3.3. Phase and Amplitude Errors of 1-D Advection Equation

Reading: Duran section 2.4.2. Tannehill et al section 4.1.2.

The following example F.D. solutions of a 1D advection equation show errors in both the wave amplitude and phase.

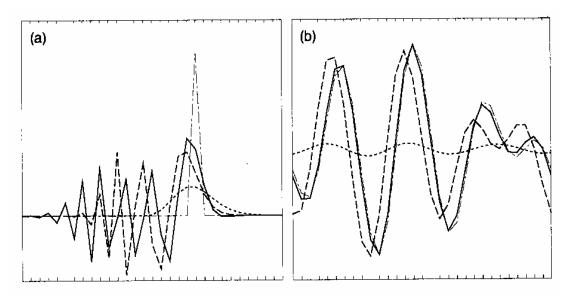


FIGURE 2.13. Exact solution and differential-difference solutions for (a) advection of a spike over a distance of five grid points, and (b) advection of the sum of equal-amplitude $7.5\Delta x$ and $10\Delta x$ sine waves over a distance of twelve grid points. Exact solution (dot-dashed), one-sided first-order (short-dashed), centered second-order (long-dashed), and centered fourth-order (solid). The distribution is translating to the right. Grid-point locations are indicated by the tick marks at the top and bottom of the plot.

In this section, we will examine the truncation errors and try to understand their behaviors.

3.3.1. Modified equation

The 1D advection equation is

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0.$$
(5)

Upwind or Donor-Cell Approximation

We have discussed earlier the stability of the forward-in-time upstream-in-space approximation to the 1D advection equation, using the energy method. The FDE is

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$$
(6)

Here we assume c>0, therefore the scheme is <u>upstream</u> in space.

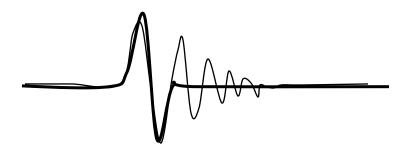
We can find from (6) that

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = -\frac{\Delta t}{2}u_{tt} + \frac{c\Delta x}{2}u_{xx} - \frac{(\Delta t)^2}{6}u_{ttt} - \frac{c(\Delta x)^2}{6}u_{xxx} + O(\Delta x^3 + \Delta t^3)$$
(7)

and the right hand side is the truncation error. The scripts x and t denote partial derivative.

An analysis of τ can reveal a lot about the expected behavior of the numerical solution, and to investigate, we develop what is known as the <u>Modified Equation</u>. In this method, we write τ so as to illustrate the anticipated error types.

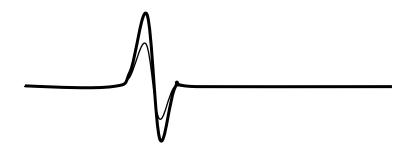
<u>**Dispersion Error**</u> – occurs when the leading terms in τ have <u>odd-order</u> derivatives. They are characterized by oscillations or small wiggles in the solution, mostly in the form of moving waves.



In the above example, the thick line is the true solution and thin line is the numerical solution.

It's called dispersion error because waves of different wavelengths propagate at different speed (i.e., wave speed = a function of k) due to numerical approximations – causing <u>dispersion</u> of waves. For the PDE, all Fourier components described by Eq.(5) should move at the same speed, c.

Dissipation Error – occurs when the leading terms int have <u>even-order derivatives</u>. They are characterized by a loss of wave amplitude. The effect is also called <u>artificial viscosity</u> and is implicit in the numerical solution.



The combined effect of dissipation and dispersion is often called diffusion.

To isolate these errors, we derive the <u>Modified Equation</u>, which is the PDE that is actually solved when a FD scheme is applied to the PDE.

The modified equation is obtained by replacing time derivatives in the truncation error by the spatial derivatives. Let's do this for Eq.(7).

To replace u_{tt} in right hand side of (7), we take (Eq.(7))_t [note here we use the FDE not the PDE] \rightarrow

$$u_{tt} + cu_{xt} = -\frac{\Delta t}{2}u_{ttt} + \frac{c\Delta x}{2}u_{xxt} - \frac{(\Delta t)^2}{6}u_{ttt} - \frac{c(\Delta x)^2}{6}u_{xxxt} + \dots$$
(8)

and $-c (Eq(7))_x$

$$-cu_{tx} - c^{2}u_{xx} = \frac{c\Delta t}{2}u_{tx} - \frac{c^{2}\Delta x}{2}u_{xxx} + \frac{c(\Delta t)^{2}}{6}u_{ttx} + \frac{c^{2}(\Delta x)^{2}}{6}u_{xxxx} + \dots$$
(9)

then add (8) and (9) \rightarrow

$$u_{tt} = c^{2}u_{xx} + \Delta t \left(\frac{-u_{ttt}}{2} + \frac{c}{2}u_{ttx} + O(\Delta t)\right) + \Delta x \left(\frac{c}{2}u_{xxt} - \frac{c^{2}}{2}u_{xxx} + O(\Delta x)\right).$$
(10)

Similarly, we can obtain other time derivatives, u_{ttt} found in (7) and (10) and u_{ttx} and u_{xxt} found in (10). They are (see Table 4.1 of Dannehill et al):

$$u_{ttt} = -c^{3}u_{xxx} + O(\Delta x + \Delta t)$$

$$u_{tx} = c^{2}u_{xxx} + O(\Delta x + \Delta t)$$

$$u_{xxt} = -cu_{xxx} + O(\Delta x + \Delta t)$$
(11)

Combining (7), (10) and (11) \rightarrow

$$u_{t} + cu_{x} = \frac{c\Delta t}{2} (1 - \mu) u_{xx} - \frac{c(\Delta x)^{2}}{6} (2\mu^{2} - 3\mu + 1) u_{xxx} + O(\Delta x^{3}, \Delta x^{2}\Delta t, \Delta t^{2}\Delta x, \Delta t^{3})$$
(12)

where $\mu = \frac{c\Delta t}{\Delta x}$.

Eq.(12) is the modified equation, which shows the error terms relative to the original PDE.

Note that the leading term has as form of $K \frac{\partial^2 u}{\partial x^2}$ which, for 1- $\mu > 0$, represent the dissipation (or diffusion as we often call it) process and therefore the dominant error is of a <u>dissipation</u> nature.

Note that if we had used CTCS scheme $\delta_{2t} + c \delta_{2x} u = 0$, then the leading error term in the modified equation would be

$$\frac{c(\Delta x)^2}{6} \Big[\mu^2 - 1 \Big] \frac{\partial^3 u}{\partial x^3}.$$
(12)

It contains the third (odd) order derivative, and the dominant error is of the dispersive nature.

Returning to the upstream scheme, we find that when $\mu = c \Delta t/\Delta x = 1$, the scheme is exact!! The coefficient of the leading error term, $\frac{c\Delta t}{2}(1-\mu)$, is called the <u>artificial viscosity</u>, and when $\mu \neq 1$, causes severe damping of the computational solution (see figure shown earlier). In fact, the Doner-Cell is well known for its strong damping. Read Tannehill et al, Section 4.1.2.

3.3.2. Quantitative Estimate of Phase and Amplitude Errors

Reading: Sections 4.1.2 – 4.1.12 of Tannehill et al. Sections 2.5.1 and 2.5.2 of Durran.

By examining the leading order error in the modified equation, we can find the basic nature of the error. To estimate the error quantitatively, we use either <u>analytical</u> (as part of the stability analysis) or <u>numerical</u> method. We will first look at the former.

With the stability analysis, we were already examining the <u>amplitude</u> of waves in the numerical solution. For a linear advection equation, we want the <u>amplification factor</u> to be 1, so that the wave does not grow or decay in time. The von Neumann stability analysis actually also provides the information about propagation (phase) speed of the waves. Any difference between the numerical phase speed and true phase speed is the <u>phase error</u>.

Going back to the figure we showed at the beginning of this section (section 3.3) and reproduced in the following, we can see that the first-order FTUS scheme has strong amplitude error but little phase error, while the 2nd-order CTCS scheme has large phase error but small amplitude error. The 4th-order CTCS scheme has a smaller phase error than its 2nd-order counterpart.

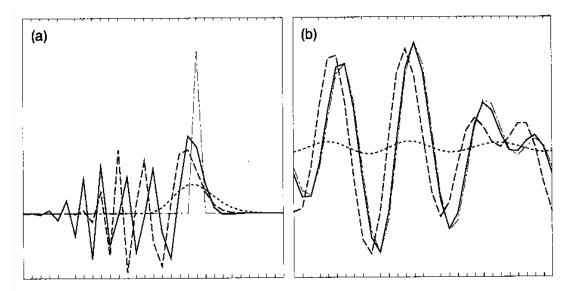


FIGURE 2.13. Exact solution and differential-difference solutions for (a) advection of a spike over a distance of five grid points, and (b) advection of the sum of equal-amplitude $7.5\Delta x$ and $10\Delta x$ sine waves over a distance of twelve grid points. Exact solution (dot-dashed), one-sided first-order (short-dashed), centered second-order (long-dashed), and centered fourth-order (solid). The distribution is translating to the right. Grid-point locations are indicated by the tick marks at the top and bottom of the plot.

Amplitude Error

Recall that in the Neumann stability analysis, the frequency $\underline{\omega}$ can be complex, and <u>if it is</u>, there will be either <u>decay or growth</u> in amplitude – which is entirely <u>computational</u> for a pure advection problem. This is so because

if ω is real,

 $|\lambda| = |\exp(-i\omega\Delta t)| = |\cos(\omega\Delta t) + i\sin(\omega\Delta t)| = 1 \rightarrow \text{ no change in amplitude.}$

if ω is complex, i.e., $\omega = \omega_R + i \omega_I$,

 $|\lambda| = |\exp(-i\omega\Delta t)| = |\exp(-i\omega_R \Delta t) \exp(\omega_I \Delta t)| = |\exp(\omega_I \Delta t)| \neq 1 \text{ most of the time.}$

When $\omega_I > 0$, $|\lambda| > 1$, the wave grows and when $\omega_I < 0$, $|\lambda| < 1$ the wave decays (is damped). $|\lambda|$ is the amplitude change per time step and $|\lambda|^N$ is the <u>total</u> amplitude change after *N* steps.

If, e.g., $|\lambda| = 0.95$, then after 100 steps, the amplitude becomes 5.92 x 10⁻³!

Remember for <u>PDE</u> $u_x + c u_x = 0$, the frequency ω is always real. Assuming wave solution $u = U \exp[i(kx - \omega t)]$, you can find $\omega = kc$, which is called the dispersion relation in wave dynamics. For the current problem the phase speed of waves is $\omega/k = c$ which is the same for all wave components. Therefore the analytic waves are non-dispersive.

Phase Error

For convenience, let's define

 ω_a = frequency of the <u>analytical</u> solution (PDE) ω_d = frequency of <u>discrete</u> solution (FDE)

then

 $\lambda_a \equiv \exp(-i\omega_a \Delta t), \ \lambda_d \equiv \exp(-i\omega_d \Delta t).$

Recall that if z = x + i y ($i = \sqrt{-1}$), we can use the polar form and write

 $z = |z| \exp(i \theta)$ or $z = |z| (\cos\theta + i \sin\theta)$

where $|z| = (x^2 + y^2)^{1/2}$ is called the modulus of z.

Thus,

 $\lambda_a = |\lambda_a| exp(i \theta_a) = exp(i \theta_a)$ (because $|\lambda_a| = 1$ for advection problem).

We define θ_a = the <u>phase change per time step</u> of the analytic solution

= - $\omega_a \Delta t$ ~ frequency × time step size

For the finite difference solution, ω will, in general, be complex, i.e., ω has an imaginary part:

$$\omega_d = (\omega_d)_R + i (\omega_d)_I$$

$$\therefore \qquad \lambda_d = exp[(\omega_d)_I \Delta t] exp[-i(\omega_d)_R \Delta t] = |\lambda_d| exp(i \theta_d) \rightarrow$$
(13)

 $\theta_d \equiv -(\omega_d)_R \Delta t$ is the <u>phase change per time step</u> associated with the F.D. scheme. $|\lambda_d|$ is not necessarily 1 here.

From (13), we can see that
$$\theta_d = \operatorname{atan} \frac{\operatorname{Im}\{\lambda_d\}}{\operatorname{Re}\{\lambda_d\}}$$
. (14)
Taking the radio, $\frac{\theta_d}{\theta_a} = \frac{-(\omega_d)_R \Delta t}{-\omega_a \Delta t} = \frac{kc_d}{kc_a} = \frac{c_d}{c_a}$

for the same wave number, and the ratio tells us about the relative phase error.

If $c_d / c_a < 1$, the F.D. solution <u>lags</u> the analytic solution (moves slower) If $c_d / c_a > 1$, the F.D. solution <u>leads</u> the analytic solution (moves faster) If $c_d / c_a = 1$, the F.D. solution has no phase error

a) First-order upwind scheme

Let's now apply these notations of phase and amplitude error to the first-order upwind (donor-cell) scheme.

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$$
(15)

Using Neumann method, assume that $u_i^n = U \lambda_d^n e^{ikx_i}$, you can show for yourself that

$$\lambda_d = 1 - \mu + \mu \cos(k\Delta x) - i \,\mu \sin(k\Delta x) \tag{16}$$

where $\mu = c\Delta t / \Delta x$ is the Courant number.

$$|\lambda_d|^2 = 1 + 2\mu(\mu - 1) [1 - \cos(k\Delta x)]$$

since 1-cos($k \Delta x \ge 0$,

 $|\lambda_d| \leq 1$ when $\mu \leq 1$.

Look at the $2\Delta x$ wave, $k\Delta x = 2\pi/w.l$. $\Delta x = 2\pi/(2\Delta x) \Delta x = \pi$

$$|\lambda_d|^2 = 1 + 2\mu(\mu - 1) [1+1] = 1 + 4\mu(\mu - 1).$$
(17)

When $\mu = 1$, $|\lambda_d| = 1$, there is no amplitude error.

When $\mu = 0.5$, $|\lambda_d| = 0$, the 2 Δx wave is completed damped in one time step!!

For a $4\Delta x$ wave and when $\mu = 0.5$, $|\lambda_d| = 0.5 \rightarrow 4\Delta x$ waves are damped by half in one time step!

Therefore, the upwind advection scheme is strongly <u>damping</u>. It should not be used except for some special reason.

The following figure shows the amplification modulus for the upwind scheme plotted for different values of μ (υ in the figure), the Courant number.

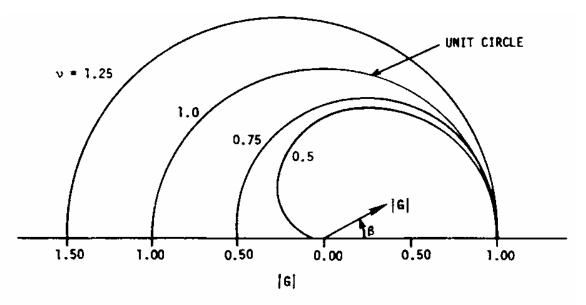


Figure 4.2 Amplification factor modulus for upstream differencing scheme.

 β in the figure is our $k\Delta x$, and $\pi\Delta x/L \le k\Delta x \le \pi$. The lower and upper limits of $k\Delta x$ correspond to 2L and $2\Delta x$ waves, respectively. *L* is the length of the computational domain.

This is so because the shortest wave supported is $2\Delta x$ in wavelength, \rightarrow

 $k\Delta x = 2\pi/(2\Delta x) \Delta x = \pi$

The longest wave supported by a domain of length L is 2L in wavelength \rightarrow

 $k \Delta x = 2 \pi / (2L) \Delta x = \pi \Delta x / L$

 $k \Delta x \rightarrow 0$ when $L \rightarrow \infty$.

For example, for a $4\Delta x$ wave, $k\Delta x = \pi/2$

From the figure, we see that:

When $\mu = 1$, the amplification factor is 1, there is <u>no amplitude error</u> for all values of $k\Delta x$ (β), i.e., for all waves.

When $\mu > 1$, the amplification factor is > 1 for all $k\Delta x$ except for wave number zero. The amplification factor is the largest for the shortest wave ($k\Delta x = \pi$), implying that the $2\Delta x$ wave will grow the fastest when $\mu > 1$, in another word, the $2\Delta x$ wave is most unstable.

This is why we see grid-scale noises when the solution blows up!

When $\mu < 1$, all waves are stable but are significantly <u>damped</u>. Again, the amplitude error is larger for shorter waves (larger $k\Delta x$). For Courant number of 0.75, the amplitude of the $2\Delta x$ wave is reduced by half after one single time step. The error is even bigger when $\mu = 0.5$.

From the above, we can see that the numerical <u>solution</u> is <u>poorest</u> for <u>the shortest waves</u>, and as the wavelength increases, the solution becomes increasingly accurate. This is so because longer waves are sampled by a large number of grid points and are, therefore, <u>well resolved</u>.

 $2\Delta x$ wave is special in that it is often the most unstable when stability criterion is violated, and when the solution is stable it tends to be most inaccurate.

For general cases, it is impossible to ensure $\mu = 1$ everywhere unless the advection speed is constant. Therefore, strong damping is inevitable with the upwind scheme. You will see severely smoothed solution when using this scheme.

The damping behavior of the upwind scheme can also be understood from the modified equation (13) discussed earlier. The leading error term is of the form $K \frac{\partial^2 u}{\partial x^2}$ which represents dissipation/diffusion.

Now, let's examine the dispersion (phase) error of the upwind scheme.

According to earlier definitions and (16)

 $\theta_a = -\omega_a \Delta t = -c k\Delta t = -\mu k\Delta x$

$$\theta_d = \operatorname{atan} \frac{\operatorname{Im}\{\lambda_d\}}{\operatorname{Re}\{\lambda_d\}} = \operatorname{atan} \frac{-\mu \sin(k\Delta x)}{1 - \mu + \mu \cos(k\Delta x)}$$

From the above, the ratio of the numerical to analytic phase speed, $\frac{\theta_d}{\theta_a}$, can be calculated.

In the following figure this ratio is plotted as a function of $\beta(k\Delta x)$ for $\mu(v)$ in the figure) = 0.25, 0.5 and 0.75.

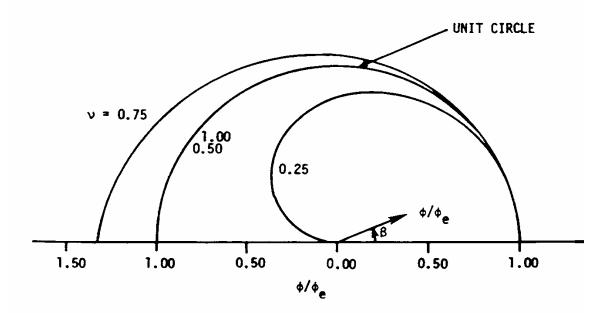


Figure 4.3 Relative phase error of upstream differencing scheme.

We can see that there is no phase error (corresponding to the unit circle) when $\mu = 0.5$.

All waves are slowed down when $\mu < 0.5$. All waves are accelerated when $0.5 < \mu < 1.0$.

Again the phase error is larger for short waves (larger β , i.e., $k\Delta x$). The error is greatest for the $2\Delta x$ wave.

For $\mu=0.25$, $\theta_d \rightarrow 0$ when $k\Delta x \rightarrow \pi$, i.e., $2\Delta x$ does not move at all!

Because the F.D. phase speed is dependent on wavenumber k, the numerical solution is <u>dispersive</u>, whereas the analytical solution is not.

From the above discussions, we see that when using the upwind scheme the waves that move too slow are also strongly damped.

The upwind advection scheme is actually a <u>monotonic</u> scheme – it <u>does not generate new extrema</u> (minimum or maximum) that are not already in the field. For a positive field such as density, it will not generate negative values. We will discuss more about the monotonicity of numerical schemes later.

Note that for practical problems, *c* can change sign in a computational domain. In that case, which point (on the right or left) to use in the spatial difference depends on the local sign of c:

$$\frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} + c \frac{u_{i}^{n} - u_{i-1}^{n}}{\Delta x} = 0 \qquad \text{when } c > 0$$

$$\frac{u_{i}^{n+1} - u_{i}^{n}}{\Delta t} + c \frac{u_{i+1}^{n} - u_{i}^{n}}{\Delta x} = 0 \qquad \text{when } c < 0 \qquad (18)$$

Using the following definitions:

$$c^+ = (c + |c|)/2, c^- = (c - |c|)/2,$$

the upwind scheme in (19) can be written into a single expression

$$u_i^{n+1} = u_i^n + \frac{\Delta t}{\Delta x} \Big[c^+ (u_i^n - u_{i-1}^n) + c^- (u_{i+1}^n - u_i^n) \Big]$$
(19)

Substituting c^+ and c^- into (18) yields

$$u_i^{n+1} = u_i^n + \Delta t \frac{c(u_{i+1}^n - u_{i-1}^n)}{2\Delta x} + \frac{\Delta t \Delta x | c | (u_{i+1}^n - 2u_i^n + u_{i-1}^n)}{\Delta x^2}.$$
 (20)

One can see that the 2nd term on RHS is the advection term in centered difference form and the 3rd term has a form of diffusion. If one uses forward-in-time centered-in-space scheme to discretize equation (5), one will get a FDE like (2) except for the 3rd term on RHS. The scheme is known as the <u>Euler explicit scheme</u>, and the stability analysis tells us that it is <u>absolutely unstable</u>. So it should never be used. Apparently, the 'diffusion term' included in the upwind scheme stabilizes the upwind scheme – it is achieved by damping the otherwise growing short waves.

The included 'diffusion term' also introduces excessively damping to the short waves, as seen earlier. One possible remedy is to attempt to remove this excessive diffusion through one or several corrective steps. This is exactly what is done in the Smolarkiewicz (1983, 1984) scheme, which is rather popular in the field of meteorology.

Because Smolarkiewicz scheme is based on the upwind scheme, it maintains the positive definiteness of the advected fields therefore is a good choice for advecting mass and water variables.

References:

Smolarkiewicz, P. K., 1983: A simple positive definite advection scheme with small implicit diffusion. *Mon. Wea. Rev.*, **111**, 479-486.

Smolarkiewicz, P. K., 1984: A fully multidimensional positive definite advection transport algorithm with small implicit diffusion. *J. Comput. Phys.*, **54**, 325-362.

b). Leapfrog scheme for advection

In this section, we examine a perhaps most commonly used scheme in atmospheric models – the leapfrog centered advection scheme.

Here leapfrog refers to finite difference in time – the frog leaps over time level n from n-1 to n+1 – it is a name for the second-order centered difference in time.

Leapfrog scheme is usually used together with centered difference in space – and the latter can be of 2nd or higher order.

The leapfrog scheme gives us second order accuracy in time.

The PDE is

$$\frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t} + c \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0$$

$$\tau = O(\Delta x^2, \Delta t^2)$$
(21)

and (show it yourself)

 $\lambda_{+} = -i\mu\sin(k\Delta x) \pm [1 - \mu^{2}\sin^{2}(k\Delta x)]^{1/2}$ (22)

If $1 - \mu^2 \sin^2(k\Delta x) \ge 0$, then $|\lambda_{\pm}| = 1$ and there is <u>no amplitude error</u> for all waves. This is the most attractive property of the leapfrog scheme.

In (22), we see that there are two roots for λ - one of them is actually non-physical and is known as the <u>computational mode</u>.

Which one is computational and how does it behave?

Let's look at the positive root λ_+ first:

$$\lambda_{+} = | \lambda_{+} | \exp(-i \beta_{+})$$

where $\beta_+ = -\theta_d$ (θ_d is the phase change in one time step for the discretized scheme, as defined earlier). If $\mu \le 1$, $|\lambda_+| = 1$.

$$\lambda_{+} = \cos(\beta_{+}) - i\sin(\beta_{+}) = -ia + [1 - a^{2}]^{1/2}$$

where $a = \mu \sin(k\Delta x)$, therefore

$$\beta_{+} = \sin^{-1}[\mu \sin(k\Delta x)].$$

Now consider the <u>negative root</u> λ_{-} :

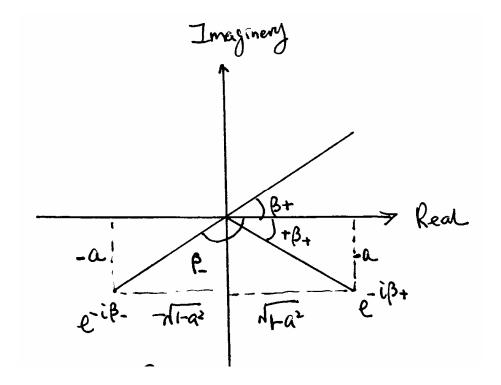
 $\lambda_{-} = |\lambda_{-}| \exp(-i\beta_{-})$

If $\mu \le 1$, $|\lambda_{-}| = 1$.

$$\lambda_{-} = \cos(\beta_{-}) - i\sin(\beta_{-}) = -ia - [1 - a^{2}]^{1/2}$$

with the aid of the following schematics, we can see that

$$\beta_{-} + \beta_{+} = -\pi \quad \Rightarrow \quad -\beta_{-} = \pi + \beta_{+}.$$



We see that the phase of the negative root is the same as that of the positive root shifted by π then multiplied by -1.

What does all this mean then?

For a single wave k, we can write the solution as a linear combination of these two modes (since both modes are present):

$$u_i^n = (A\lambda_+^n + B\lambda_-^n)e^{ikx_i}$$

= $[Ae^{-in\beta_+} + Be^{in(\pi+\beta_+)}]e^{ikx_i}$
= $[Ae^{-in\beta_+} + B(-1)^n e^{in\beta_+}]e^{ikx_i}$ (23)

where A and B are the amplitude of these two modes at time 0.

Which root corresponds to the computational mode then? The negative one, the one that give rises to the second term in (23), because of the following observations:

- (1) The computational mode <u>changes sign every time step</u>. The period of oscillation is $2\Delta t$.
- (2) It has a phase opposite to the physical mode, therefore it propagates in the opposite direction from the physical mode.
- (3) Because of the 2∆t period, the computational mode can be damped effectively using a time filter, which will be discussed in next section.
- (4) The presence of the computational mode is due to the use of three time levels, which requires two initial conditions instead of one the first and second time step integrations start from time level –1 and 0 respectively, which are two different initial conditions.

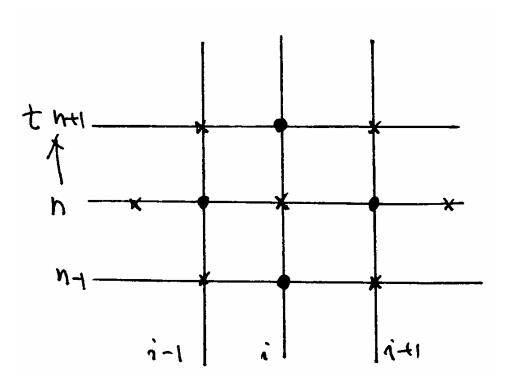
In practice, we usually have only one initial condition – we often start the time integration by using forward-intime scheme for the first step, i.e., for the first step, we do

$$\frac{u_i^1 - u_i^0}{\Delta t} = -c \frac{u_{i+1}^0 - u_{i-1}^0}{2\Delta x}$$

and for the second, we do

$$\frac{u_i^2 - u_i^0}{2\Delta t} + c \frac{u_{i+1}^1 - u_{i-1}^1}{2\Delta x} = 0.$$

An additional note: when $u_i^{n+1} = u_i^{n-1} - \frac{c\Delta t}{\Delta x}(u_{i+1}^n - u_{i-1}^n)$ is used to integrate the advection equation, we can experience the grid separation problem, as show schematically below:



Due to the layout of the computational stencil, the solution at cross points never knows what's going on at the dot points. As the solution march forward in time, the solutions at neighboring points can <u>split</u> away from each other. This problem is also related to the use of three time levels, and can be alleviated by the use of Asselin time filter. An artificial spatial smoothing term of the form of $K\partial^2 u/\partial x^2$ will also help. In practice, other forcing terms in the equation can also couple the solutions together.

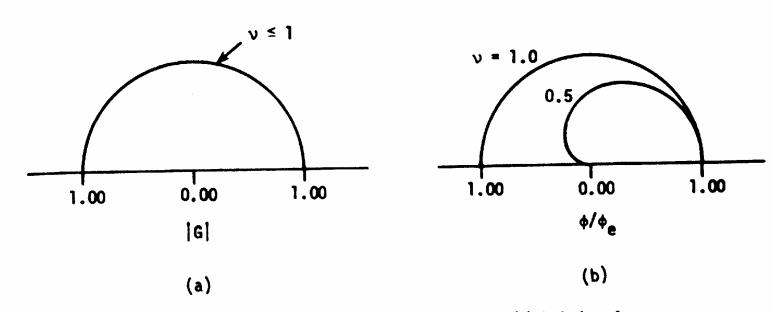


Figure 4.7 Leap frog method. (a) Amplification factor modulus. (b) Relative phase error.

c) Asselin Time Filter

The Asselin (also called Robert-Asselin) time filter (Robert 1966; Asselin 1972) is designed to re-couple of the splitting solutions in time and damp the computational mode found with the leapfrog scheme and others.

It is a two-step process:

(1) u is integrated to time level n+1 using the regular leapfrog scheme,

$$u_i^{*n+1} = u_i^{n-1} - \mu (u_{i+1}^{*n} - u_{i-1}^{*n})$$
(24)

where * indicates values that have not been 'smoothed'.

(2) a filter is then applied to three time levels of data

$$u_i^n = u_i^{*n} + \varepsilon \left(u_i^{*n+1} - 2u_i^{*n} + u_i^{n-1} \right).$$
(25)

Note that the term in second term in (15) is a finite difference version of $\partial^2 u/\partial t^2$ - the diffusion in time which tends to damp high-frequency oscillations.

If we use (25) in (24), we can do a stability analysis and examine the impact of the time filter on solution accuracy:

$$\lambda_{\pm} = -ia + \varepsilon \pm [b - a^2]^{1/2} \tag{26}$$

where $a = \mu \sin(k\Delta x)$ and $b = (1-\varepsilon)^2$ [compare (22) with (26)].

If $b - a^2 \ge 0$ (note that this stability condition has also changed), we have

 $|\lambda|^{2} = (\epsilon^{2} + b) \pm 2\epsilon (b - a^{2})^{1/2}.$

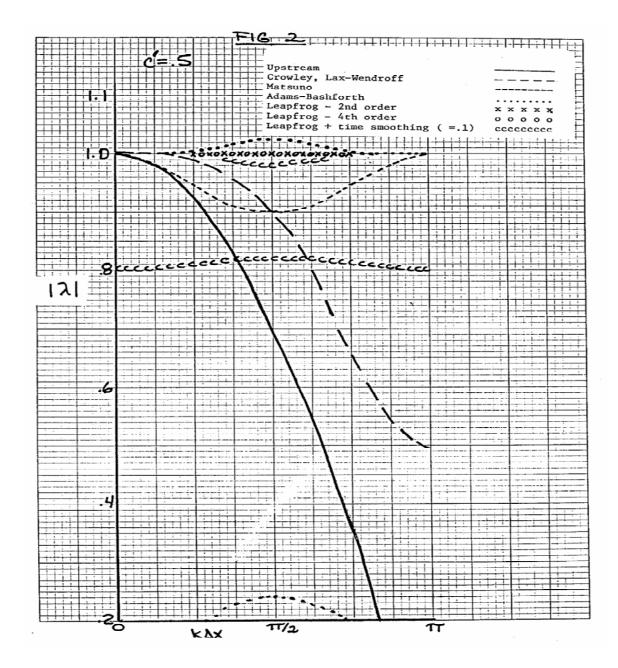
We can plot this to determine its effect on the solution.

We will find that:

(1) amplitude error is introduced by the time filter;

(2) the time filter reduces the time integration scheme from second-order accurate to first-order accuracy only

(3) the filter makes the stability condition more restrictive (can use smaller Δt now).



We want to use as small a ε as possible. Typically $\varepsilon = 0.05$ to 0.1.

The leapfrog (2nd or 4th-order) centered difference scheme combined with the Asselin filter is used in the ARPS for the advective process (more complex monotonic advection schemes are also available for scalar advection).

Reference:

Robert, A. J., 1966: The integration of a low order spectral form of the primitive meteorological equations. *J. Meteor. Soc. Japan*, **44**, 237-245.

Asselin, R., 1972: Frequency filter for time integration. Mon. Wea Rev., 100, 487-490.

Reading: Durran Section 2.3.5.

d) Adam-Bashforth schemes

Second-order Adam-Bashforth Scheme

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -c \left[\frac{3}{2} \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} - \frac{1}{2} \frac{u_{i+1}^{n-1} - u_{i-1}^{n-1}}{2\Delta x} \right]$$

- The RHS is a linear extrapolation of δ_{2x} u from n-1 and n to n+1/2, so that the scheme is "centered" in time at n+1/2.
- Second order in time and space
- Stability analysis shows that

$$\lambda_{\pm} = \frac{1}{2} \left[1 - \frac{3}{2} is \pm \left(1 - \frac{9}{4} s^2 - is \right)^{1/2} \right]$$

where $s = \mu \sin(k\Delta x)$.

Note that this scheme is also a 3 time level scheme and 3 time level schemes always have two modes – one physical and one computational. We can see that for the physical mode (+ case), $\lambda \rightarrow 1$ as s $\rightarrow 0$, and for the computational mode (minus sign case), $\lambda \rightarrow 0$ as s $\rightarrow 0$.

If $s \ll 1$, we can show that

 $|\lambda_{+}| \approx (1 + s^{4}/4)^{1/2}$

 $|\lambda_{-}| \approx 0.5 \text{ s}(1 + \text{s}^2)^{1/2}$

(You can show it by performing binomial expansion).

Clearly $|\lambda_+| > 1$ for $s \neq 0$ therefore the scheme is absolutely unstable.

However, for small enough values of s (i.e., Courant number), because s is raised to the 4th power, $|\lambda_+|$ can be close enough to 1 so that the growth rate is small enough for the scheme to be still usable (especially computational diffusion is added to the equation).

One can estimate the growth rate in terms of e-folding time -i.e., the time taken for a wave to growth by a factor of e.

However, it is the higher-order Adam-Bashforth (AB) schemes that we are more interested in. The higher-order AB scheme can be obtained by extrapolating the right hand side of the equation (i.e., F in $u_t = F$) to time level n+1/2, as we do for the 2nd-order AB scheme, but using high-order (e.g., 2nd-order) polynomials, which will also involve more time levels.

Third-order Adam-Bashforth Scheme

The 3rd-order AB scheme thus obtained has the form of

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{c}{12} [23\delta_{2x}u^n - 16\delta_{2x}u^{n-1} + 5\delta_{2x}u^{n-2}]$$

- It involves data at four time levels require more storage space.
- And it has two computational modes and one physical mode.

• The computational modes are strongly damped, however, unlike the leapfrog scheme, so there is no need for time filtering.

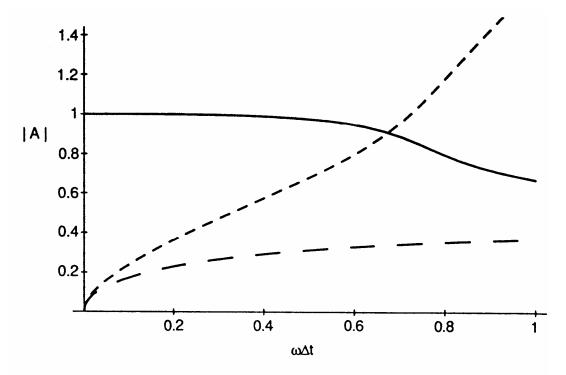


FIG. 1. Magnitude of the amplification factor for the third-order Adams-Bashforth scheme plotted as a function of $\omega \Delta t$. Solid line is the physical mode; dashed curves are the two computational modes.

• Most accurate results are obtained for μ near stability limit. This is not true for the leapfrog 4th-order centered in space scheme. That solution is more accurate for $\mu < 0.5$ where certain cancellation between time and space truncation errors occur.

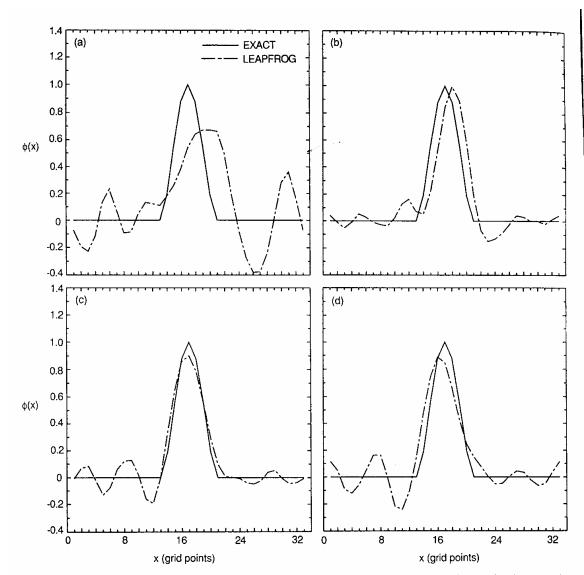


FIG. 3. Effect of leapfrog stepsize on the accuracy of fourth-order centered-difference solution to the advection equation. Shown are the exact and numerical solutions computed using Courant numbers of (a) 0.7272, (b) 0.5, (c) 0.3, and (d) 0.1. All results are for a nondimensional time of 3.

• Durran (1991 MWR) shows that 3rd-order AB time difference combined with 4th-order spatial difference is a good choice – it is in general more accurate than the commonly used leapfrog 4th-order centered-in-space scheme.

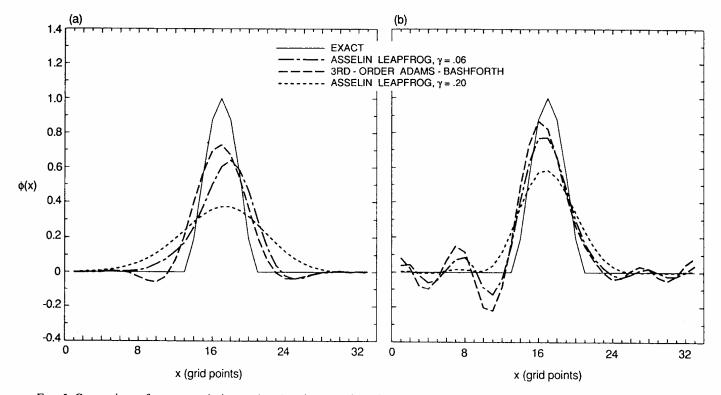
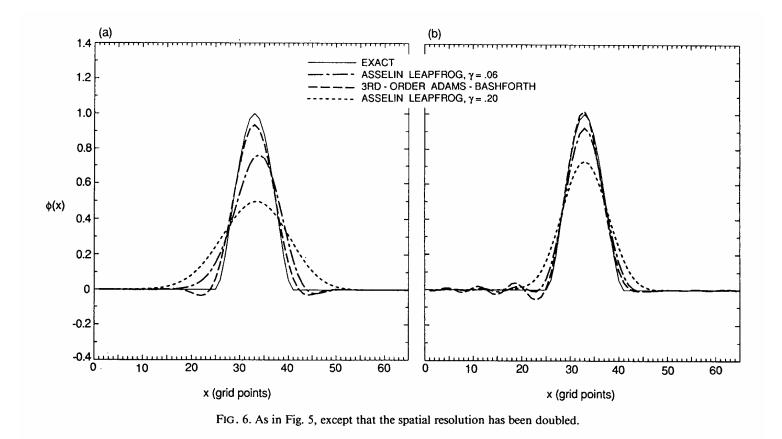


FIG. 5. Comparison of an exact solution to the advection equation with results obtained using Adams-Bashforth and Asselin-filtered leapfrog time differencing in a fourth-order finite-difference model at a nondimensional time of 3, for (a) $\mu = 0.5$ and (b) $\mu = 0.2$.



e) Other schemes

There are many other schemes for solving the advection equation. In the following are some of them, given together with brief discussions on their important properties.

Euler explicit (Euler refers to forward in time)

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_{i+1}^n - u_i^n}{\Delta x} = 0, \quad c > 0 \quad \text{- forward-in-time, downstream in space}$$
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0 \quad \text{- forward-in-time, centered in space}$$

- Both schemes are absolutely unstable. You can show it for yourself.
- They are of no use.

Lax Method

$$\frac{u_i^{n+1} - (u_{i+1}^n + u_{i-1}^n)/2}{\Delta t} + c \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0$$

- 1st-order in time, 2nd-order in space.
- Stable when $|\mu| \le 1$.
- Large dissipation error.
- Significant leading phase error waves propagate faster. $2\Delta x$ waves twice as fast when $\mu=0.2$.

Lax-Wendroff

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -c \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} + \frac{c^2 \Delta t}{2} \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}$$

• Effectively an Euler explicit (FTCS) scheme plus a diffusion term.

Its derivation is interesting – it's based the Taylor series expansion in time first:

$$u_i^{n+1} = u_i^n + \Delta t u_t + \frac{1}{2} (\Delta t)^2 u_{tt} + O(\Delta t^3)$$

and use $u_t = -c u_x$ and $u_{tt} = c^2 u_{xx}$ to rewrite it as

$$u_i^{n+1} = u_i^n - c\Delta t u_x + \frac{1}{2}c^2(\Delta t)^2 u_{xx} + O(\Delta t^3).$$

It is then discretized in space.

- Stable when $|\mu| \le 1$
- Amplitude (dissipation) error for short waves
- Mostly lagging phase error, for short waves. Leading phase error for shortest waves when μ is near 0.75.

We have actually obtained this scheme before based on characteristics and second order interpolation. See Section 2.3.

MacCormack (an example of two-step predictor-corrector method)

Predictor: $(u_i^{n+1})^* = u_i^n - c\Delta t \frac{u_{i+1}^n - u_i^n}{\Delta x}$

Corrector:
$$u_i^{n+1} = \frac{1}{2} \left[u_i^n + (u_i^{n+1})^* - c\Delta t \frac{(u_i^{n+1})^* - (u_{i-1}^{n+1})^*}{\Delta x} \right]$$

- Combination of upwind and downwind steps
- Intermediate prediction is used in the second corrector step
- In the corrector step, the time difference is 'backward in time'
- For linear advection equation, this scheme is <u>equivalent</u> to (you can show this by substituting the 1st eq. into the 2nd), therefore its properties are the same as, the Lax-Wendroff scheme.

Euler Implicit (Euler refers to forward in time)

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2\Delta x} = 0$$

- 1st-order in time and 2nd-order in space.
- Unconditionally stable.
- Relatively small dissipation error, only for intermediate wave lengths. No dissipation error for longest and shortest waves.
- Significant lagging phase error for short waves.
- Need to solve a coupled system of equations. Tridiagonal in 1-D. Block trigiagonal in 2-D.

Time-centered Implicit (Trapezoidal)

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{c}{2} \left[\frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2\Delta x} + \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} \right] = 0$$

• 2nd-order in both time and space.

- Absolutely stable.
- No dissipation error for all waves (similar to leapfrog scheme which is also 2nd-order accurate in time)
- Significant lagging phase error for short waves, similar to Euler implicit.

Matsuno (forward-backward two-step) Scheme

$$\frac{(u_i^{n+1})^* - u_i^n}{\Delta t} + c \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0$$
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{(u_{i+1}^{n+1})^* - (u_{i-1}^{n+1})^*}{2\Delta x} = 0$$

- 1st-order in time, second order in space
- Stable when $\mu \leq 1$.
- Relatively large dissipation and phase error

Leapfrog Fourth-order Centered-in-Space Scheme

$$\frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t} + c \left[\frac{4}{3} \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} - \frac{1}{3} \frac{u_{i+2}^n - u_{i-2}^n}{4\Delta x} \right] = 0$$

- 2nd-order in time and 4th-order in space
- Stable for $\mu \le 0.728$ (more restrictive than 2nd-order)
- No dissipation error without time filter
- Also contains computational mode, as all three-time level schemes do
- Smaller phase error than 2nd-order centered-in-space counterpart

• Leapfrog scheme can be combined with centered spatial difference schemes of even higher order

Second and third-order Rouge-Kutta Scheme

One possible form (there is more than one form that is second-order accurate) of 2nd-order Rouge-Kutta scheme with centered spatial difference is

$$u_{i}^{*} = u_{i}^{n} - \frac{\Delta t}{2} c \frac{u_{i+1}^{n} - u_{i-1}^{n}}{2\Delta x}$$
$$u_{i}^{n+1} = u_{i}^{n} - \Delta t c \frac{u_{i+1}^{*} - u_{i-1}^{*}}{2\Delta x}$$

This scheme is absolutely unstable although the stability is weak. It can be combined with upwind biased advection to yield a stable time integration scheme, however. Wicker and Skamarock (1998) discusses applying such a scheme to solve a compressible system of equations.

One possible form of 3rd-order Rouge-Kutta scheme with centered spatial difference is

$$u_{i}^{*} = u_{i}^{n} - \frac{\Delta t}{3} c \frac{u_{i+1}^{n} - u_{i-1}^{n}}{2\Delta x}$$
$$u_{i}^{**} = u_{i}^{n} - \frac{\Delta t}{2} c \frac{u_{i+1}^{*} - u_{i-1}^{*}}{2\Delta x}$$
$$u_{i}^{n+1} = u_{i}^{n} - \Delta t c \frac{u_{i+1}^{**} - u_{i-1}^{**}}{2\Delta x}$$

The scheme involves three steps, therefore three evaluations of the advection term. The increased cost is somewhat offset by its better stability property. As discussed by Durran (page 68-69), for oscillation equations, it is stable for $k\Delta t < 1.73$ while the leapfrog scheme requires $k\Delta t < 1$ therefore the time step size can be 1.73 times larger. Perhaps more attractively, when the 3rd-order Rouge-Kutta scheme is combined with high-order spatial difference for the advection term, the maximum stable Courant number is not as much reduced as in the leapfrog case. The following table is from Wicker and Skamarock (2002).

	Spatial order				
Time scheme	3rd	4th	5th	6th	
Leapfrog	U	0.72	U	0.62	
RK2	0.88	U	0.30	U	
RK3	1.61	1.26	1.42	1.08	

TABLE 1. Maximum stable Courant number for one-dimensional linear advection. Here, U indicates the scheme is unstable.

The ability for the scheme to be combined with high odd order spatial difference and be used in split-explicit time integration for compressible system of equation, and allowing relatively large time step size is attractive. Third-order Rouge-Kutta scheme is used in the new Weather Research and Forecast (WRF, http://wrf-model.org) model.

See Durran Section 2.3.6, and Wicker and Skamarock (1998, 2002).

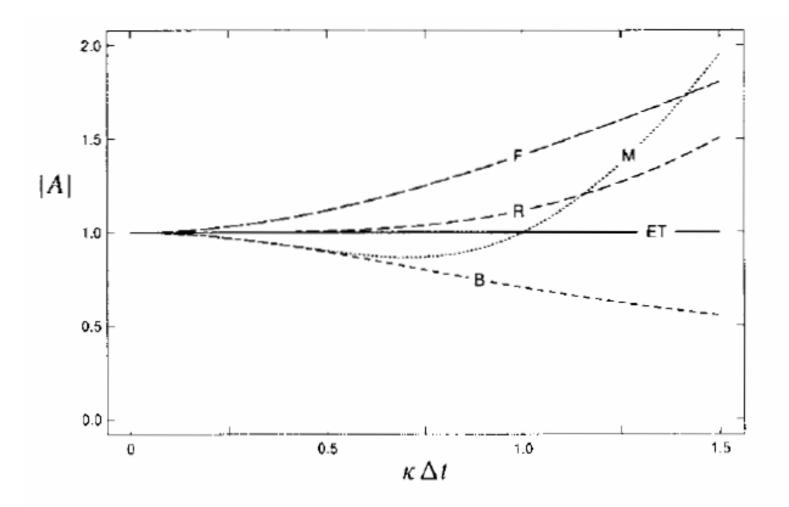


FIGURE 2.2. The modulus of the amplification factor |A| as a function of temporal resolution $\kappa \Delta t$ for the true solution and five two-level schemes: exact solution and trapezoidal method (ET), forward differencing (F), backward differencing (B), second-order Runge-Kutta (R), and Matsuno (M).

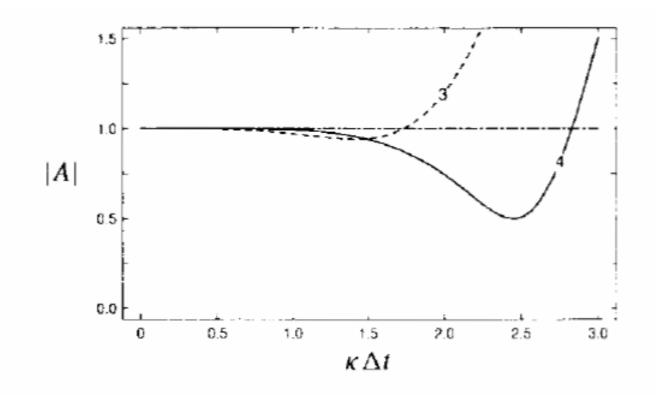
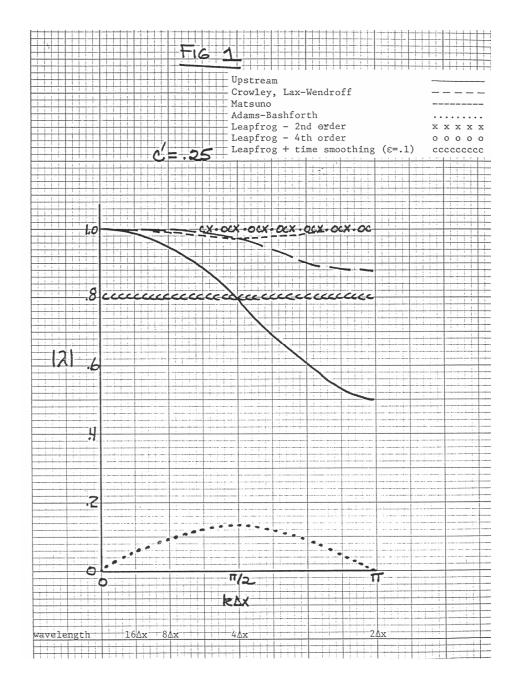
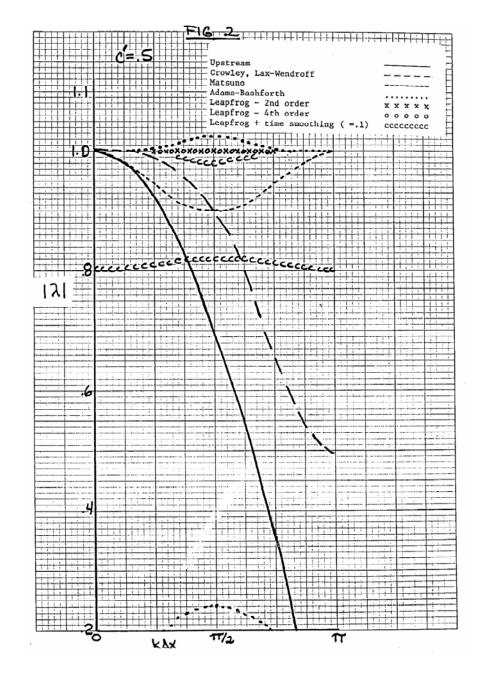


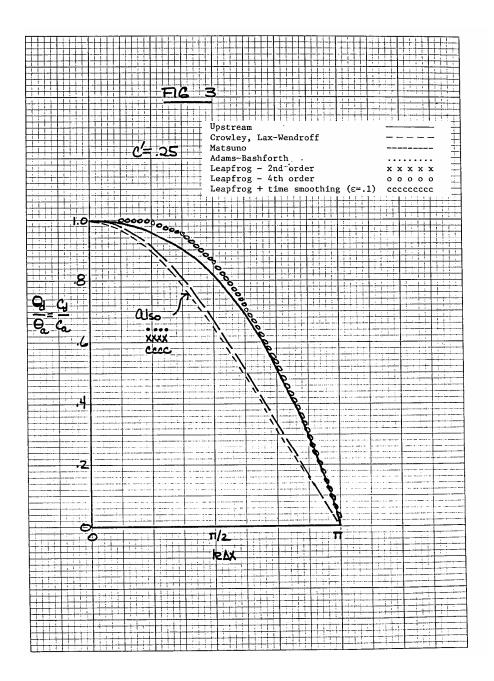
FIGURE 2.8. Modulus of the amplification factor plotted as a function of temporal resolution $\kappa \Delta t$ for higher-order Runge-Kutta solutions to the oscillation equation. Dashed line: third-order scheme; solid line: fourth-order method.

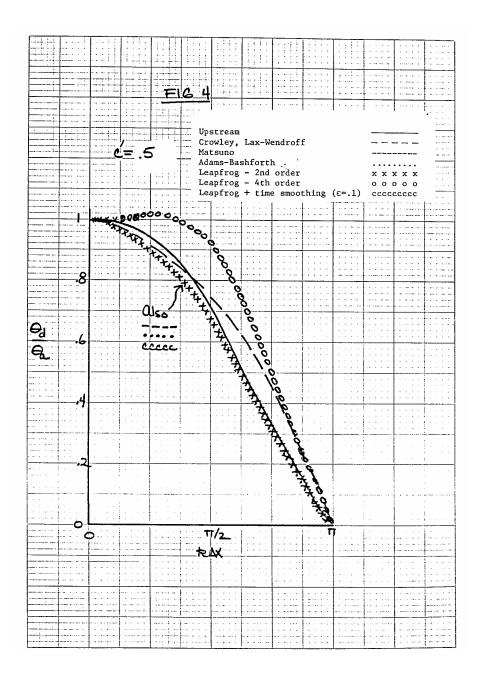


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List of commonly used time difference schemes and their basic properties (from Durran):

Method	Order	Formula			
Forward	1	$\phi^{n+1} = \phi^n + hF(\phi^n)$			
Backward	1	$\phi^{n+1} = \phi^n + hF(\phi^{n+1})$			
Asselin Leapfrog	1	$\phi^{n+1} = \overline{\phi^{n-1}} + 2hF(\phi^n)$ $\overline{\phi^n} = \phi^n + \gamma(\overline{\phi^{n-1}} - 2\phi^n + \phi^{n+1})$			
Leapfrog	2	$\phi^{n+1} = \phi^{n-1} + 2hF(\phi^n)$			
Adams– Bashforth	2	$\phi^{n+1} = \phi^n + \frac{h}{2} \left[3F(\phi^n) - F(\phi^{n-1}) \right]$			
Trapezoidal	2	$\phi^{n+1} = \phi^n + \frac{h}{2} \left[F(\phi^{n+1}) + F(\phi^n) \right]$			
Runge-Kutta	2	$q_1 = hF(\phi^n),$ $\phi_1 = \phi^n + q_1$ $q_2 = hF(\phi_1) - q_1,$ $\phi^{n+1} = \phi_1 + q_2/2$			
Magazenkov	2	$\phi^{n} = \phi^{n-2} + 2hF(\phi^{n-1})$ $\phi^{n+1} = \phi^{n} + \frac{h}{2} \left[3F(\phi^{n}) - F(\phi^{n-1}) \right]$			

Leapfrog– Trapezoidal	2	$\phi_1 = \phi^{n-1} + 2hF(\phi^n)$ $\phi^{n+1} = \phi^n + \frac{h}{2} \left[F(\phi_1) + F(\phi^n) \right]$
Adams– Bashforth	3	$\phi^{n+1} = \phi^n + \frac{h}{12} \left[23F(\phi^n) - 16F(\phi^{n-1}) + 5F(\phi^{n-2}) \right]$
Adams– Moulton	3	$\phi^{n+1} = \phi^n + \frac{h}{12} \left[5F(\phi^{n+1}) + 8F(\phi^n) - F(\phi^{n-1}) \right]$
ABM Predictor- Corrector	3	$\phi_1 = \phi^n + \frac{h}{2} \left[3F(\phi^n) - F(\phi^{n-1}) \right]$ $\phi^{n+1} = \phi^n + \frac{h}{12} \left[5F(\phi_1) + 8F(\phi^n) - F(\phi^{n-1}) \right]$
Runge–Kutta	3	$q_{1} = hF(\phi^{n}), \qquad \phi_{1} = \phi^{n} + q_{1}/3$ $q_{2} = hF(\phi_{1}) - 5q_{1}/9, \qquad \phi_{2} = \phi_{1} + 15q_{2}/16$ $q_{3} = hF(\phi_{2}) - 153q_{2}/128, \qquad \phi^{n+1} = \phi_{2} + 8q_{3}/15$
Runge–Kutta	4	$q_{1} = hF(\phi^{n}), \qquad q_{2} = hF(\phi^{n} + q_{1}/2) q_{3} = hF(\phi^{n} + q_{2}/2), \qquad q_{4} = hF(\phi^{n} + q_{3}) \phi^{n+1} = \phi^{n} + (q_{1} + 2q_{2} + 2q_{3} + q_{4})/6$

TABLE 2.1. Summary of methods for the solution of ordinary differential equations. The second- and third-order Runge-Kutta methods are low-storage variants; $h = \Delta t$.

Method	Storage Factor	Efficiency Factor	Amplification Factor	Phase Error	Max s
Forward	2	0	$1 + \frac{s^2}{2}$	$1-\frac{s^2}{3}$	0
Backward	*	∞	$1-\frac{s^2}{2}$	$1 - \frac{s^2}{3}$	œ
Asselin Leapfrog	3	< 1	$1-\frac{\gamma s^2}{2(1-\gamma)}$	$1+\frac{(1+2\gamma)s^2}{6(1-\gamma)}$	< 1
Leapfrog	2	1	1	$1+\frac{s^2}{6}$	1
Adams– Bashforth–2	3	0	$1+\frac{s^4}{4}$	$1+\frac{5}{12}s^2$	0
Trapezoidal	*	∞	1	$1 - \frac{s^2}{12}$	00
Runge–Kutta–2	2	0	$1 + \frac{s^4}{8}$	$1+\frac{s^2}{6}$	0
Magazenkov	3	0.67	$1-\frac{s^4}{4}$	$1 + \frac{s^2}{6}$	0.67

Leapfrog– Trapezoidal	3	0.71	$1-\frac{s^4}{4}$	$1-\frac{s^2}{12}$	1.41
Adams– Bashforth–3	4	0.72	$1-\frac{3}{8}s^4$	$1 + \frac{289}{720}s^4$	0.72
Adams– Moulton–3	*	0	$1 + \frac{s^4}{24}$	$1 - \frac{11}{720}s^4$	0
ABM Predictor- Corrector-3	4	0.60	$1 - \frac{19}{144}s^4$	$1 + \frac{1243}{8640}s^4$	1.20
Runge-Kutta-3	2	0.58	$1-rac{s^4}{24}$	$1 + \frac{s^4}{30}$	1.73
Runge–Kutta–4	4 [†]	0.70	$1-\frac{s^6}{144}$	$1 - \frac{s^4}{120}$	2.82

[†]A storage factor of 3 may be achieved following the algorithm of Blum (1962).

TABLE 2.2. Characteristics of the schemes listed in Table 2.1. The amplification factor and relative phase change are for well-resolved solutions to the oscillation equation, and $s = \kappa \Delta t$. "Max s" is the maximum value of $\kappa \Delta t$ for which the solution is nonamplifying. The storage and efficiency factors are defined in the text. No storage factor is given for implicit schemes.

3.3.3. Practical Measures of Dissipation and Dispersion Errors

Takacs (1985 MWR) proposed a practical measure for estimating dissipation and dispersion errors based on numerical solutions. The methods divide the total mean square error into two parts, one indicative of dissipation error and one the dispersion error.

The total mean square error is given as

$$\tau = \frac{1}{N} \sum_{i}^{N} (u_a - u_d)^2 \,. \tag{27}$$

 u_a is the analytical solution and u_d the numerical (discrete) solution.

It can be rewritten as (show it yourself):

$$\tau = \sigma^2(u_a) + \sigma^2(u_d) - 2\rho\sigma(u_a)\sigma(u_d) + (\overline{u}_a - \overline{u}_d)^2$$
(28)

where $\sigma^2(u_a) = \frac{1}{N} \sum_{i}^{N} (u_a - \overline{u}_a)^2$, $\sigma^2(u_d) = \frac{1}{N} \sum_{i}^{N} (u_d - \overline{u}_d)^2$ are the <u>variance</u> of the u_a and u_d, respectively. $\operatorname{cov}(u_a, u_d) = \frac{1}{N} \sum_{i}^{N} (u_a - \overline{u}_a)(u_d - \overline{u}_d)$ is the <u>co-variance</u> between u_a and u_d and $\rho = \frac{\operatorname{cov}(u_a, u_d)}{\sigma(u_a)\sigma(u_d)}$ is the <u>correlation</u> <u>coefficient</u>.

(28) can be rewritten as

$$\tau = [\sigma(u_a) - \sigma(u_d)]^2 + (\overline{u}_a - \overline{u}_d)^2 + 2(1 - \rho)\sigma(u_a)\sigma(u_d)$$
(29)

Takacs definite the first two terms of the RHS of (29) as the dissipation error and the third term as the dispersion error, i.e.,

$$\tau_{DISS} = [\sigma(u_a) - \sigma(u_d)]^2 + (\overline{u}_a - \overline{u}_d)^2$$
(30a)

$$\tau_{DISP} = 2(1 - \rho)\sigma(u_a)\sigma(u_d) \tag{30b}$$

We can see that when two wave patterns differ only in amplitude but not in phase, their correlation coefficient ρ should be 1. According to (30a), $\tau_{DISP} = 0$. That's a reasonable result.