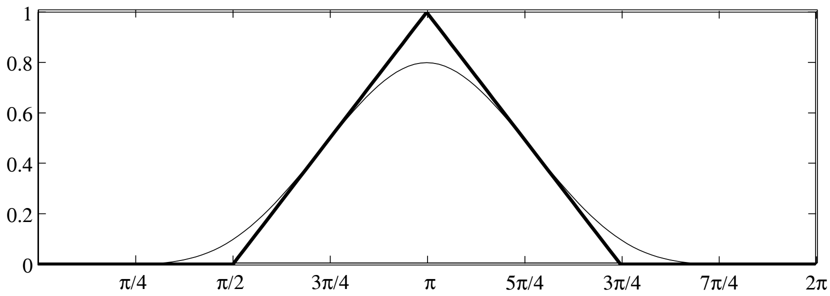

Fig. 2.5 Results of calculations with upwind scheme with $\Delta x = 2\pi/128$ and $\lambda = 0.5$. Legend as before.

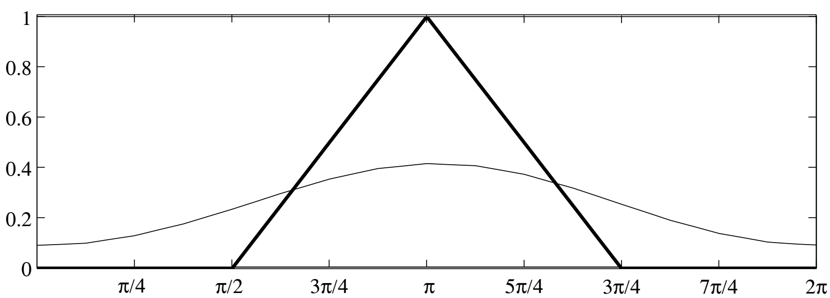

Fig. 2.6 Result of computation with the Lax–Friedrichs scheme with $\Delta x = 2\pi/32$ and $\lambda = 0.5$. Legend as before.

This is sometimes known as the Lax–Friedrichs scheme. The results of applying this scheme are shown in Figure 2.6. From that figure, we see that, as in the case of the upwind scheme, the result is of the correct order of magnitude, and has the correct general shape, but the approximate solution is unrealistically damped, to even a greater extent than the result from the upwind scheme with the same Δx and Δt. So the way we discretize something makes a great deal of difference. In the next section, we will use analytical techniques to investigate the effects of discretization.

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2.2 Analysis of numerical results

2.2.1 Consistency, stability, convergence: the fundamentals

We began this chapter by taking a simple partial differential equation and approximating the partial derivatives by divided differences. All of the schemes we tried out were *consistent*, i.e., each individual difference quotient would converge to the derivative it was intended to approximate as Δt and Δx decreased. It is easy enough to formalize this. Let $v(x,t)$ be a solution of (2.1). We may write the scheme (2.3) as

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = 0.$$

We may now expand v in Taylor series:

$$\begin{aligned} v[j\Delta x, (n+1)\Delta t] &= v(j\Delta x, n\Delta t) + \Delta t v_t(j\Delta x, n\Delta t) + 0(\Delta t^2) \\ v[(j+1)\Delta x, n\Delta t] &= v(j\Delta x, n\Delta t) + \Delta x v_x(j\Delta x, n\Delta t) \\ &\qquad + \frac{1}{2}\Delta x^2 v_{xx}(j\Delta x + n\Delta t) + 0(\Delta x^3), \end{aligned}$$

which gives us

$$\frac{v[j\Delta x, (n+1)\Delta t] - v(j\Delta x, n\Delta t)}{\Delta t} + \frac{v[(j+1)\Delta x, n\Delta t] - v[(j-1)\Delta x, n\Delta t]}{2\Delta x} = v_t + v_x + 0(\Delta t) + 0(\Delta x^2).$$

In the limit as Δt and Δx approach zero, the solution of the difference equations approaches the solution of the differential equation at any fixed x and t. We have seen that consistency is not enough. All of the schemes in Section 2.1 were consistent, yet some were obviously unsatisfactory.

The troubles illustrated in Figures 2.2 and 2.4 can be avoided if we choose schemes that are *stable*. A scheme for solution of an initial value problem is stable if small changes in the initial condition result in small changes in the result at some fixed time, say $t = 2\pi$, as in the cases shown in the previous section. To make this precise, we must say what we mean by "small."

We begin by writing the approximate solution after n time steps as the vector $\mathbf{v}^n$, whose jth component is the value v_j^n of the approximate solution at the jth grid point after n time steps. We decide whether a vector is large or small by assigning a *norm* to it. A norm of $\mathbf{v}$ is a scalar valued function written $\|\mathbf{v}\|$ which is positive definite, i.e.,

$$\|\mathbf{v}\| \geq 0, \tag{2.7}$$

with equality holding if and only if $\mathbf{v} = 0$ and obeys the triangle inequality

$$\|\mathbf{v} + \mathbf{w}\| \leq \|\mathbf{v}\| + \|\mathbf{w}\| \tag{2.8}$$

for any pair of vectors $\mathbf{v}$ and $\mathbf{w}$. A norm is a general notion of length. The ordinary Euclidean length of a vector, given by $(\sum_j v_j^2)^{1/2}$, is an example of a norm. There are times when other norms are more convenient to use or give rise to more enlightening results.

We may formulate a definition of stability in a number of ways. The following is standard for linear difference schemes.

Let $\mathbf{v}^n$ be the discrete solution at time $n\Delta t$, and let the difference scheme be given by

$$\mathbf{v}^{n+1} = L(\Delta t)\mathbf{v}^n.$$

All of the schemes in Section 2.1 can be written in this form. Our definition of stability will be given in terms of a norm of the matrix L. Here we assign a norm to a matrix by saying that the norm of a matrix L is large if there is some unit vector $\mathbf{v}$ such that the norm of the product $L\mathbf{v}$ is large, i.e., given a vector norm $\|\cdot\|$, the norm of the matrix L is the maximum over all vectors $\mathbf{u}$ of $\|L\mathbf{u}\|/\|\mathbf{u}\|$. This norm is referred to as the matrix norm *induced* by $\|\cdot\|$. The scheme is said to be stable if

$$\|L\| \leq 1 + 0(\Delta t).$$

Note that solutions to a stable scheme may grow at most exponentially. Fix some time $T = n\Delta t$, and let $L(\Delta t)$ be stable. Then

$$\mathbf{v}^n = L^n\mathbf{v}^0$$

and

$$\|\mathbf{v}^n\| = \|L^n\mathbf{v}^0\| \leq \|L\|^n\|\mathbf{v}^0\| \leq (1 + k\Delta t)^n\|\mathbf{v}_0\|$$

for some k, if Δt is sufficiently small. Therefore

$$\|\mathbf{v}^n\| = \left(1 + \frac{kT}{n}\right)^n \|\mathbf{v}_0\| \leq \mathrm{e}^{kT}\|\mathbf{v}_0\|.$$

On the other hand, if $\|L\| > 1$ independent of Δt, the solution will obviously blow up as $n \to \infty$.

For nonlinear systems, this definition is not so hard to generalize. We wish stability of a numerical scheme to mean the same thing as stability of anything else: the effect of small perturbations should remain bounded for finite time. So if $\mathbf{v}$ and $\mathbf{w}$ are solutions to a given difference scheme at time T with initial conditions $\mathbf{v}^0$ and $\mathbf{w}^0$ respectively, we wish $\|\mathbf{v}-\mathbf{w}\|$ to be bounded in terms of $\|\mathbf{v}^0-\mathbf{w}^0\|$, independent of Δt. This condition is usually very hard to verify.

We have seen that the exact solution to (2.1) can be found by examining the characteristics, and we found that in this case, the solution to (2.1) at any point depends only on the initial value at a single point on the x-axis. We say the *domain of dependence* for the solution of an initial value problem at the point $(\hat{x},\hat{t})$ is that set of points on the x-axis at which the initial values influence the solution at $(\hat{x},\hat{t})$. In this simple case, the domain of dependence consists of a single point $x=\hat{x}-\hat{t}$. We may define a *numerical domain of dependence* at the point $(j\Delta x,\ n\Delta t)$ analogously. The Courant–Friedrichs–Lewy (CFL) theorem states that in order for a numerical method to be stable, the numerical domain of dependence must contain the domain of dependence for the differential equation. This condition is necessary but not sufficient.

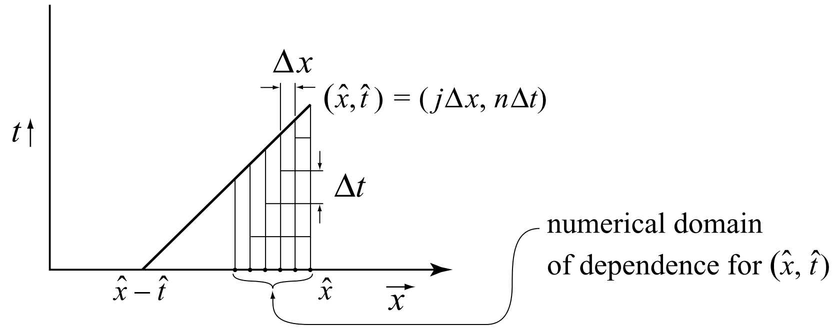

Fig. 2.7 Schematic diagram of the upwind scheme in the characteristic plane for $\lambda \approx 2$.

Let us consider the upwind scheme (2.4). The behavior of the scheme in the characteristic plane is illustrated in Figure 2.7. The leftmost point in the numerical domain of dependence is $j\Delta x-(n/\lambda)\Delta t$; the CFL criterion for stability is then $j\Delta x-(n/\lambda)\Delta t < j\Delta x - n\Delta t$, or $\lambda \le 1$. So if $\lambda > 1$, the solution to the numerical scheme cannot converge to the solution of the PDE, no matter how small Δx and Δt are. This explains the behavior of the upwind scheme (2.4), but a similar analysis shows