engineering; these methods allow considerable freedom in putting computational elements where you want them, important when dealing with highly irregular geometries. Spectral methods [13-15] are preferred for very regular geometries and smooth functions; they converge more rapidly than finite-difference methods (cf. §19.4), but they do not work well for problems with discontinuities.

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19.1 Flux-Conservative Initial Value Problems

A large class of initial value (time-evolution) PDEs in one space dimension can be cast into the form of a *flux-conservative equation*,

$$\frac{\partial \mathbf{u}}{\partial t} = -\frac{\partial \mathbf{F}(\mathbf{u})}{\partial x} \tag{19.1.1}$$

where **u** and **F** are vectors, and where (in some cases) **F** may depend not only on **u** but also on spatial derivatives of **u**. The vector **F** is called the *conserved flux*.

For example, the prototypical hyperbolic equation, the one-dimensional wave equation with constant velocity of propagation v

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} \tag{19.1.2}$$

can be rewritten as a set of two first-order equations

$$\begin{aligned}\frac{\partial r}{\partial t} &= v\frac{\partial s}{\partial x}\\ \frac{\partial s}{\partial t} &= v\frac{\partial r}{\partial x}\end{aligned} \tag{19.1.3}$$

where

$$\begin{aligned}r &\equiv v\frac{\partial u}{\partial x}\\ s &\equiv \frac{\partial u}{\partial t}\end{aligned} \tag{19.1.4}$$

In this case r and s become the two components of $\mathbf{u}$, and the flux is given by the linear matrix relation

$$\mathbf{F}(\mathbf{u}) = \begin{pmatrix} 0 & -v \\ -v & 0 \end{pmatrix} \cdot \mathbf{u} \tag{19.1.5}$$

(The physicist-reader may recognize equations (19.1.3) as analogous to Maxwell's equations for one-dimensional propagation of electromagnetic waves.)

We will consider, in this section, a prototypical example of the general flux-conservative equation (19.1.1), namely the equation for a scalar u,

$$\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x} \tag{19.1.6}$$

with v a constant. As it happens, we already know analytically that the general solution of this equation is a wave propagating in the positive x-direction,

$$u = f(x - vt) \tag{19.1.7}$$

where f is an arbitrary function. However, the numerical strategies that we develop will be equally applicable to the more general equations represented by (19.1.1). In some contexts, equation (19.1.6) is called an *advective* equation, because the quantity u is transported by a "fluid flow" with a velocity v.

How do we go about finite differencing equation (19.1.6) (or, analogously, 19.1.1)? The straightforward approach is to choose equally spaced points along both the t- and x-axes. Thus denote

$$\begin{aligned}x_j &= x_0 + j\Delta x, \qquad & j &= 0, 1, \ldots, J\\ t_n &= t_0 + n\Delta t, \qquad & n &= 0, 1, \ldots, N\end{aligned} \tag{19.1.8}$$

Let u_j^n denote $u(t_n, x_j)$. We have several choices for representing the time derivative term. The obvious way is to set

$$\left.\frac{\partial u}{\partial t}\right|_{j,n} = \frac{u_j^{n+1} - u_j^n}{\Delta t} + O(\Delta t) \tag{19.1.9}$$

This is called *forward Euler* differencing (cf. equation 16.1.1). While forward Euler is only first-order accurate in Δt, it has the advantage that one is able to calculate

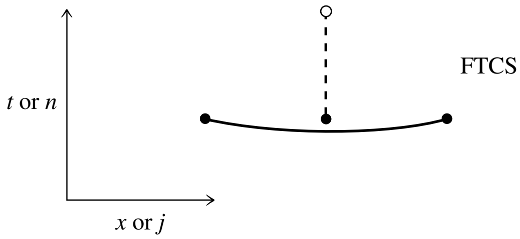

Figure 19.1.1. Representation of the Forward Time Centered Space (FTCS) differencing scheme. In this and subsequent figures, the open circle is the new point at which the solution is desired; filled circles are known points whose function values are used in calculating the new point; the solid lines connect points that are used to calculate spatial derivatives; the dashed lines connect points that are used to calculate time derivatives. The FTCS scheme is generally unstable for hyperbolic problems and cannot usually be used.

quantities at timestep $n + 1$ in terms of only quantities known at timestep n. For the space derivative, we can use a second-order representation still using only quantities known at timestep n:

$$\left.\frac{\partial u}{\partial x}\right|_{j,n} = \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} + O(\Delta x^2) \tag{19.1.10}$$

The resulting finite-difference approximation to equation (19.1.6) is called the FTCS representation (Forward Time Centered Space),

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right) \tag{19.1.11}$$

which can easily be rearranged to be a formula for u_j^{n+1} in terms of the other quantities. The FTCS scheme is illustrated in Figure 19.1.1. It's a fine example of an algorithm that is easy to derive, takes little storage, and executes quickly. Too bad it doesn't work! (See below.)

The FTCS representation is an *explicit* scheme. This means that u_j^{n+1} for each j can be calculated explicitly from the quantities that are already known. Later we shall meet *implicit* schemes, which require us to solve implicit equations coupling the u_j^{n+1} for various j. (Explicit and implicit methods for ordinary differential equations were discussed in §16.6.) The FTCS algorithm is also an example of a *single-level* scheme, since only values at time level n have to be stored to find values at time level $n + 1$.

von Neumann Stability Analysis

Unfortunately, equation (19.1.11) is of very limited usefulness. It is an *unstable* method, which can be used only (if at all) to study waves for a short fraction of one oscillation period. To find alternative methods with more general applicability, we must introduce the *von Neumann stability analysis*.

The von Neumann analysis is local: We imagine that the coefficients of the difference equations are so slowly varying as to be considered constant in space and time. In that case, the independent solutions, or *eigenmodes*, of the difference equations are all of the form

$$u_j^n = \xi^n e^{ikj\Delta x} \tag{19.1.12}$$

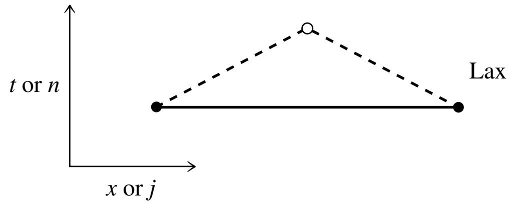

Figure 19.1.2. Representation of the Lax differencing scheme, as in the previous figure. The stability criterion for this scheme is the Courant condition.

where k is a real spatial wave number (which can have any value) and $\xi = \xi(k)$ is a complex number that depends on k. The key fact is that the time dependence of a single eigenmode is nothing more than successive integer powers of the complex number ξ. Therefore, the difference equations are unstable (have exponentially growing modes) if $|\xi(k)| > 1$ for *some* k. The number ξ is called the *amplification factor* at a given wave number k.

To find $\xi(k)$, we simply substitute (19.1.12) back into (19.1.11). Dividing by ξ^n, we get

$$\xi(k) = 1 - i\frac{v\Delta t}{\Delta x}\sin k\Delta x \tag{19.1.13}$$

whose modulus is > 1 for *all* k; so the FTCS scheme is unconditionally unstable.

If the velocity v were a function of t and x, then we would write v_j^n in equation (19.1.11). In the von Neumann stability analysis we would still treat v as a constant, the idea being that for v slowly varying the analysis is local. In fact, even in the case of strictly constant v, the von Neumann analysis does not rigorously treat the end effects at $j = 0$ and $j = N$.

More generally, if the equation's right-hand side were nonlinear in u, then a von Neumann analysis would linearize by writing $u = u_0 + \delta u$, expanding to linear order in δu. Assuming that the u_0 quantities already satisfy the difference equation exactly, the analysis would look for an unstable eigenmode of δu.

Despite its lack of rigor, the von Neumann method generally gives valid answers and is much easier to apply than more careful methods. We accordingly adopt it exclusively. (See, for example, [1] for a discussion of other methods of stability analysis.)

Lax Method

The instability in the FTCS method can be cured by a simple change due to Lax. One replaces the term u_j^n in the time derivative term by its average (Figure 19.1.2):

$$u_j^n \to \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right) \tag{19.1.14}$$

This turns (19.1.11) into

$$u_j^{n+1} = \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right) - \frac{v\Delta t}{2\Delta x}\left(u_{j+1}^n - u_{j-1}^n\right) \tag{19.1.15}$$

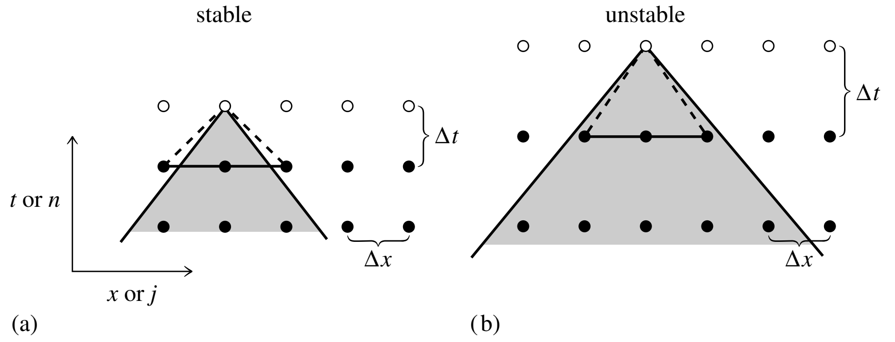

Figure 19.1.3. Courant condition for stability of a differencing scheme. The solution of a hyperbolic problem at a point depends on information within some domain of dependency to the past, shown here shaded. The differencing scheme (19.1.15) has its own domain of dependency determined by the choice of points on one time slice (shown as connected solid dots) whose values are used in determining a new point (shown connected by dashed lines). A differencing scheme is Courant stable if the differencing domain of dependency is larger than that of the PDEs, as in (a), and unstable if the relationship is the reverse, as in (b). For more complicated differencing schemes, the domain of dependency might not be determined simply by the outermost points.

Substituting equation (19.1.12), we find for the amplification factor

$$\xi = \cos k\Delta x - i\frac{v\Delta t}{\Delta x}\sin k\Delta x \tag{19.1.16}$$

The stability condition $|\xi|^2 \leq 1$ leads to the requirement

$$\frac{|v|\Delta t}{\Delta x} \leq 1 \tag{19.1.17}$$

This is the famous Courant-Friedrichs-Lewy stability criterion, often called simply the *Courant condition*. Intuitively, the stability condition can be understood as follows (Figure 19.1.3): The quantity u_j^{n+1} in equation (19.1.15) is computed from information at points $j-1$ and $j+1$ at time n. In other words, x_{j-1} and x_{j+1} are the boundaries of the spatial region that is allowed to communicate information to u_j^{n+1}. Now recall that in the continuum wave equation, information actually propagates with a maximum velocity v. If the point u_j^{n+1} is outside of the shaded region in Figure 19.1.3, then it requires information from points more distant than the differencing scheme allows. Lack of that information gives rise to an instability. Therefore, Δt cannot be made too large.

The surprising result, that the simple replacement (19.1.14) stabilizes the FTCS scheme, is our first encounter with the fact that differencing PDEs is an art as much as a science. To see if we can demystify the art somewhat, let us compare the FTCS and Lax schemes by rewriting equation (19.1.15) so that it is in the form of equation (19.1.11) with a remainder term:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right) + \frac{1}{2}\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta t}\right) \tag{19.1.18}$$

But this is exactly the FTCS representation of the equation

$$\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2\Delta t}\nabla^2 u \tag{19.1.19}$$

where $\nabla^2 = \partial^2/\partial x^2$ in one dimension. We have, in effect, added a diffusion term to the equation, or, if you recall the form of the Navier-Stokes equation for viscous fluid flow, a dissipative term. The Lax scheme is thus said to have *numerical dissipation*, or *numerical viscosity*. We can see this also in the amplification factor. Unless $|v|\Delta t$ is exactly equal to Δx, $|\xi| < 1$ and the amplitude of the wave decreases spuriously.

Isn't a spurious decrease as bad as a spurious increase? No. The scales that we hope to study accurately are those that encompass many grid points, so that they have $k\Delta x \ll 1$. (The spatial wave number k is defined by equation 19.1.12.) For these scales, the amplification factor can be seen to be very close to one, in both the stable and unstable schemes. The stable and unstable schemes are therefore about equally accurate. For the unstable scheme, however, short scales with $k\Delta x \sim 1$, *which we are not interested in*, will blow up and swamp the interesting part of the solution. Much better to have a stable scheme in which these short wavelengths die away innocuously. Both the stable and the unstable schemes are *inaccurate* for these short wavelengths, but the inaccuracy is of a tolerable character when the scheme is stable.

When the independent variable **u** is a vector, then the von Neumann analysis is slightly more complicated. For example, we can consider equation (19.1.3), rewritten as

$$\frac{\partial}{\partial t}\begin{bmatrix} r \\ s \end{bmatrix} = \frac{\partial}{\partial x}\begin{bmatrix} vs \\ vr \end{bmatrix} \tag{19.1.20}$$

The Lax method for this equation is

$$\begin{aligned} r_j^{n+1} &= \frac{1}{2}(r_{j+1}^n + r_{j-1}^n) + \frac{v\Delta t}{2\Delta x}(s_{j+1}^n - s_{j-1}^n) \\ s_j^{n+1} &= \frac{1}{2}(s_{j+1}^n + s_{j-1}^n) + \frac{v\Delta t}{2\Delta x}(r_{j+1}^n - r_{j-1}^n) \end{aligned} \tag{19.1.21}$$

The von Neumann stability analysis now proceeds by assuming that the eigenmode is of the following (vector) form,

$$\begin{bmatrix} r_j^n \\ s_j^n \end{bmatrix} = \xi^n e^{ikj\Delta x}\begin{bmatrix} r^0 \\ s^0 \end{bmatrix} \tag{19.1.22}$$

Here the vector on the right-hand side is a constant (both in space and in time) eigenvector, and ξ is a complex number, as before. Substituting (19.1.22) into (19.1.21), and dividing by the power ξ^n, gives the homogeneous vector equation

$$\begin{bmatrix} (\cos k\Delta x) - \xi & i\dfrac{v\Delta t}{\Delta x}\sin k\Delta x \\ i\dfrac{v\Delta t}{\Delta x}\sin k\Delta x & (\cos k\Delta x) - \xi \end{bmatrix} \cdot \begin{bmatrix} r^0 \\ s^0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{19.1.23}$$

This admits a solution only if the determinant of the matrix on the left vanishes, a condition easily shown to yield the two roots ξ

$$\xi = \cos k\Delta x \pm i\frac{v\Delta t}{\Delta x}\sin k\Delta x \tag{19.1.24}$$

The stability condition is that both roots satisfy $|\xi| \le 1$. This again turns out to be simply the Courant condition (19.1.17).

Other Varieties of Error

Thus far we have been concerned with *amplitude error*, because of its intimate connection with the stability or instability of a differencing scheme. Other varieties of error are relevant when we shift our concern to accuracy, rather than stability.

Finite-difference schemes for hyperbolic equations can exhibit dispersion, or *phase errors*. For example, equation (19.1.16) can be rewritten as

$$\xi = e^{-ik\Delta x} + i\left(1 - \frac{v\Delta t}{\Delta x}\right)\sin k\Delta x \tag{19.1.25}$$

An arbitrary initial wave packet is a superposition of modes with different k's. At each timestep the modes get multiplied by different phase factors (19.1.25), depending on their value of k. If $\Delta t = \Delta x/v$, then the exact solution for each mode of a wave packet $f(x - vt)$ is obtained if each mode gets multiplied by $\exp(-ik\Delta x)$. For this value of Δt, equation (19.1.25) shows that the finite-difference solution gives the exact analytic result. However, if $v\Delta t/\Delta x$ is not exactly 1, the phase relations of the modes can become hopelessly garbled and the wave packet disperses. Note from (19.1.25) that the dispersion becomes large as soon as the wavelength becomes comparable to the grid spacing Δx.

A third type of error is one associated with nonlinear hyperbolic equations and is therefore sometimes called *nonlinear instability*. For example, a piece of the Euler or Navier-Stokes equations for fluid flow looks like

$$\frac{\partial v}{\partial t} = -v\frac{\partial v}{\partial x} + \dots \tag{19.1.26}$$

The nonlinear term in v can cause a transfer of energy in Fourier space from long wavelengths to short wavelengths. This results in a wave profile steepening until a vertical profile or "shock" develops. Since the von Neumann analysis suggests that the stability can depend on $k\Delta x$, a scheme that was stable for shallow profiles can become unstable for steep profiles. This kind of difficulty arises in a differencing scheme where the cascade in Fourier space is halted at the shortest wavelength representable on the grid, that is, at $k \sim 1/\Delta x$. If energy simply accumulates in these modes, it eventually swamps the energy in the long wavelength modes of interest.

Nonlinear instability and shock formation is thus somewhat controlled by numerical viscosity such as that discussed in connection with equation (19.1.18) above. In some fluid problems, however, shock formation is not merely an annoyance, but an actual physical behavior of the fluid whose detailed study is a goal. Then, numerical viscosity alone may not be adequate or sufficiently controllable. This is a complicated subject which we discuss further in the subsection on fluid dynamics, below.

For wave equations, propagation errors (amplitude or phase) are usually most worrisome. For advective equations, on the other hand, *transport errors* are usually of greater concern. In the Lax scheme, equation (19.1.15), a disturbance in the advected quantity u at mesh point j propagates to mesh points $j + 1$ and $j - 1$ at the next timestep. In reality, however, if the velocity v is positive then only mesh point $j + 1$ should be affected.

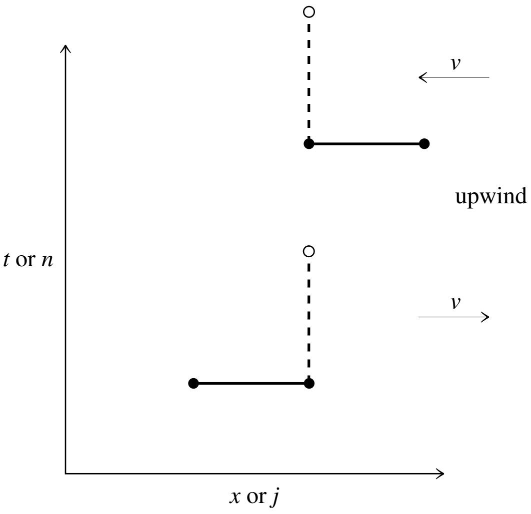

Figure 19.1.4. Representation of upwind differencing schemes. The upper scheme is stable when the advection constant v is negative, as shown; the lower scheme is stable when the advection constant v is positive, also as shown. The Courant condition must, of course, also be satisfied.

The simplest way to model the transport properties "better" is to use *upwind differencing* (see Figure 19.1.4):

$$\frac{u_j^{n+1}-u_j^n}{\Delta t} = -v_j^n \begin{cases} \dfrac{u_j^n - u_{j-1}^n}{\Delta x}, & v_j^n > 0 \\ \dfrac{u_{j+1}^n - u_j^n}{\Delta x}, & v_j^n < 0 \end{cases} \tag{19.1.27}$$

Note that this scheme is only first-order, not second-order, accurate in the calculation of the spatial derivatives. How can it be "better"? The answer is one that annoys the mathematicians: The goal of numerical simulations is not always "accuracy" in a strictly mathematical sense, but sometimes "fidelity" to the underlying physics in a sense that is looser and more pragmatic. In such contexts, some kinds of error are much more tolerable than others. Upwind differencing generally adds fidelity to problems where the advected variables are liable to undergo sudden changes of state, e.g., as they pass through shocks or other discontinuities. You will have to be guided by the specific nature of your own problem.

For the differencing scheme (19.1.27), the amplification factor (for constant v) is

$$\xi = 1 - \left|\frac{v\Delta t}{\Delta x}\right|(1-\cos k\Delta x) - i\frac{v\Delta t}{\Delta x}\sin k\Delta x \tag{19.1.28}$$

$$|\xi|^2 = 1 - 2\left|\frac{v\Delta t}{\Delta x}\right|\left(1-\left|\frac{v\Delta t}{\Delta x}\right|\right)(1-\cos k\Delta x) \tag{19.1.29}$$

So the stability criterion $|\xi|^2 \le 1$ is (again) simply the Courant condition (19.1.17).

There are various ways of improving the accuracy of first-order upwind differencing. In the continuum equation, material originally a distance $v\Delta t$ away

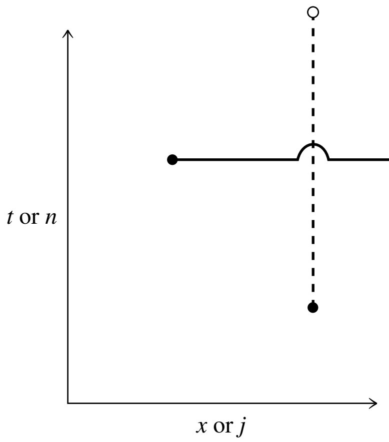

Figure 19.1.5. Representation of the staggered leapfrog differencing scheme. Note that information from two previous time slices is used in obtaining the desired point. This scheme is second-order accurate in both space and time.

arrives at a given point after a time interval Δt. In the first-order method, the material always arrives from Δx away. If $v\Delta t \ll \Delta x$ (to insure accuracy), this can cause a large error. One way of reducing this error is to interpolate u between $j-1$ and j before transporting it. This gives effectively a second-order method. Various schemes for second-order upwind differencing are discussed and compared in [2-3].

Second-Order Accuracy in Time

When using a method that is first-order accurate in time but second-order accurate in space, one generally has to take $v\Delta t$ significantly smaller than Δx to achieve desired accuracy, say, by at least a factor of 5. Thus the Courant condition is not actually the limiting factor with such schemes in practice. However, there are schemes that are second-order accurate in both space and time, and these can often be pushed right to their stability limit, with correspondingly smaller computation times.

For example, the *staggered leapfrog* method for the conservation equation (19.1.1) is defined as follows (Figure 19.1.5): Using the values of u^n at time t^n, compute the fluxes F_j^n. Then compute new values u^{n+1} using the time-centered values of the fluxes:

$$u_j^{n+1} - u_j^{n-1} = -\frac{\Delta t}{\Delta x}(F_{j+1}^n - F_{j-1}^n) \tag{19.1.30}$$

The name comes from the fact that the time levels in the time derivative term "leapfrog" over the time levels in the space derivative term. The method requires that u^{n-1} and u^n be stored to compute u^{n+1}.

For our simple model equation (19.1.6), staggered leapfrog takes the form

$$u_j^{n+1} - u_j^{n-1} = -\frac{v\Delta t}{\Delta x}(u_{j+1}^n - u_{j-1}^n) \tag{19.1.31}$$

The von Neumann stability analysis now gives a quadratic equation for ξ, rather than a linear one, because of the occurrence of three consecutive powers of ξ when the form (19.1.12) for an eigenmode is substituted into equation (19.1.31),

$$\xi^2 - 1 = -2i\xi \frac{v\Delta t}{\Delta x} \sin k\Delta x \tag{19.1.32}$$

whose solution is

$$\xi = -i\frac{v\Delta t}{\Delta x} \sin k\Delta x \pm \sqrt{1 - \left(\frac{v\Delta t}{\Delta x} \sin k\Delta x\right)^2} \tag{19.1.33}$$

Thus the Courant condition is again required for stability. In fact, in equation (19.1.33), $|\xi|^2 = 1$ for any $v\Delta t \leq \Delta x$. This is the great advantage of the staggered leapfrog method: There is no amplitude dissipation.

Staggered leapfrog differencing of equations like (19.1.20) is most transparent if the variables are centered on appropriate half-mesh points:

$$\begin{aligned} r^n_{j+1/2} &\equiv v \left.\frac{\partial u}{\partial x}\right|^n_{j+1/2} = v\frac{u^n_{j+1} - u^n_j}{\Delta x} \\ s^{n+1/2}_j &\equiv \left.\frac{\partial u}{\partial t}\right|^{n+1/2}_j = \frac{u^{n+1}_j - u^n_j}{\Delta t} \end{aligned} \tag{19.1.34}$$

This is purely a notational convenience: we can think of the mesh on which r and s are defined as being twice as fine as the mesh on which the original variable u is defined. The leapfrog differencing of equation (19.1.20) is

$$\begin{aligned} \frac{r^{n+1}_{j+1/2} - r^n_{j+1/2}}{\Delta t} &= \frac{s^{n+1/2}_{j+1} - s^{n+1/2}_j}{\Delta x} \\ \frac{s^{n+1/2}_j - s^{n-1/2}_j}{\Delta t} &= v\frac{r^n_{j+1/2} - r^n_{j-1/2}}{\Delta x} \end{aligned} \tag{19.1.35}$$

If you substitute equation (19.1.22) in equation (19.1.35), you will find that once again the Courant condition is required for stability, and that there is no amplitude dissipation when it is satisfied.

If we substitute equation (19.1.34) in equation (19.1.35), we find that equation (19.1.35) is equivalent to

$$\frac{u^{n+1}_j - 2u^n_j + u^{n-1}_j}{(\Delta t)^2} = v^2 \frac{u^n_{j+1} - 2u^n_j + u^n_{j-1}}{(\Delta x)^2} \tag{19.1.36}$$

This is just the "usual" second-order differencing of the wave equation (19.1.2). We see that it is a two-level scheme, requiring both u^n and u^{n-1} to obtain u^{n+1}. In equation (19.1.35) this shows up as both $s^{n-1/2}$ and r^n being needed to advance the solution.

For equations more complicated than our simple model equation, especially nonlinear equations, the leapfrog method usually becomes unstable when the gradients get large. The instability is related to the fact that odd and even mesh points are completely decoupled, like the black and white squares of a chess board, as shown

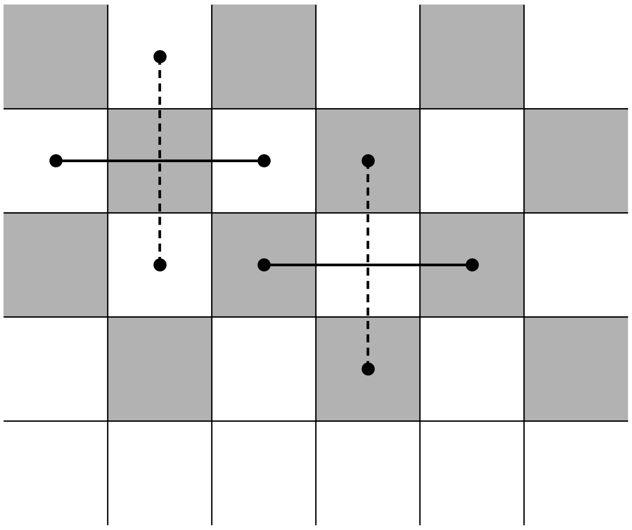

Figure 19.1.6. Origin of mesh-drift instabilities in a staggered leapfrog scheme. If the mesh points are imagined to lie in the squares of a chess board, then white squares couple to themselves, black to themselves, but there is no coupling between white and black. The fix is to introduce a small diffusive mesh-coupling piece.

in Figure 19.1.6. This mesh drifting instability is cured by coupling the two meshes through a numerical viscosity term, e.g., adding to the right side of (19.1.31) a small coefficient ($\ll 1$) times $u_{j+1}^n - 2u_j^n + u_{j-1}^n$. For more on stabilizing difference schemes by adding numerical dissipation, see, e.g., [4].

The *Two-Step Lax-Wendroff* scheme is a second-order in time method that avoids large numerical dissipation and mesh drifting. One defines intermediate values $u_{j+1/2}$ at the half timesteps $t_{n+1/2}$ and the half mesh points $x_{j+1/2}$. These are calculated by the Lax scheme:

$$u_{j+1/2}^{n+1/2} = \frac{1}{2}(u_{j+1}^n + u_j^n) - \frac{\Delta t}{2\Delta x}(F_{j+1}^n - F_j^n) \tag{19.1.37}$$

Using these variables, one calculates the fluxes $F_{j+1/2}^{n+1/2}$. Then the updated values u_j^{n+1} are calculated by the properly centered expression

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2}^{n+1/2} - F_{j-1/2}^{n+1/2}\right) \tag{19.1.38}$$

The provisional values $u_{j+1/2}^{n+1/2}$ are now discarded. (See Figure 19.1.7.)

Let us investigate the stability of this method for our model advective equation, where $F = vu$. Substitute (19.1.37) in (19.1.38) to get

$$\begin{aligned} u_j^{n+1} = u_j^n - \alpha \biggl[&\frac{1}{2}(u_{j+1}^n + u_j^n) - \frac{1}{2}\alpha(u_{j+1}^n - u_j^n) \\ &- \frac{1}{2}(u_j^n + u_{j-1}^n) + \frac{1}{2}\alpha(u_j^n - u_{j-1}^n)\biggr] \end{aligned} \tag{19.1.39}$$

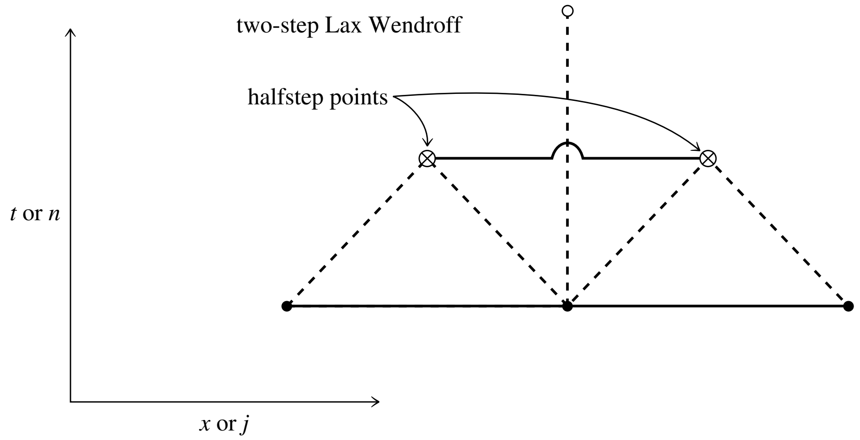

Figure 19.1.7. Representation of the two-step Lax-Wendroff differencing scheme. Two halfstep points ($\otimes$) are calculated by the Lax method. These, plus one of the original points, produce the new point via staggered leapfrog. Halfstep points are used only temporarily and do not require storage allocation on the grid. This scheme is second-order accurate in both space and time.

where

$$\alpha \equiv \frac{v\Delta t}{\Delta x} \tag{19.1.40}$$

Then

$$\xi = 1 - i\alpha \sin k\Delta x - \alpha^2(1 - \cos k\Delta x) \tag{19.1.41}$$

so

$$|\xi|^2 = 1 - \alpha^2(1 - \alpha^2)(1 - \cos k\Delta x)^2 \tag{19.1.42}$$

The stability criterion $|\xi|^2 \leq 1$ is therefore $\alpha^2 \leq 1$, or $v\Delta t \leq \Delta x$ as usual. Incidentally, you should not think that the Courant condition is the only stability requirement that ever turns up in PDEs. It keeps doing so in our model examples just because those examples are so simple in form. The method of analysis is, however, general.

Except when $\alpha = 1$, $|\xi|^2 < 1$ in (19.1.42), so some amplitude damping does occur. The effect is relatively small, however, for wavelengths large compared with the mesh size Δx. If we expand (19.1.42) for small $k\Delta x$, we find

$$|\xi|^2 = 1 - \alpha^2(1 - \alpha^2)\frac{(k\Delta x)^4}{4} + \dots \tag{19.1.43}$$

The departure from unity occurs only at fourth order in k. This should be contrasted with equation (19.1.16) for the Lax method, which shows that

$$|\xi|^2 = 1 - (1 - \alpha^2)(k\Delta x)^2 + \dots \tag{19.1.44}$$

for small $k\Delta x$.

In summary, our recommendation for initial value problems that can be cast in flux-conservative form, and especially problems related to the wave equation, is to use the staggered leapfrog method when possible. We have personally had better success with it than with the Two-Step Lax-Wendroff method. For problems sensitive to transport errors, upwind differencing or one of its refinements should be considered.

Fluid Dynamics with Shocks

As we alluded to earlier, the treatment of fluid dynamics problems with shocks has become a very complicated and very sophisticated subject. All we can attempt to do here is to guide you to some starting points in the literature.

There are basically three important general methods for handling shocks. The oldest and simplest method, invented by von Neumann and Richtmyer, is to add *artificial viscosity* to the equations, modeling the way Nature uses real viscosity to smooth discontinuities. A good starting point for trying out this method is the differencing scheme in §12.11 of [1]. This scheme is excellent for nearly all problems in one spatial dimension.

The second method combines a high-order differencing scheme that is accurate for smooth flows with a low order scheme that is very dissipative and can smooth the shocks. Typically, various upwind differencing schemes are combined using weights chosen to zero the low order scheme unless steep gradients are present, and also chosen to enforce various "monotonicity" constraints that prevent nonphysical oscillations from appearing in the numerical solution. References [2-3,5] are a good place to start with these methods.

The third, and potentially most powerful method, is Godunov's approach. Here one gives up the simple linearization inherent in finite differencing based on Taylor series and includes the nonlinearity of the equations explicitly. There is an analytic solution for the evolution of two uniform states of a fluid separated by a discontinuity, the Riemann shock problem. Godunov's idea was to approximate the fluid by a large number of cells of uniform states, and piece them together using the Riemann solution. There have been many generalizations of Godunov's approach, of which the most powerful is probably the PPM method [6].

Readable reviews of all these methods, discussing the difficulties arising when one-dimensional methods are generalized to multidimensions, are given in [7-9].

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19.2 Diffusive Initial Value Problems

Recall the model parabolic equation, the diffusion equation in one space dimension,

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right) \tag{19.2.1}$$

where D is the diffusion coefficient. Actually, this equation is a flux-conservative equation of the form considered in the previous section, with

$$F = -D\frac{\partial u}{\partial x} \tag{19.2.2}$$

the flux in the x-direction. We will assume $D \geq 0$, otherwise equation (19.2.1) has physically unstable solutions: A small disturbance evolves to become more and more concentrated instead of dispersing. (Don't make the mistake of trying to find a stable differencing scheme for a problem whose underlying PDEs are themselves unstable!)

Even though (19.2.1) is of the form already considered, it is useful to consider it as a model in its own right. The particular form of flux (19.2.2), and its direct generalizations, occur quite frequently in practice. Moreover, we have already seen that numerical viscosity and artificial viscosity can introduce diffusive pieces like the right-hand side of (19.2.1) in many other situations.

Consider first the case when D is a constant. Then the equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \tag{19.2.3}$$

can be differenced in the obvious way:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = D\left[\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}\right] \tag{19.2.4}$$

This is the FTCS scheme again, except that it is a second derivative that has been differenced on the right-hand side. But this makes a world of difference! The FTCS scheme was unstable for the hyperbolic equation; however, a quick calculation shows that the amplification factor for equation (19.2.4) is

$$\xi = 1 - \frac{4D\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right) \tag{19.2.5}$$

The requirement $|\xi| \leq 1$ leads to the stability criterion

$$\frac{2D\Delta t}{(\Delta x)^2} \leq 1 \tag{19.2.6}$$