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Note

Some Extensions of the Lax–Wendroff Method

Lax and Wendroff [1] gave a well-known difference scheme of second order accuracy for solving a system of equations in conservation law form. But not all systems of partial differential equations are, or can easily be put, in conservation form. For instance, although the Eulerian equations of fluid dynamics in one space variable occur naturally in conservation form, the Lagrangian equations do not. And the Lagrangian form is often the more natural description to use in physical applications. For instance, the ideas contained in this note first arose in connection with integrations of the collapse of a spherical cloud under the influence of its own gravity. A Lagrangian description is then very appropriate, both because it collapses along with the flow, and also because it allows a simple expression for the gravitational forces. Richtmyer and Morton [2, Sect. 12.7] have shown how the Lagrangian equations can be converted to conservation-law form in the planar case. However, their device involves the elimination of the particle displacement R, and does not work for cylindrically or spherically symmetric flows. (The Eulerian equations for cylindrically and spherically symmetric flows also lack conservation form.) In any case, a major reason for using a Lagrangian formulation in the first place normally is that it gives particle displacements directly.

The Taylor series expansion in time that Lax and Wendroff used to derive their algorithm can clearly be applied to equations that are not in conservation law form. This note considers certain specific applications in fluid dynamics, and shows that such expansions can lead to unstable difference schemes. Fortunately, the difference schemes can also be recast in stable forms. Interestingly, the instabilities that may occur are not primarily due to the fact that the equations involved lack conservation form. Similar instabilities can also arise with equations of conservation form when staggered grids are used.

Consider now the Lagrangian equations for the spatially symmetric flow of a barotropic fluid in α dimensions which, using the notation of Richtmyer and Morton, are

$$\frac{\partial R(r, t)}{\partial t} = u(r, t), \quad \frac{\partial u}{\partial t} = -V_0 \left[\frac{R}{r}\right]^{\alpha-1} \frac{\partial p}{\partial r}, \quad \frac{1}{\rho(r, t)} = V_0 \left[\frac{R}{r}\right]^{\alpha-1} \frac{\partial R}{\partial r}, \quad p = p(\rho). \tag{1}$$

Richtmyer and Morton [2, Eqs. (12.10)] give a difference scheme of the leapfrog type for solving these equations, in which the thermodynamic variables are evaluated at

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midpoints of the spatial grid. The equation of mass conservation, for instance, is approximated as

$$\frac{1}{\rho^n_{j+1/2}} = V_0 \frac{(R^n_{j+1})^\alpha - (R_j{}^n)^\alpha}{(r_{j+1})^\alpha - (r_j)^\alpha}. \tag{2}$$

Richtmyer and Morton's scheme has second order accuracy when $p = p(\rho)$, though not when a more general energy equation must be used. However, as their Fig. 12.4 shows, their scheme cannot handle shock waves. This defect can be remedied by the addition of an artificial viscosity, but they state that they regard this device as superseded by the Lax-Wendroff method [2, p. 320]. This latter method is inherently dissipative, and can handle shocks implicitly.

To obtain an alternative and dissipative difference scheme of second order accuracy for the Lagrangian Eqs. (1), we can follow Lax and Wendroff and expand in time:

$$\begin{aligned} R_j^{n+1} &= R_j{}^n + u_j{}^n \Delta t + \frac{1}{2}\left(\frac{\partial u}{\partial t}\right)_j^n (\Delta t)^2, \\ u_j^{n+1} &= u_j{}^n + \left(\frac{\partial u}{\partial t}\right)_j^n \Delta t + \frac{1}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)_j^n (\Delta t)^2. \end{aligned} \tag{3}$$

The first derivative $\partial u/\partial t$ can be evaluated as in [2],

$$\left(\frac{\partial u}{\partial t}\right)_j^n = -V_0 \left(\frac{R_j{}^n}{r_j}\right)^{\alpha-1} \frac{p^n_{j+1/2} - p^n_{j-1/2}}{\Delta r}, \tag{4}$$

The density ρ can be found using Eq. (2), and p can be found from the known function $p = p(\rho)$. The second derivative $\partial^2 u/\partial t^2$ can be evaluated by differentiating the second of Eqs. (1), and then differencing in the same style:

$$\begin{aligned} \left(\frac{\partial^2 u}{\partial t^2}\right)_j^n = &-(\alpha - 1)\, V_0 \frac{(R_j{}^n)^{\alpha-2}\, u_j{}^n}{(r_j)^{\alpha-1}} \frac{p^n_{j+1/2} - p^n_{j-1/2}}{\Delta r} \\ &- V_0 \left(\frac{R_j{}^n}{r_j}\right)^{\alpha-1} \frac{(\partial p/\partial t)^n_{j+1/2} - (\partial p/\partial t)^n_{j-1/2}}{\Delta r}. \end{aligned} \tag{5}$$

The derivative $\partial p/\partial t$ needed here is equal to $p'(\rho)\, \partial\rho/\partial t$, and can be evaluated from the time derivative of the equation of mass conservation, in a manner similar to the way in which ρ is evaluated from the original equation, as

$$-\frac{1}{(\rho^n_{j+1/2})^2}\left(\frac{\partial \rho}{\partial t}\right)^n_{j+1/2} = \alpha V_0 \frac{(R^{\alpha-1}u)^n_{j+1} - (R^{\alpha-1}u)^n_j}{(r_{j+1})^\alpha - (r_j)^\alpha}. \tag{6}$$

But the resulting explicit difference scheme is anti-dissipative and unstable. This is easily seen by applying the usual kind of approximate local stability analysis, in which coefficient variations are ignored. Also, since the analysis is local, we ignore spatial divergences by setting $\alpha = 1$ and simply considering the plane case. The terms in ρ and

p can be eliminated, and we can look for separable solutions of the difference equations of the form

$$R_j^n = A\xi^n e^{ijk\Delta r}, \quad u_j^n = B\xi^n e^{ijk\Delta r}, \tag{7}$$

for some constants A and B. Equations (3) then yield the relations

$$\begin{aligned} \xi A &= A + B\,\Delta t + A\left(\frac{c\rho V_0\,\Delta t}{\Delta r}\right)^2(\cos\theta - 1), \\ \xi B &= B + \left(\frac{c\rho V_0\,\Delta t}{\Delta r}\right)^2(\cos\theta - 1)\left(\frac{2A}{\Delta t} + B\right), \qquad \theta = k\,\Delta r. \end{aligned} \tag{8}$$

Here c is the velocity of sound. If we introduce the symbol μ:

$$\mu = \frac{cV_0\rho\,\Delta t}{\Delta r},$$

then the two solutions for ξ given by Eqs. (8) are

$$\xi = 1 - 2\mu^2\sin^2(\theta/2) \pm 2i\mu\sin(\theta/2). \tag{9}$$

The magnitude of both roots is $[1 + 4\mu^4\sin^4(\theta/2)]^{1/2}$, and hence, unlike the Lax-Wendroff scheme, this scheme is unstable.

However, a stable scheme can be obtained by the simple expedient of replacing the first of Eqs. (3) by the equally accurate relation

$$R_j^{n+1} = R_j^n + u_j^{n+1}\,\Delta t - \frac{1}{2}\left(\frac{\partial u}{\partial t}\right)_j^n(\Delta t)^2. \tag{10}$$

The finite difference scheme is still explicit if one calculates in order for u, r, ρ and $\partial\rho/\partial t$ at each time step. It may now also be stable, because the equation for ξ is modified to

$$\xi^2 - 2\xi[1 - 2\mu^2\sin^2(\theta/2)] + [1 - 4\mu^4\sin^4(\theta/2)] = 0. \tag{11}$$

The roots of Eq. (11) are a complex conjugate pair for which $|\,\xi\,|^2 = 1 - 4\mu^4\sin^4(\theta/2)$ if $0 < 2\mu^2\sin^2(\theta/2) < 1$, and are both zero when $\mu^2\sin^2(\theta/2) = 1/2$. The roots are real and of opposite sign for larger values of $\mu^2\sin^2(\theta/2)$. The root that is larger in magnitude becomes -1 when $2\mu^2\sin^2(\theta/2) = 5^{1/2} - 1$. Hence, the difference scheme is stable, and is also dissipative of fourth order, provided

$$0 < \mu = \frac{c\rho V_0\,\Delta t}{\Delta r} < \left[\frac{1}{2}(5^{1/2} - 1)\right]^{1/2} = 0.7862. \tag{12}$$

This condition is akin to the Courant-Friedrichs-Lewy condition [3], because $\rho V_0/\Delta r$

is the spatial separation between two Lagrangian grid points, though more restrictive than it because of the presence of the numerical factor 0.7862 in place of 1.

The instability that we have just encountered might appear to be a consequence of the fact that $u = \partial R/\partial t$ and, in this plane case, $\partial u/\partial t = \rho^2 c^2 V_0{}^2 \partial^2 R/\partial r^2$. This pair of equations is of a form that Richtmyer and Morton advise against [2, p. 294]. However, a more fundamental cause appears to be the use of the staggered grid that is implicitly involved in our analysis. To see this, consider the more general case of plane adiabatic flow, for which the $p = p(\rho)$ relation is replaced by the differential equation

$$\frac{\partial p}{\partial t} = c^2 \frac{\partial \rho}{\partial t} = -c^2 \rho^2 V_0 \frac{\partial u}{\partial r}. \tag{13}$$

We can continue using the same kind of staggered grid differencing, but now also need an equation for predicting the pressure, such as

$$p_{j+1/2}^{n+1} = p_{j+1/2}^{n} + \left(\frac{\partial p}{\partial t}\right)_{j+1/2}^{n} \Delta t + \frac{1}{2}\left(\frac{\partial^2 p}{\partial t^2}\right)_{j+1/2}^{n} (\Delta t). \tag{14}$$

An equation for $\partial^2 p/\partial t^2$ can of course be derived by differentiating that for $\partial p/\partial t$, and Eqs. (3) and (14) then together give sufficient relations for advancing the integration. But, as Eqs. (1) and (13) show, the variable R is not directly involved in the interrelation between p and u. A further stability analysis in which we set $p_{j+1/2}^{n} = C\xi^n e^{i(j+1/2)k\Delta r}$ in addition to Eqs. (7) yields

$$\begin{aligned}
\xi A &= A + B\,\Delta t - \frac{iV_0 C(\Delta t)^2}{\Delta r} \sin\left(\frac{\theta}{2}\right), \\
\xi B &= B - \frac{2iV_0 C\,\Delta t}{\Delta r} \sin\left(\frac{\theta}{2}\right) + \mu^2 B(\cos\theta - 1), \\
\xi C &= C - \frac{2ic^2\rho^2 V_0 B\,\Delta t}{\Delta r} \sin\left(\frac{\theta}{2}\right) + \mu^2 C(\cos\theta - 1),
\end{aligned} \tag{15}$$

and the second and third equations are independent of the first. They yield precisely the eigenvalues of Eq. (9). Hence we again have an unstable difference scheme, but again it may be stabilized by replacing *one* of the Taylor series expansions for advancing u and p by an expansion modeled after Eq. (10) in which the first derivative term is evaluated at the forward time. The third eigenvalue of Eqs. (15) is $\xi = 1$, so that the scheme that we have just proposed is dissipative of fourth order only for p and u, but not for R.

The fact that it is really the staggered grid that is causing the instabilities can be confirmed by considering a slight variant of the Lax-Wendroff procedure for the equations

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}\frac{\partial \mathbf{U}}{\partial x} = \mathbf{0}, \tag{16}$$

where **A** is a constant matrix. Suppose that a staggered grid is used for evaluating the first time derivatives via the first space derivatives to give

$$\mathbf{U}_j^{n+1} = \mathbf{U}_j^n - \frac{\Delta t}{\Delta x} \mathbf{A}(\mathbf{U}_{j+1/2}^n - \mathbf{U}_{j-1/2}^n) + \frac{1}{2}\left(\frac{\Delta t}{\Delta x} \mathbf{A}\right)^2 (\mathbf{U}_{j+1}^n - 2\mathbf{U}_j^n + \mathbf{U}_{j-1}^n). \quad (17)$$

Then with the same definition of θ as before, the eigenvalue g of the amplification matrix corresponding to an eigenvalue λ of **A** is

$$g = 1 - \frac{2i\lambda\, \Delta t}{\Delta x} \sin\frac{\theta}{2} - \left(\frac{\lambda\, \Delta t}{\Delta x}\right)^2 (1 - \cos\theta). \quad (18)$$

The presence of the term $2\sin(\theta/2)$, in place of the $\sin\theta$ of the original scheme, has the effect of changing stability to instability because Eq. (18) is of the same form as Eq. (9). This fact does not appear to have been noted before, presumably because the scheme of Eq. (17) is not practical for general forms of Eq. (16). It does become practical if the components of **U** fall into two equal sets, with the x-derivatives of one being related to the t-derivatives of the other. This essentially is what happens for the

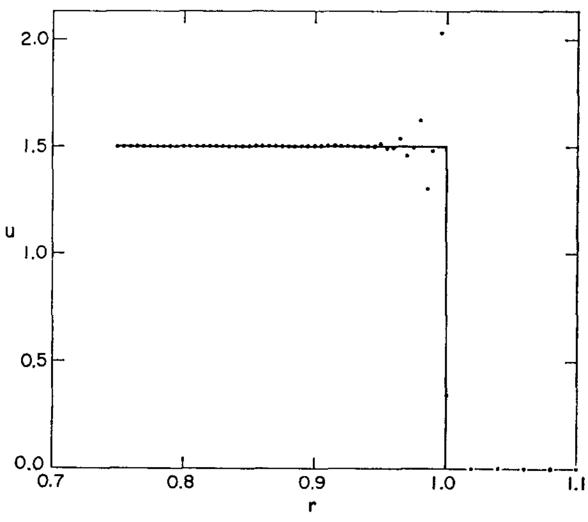

FIG. 1. An instantaneous increase in pressure by a factor 4 at the boundary $r = 0$ of an initially uniform plane slab of isothermal gas causes a shock to propagate into the undisturbed gas with velocity 2, in units of the velocity of sound. The condensed gas behind the shock moves with velocity 3/2. The filled circles show the solution for u at time $t = 0.5$ of a 100 point Lagrangian calculation performed using the methods described in the paper. There is a rigid wall at $t = 2$, and the exact solution is marked by solid lines. The nth Lagrangian point is initially at $r = 0.2(n - 1)$, and the values of $\rho_{1/2}$ and $(\partial\rho/\partial t)_{1/2}$ needed for the finite difference scheme are obtained using simple extrapolation formulas of second order accuracy. The maximum time step consistent with Eq. (12), applied for each interval, was used. The error in the computed position of the left hand free boundary is 2×10^{-5}. The points adjacent to the shock front show the characteristic oscillations, but the discontinuity is clearly and accurately marked.

Lagrangian equations of fluid flow. Then staggered spatial grids can be used, provided values updated in time are used in half of the extrapolation formulae as above.

The type of difference scheme proposed in this paper has been used extensively and successfully for integrations of the collapse of isothermal self-gravitating spheres [4]. The Richtmyer-Morton scheme was satisfactory for smoothly generated collapses, but not for the collapses generated by a sudden increase in pressure at the outer boundary of the sphere. Such an increase causes a shock to be formed instantly at the outer boundary, and to then propagate inwards. A simple test problem for the new difference scheme is the calculation of the isothermal shock for the corresponding problem with a uniform plane slab of gas, for which an exact analytical solution is easily found. Figure 1 shows a comparison between a numerical and an analytical solution, and is qualitatively very similar to Fig. 12.6 of [2], which displays a shock calculation performed using the original Lax-Wendroff scheme applied to Eulerian equations of motion.

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C. Hunter*

Joint Institute for Laboratory Astrophysics
University of Colorado and National Bureau of Standards
Boulder, Colorado 80309

* JILA Visiting Fellow 1976–1977, on leave from Florida State University.