PHYS 410 Finite Difference Methods November 2–7 2000
Notes on the 1-d Wave Equation

Recall that we are considering the following problem (1-d wave equation with unit speed ($c^2 = 1$) and fixed (Dirichlet) boundary conditions):

$$u_{tt}(x,t) = u_{xx}(x,t)\,, \tag{1}$$

on the domain

$$0 \le x \le 1 \qquad t \ge 0\,,$$

with initial and boundary conditions:

$$\begin{aligned} u(x,0) &= f(x), & (2)\\ u_t(x,0) &= g(x), & (3)\\ u(0,t) &= u(1,t) = 0\,. & (4) \end{aligned}$$

Continuum Solution

Assume for a moment that we are solving (1) on an *infinite* spatial domain:

$$-\infty < x < +\infty \qquad t > 0\,.$$

In this case, the general solution can be written as the *superposition* of an arbitrary *left-moving* "profile" ($v = -c = -1$) and an arbitrary *right-moving* "profile" ($v = +c = +1$), i.e.

$$u(x,t) = l(x+t) + r(x-t)\,. \tag{5}$$

The function $l(x,t) = l(x+t)$ is constant along the "left-directed" *characteristics* of the wave equation, while the function $r(x,t) = r(x-t)$ is constant along the "right-directed" characteristics

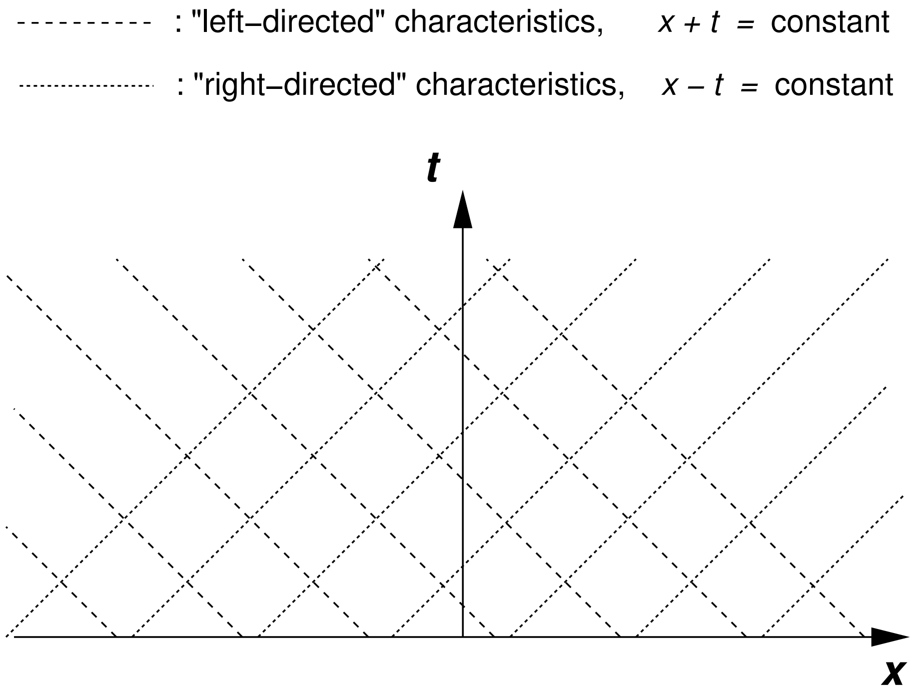

Figure 1: Characteristics of the wave equation: $u_{xx} = u_{tt}$. Signals (disturbances) travel along the characteristics (dashed and dotted lines.)

In fact, it is often convenient to specify the initial conditions for a wave equation, such as (1), in terms of the initially left-going and initially right-going parts of the solution. In particular, given the arbitrary profiles (functions), $l(x)$ and $r(x)$, we specify

$$
\begin{aligned}
u(x,0) &= l(x) + r(x)\,, && (6)\\
u_t(x,0) &= l'(x) - r'(x)\,. && (7)
\end{aligned}
$$

where $'$ denotes ordinary differentiation (i.e. $l' \equiv dl/dx$, etc.).

Generating Initial Data for The FDA

We first re-introduce the notation wherein a caret (hat) denotes a quantity which satisfies a difference equation. Thus, $\hat{u}^n_j$ is the quantity which satisfies the usual $O(h^2)$ approximation of (1):

$$\frac{\hat{u}^{n+1}_j - 2\hat{u}^n_j + \hat{u}^{n-1}_j}{\triangle t^{\,2}} = \frac{\hat{u}^n_{j+1} - 2\hat{u}^n_j + \hat{u}^n_{j-1}}{\triangle x^{\,2}}, \tag{8}$$

while u^n_j satisfies the *differential* (continuum) equation, i.e.

$$(u_{tt})^n_j = (u_{xx})^n_j, \qquad j = 1, 2, \cdots, J \qquad n = 0, 1, 2, \cdots .$$

(since the differential equation holds *everywhere*, it must, in particular, hold at all "grid points" (x_j, t^n)). We initialize (8) by specifying

$$\hat{u}^0_j, \qquad \hat{u}^1_j, \qquad j = 1, 2, \cdots, J$$

freely, but in a manner consistent with the boundary conditions

$$\hat{u}^0_1 = \hat{u}^0_J = \hat{u}^1_1 = \hat{u}^1_J = 0.$$

We now assume that our difference solution will admit a Richardson expansion (why?)

$$\hat{u}(x,t) = u(x,t) + h^2 e_2(x,t) + h^4 e_4(x,t) + \cdots , \tag{9}$$

$\hat{u}_j^0$ and $\hat{u}_j^1$. First recall that the problem prescription includes the initial conditions:

$$u\,(x,0) = f\,(x)\ , \qquad\qquad u_t\,(x,0) = g\,(x)\ .$$

Clearly then, we can (and might as well) specify $\hat{u}_j^0$ exactly:

$$\hat{u}_j^0 = f_j\,,$$

which implies (of course) that $e_2(x,0) = 0$. Then in order for (9) to hold, we must have

$$\begin{aligned}
\hat{u}_j^1 &\equiv \hat{u}(x_j,\, \triangle t\,) \\
&= u(x_j,\, \triangle t\,) + h^2 e_2(x_j,\, \triangle t\,) + O(h^4)\,,
\end{aligned}$$

which implies that

$$\hat{u}(x_j,\, \triangle t\,) - u(x_j,\, \triangle t\,) = h^2 e_2(x_j,\, \triangle t\,) + O(h^4)\,.$$

But

$$
\begin{aligned}
e_2(x_j,\, \triangle t\,) &= e_2(x_j,0) + \triangle t\, \frac{\partial e_2}{\partial t}(x_j,0) \,+\, O(\,\triangle t^{\,2}) \\
&= \triangle t\, \frac{\partial e_2}{\partial t}(x_j,0) + O(\,\triangle t^{\,2}) = \lambda h \frac{\partial e_2}{\partial t}(x_j,0) + O(\,\triangle t^{\,2})
\end{aligned}
$$

Thus,

$$
\hat{u}(x_j,\, \triangle t\,) - u(x_j,\, \triangle t\,) = h^2 \left(\lambda h \frac{\partial e_2}{\partial t}(x_j,0) \right) \,+\, \cdots = O(h^3)\,,
$$

and *we see that we must specify* $\hat{u}_j^1$ *to* $O(h^3)$ *accuracy in order for our solution to be (globally)* $O(h^2)$ *accurate.*

In this example (and elsewhere) we can readily initialize $\hat{u}_j^1$ to $O(h^3)$ accuracy simply by Taylor-expanding to sufficiently high order, and then using the equations of motion to eliminate higher time derivatives:

$$
\begin{aligned}
u(x_j,\, \triangle t\,) &= u(x_j,0) + \triangle t\ u_t(x_j,0) + \frac{1}{2}\triangle t^{\,2}\, u_{tt}(x_j,0) + O(\,\triangle t^{\,3}) \\
&= u(x_j,0) + \triangle t\ u_t(x_j,0) + \frac{1}{2}\triangle t^{\,2}\, u_{xx}(x_j,0) + O(h^3)\,.
\end{aligned}
$$

Recalling (6-7), where we specified the initial conditions in terms of initially left-moving and right-moving profiles, $l(x)$ and $r(x)$, and their derivatives, $l'(x)$ and $r'(x)$:

$$
\begin{aligned}
u\,(x,0) &= l\,(x) + r\,(x)\ , \\
u_t\,(x,0) &= l'\,(x) - r'\,(x)\ ,
\end{aligned}
$$

and noting that

$$
u_{tt}\,(x,0) = l''\,(x) + r''\,(x)\ ,
$$

we have for our initialization:

$$
\begin{aligned}
\hat{u}_j^0 &= l_j + r_j\,, && (10) \\
\hat{u}_j^1 &= l_j + r_j + \triangle t\ \left(l'_{\,j} - r'_{\,j}\right) + \frac{1}{2}\triangle t^{\,2}\left(l''_{\,j} + r''_{\,j}\right)\ . && (11)
\end{aligned}
$$

Implementation Notes

In treating time-dependent PDEs using FD techniques, it is generally not feasible (even in 1-d) to store *all* of the data which is generated during the evolution—i.e., in the current case, all of the u_j^n for $n = 0, 1, \cdots$.

Indeed, for multi-dimensional problems (3-d calculations in particular), computations are often *memory-limited* or *memory-bound*, and then it becomes important to implement the FD algorithm using as *little* storage as possible, using periodic output (usually to a file) to save the generated data from intermediate time-steps. A natural way to represent (store) u_j^{n-1}, u_j^n and u_j^{n+1} is to use a two dimensional array:

```
real*8     u(maxj,ntlevs)
```

where the constant `maxj` is the maximum number of spatial grid points allowed, and the constant `ntlevs` is the number of time-levels of data stored at any instant. Superficial investigation of the difference equation (8) suggests that we need `ntlevs = 3`, but we can actually code (8) using storage for only *two* levels (level n and level $n+1$) since u_j^{n-1} is only referenced just before u_j^{n+1} is computed.

The following code segment also illustrates a technique wherein we use integer variables `n`, `nm1` and `np1` as "pointers" to whichever columns of the array `u` currently hold the levels n, $n-1$ and $n+1$ data respectively. Using this mechanism we can effect (implement) a time-step advance—wherein the level n data becomes level $n-1$ and level $n+1$ becomes level n—simply be redefining the scalars `n`, `nm1` and `np1`. In particular, with this approach there is no need to *copy* any of the grid function data to advance from $t = t^n$ to $t = t^{n+1}$.

```
      real*8      u(maxj,2)
      integer     n,   nm1,    np1,   nswap

      n   = 2       ! Initialize "pointers"---note 'n-1' and 'n+1'
      nm1 = 1       ! storage is shared; only possible due to
      np1 = 1       ! explicit nature of FDA

c     Section of code which initializes  u(j,nm1) and u(j,n)
c     goes here.

      do it = 2 , nt       ! Begin time-step loop
         u(1,np1) = 0.0d0
         do j = 2 , nx - 1
            u(j,np1) = 2.0d0 * u(j,n) - u(j,nm1) +
     &          lamsq * (u(j+1,n) - 2.0d0 * u(j,n) + u(j-1,n))
         end do
         u(nx,np1) = 0.0d0

c        Periodic output of u(j,np1) goes here

c        Swap time level pointers (time step advance)

         nswap = np1
         np1   = n
         n     = nswap
         nm1   = np1
      end do               ! End time step loop
```

Stability Analysis

One of the most frustrating—yet fascinating—features of FD solutions of time dependent problems, is that the discrete solutions often "blow up"—e.g. floating-point overflows are generated at some point in the evolution. Although "blow-ups" can sometimes be caused by legitimate (!) "bugs"—i.e. an incorrect implementation—at other times it is simply the *nature of the FD scheme* which causes problems. We are thus lead to consider the *stability* of solutions of difference equations (as well as their differential-equation progenitors).

Let us again consider our prototypical time-dependent differential equation (1), and let us now remark that this is a *linear, non-dispersive* wave equation, a consequence of which is the fact that the "size" of the waves does *not* change with time:

$$\|u(x,t)\| \sim \|u(x,0)\| \,, \tag{12}$$

where $\|\cdot\|$ is an suitable norm, such as the L_2 norm:

$$\|u(x,t)\| \equiv \left(\int_0^1 u(x,t)^2\,dx\right)^{1/2} . \tag{13}$$

We will use the property captured by (12) as our working definition of stability. In particular, if you believe (12) is true for the wave equation, then you believe the wave equation is stable.

Fundamentally, if our FDA approximation *converges*, then we expect the same behaviour for the difference solution (note that in this section, we drop the carets on solutions of difference equations):

$$\| u_j^n \| \sim \| u_j^0 \| \,. \tag{14}$$

Now, we construct our FD solution by *iterating in time*, generating

$$u_j^0,\ u_j^1,\ u_j^2,\ u_j^3,\ u_j^4,\ \cdots$$

in succession, using the FD equation

$$u_j^{n+1} = 2u_j^n - u_j^{n-1} + \lambda^2 \left(u_{j+1}^n - 2u_j^n + u_{j-1}^n \right) \,.$$

As it turns out, we are *not* guaranteed that (14) holds for all values of $\lambda \equiv \triangle t \,/\, \triangle x$. In fact, for certain λ (all $\lambda > 1$, as we shall see), we have

$$\| u_j^n \| \gg \| u_j^0 \| \,,$$

and for those λ, $\| u^n \|$ *diverges* from u, even (especially!) as $h \to 0$—that is, the difference scheme is *unstable*.

In fact, for many wave problems (including all linear problems), given that a FD scheme is *consistent* (i.e. so that $\hat{\tau} \to 0$ as $h \to 0$), stability is the necessary and sufficient condition for convergence (and vice versa).

Let us write a general time-dependent FDA in the form

$$\mathbf{u}^{n+1} = \mathbf{G}[\mathbf{u}^n]\,, \tag{15}$$

where $\mathbf{G}$ is some *update operator* (linear in our example problem), and $\mathbf{u}$ is a column vector containing sufficient unknowns to write the problem in first-order-in-time form. For example, if we introduce a new, auxiliary set of unknowns, v_j^n, defined by

$$v_j^n = u_j^{n-1}\,,$$

then we can rewrite the differenced-wave-equation (8) as

$$\begin{aligned} u_j^{n+1} &= 2u_j^n - v_j^n + \lambda^2 \left(u_{j+1}^n - 2u_j^n + u_{j-1}^n \right)\,, &(16)\\ v_j^{n+1} &= u_j^n\,, &(17) \end{aligned}$$

so with

$$\mathbf{u}^n = [u_1^n, v_1^n,\ u_2^n, v_2^n,\ \cdots\ u_J^n, v_J^n]\,,$$

(for example), (16-17) is clearly of the form (15).

Equation (15) provides us with a compact way of describing the solution of the FDA. Given initial data, $\mathbf{u}^0$, the solution after n time-steps is

$$\mathbf{u}^n = \mathbf{G}^n \mathbf{u}^0\,, \tag{18}$$

where $\mathbf{G}^n$ is the n-th power of the matrix $\mathbf{G}$. Now, assume that $\mathbf{G}$ has a complete set of orthonormal eigenvectors

$$\mathbf{e}_k, \quad k = 1, 2, \cdots J\,,$$

and corresponding eigenvalues

$$\mu_k, \quad k = 1, 2, \cdots J\,,$$

so that

$$\mathbf{G}\,\mathbf{e}_k = \mu_k\,\mathbf{e}_k, \quad k = 1, 2, \cdots J\,.$$

We can then write the initial data as (spectral decomposition):

$$\mathbf{u}^0 = \sum_{k=1}^{J} c_k^0 \, \mathbf{e}_k \,,$$

where the c_k^0 are coefficients. Using (18), the solution at time-step n is then

$$\begin{aligned} \mathbf{u}^n &= \mathbf{G}^n \left(\sum_{k=1}^{J} c_k^0 \, \mathbf{e}_k \right) && (19) \\ &= \sum_{k=1}^{J} c_k^0 \, (\mu_k)^n \, \mathbf{e}_k \,. && (20) \end{aligned}$$

Clearly, if the difference scheme is to be stable, we must have

$$\boxed{|\mu_k| \leq 1 \qquad k = 1, 2, \cdots J} \tag{21}$$

(Note: μ_k will be complex in general, so $|\mu|$ denotes complex modulus, $|\mu| \equiv \sqrt{\mu\mu^\star}$).

Geometrically, then, the eigenvalues of the update matrix must lie on or within the unit circle (see Figure 2).

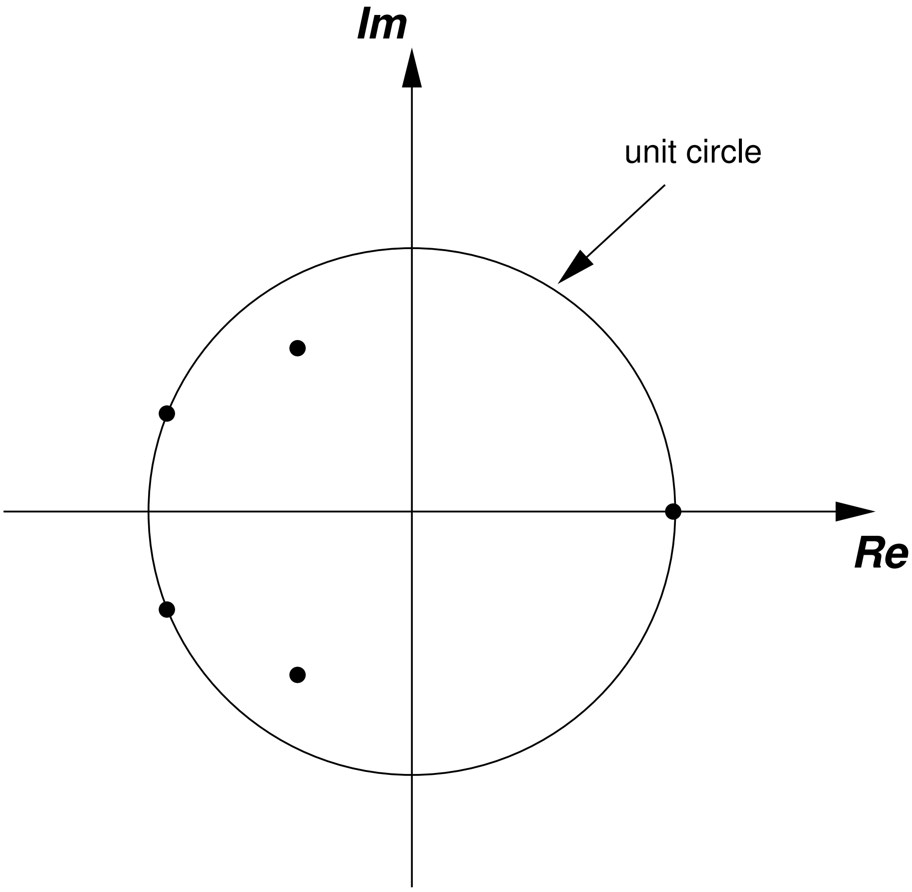

Figure 2: Schematic illustration of location in complex plane of eigenvalues of update matrix G. In this case, all eigenvalues (dots) lie on or within the unit circle, indicating that the corresponding finite difference scheme is stable.

Von-Neumann (Fourier) Stability Analysis

Von-Neumann stability analysis is based on the ideas sketched above, but additionally assumes that the difference equation is linear with constant coefficients, and that the boundary conditions are periodic. We can then use Fourier analysis, which has the same benefits in the discrete domain—difference operators in real-space variable $x \longrightarrow$ algebraic operations in Fourier-space variable k—as it does in the continuum Schematically, instead of writing

$$\mathbf{u}^{n+1}(x) = \mathbf{G}[\mathbf{u}^{n}(x)]\,,$$

we consider the Fourier-domain equivalent:

$$\tilde{\mathbf{u}}^{n+1}(k) = \tilde{\mathbf{G}}[\tilde{\mathbf{u}}^{n}(k)]\,,$$

where k is the wave-number (Fourier-space variable) and $\tilde{\mathbf{u}}$ and $\tilde{\mathbf{G}}$ are the Fourier-transforms of $\mathbf{u}$ and $\mathbf{G}$, respectively.

Specifically, we define the Fourier-transformed grid function via

$$\tilde{\mathbf{u}}^n(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ikx}\, \mathbf{u}^n(x)\, dx\,. \tag{22}$$

For a general difference scheme, we will find that

$$\tilde{\mathbf{u}}^{n+1}(k) = \tilde{\mathbf{G}}(\xi)\, \tilde{\mathbf{u}}^n(k)\,,$$

where $\xi \equiv kh$, and we will have to show that $\tilde{\mathbf{G}}(\xi)$'s eigenvalues lie within or on the unit circle for all conceivable ξ. The appropriate range for ξ is

$$-\pi \leq \xi \leq \pi\,,$$

since the shortest wavelength representable on a uniform mesh with spacing h is $\lambda = 2h$ (Nyquist limit), corresponding to a maximum wave number $k = (2\pi)/\lambda = \pm\pi/h$.

Let us consider the application of the Von-Neumann stability analysis to our current model problem. We first define a (non-divided) difference operator D^2 as follows:

$$D^2\, u(x) = u(x+h) - 2u(x) + u(x-h)\,.$$

Then, suppressing the spatial grid index, we can write the first-order form of the difference equation (16-17) as

$$\begin{aligned} u^{n+1} &= 2u^n - v^n + \lambda^2\, D^2\, u^n\,, \\ v^{n+1} &= u^n\,, \end{aligned}$$

or

$$\begin{bmatrix} u \\ v \end{bmatrix}^{n+1} = \begin{bmatrix} 2+\lambda^2\, D^2 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}^{n}. \tag{23}$$

In order to perform the Fourier transform, we need to know the action of D^2 in Fourier-space. Using the transform inverse to (22) we have

$$u(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ikx} \, \tilde{u}(k) \, dk \,,$$

so

$$\begin{aligned} D^2 \, u(x) = u(x+h) - 2u(x) + u(x-h) \; &= \; \int_{-\infty}^{+\infty} \left(e^{ikh} - 2 + e^{-ikh}\right) e^{ikx} \, \tilde{u}(k) \, dk \\ &= \; \int_{-\infty}^{+\infty} \left(e^{i\xi} - 2 + e^{-i\xi}\right) e^{ikx} \, \tilde{u}(k) \, dk \,. \end{aligned}$$

Now consider the quantity $-4\sin^2(\xi/2)$:

$$\begin{aligned} -4\sin^2\frac{\xi}{2} \; &= \; -4\left(\frac{e^{i\xi/2} - e^{-i\xi/2}}{2i}\right)^2 \\ &= \; \left(e^{i\xi/2} - e^{-i\xi/2}\right)^2 = e^{i\xi} - 2 + e^{-i\xi} \,, \end{aligned}$$

so

$$D^2 \, u(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left(-4\sin^2\frac{\xi}{2}\right) e^{ikx} \, \tilde{u}(k) \, dk \,.$$

In summary, under Fourier transformation, we have

$$\begin{aligned} \mathbf{u}(x) &\longrightarrow \tilde{\mathbf{u}}(k)\,, \\ D^2\mathbf{u}(x) &\longrightarrow -4\sin^2\frac{\xi}{2}\tilde{\mathbf{u}}(k)\,. \end{aligned}$$

Using this result in the Fourier transform of (23), we see that we need to compute the eigenvalues of

$$\begin{bmatrix} 2-4\lambda^2\sin^2(\xi/2) & -1 \\ 1 & 0 \end{bmatrix},$$

and determine the conditions under which the eigenvalues lie on or within the unit circle. The characteristic equation (whose roots are the eigenvalues) is

$$\begin{vmatrix} 2-4\lambda^2\sin^2(\xi/2)-\mu & -1 \\ 1 & -\mu\,, \end{vmatrix} = 0$$

or

$$\mu^2 + \left(4\lambda^2\sin^2\frac{\xi}{2} - 2\right)\mu + 1 = 0\,.$$

This equation has roots

$$\mu(\xi) = \left(1 - 2\lambda^2 \sin^2 \frac{\xi}{2}\right) \pm \left(\left(1 - 2\lambda^2 \sin^2 \frac{\xi}{2}\right)^2 - 1\right)^{1/2}.$$

We now need to find sufficient conditions for

$$|\mu(\xi)| \leq 1,$$

or equivalently

$$|\mu(\xi)|^2 \leq 1.$$

To this end, we note that we can write

$$\mu(\xi) = (1 - Q) \ \pm \ ((1 - Q)^2 - 1)^{1/2},$$

where the quantity, Q

$$Q \equiv 2\lambda^2 \sin^2 \frac{\xi}{2},$$

is *real* and *non-negative* ($Q \geq 0$).

There are now two cases to consider:

1. $(1-Q)^2 - 1 \leq 0$,
2. $(1-Q)^2 - 1 > 0$.

In the first case, $((1-Q)^2 - 1)^{1/2}$ is purely imaginary, so we have

$$|\mu(\xi)|^2 = (1-Q)^2 + (1-(1-Q)^2) = 1 \, .$$

In the second case, $(1-Q)^2 - 1 > 0 \longrightarrow (1-Q)^2 > 1 \longrightarrow Q > 2$, and then we have

$$1 - Q - ((1-Q^2) - 1)^{1/2} \, < \, -1 \, ,$$

so, in this case, our stability criterion will *always* be violated. We thus conclude that a necessary condition for Von-Neumann stability is

$$(1-Q)^2 - 1 \leq 0 \longrightarrow (1-Q)^2 \leq 1 \longrightarrow Q \leq 2 \, .$$

Since $Q \equiv 2\lambda \sin^2(\xi/2)$ and $\sin^2(\xi/2) \leq 1$, we must therefore have

$$\lambda \equiv \frac{\triangle t}{\triangle x} \leq 1 \, ,$$

for stability of our scheme (8).

This condition is often called the CFL condition—after Courant, Friedrichs and Lewy who derived it in 1928 (the ratio $\lambda = \triangle x \,/\, \triangle t$ is also frequently called the *Courant number*).

In practical terms, we must limit time-discretization scale , $\triangle t$, to values no larger than the space-discretization scale, $\triangle x$.

Furthermore, this type of instability has a "physical" interpretation, often summarized by the statement *the numerical domain of dependence of an explicit difference scheme must contain the physical domain of dependence.*