

## Ch. 3 Lecture Note - Numerical Methods

[Based on Ch. 12: Numerical Methods of "*Mesoscale Dynamics*" by Y.-L. Lin, Cambridge University Press 2007, 630pp]

### Chapter 12 Numerical Methods

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(Equation editor:  $\frac{Du}{Dt} - fv = -\frac{1}{\rho} \frac{\partial p}{\partial x} + F_{rx}$ )

## 3.1 Introduction

- Available **analytical solutions of nonlinear PDEs** (partial differential equations) are rare, such as the
  - **Burger equation** (see Project 2)
  - **Long's equation** for idealized flow over a bell-shaped mountain (see **Lin and Wang (1996)** or Ch. 5 of Lin (2007))
  - **KdV equation** for solitary waves or solitons
  - **Schrodinger equation** for propagation of light in nonlinear optical fibers and planar waveguides and to Bose-Einstein condensates, and
  - **nonlinear dynamical system** for strange (Lorenz) attractor etc.,

and are normally limited by having to make small-perturbation (linear) assumption and apply analytical methods.

- For large scale flow, quasi-geostrophic approximation or geostrophic momentum approximation are often adopted for simplifying the governing equations. However, this does not work for mesoscale flow since the Rossby number is not small enough.
- For small scale flow, the Coriolis force can be ignored, but nonhydrostatic and compressibility often has to be included to add the complexity to the governing equations.
- An option to solve those nonlinear equations or a set of nonlinear equations is by applying numerical approximations on certain grid points in space and time.
- **Advantages of numerical simulations or experiments:**
  - (a) The full set of nonlinear PDE's can be solved approximately.
  - (b) It provides a powerful way in setting the environments for testing different forcing or physical processes, such as deactivating nonlinearity, orography, PBL, latent heating, radiation, etc. This is called “**sensitivity test**” or “**sensitivity experiment**”.
- **Important questions to ask in numerical modeling:**
  - Does the approximate equation converge to the real differential equation when the time and grid intervals approach zero?
  - Is the numerical solution well-behaved in time, or more precisely speaking, is it *stable numerically*?

- How well do the amplitude and phases of the approximated waves or disturbances represent those of the exact solution?
- **Major numerical methods used in NWP modeling:**
  - (1) *Finite difference methods*
  - (2) *Galerkin methods*
  - (3) *Lagrangian methods*
- ***Finite Difference Methods* (most popular in NWP models)**
  - Dependent variables are defined at certain grid points in space and time, and the derivatives in the equations are approximated using the Taylor series expansion.
  - Since finite area is used, mesoscale and NWP models are often referred to as *limited-area numerical models*.
  - Initial conditions and boundary conditions are needed for integrating the PDE's.
- ***Galerkin Methods***
  - Dependent variables are represented by a sum of functions that have a prescribed spatial structure.
  - The coefficient associated with each function is normally a function of time.
  - A partial differential equation is transformed into a set of ordinary differential equations (in time) for the coefficients. These equations are usually solved with finite difference approximations in time.

*Galerkin methods* may be divided into two major categories: (a) *spectral method* and (b) *finite element method*.

- (a) In *spectral methods*, dependent variables are represented by orthogonal, global basis functions, such as sinusoidal functions used in Fourier transform.
- Less popular in mesoscale or NWP models because it is more difficult to handle the nonperiodic lateral boundary condition.
  - More popular in large-scale and global models due to the periodic nature of the boundary conditions.
- (b) *Finite element methods* are similar to spectral method except it uses local basis functions, instead of globally (in terms of the integration domain) basis functions, such as the chapeau or tent function.
- Advantages: their accuracy and the flexibility of treating irregular geometry of the internal and external boundaries.
  - Disadvantages: requiring a significant amount of computing time to invert a large matrix at every time step.

- **Lagrangian methods**

- The PDE's are solved by following a fixed set of particles throughout the period of integration.
- Advantages: treating the total derivative at once, instead of having to treat the individual terms, such as the local rate of change and advection terms.
- Practically, it is very difficult to trace the air parcels at the next time step since they normally are distributed randomly in the

computational domain, instead of located right at regularly distributed grid points.

- In order to avoid this problem, the fluid variables at the predicted time step are defined at the regular grids and traced back to where at the previous time steps. This is called the *[semi-Lagrangian method](#)*.
- Semi-Lagrangian method is getting more popular since a relatively large time interval for integration can be used due to its unconditional stability.
- There are some other numerical methods, such as *[upstream interpolation methods](#)* and *[finite-volume methods](#)* etc.
  - In an *[interpolation method](#)*, dependent variables at grid points are used to derive interpolation formulae for the spaces between as well as at the grid points.
  - In a *[finite-volume method](#)*, the grid-point value  $f_i$  represents the average of the function  $f(x)$  over the grid cell  $[(i-1/2)\Delta x, (i+1/2)\Delta x]$ .
    - Finite-volume methods are very useful for approximating solutions that contain discontinuities.
    - Finite-volume methods generate approximations to the grid-interval or grid-cell average.

### 3.2 Finite Difference Approximations of Derivatives

- *[Forward difference scheme](#)*

Consider the *[Taylor series](#)* to approximate  $f(x)$  at  $x + \Delta x$ ,

$$f(x + \Delta x) = f(x) + f'(x)\Delta x + f''(x)\frac{\Delta x^2}{2!} + f'''(x)\frac{\Delta x^3}{3!} + \dots \quad (12.2.1)$$

where  $\Delta x (>0)$ : *spatial increment or grid interval*.

Thus, the derivative of  $f'(x)$  can be solved,

$$f'(x) = \frac{f(x + \Delta x) - f(x)}{\Delta x} + R(x, \Delta x), \quad (12.2.2)$$

where

$$R(x, \Delta x) \equiv \Delta x \left\{ -\frac{f''(x)}{2!} - \frac{f'''(x)\Delta x}{3!} - \dots \right\}$$

In the above expression,  $R$  is called the *remainder term*, which has a magnitude of  $O(\Delta x)$ .

If the remainder term is much smaller than the first term on the right hand side of Eq. (12.2.2), then the above equation may be approximated by

$$f'(x) = \frac{f(x + \Delta x) - f(x)}{\Delta x}. \quad (12.2.3)$$

- The above equation is called a *finite difference equation* or *difference equation*.
- The scheme is called a *forward difference scheme* on the order of  $\Delta x$  (*first order scheme*).

➤ The remainder term ( $R$ ) is the *truncation error* (on the order of  $\Delta x$  or *first order of accuracy*).

- *Review of the concept of numerical modeling*

Consider Newton's second law of motion:

$$F = ma$$

$$a = \frac{du}{dt} = \frac{F}{m}.$$

For an object with constant mass pushed by a constant force,  $F/m = c$ , the above equation of motion reduces to

$$\frac{du}{dt} = c.$$

Q: How do you calculate or “predict” the speed of the object (i.e.,  $u$ ) at certain time  $t$  later?

Based on (12.2.2), there are two ways to reduce the truncation error:

- (a) reduce the space interval ( $\Delta x$ ) or
- (b) use a higher-order approximation method.

This also can be seen from the sketch in Fig. 12.1.

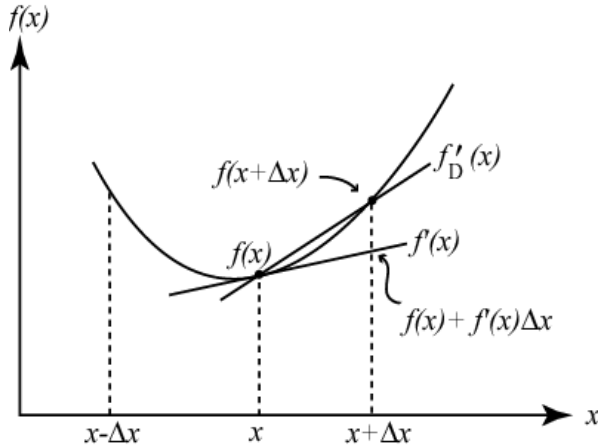


Fig. 12.1: A sketch of the forward finite difference scheme, as shown in Eq. (12.2.3). The actual derivative,  $f'(x)$ , is approximated by the slope  $f'_D(x)$ .

The distance between  $f(x + \Delta x)$  and  $f(x) + f'(x)\Delta x$  at  $x + \Delta x$  is  $-R\Delta x$ .

When  $\Delta x$  is reduced, the approximated derivative  $f'(x)$  (i.e., the R.H.S. of (12.2.3) is closer to the real derivative.

- **Backward difference scheme**

Similarly, the **Taylor series expansion** may also be expanded in a **backward** manner,

$$f(x - \Delta x) = f(x) - f'(x)\Delta x + f''(x)\frac{\Delta x^2}{2!} - f'''(x)\frac{\Delta x^3}{3!} + \dots, \quad (12.2.4)$$

which may also be rearranged in the following form,

$$f'(x) = \frac{f(x) - f(x - \Delta x)}{\Delta x} + \Delta x \left\{ \frac{f''(x)}{2!} - \frac{f'''(x)\Delta x}{3!} + \dots \right\}. \quad (12.2.5)$$



Eq. (12.2.5) may be approximated by the *backward difference scheme*,

$$f'(x) = \frac{f(x) - f(x - \Delta x)}{\Delta x}. \quad (12.2.6)$$

The meaning of Eq. (12.2.6) can be easily understood by replacing  $x + \Delta x$  and  $x$  by  $x$  and  $x - \Delta x$ , respectively, in Fig. 12.1.

Similar to the forward difference scheme, the backward scheme has accuracy on the order of  $\Delta x$  or is referred to as the *first order of accuracy*.

- ***Centered difference scheme***

An alternative way to approximate the derivative can be obtained by subtracting (12.2.4) from (12.2.1),

$$f(x + \Delta x) - f(x - \Delta x) = 2f'(x)\Delta x + 2f'''(x)\frac{\Delta x^3}{3!} + \dots \quad (12.2.7)$$

The derivative,  $f'(x)$ , may then be solved,

$$f'(x) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x} + R \quad (12.2.8)$$

The remainder term is on the order of  $\Delta x^2$ ,

$$R = \Delta x^2 \left\{ -\frac{f'''(x)}{3!} - \frac{f^{(5)}(x)}{5!} \Delta x - \dots \right\}. \quad (12.2.9)$$

Neglecting the remainder term leads to the centered difference scheme,

$$f'(x) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x}. \quad (12.2.10)$$

Based on (12.2.9), the centered difference scheme has accuracy on the order of  $\Delta x^2$  or the second order of accuracy and the numerical method is called second-order scheme.

The mathematical meaning of the scheme is depicted in Fig. 12.2.

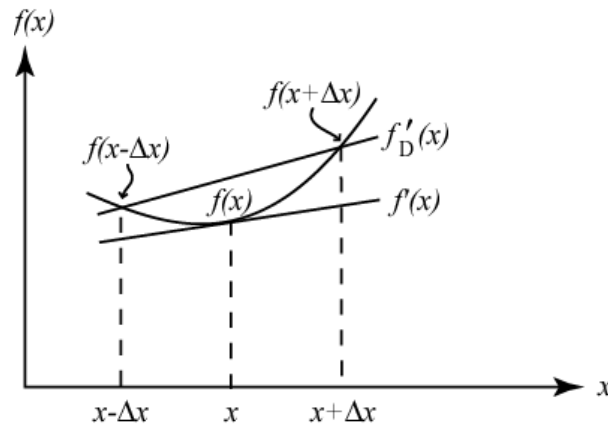


Fig. 12.2: A sketch of the relationship of  $f'(x)$  and its centered difference approximation,  $f'_D(x)$ .

Comparing with Fig. 12.1, the centered difference scheme is more accurate than the forward or backward finite difference scheme.

- Approximation of the second-order derivative,  $f''(x)$ :

Adding Eq. (12.2.4) to Eq. (12.2.1),

$$f''(x) = \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} + O(\Delta x^2). \quad (12.2.11)$$

Again,  $f''(x)$  may be approximated by the first term on the right-hand side of the above equation.

- *Two questions may be raised for the above 1<sup>st</sup> and 2<sup>nd</sup> order finite difference schemes:*

- *How accurate are they?*

- *Are these numerical solutions well-behaved, or say, are they stable?*

- *Accuracy of a finite difference scheme*

To find the accuracy of the finite difference methods, we may consider the centered difference approximation to the first derivative of the sine function,

$$f(x) = A \sin \frac{2\pi x}{L}. \quad (12.2.12)$$

The first-order derivative may be easily obtained analytically,

$$f'(x) = \frac{2\pi A}{L} \cos \frac{2\pi x}{L}. \quad (12.2.13)$$

Now, we can apply the centered difference scheme, Eq. (12.2.10), to  $f'(x)$ ,

$$f_D'(x) = \frac{A \sin\left(\frac{2\pi(x + \Delta x)}{L}\right) - A \sin\left(\frac{2\pi(x - \Delta x)}{L}\right)}{2\Delta x}, \quad (12.2.14)$$

which may be rearranged to be

$$f_D'(x) = \frac{A \cos\left(\frac{2\pi x}{L}\right) \sin\left(\frac{2\pi \Delta x}{L}\right)}{\Delta x}. \quad (12.2.15)$$

Dividing the above approximation by  $f'(x)$  yields

$$\frac{f_D'(x)}{f'(x)} = \frac{\sin(2\pi \Delta x / L)}{2\pi \Delta x / L}. \quad (12.2.16)$$

The relationship between  $f_D'(x)$  and  $f'(x)$  is also sketched in Fig. 12.2.

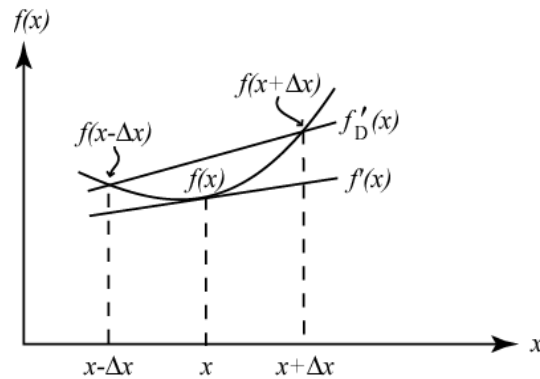


Fig. 12.2: A sketch of the relationship of  $f'(x)$  and its centered difference approximation,  $f_D'(x)$ .

From the above expression, we obtain

$$\frac{f_D'(x)}{f'(x)} \rightarrow 1 \quad \text{as} \quad \frac{2\pi\Delta x}{L} \rightarrow 0, \quad (12.2.17)$$

because  $\sin \theta \rightarrow \theta$  when the angle  $\theta$  approaches 0, based on the [Taylor series of expansion](#) of  $\sin \theta$ .

In other words, the truncation error of the center difference scheme approaches 0 when  $\Delta x \ll L$ . Thus, in order to have a good approximation, the grid interval chosen should be much smaller than wavelength.

- ***For a wave*** with  $L = 2\Delta x$  (also called  $2\Delta x$  wave).

Substituting  $L = 2\Delta x$  into the right side of Eq. (12.2.16) leads to

$$\frac{f_D'(x)}{f'(x)} = \frac{\sin \pi}{\pi} = 0. \quad (12.2.18)$$

The above equation implies that [the centered difference scheme fails to resolve a  \$2\Delta x\$  wave](#).

It also can be shown that for a fixed grid interval, shorter waves are poorly resolved by the centered difference scheme, while longer waves are reasonably well resolved.

- ***Formulas for Finite Difference Approximations of Derivatives*** (Adapted from Gerald and Wheatley 2003; see Lin 2007)

**Formulas for the first derivatives:**

$$f'(x) = \frac{f(x + \Delta x) - f(x)}{\Delta x} + O(\Delta x), \quad (\text{forward difference})$$

$$f'(x) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x} + O(\Delta x^2), \quad (2^{\text{nd}}\text{-order centered difference})$$

$$f'(x) = \frac{-f(x + 2\Delta x) + 4f(x + \Delta x) - 3f(x)}{2\Delta x} + O(\Delta x^2), \quad (\text{one-sided } 2^{\text{nd}}\text{-order centered difference})$$

$$f'(x) = \frac{-f(x + 2\Delta x) + 8f(x + \Delta x) - 8f(x - \Delta x) + f(x - 2\Delta x)}{12\Delta x} + O(\Delta x^4). \quad (4^{\text{th}}\text{-order centered difference})$$

**Formulas for the second derivatives:**

$$f''(x) = \frac{f(x + 2\Delta x) - 2f(x + \Delta x) + f(x)}{\Delta x^2} + O(\Delta x), \quad (\text{forward difference})$$

$$f''(x) = \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} + O(\Delta x^2), \quad (2^{\text{nd}}\text{-order centered difference})$$

$$f''(x) = \frac{-f(x + 3\Delta x) + 4f(x + 2\Delta x) - 5f(x + \Delta x) + 2f(x)}{\Delta x^2} + O(\Delta x^2), \quad (\text{one-sided})$$

$$f''(x) = \frac{-f(x + 2\Delta x) + 16f(x + \Delta x) - 30f(x) + 16f(x - \Delta x) - f(x - 2\Delta x)}{12\Delta x^2} + O(\Delta x^4). \quad (4^{\text{th}}\text{-order centered difference})$$

**Formulas for the third derivatives:**

$$f'''(x) = \frac{f(x + 3\Delta x) - 3f(x + 2\Delta x) + 3f(x + \Delta x) - f(x)}{\Delta x^3} + O(\Delta x),$$

$$f'''(x) = \frac{f(x + 2\Delta x) - 2f(x + \Delta x) + 2f(x - \Delta x) - f(x - 2\Delta x)}{2\Delta x^3} + O(\Delta x^2). \quad (\text{averaged differences})$$

**Formulas for the fourth derivatives:**

$$f^{iv}(x) = \frac{f(x + 4\Delta x) - 4f(x + 3\Delta x) + 6f(x + 2\Delta x) - 4f(x + \Delta x) + f(x)}{\Delta x^4} + O(\Delta x),$$

$$f^{iv}(x) = \frac{f(x + 2\Delta x) - 4f(x + \Delta x) + 6f(x) - 4f(x - \Delta x) + f(x - 2\Delta x)}{\Delta x^4} + O(\Delta x^2). \quad (\text{centered difference})$$

### 3.3 Finite Difference Approximations of the Advection Equation

- One of the simplest finite difference models is the one-dimensional advection equation with a constant advection velocity ( $c$ ), which composes only one dependent variable, one time derivative and one spatial derivative,

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0, \quad (12.3.1)$$

where  $u$  is the horizontal velocity.

If  $c$  is replaced by  $u$  in Eq. (12.3.1), then it is called the **inviscid Burger equation**. The inviscid Burger equation has also been adopted as a model for fluid dynamical systems.

[An analytical solution of Eq. \(12.3.1\) can be found,](#)

$$u(x, t) = f(x - ct), \quad (12.3.2)$$

where  $f$  is an arbitrary function, which determines  $u$  at  $t = 0$ , or say, the *initial condition*,  $f_i(x)$ .

For example, if

$$f_i(x) = \frac{u_o a^2}{x^2 + a^2}, \quad (12.3.3)$$

then

$$u(x, t) = f_i(x - ct) = \frac{u_o a^2}{(x - ct)^2 + a^2}. \quad (12.3.4)$$

If the advection velocity ( $c$ ) is positive (negative), then the wave propagates to the right (left).

- Note that Eq. (12.3.3) is called the *bell-shaped function* which has amplitude  $u_o$  and a half-width  $a$ . It is also called the *Witch of Agnesi*.
- **Physical meaning of Eq. (12.3.4)**

The solution  $u(x,t)$  always keeps its initial shape along the *phase line*  $x-ct=constant$ .

That is, the wave or disturbance propagates along a constant phase line  $x-ct$ , the characteristics of the advection equation or the wave propagates at the speed  $c$ .

This wave or disturbance propagation along a constant phase line is illustrated in Fig. 12.3.

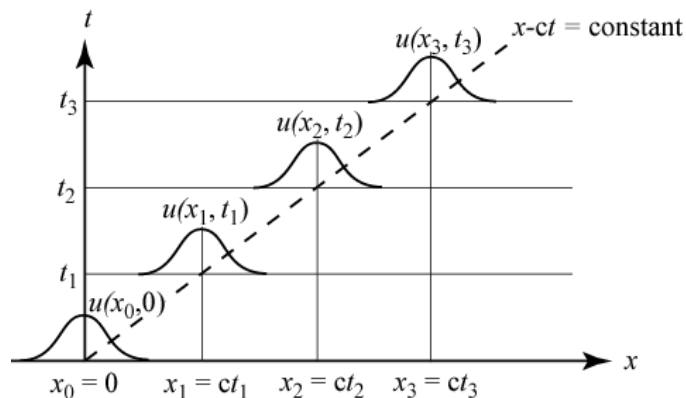


Fig. 12.3: A sketch of the propagation of  $u(x,t)$  along a constant phase line,  $x-ct=constant=0$ . [From Lin 2007 – Mesoscale Dynamics, Cambridge Univ. Press]

- In the following, we will discuss some major numerical approximations of the advection equation, which have been adopted in mesoscale numerical models, and their characteristics.



- Based on the levels of time integration, the major methods which have been adopted in NWP may be categorized as *two-time-level schemes* and *three-time-level schemes*.

### 3.3.1 Two-Time-Level schemes

- The finite difference schemes for approximating  $f'(x)$ , as discussed in the previous subsection, may also be applied to the time derivative.
- Similarly, one may choose to adopt the *forward*, *backward*, or *centered* difference approximations in time.
- If one chooses to use *forward or backward finite difference in time*, then the method belongs to the so-called *two-time-level schemes* since there are only two time steps involved at each time of integration.
- On the other hand, if one chooses to use the *second-order centered difference in time* (or known as *leapfrog*), and then the method belongs to the so-called *three-time-level schemes* since there are three times involved at each time step of integration.

#### (a) Forward in time and centered in space scheme and its computational instability

The derivatives in the advection equation, Eq. (12.3.1), may be approximated by a combination of forward difference of the time derivative and center difference of the spatial derivative on a time-spatial grid system

$$\frac{u_i^{\tau+1} - u_i^\tau}{\Delta t} + c \left( \frac{u_{i+1}^\tau - u_{i-1}^\tau}{2\Delta x} \right) = 0, \quad (12.3.5)$$

where

$\tau$  : time step,

$i$  : grid point in space.

What we are really interested in predicting is  $u$  at *grid point*  $i$  and *time step*  $\tau + 1$ , i.e.  $u_i^{\tau+1}$ , which can be obtained from the above equation,

$$u_i^{\tau+1} = u_i^\tau - \left( \frac{c\Delta t}{2\Delta x} \right) (u_{i+1}^\tau - u_{i-1}^\tau). \quad (12.3.6)$$

- Eq. (12.3.5) or Eq. (12.3.6) is called the *difference equation for the advection equation* under the *scheme of forward in time and centered in space (FTCS)*.
- The algorithm of the scheme is sketched in the following figure.

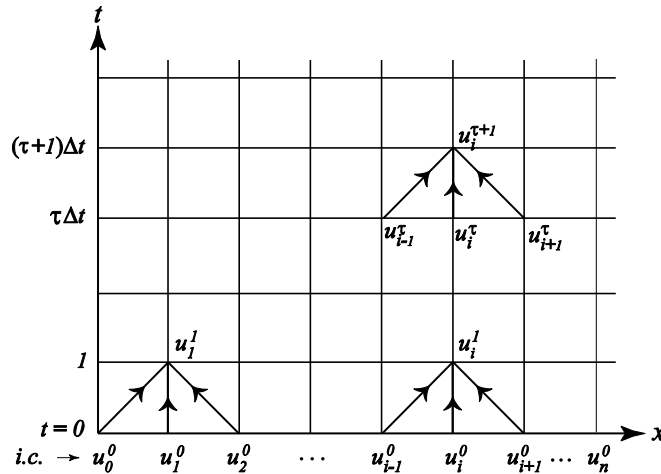


Fig. 12.4: The grid system and algorithm for forward-in-time and centered-in-space finite difference scheme of the advection equation. The values of  $u$  at  $t=0$  are provided by the

- initial condition (*i.c.*) and the values at the left and right boundaries are determined by the boundary conditions (*b.c.*).
- The **interior points**  $u_i$ ,  $i = 1, 2, 3, n-1$ , at time step  $\tau + 1$  are predicted by Eq. (12.3.6) using the values of  $u_{i-1}$ ,  $u_i$ ,  $u_{i+1}$  at time step  $\tau$ .
  
  - Note that **initial condition is needed** for obtaining values at time step 2. **Boundary conditions are also needed at both the left and right boundary points.** The values at the boundary points, **i.e.**  $u_0^{\tau+1}$  and  $u_n^{\tau+1}$ , are determined by the boundary conditions.
  
  - Although many schemes exist to approximate a differential equation, there is **no guaranty that every numerical solution is well behaved.**
  
  - In other words, the numerical solution may not necessarily converge to the real solution of the differential equation when  $\Delta t$  and  $\Delta x$  approach 0.

When this occurs, the scheme is called *numerically or computationally unstable*. Otherwise, the scheme is *numerically stable*. Now, let us check to see whether this natural choice of numerical method, i.e. forward-in-time and centered-in-space scheme is numerically stable or not.

- **Numerical stability of the forward-in-time and centered-in-space scheme**

Consider the following sinusoidal wave in both  $t$  and  $x$  directions,

$$u(x, t) = \hat{u}(k, \omega) e^{i(kx - \omega t)}, \quad (12.3.7)$$

$\hat{u}$  : wave amplitude

$k$  : wave number

$\omega$  : wave frequency.

All of  $\hat{u}, k, \omega$  are complex numbers.

Both  $x$  and  $t$  are represented by the grid interval and time interval, respectively,

$$x = n\Delta x, \text{ and } t = \tau\Delta t,$$

$n$  : number of grid intervals

$\tau$  : number of time intervals

Thus, Eq. (12.3.7) can be rewritten as

$$u(x, t) = u(n\Delta x, \tau\Delta t) = \hat{u}(k, \omega) e^{i(kn\Delta x - \omega\tau\Delta t)}. \quad (12.3.8)$$

Substituting (12.3.8) into the finite difference equation, (12.3.5), yields

$$\begin{aligned} \hat{u}(k, \omega) \left\{ e^{i[kn\Delta x - \omega(\tau+1)\Delta t]} - e^{i[kn\Delta x - \omega\tau\Delta t]} \right\} \\ + \frac{c\Delta t}{2\Delta x} \hat{u}(k, \omega) \left\{ e^{i[k(n+1)\Delta x - \omega\tau\Delta t]} - e^{i[k(n-1)\Delta x - \omega\tau\Delta t]} \right\} = 0, \end{aligned} \quad (12.3.9)$$

or

$$e^{-i\omega\Delta t} = 1 - C [i \sin k\Delta x], \quad (12.3.10)$$

where

$$C = \frac{c\Delta t}{\Delta x}, \quad (12.3.11)$$

is called the *Courant number*.

Substituting  $\omega = \omega_r + i\omega_i$  into the left side of (12.3.10) yields

$$e^{-i\omega\Delta t} = \underbrace{e^{\omega_i\Delta t}}_{(1)} \underbrace{e^{-i\omega_r\Delta t}}_{(2)}. \quad (12.3.12)$$

Term (1): wave amplitude change in one time step  $\Delta t$ .

Term (2): phase change.

Since the first term is a real number and the second term is an imaginary number. If we let  $\lambda = e^{\omega_i\Delta t}$ , then Eq. (12.3.10) becomes

$$\lambda e^{-i\omega_r\Delta t} = 1 - i C \sin k\Delta x, \quad \lambda = e^{\omega_i\Delta t}. \quad (12.3.13)$$

Equating the real and imaginary parts yields

$$\begin{aligned} \lambda \cos \omega_r \Delta t &= 1, \text{ and} \\ \lambda \sin \omega_r \Delta t &= C \sin k\Delta x. \end{aligned} \quad (12.3.14)$$

Summing the squares of the above two equations gives

$$\lambda = \pm \sqrt{1 + C^2 \sin^2 k\Delta x}. \quad (12.3.15)$$

Combining Eqs. (12.3.8), (12.3.12) and (12.3.13) lead to

$$u(x, t) = \hat{u}(k, \omega) \left( e^{ikn\Delta x} e^{-i\omega_r \tau \Delta t} \right) \lambda^\tau. \quad (12.3.16)$$

Term  $\left( e^{ikn\Delta x} e^{-i\omega_r \tau \Delta t} \right)$ : can only change the phase of these waves

Term  $\lambda^\tau$  : may change the amplitude as time proceeds.

In order to have a converged solution, or numerical stability, of Eq. (12.3.16), it requires  $|\lambda| < 1$ .

- However, Eq. (12.3.15) implies that the absolute value of  $\lambda$  is always greater than 1. Thus, surprisingly, the amplitude will grow with time and *the scheme of forward-in-time and centered-in-space is unconditionally unstable* since any small perturbations will grow fictitiously.
- This type of analysis is called *stability analysis*, which determines whether the scheme is stable or not, should be made before a numerical scheme is adopted for approximating a differential equation.

In general,

$$\begin{aligned} u(x, t) &= \hat{u}(k, \omega) e^{i(kx - \omega t)} = \hat{u}(k, \omega) e^{ikx} e^{-i\omega t} \\ &= \hat{u}(k, \omega) e^{ikx} e^{-i(\omega_r + i\omega_i)t} = \hat{u}(k, \omega) e^{ikx} e^{-i\omega_r t} e^{\omega_i t} \end{aligned}$$

$$\begin{aligned}
u(n\Delta x, \tau\Delta t) &= \hat{u}(k, \omega) e^{i(kn\Delta x - \omega_r \tau\Delta t)} e^{i\omega_i \tau\Delta t} \\
&= \hat{u}(k, \omega) e^{i(kn\Delta x - \omega_r \tau\Delta t)} \left( e^{i\omega_i \Delta t} \right)^\tau \\
&= \hat{u}(k, \omega) e^{i(kn\Delta x - \omega_r \tau\Delta t)} \lambda^\tau
\end{aligned}$$

where  $\lambda = e^{i\omega_i \Delta t}$  is different for different numerical scheme. In order to have a stable numerical solution, i.e., numerical stability, we require  $\lambda \leq 1$ .

**(b) Forward in time and upstream (upwind) in space scheme**

Under this scheme, the advection equation is approximated by

$$\frac{u_i^{\tau+1} - u_i^\tau}{\Delta t} = -c \frac{u_i^\tau - u_{i-1}^\tau}{\Delta x} \quad \text{if } c > 0, \quad (12.3.17a)$$

$$= -c \frac{u_{i+1}^\tau - u_i^\tau}{\Delta x} \quad \text{if } c \leq 0. \quad (12.3.17b)$$

**Stability check:** Consider a positive constant advection velocity,  $c > 0$ , and substitute Eq. (12.3.8) into Eq. (12.3.17a)

$$\left\{ u(x, t) = u(n\Delta x, \tau\Delta t) = \hat{u}(k, \omega) e^{i(kn\Delta x - \omega_r \tau\Delta t)} \right\} \quad (12.3.8)$$

- Make sure you can perform this type of stability check, i.e. substitute (12.3.8) into any finite difference equation, such as (12.3.17a) or so, to (12.3.20) and the conclusion!

$$e^{-i(\omega_r + i\omega_i)\Delta t} = 1 - C \left[ 1 - e^{-ik\Delta x} \right], \quad C \equiv \frac{c\Delta t}{\Delta x}, \quad (12.3.18)$$

or

$$\lambda \cos \omega_r \Delta t = 1 - C [1 - \cos k \Delta x], \quad (12.3.19a)$$

$$\lambda \sin \omega_r \Delta t = C \sin k \Delta x, \quad \lambda = e^{i \omega_r \Delta t}. \quad (12.3.19b)$$

Summing the squares of the above equations yields

$$\lambda = \pm \sqrt{1 + 2C(\cos k \Delta x - 1)(1 - C)}. \quad (12.3.20)$$

Numerical or computational stability requires  $|\lambda| < 1$  or

$$2C(\cos k \Delta x - 1)(1 - C) \leq 0. \quad (12.3.21)$$

It holds if  $C \leq 1$  since  $(\cos k \Delta x - 1)$  is always negative.

Thus, it requires  $\Delta t \leq \Delta x / c$  for the *forward in time and upstream in space* scheme to be stable. This condition is called the *CFL (Courant-Friedrichs-Lewy) stability criterion*.

Thus, the scheme of forward in time and upstream in space is conditionally stable when it meets the CFL criterion.

- Note that the CFL stability criterion is just a necessary condition for numerical stability of this scheme and the sufficient condition for stability is often more restrictive and difficult to obtain.
- Beside the potential change in wave amplitude, **the phase of a wave may be changed** after applying a numerical method in solving a differential equation.



To investigate the *phase* characteristics of the *forward-in-time and upstream-in-space scheme*, we may divide (12.3.19b) by (12.3.19a)

$$\left\{ \begin{aligned} \lambda \cos \omega_r \Delta t &= 1 - C [1 - \cos k \Delta x], \quad (12.3.19a) \\ \lambda \sin \omega_r \Delta t &= C \sin k \Delta x, \quad \lambda = e^{\omega_r \Delta t}. \quad (12.3.19b) \end{aligned} \right\}$$

to obtain

$$\tan \omega_r \Delta t = \frac{C \sin k \Delta x}{1 + C(\cos k \Delta x - 1)}. \quad (12.3.22)$$

Based on the above equation and (12.3.16), the *computational phase speed* may be obtained

$$\tilde{c}_p = \frac{\omega_r}{k} = \frac{1}{k \Delta t} \tan^{-1} \left[ \frac{C \sin k \Delta x}{1 + C(\cos k \Delta x - 1)} \right]. \quad (12.3.23)$$

[A review of [dispersion relation and dispersive waves](#)  $u(x, t) = \hat{u} e^{i(kx - \omega t)}$  ]

This indicates that the *finite difference scheme of forward in time and upstream in space is dispersive* since the computational phase speed is a function of the wave number ( $k$ ).

Based on the advection equation, (12.3.1), and Eq. (12.3.7), the physical phase speed for the advection equation may be obtained,

$$c_p = \frac{\omega}{k} = c. \quad (12.3.24)$$

Thus, *the wave is physically nondispersive* since the physical phase speed is independent of the wave number.

However, the numerical method applied here does introduce a *computational wave mode, which is dispersive*. In other words, similar to the physical dispersion, waves with different wavelengths propagate at different speeds. In this way, the wave cannot preserve its original wave pattern and is called *dispersive wave*.

It is interesting to observe that wave dispersion may be induced by a numerical scheme, in addition to the physical wave dispersion.

The ratio of the *computational phase speed* ( $\tilde{c}_p$ ) to the *physical phase speed* ( $c_p$ ) is

$$\frac{\tilde{c}_p}{c_p} = \frac{1}{kc\Delta t} \tan^{-1} \left[ \frac{C \sin k\Delta x}{1 + C(\cos k\Delta x - 1)} \right], \quad (12.3.25)$$

which indicates that

$$\begin{aligned} \tilde{c}_p &> c_p \quad \text{when } 0.5 < C < 1.0 \text{ and} \\ \tilde{c}_p &< c_p \quad \text{when } 0 < C < 0.5. \end{aligned} \quad (12.3.26)$$

Example of wave dispersion:

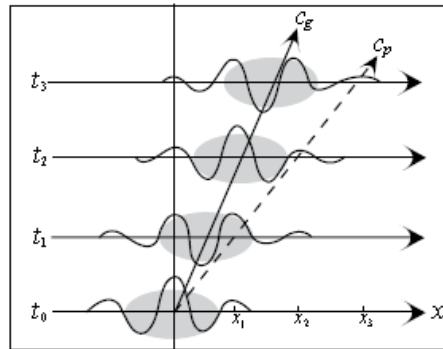


Fig. 3.1: Propagation of a wave group and an individual wave. The solid and dashed lines denote the group velocity ( $c_g$ ) and phase velocity ( $c_p$ ), respectively. Shaded oval denotes the concentration of wave energy which propagates with the group velocity. The phase speed  $c_p$  equals  $x_i/t_i$ , where  $i = 1, 2, \text{ or } 3$ .

[From Lin (2007) - Fig. 3.1]

- In addition to the *numerical instability and numerical dispersion*, a numerical method may also introduce *numerical damping*.

For example, based on Eq. (12.3.20),

$$\lambda = \pm \sqrt{1 + 2C(\cos k\Delta x - 1)(1 - C)} \quad (12.3.20)$$

when  $C=0, 1$ , or  $k \approx 0$  (very long waves), we have  $\lambda=1$ . This means that the amplitude will be kept the same, or say, there exists no damping under these special conditions ( $C=0, 1$ , or  $k \approx 0$ ).

However, this does not apply in general. Thus, the *scheme of forward in time and upstream in space* tends to damp waves in general, especially at  $C=0.5$ .

- To demonstrate the *damping* characteristics, we may use a truncated Taylor series approximation to the advection equation

$$u_i^{\tau+1} \cong u_i^{\tau} + \frac{\partial u}{\partial t} \Delta t + \frac{1}{2!} \frac{\partial^2 u}{\partial t^2} \Delta t^2, \text{ and} \quad (12.3.27)$$

$$\text{Note } \left\{ \begin{array}{l} u(t + \Delta t, x) = u(t, x) + \frac{\partial u}{\partial t} \Delta t + \frac{1}{2!} \frac{\partial^2 u}{\partial t^2} \Delta t^2 \\ \text{where } u(t + \Delta t, x) = u_i^{\tau+1} \text{ and } u(t, x) = u_i^{\tau} \end{array} \right\}$$

$$u_{i-1}^\tau \cong u_i^\tau - \frac{\partial u}{\partial x} \Delta x + \frac{1}{2!} \frac{\partial^2 u}{\partial x^2} \Delta x^2. \quad (12.3.28)$$

Substituting the above approximations into the scheme of forward in time and upstream in space, i.e. (12.3.17a),

$$\frac{u_i^{\tau+1} - u_i^\tau}{\Delta t} = -c \frac{u_i^\tau - u_{i-1}^\tau}{\Delta x} \quad \text{if } c > 0, \quad (12.3.17a)$$

gives

$$\frac{\left( u_i^\tau + \frac{\partial u}{\partial t} \Delta t + \frac{1}{2!} \frac{\partial^2 u}{\partial t^2} \Delta t^2 \right) - u_i^\tau}{\Delta t} = -c \frac{u_i^\tau - \left( u_i^\tau - \frac{\partial u}{\partial x} \Delta x + \frac{1}{2!} \frac{\partial^2 u}{\partial x^2} \Delta x^2 \right)}{\Delta x},$$

which may be rearranged to be

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} + \frac{1}{2} \frac{\partial^2 u}{\partial t^2} \Delta t - \frac{1}{2} \frac{\partial^2 u}{\partial x^2} c \Delta x = 0. \quad (12.3.29)$$

In the above derivation, we have assumed  $c > 0$  without loss of generality.

Thus, in addition to the original advection equation, **two additional terms have been artificially introduced by this particular numerical scheme**. In other words, **computational mode can be generated by the use of a numerical scheme**.

If both  $\Delta t$  and  $\Delta x$  are approaching 0, then the above equation reduces to the original differential equation. However, under normal conditions they have non-zero values, thus the computational mode would be kept in the numerical solution which differs from the physical solution.

One can easily prove that [the last two terms are related to each other since](#)

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}. \quad (12.3.30)$$

(Class: Why?)

Substituting the above equation into Eq. (12.3.29)

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} + \frac{1}{2} \frac{\partial^2 u}{\partial t^2} \Delta t - \frac{1}{2} \frac{\partial^2 u}{\partial x^2} c \Delta x = 0. \quad (12.3.29)$$

leads to

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = \nu_c \frac{\partial^2 u}{\partial x^2}, \quad \nu_c \equiv \frac{1}{2} c \Delta x (1 - C), \quad C = \frac{c \Delta t}{\Delta x} \quad (12.3.31)$$

Therefore, the computational mode tends to damp the physical wave and  $\nu_c$  is called the [numerical or computational diffusion coefficient](#).

The damping characteristics of the  $\nu_c$  term can be shown by solving Eq. (12.3.31) without the advection term by assuming a wave-like disturbance, i.e.

$$u(x, t) = \tilde{u}(k, t) \exp(ikx) \text{ or}$$
$$u(x, t) = \tilde{u}(k, t) (A \sin kx + B \cos kx).$$

- The forward-in-time and upstream-in-space scheme has been used extensively in mesoscale numerical models in earlier times of numerical model development due to its two-time-level advantage, which saves a significant amount of computer memory in simulations. However, its computational damping characteristics and failure to preserve the proper phase has generated serious criticisms.
- This technique is acceptable if the advection and wave propagation is not dominant in the conservation relations for a particular mesoscale phenomenon.

In addition, if the subgrid mixing is important,  $\nu_c$  must be less than the corresponding physically relevant turbulent exchange coefficient to avoid excess damping.

Due to the development of more accurate three-time-level schemes and the advancement of computing facility, this scheme becomes less attractive to mesoscale modelers.

Further discussions and review of this scheme may be found in Brown and Pandolfo (1980). Smolarkiewicz (1983) also presents a

scheme to reduce the implicit diffusion of the upstream difference by adding a corrective step to the calculation.

**(c) Lax-Wendroff Scheme**

This scheme is originally proposed by Lax and Wendroff (1960). The procedure for computation is based on the grid stencil shown in Fig. 12.5 and the following procedure.

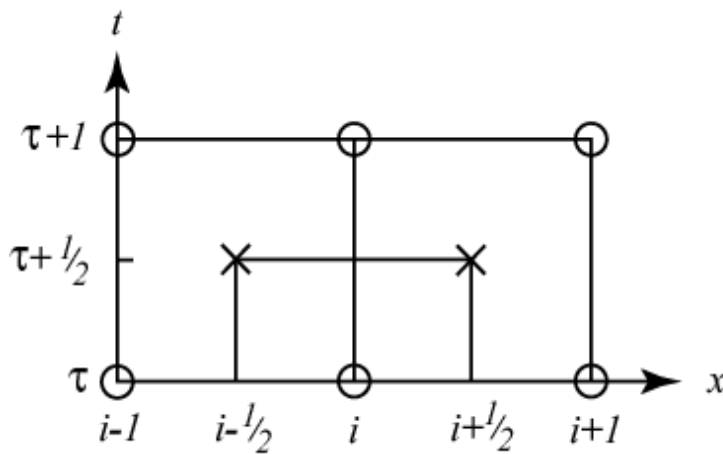


Fig. 12.5: Grid stencil for Lax-Wendroff scheme.

First, provisional values of  $u$  at provisional time step  $\tau+1/2$ , and grid points  $i-1/2$  and  $i+1/2$  are calculated at points denoted by the cross symbol applying the forward in time and centered in space scheme.

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

$$\frac{u_{i-1/2}^{\tau+1/2} - (u_i^\tau + u_{i-1}^\tau)/2}{\Delta t/2} = -c \frac{u_i^\tau - u_{i-1}^\tau}{\Delta x}. \quad (12.3.32)$$

Then, applying the **second-order centered difference scheme in both time and space** to values at grid points  $u_{i+1/2}^{\tau+1/2}$ ,  $u_{i-1/2}^{\tau+1/2}$ , and  $u_i^\tau$  gives,

$$\frac{u_i^{\tau+1} - u_i^\tau}{\Delta t} = -c \frac{u_{i+1/2}^{\tau+1/2} - u_{i-1/2}^{\tau+1/2}}{\Delta x}. \quad (12.3.33)$$

Finally, substituting the above provisional values of  $u_{i+1/2}^{\tau+1/2}$  and  $u_{i-1/2}^{\tau+1/2}$  from (12.3.32) into (12.3.33) leads to

$$u_i^{\tau+1} = u_i^\tau - \frac{C}{2} (u_{i+1}^\tau - u_{i-1}^\tau) + \frac{C^2}{2} (u_{i+1}^\tau - 2u_i^\tau + u_{i-1}^\tau). \quad (12.3.34)$$

From computational point of view,  $u_{i+1/2}^{\tau+1/2}$  and  $u_{i-1/2}^{\tau+1/2}$  are provisional since they do not show up in (12.3.34), thus there is no need to store them permanently. This saves the computer memory, just like the two-time-level schemes discussed earlier.

The Lax-Wendroff scheme has a truncation error of  $O[\Delta x^2] + O[\Delta t^2]$ . In other words, it has second-order accuracy in space and time. This is an improvement of the accuracy in two-time-level schemes.

### ➤ *Stability of the Lax-Wendroff Scheme*

It can be derived that



$$|\lambda| = \left[ 1 - 4C^2(1 - C^2) \sin^4 \frac{k\Delta x}{2} \right]^{1/2}. \quad (12.3.35)$$

Thus, the Lax-Wendroff scheme is stable if

$$C^2 \leq 1 \quad \text{or} \quad \frac{|c|\Delta t}{\Delta x} \leq 1. \quad (12.3.36)$$

That is, the *CFL stability criterion*. It can be proved that the last term of (12.3.34) serves as a damping term. In fact, the Lax-Wendroff scheme can be viewed as the modification of the forward-in-time and centered-in-space scheme with damping.

➤ *Damping characteristics of the Lax-Wendroff Scheme*

For the shortest resolvable wavelength  $2\Delta x$ , we have  $k = \pi / \Delta x$ . Substituting  $k$  into (12.3.35) yields

$$|\lambda| = |1 - 2C^2|. \quad (12.3.37)$$

For  $4\Delta x$  wave, we have

$$|\lambda| = [1 - C^2 + C^4]^{1/2}. \quad (12.3.38)$$

Therefore, the amount of damping is seen to be quite large for shorter waves.

➤ *Phase characteristics of the Lax-Wendroff Scheme:*

The phase error can also be calculated,

$$\frac{\tilde{c}_p}{c} = \frac{\tan^{-1}\left\{-C \sin k\Delta x / [1 - C^2(1 - \cos k\Delta x)]\right\}}{-C k \Delta x}. \quad (12.3.39)$$

Thus, *the Lax-Wendroff scheme is dispersive* since  $\tilde{c}_p$  is a function of wave number ( $k$ ). It has a predominantly lagging phase error except for large wave numbers with  $\sqrt{0.5} < C < 1$ .

## Modifications of the Lax-Wendroff Scheme

### (d) *The Crowley scheme*

➤ The Lax-Wendroff scheme was modified by Crowley (1968) to the following formula

$$u_i^{\tau+1} = u_i^\tau - \frac{C}{2}(u_{i+1}^\tau - u_{i-1}^\tau) + \frac{C^2}{2}(u_{i+1}^\tau - 2u_i^\tau + u_{i-1}^\tau) + \frac{C}{12}(1 - C^2)(u_{i+2}^\tau - 2u_{i+1}^\tau + 2u_{i-1}^\tau - u_{i-2}^\tau) \quad (12.3.40)$$

The above scheme is also known as *Crowley scheme*. The last term in the above equation is the *third-order space correction term*.

In order to keep the amount of damping small, Kasahara

(1969) has combined the Lax-Wendroff scheme with the leapfrog scheme (which is neutral). The Lax-Wendroff scheme is applied only once in every hundred-time step.

Schlesinger (1985) also has modified the Lax-Wendroff scheme by adding the negative of the third-order derivative in the Taylor's series expansion of its first order term.

The Lax-Wendroff scheme has been fairly widely used in earlier atmospheric models due to its two-time-level advantage, second-order accuracy, and explicit characteristics (Richmyer, 1963).

More detailed review of this scheme can also be found in Richmyer and Morton (1967) and Mesinger and Arakawa (1976).

### *(e) Warming-Kutler-Lomax (WKL) scheme*

Warming, Kutler and Lomax (1973) proposed a modified 2-time-level scheme with three 3-steps represented by

$$\text{Step 1: } u_i^* = u_i^\tau - \frac{2C}{3} (u_{i+1}^\tau - u_i^\tau),$$

$$u_{i-1}^* = u_{i-1}^\tau - \frac{2C}{3} (u_i^\tau - u_{i-1}^\tau),$$

$$u_{i+1}^* = u_{i+1}^\tau - \frac{2C}{3} (u_{i+1}^\tau - u_i^\tau)$$

$$\text{Step 2: } u_i^{**} = \frac{1}{2} \left[ u_i^\tau + u_i^* - \frac{2C}{3} (u_i^* - u_{i-1}^*) \right],$$

$$u_{i+1}^{**}$$

$$u_{i-1}^{**}$$

Step 3:

$$u_i^{\tau+1} = u_i^\tau - \frac{C}{24} \left( -2u_{i+2}^\tau + 7u_{i+1}^\tau - 7u_{i-1}^\tau + 2u_{i-2}^\tau \right) - \frac{3C}{8} \left( u_{i+1}^{**} - u_{i-1}^{**} \right) - \frac{\alpha}{24} \left( u_{i+2}^\tau - 4u_{i+1}^\tau + 6u_i^\tau - 4u_{i-1}^\tau + u_{i-2}^\tau \right), \quad (12.3.41)$$

where  $\alpha$  is a free parameter added to insure the computational stability. Note that  $u_i^{**}$  values are provisional, which do not need a permanent storage in computer memory.

The advantage of the WKL scheme is that it can save memory while increases the accuracy as a 2-time-level method.

The last term of (12.3.41) (i.e., the term with  $\alpha$ ) is analogous to the *five-point numerical smoothing or diffusion*. This will be discussed in the next chapter. It can be shown that this scheme is stable when

$$|C| \leq 1 \quad \text{and} \quad 4C^2 - C^4 \leq \alpha \leq 3. \quad (12.3.42)$$

The scheme has a minimum dissipation when

$$\alpha = \alpha_1 = 4C^2 - C^4, \quad (12.3.43)$$

and a minimum dispersion when

$$\alpha = \alpha_2 = \frac{(4C^2 + 1)(4 - C^2)}{5}. \quad (12.3.44)$$

The readers are referred to Andersen and Fattahi (1974) for more detailed review of this scheme.

### *(e) Multi-stage schemes*

The advection equation can be viewed as a special case of the following equation,

$$\frac{\partial u}{\partial t} = F(u). \quad (12.3.45)$$

The advection term is considered to be the forcing term. To improve the accuracy of two-time-level schemes, such as forward time difference, Eq. (12.3.45) may be approximated by the *multi-stage scheme*,

$$\begin{aligned} \tilde{u}^{\tau+\alpha} &= u^\tau + \alpha \Delta t F(u^\tau), \\ u^{\tau+1} &= u^\tau + \Delta t \left[ \beta F(\tilde{u}^{\tau+\alpha}) + (1 - \beta) F(u^\tau) \right]. \end{aligned} \quad (12.3.46)$$

The above method reduces to the

- (1) *Second-order Runge-Kutta schemes* when  $\alpha\beta = 1/2$   
(e.g, WRF model time differencing)
- (2) *Heun scheme* when  $\alpha = 1, \beta = 1/2$

- (3) *Forward-backward or Matsuno scheme* when  $\alpha = \beta = 1$  (Matsuno 1966).

More detailed reviews can be found in Durran (1998).  
Time integration scheme in WRF:

<http://cires.colorado.edu/science/groups/pielke/classes/at7500/wrfarw.pdf>.

### 3.3.2 Three-Time-Level Schemes

#### (a) *Leapfrog in time and centered in space schemes*

The advection equation may also be approximated by the scheme of second-order centered (leapfrog) in time and second-order centered difference in space,

$$\frac{u_i^{\tau+1} - u_i^{\tau-1}}{2\Delta t} = -c \frac{u_{i+1}^{\tau} - u_{i-1}^{\tau}}{2\Delta x} \quad (12.3.48)$$

Substituting the wave solution Eq. (12.3.8)

$$u(x, t) = u(n\Delta x, \tau\Delta t) = \hat{u}(k, \omega) e^{i(kn\Delta x - \omega \tau\Delta t)} \quad (12.3.8)$$

into Eq. (12.3.48) yields,

$$\left( \lambda e^{-i\omega_r \Delta t} - \frac{1}{\lambda e^{-i\omega_r \Delta t}} \right) = -C 2i \sin k\Delta x; \quad (12.3.49)$$

where

$$\lambda \equiv e^{i\omega_r \Delta t}; \quad C \equiv \frac{c\Delta t}{\Delta x} .$$

The above equation may be rearranged to obtain

$$\lambda^2 e^{-2i\omega_r \Delta t} + i\alpha \lambda e^{-i\omega_r \Delta t} - 1 = 0 . \quad (12.3.50)$$

Here  $\alpha$  is just a temporary parameter defined as  $2C \sin k\Delta x$ . Regarding  $\lambda e^{-i\omega_r \Delta t}$  as the unknown in the above equation, we obtain

$$\lambda e^{-i\omega_r \Delta t} = \frac{-i\alpha \pm \sqrt{4 - \alpha^2}}{2} . \quad (12.3.51)$$

There exist two possible cases, namely, (1)  $\alpha^2 \leq 4$  and (2)  $\alpha^2 > 4$ .

**Case 1:**  $\alpha^2 \leq 4$

Separating the real and imaginary parts of (12.3.51) gives

$$\lambda \cos \omega_r \Delta t = \pm \frac{1}{2} \sqrt{4 - \alpha^2} , \quad (12.3.52a)$$

$$\lambda \sin \omega_r \Delta t = \frac{\alpha}{2} . \quad (12.3.52b)$$

Summing the squares of the above two equations yields

$$|\lambda| = 1 .$$

Therefore, the amplitude of the wave or disturbance is preserved for all wavelengths when  $\alpha^2 \leq 4$ . **In other words, the scheme is *neutral* when  $\alpha^2 \leq 4$ . ( $\alpha = 2C \sin k\Delta x$ )**

**Case 2:**  $\alpha^2 > 4$

$$\lambda \cos \omega_r \Delta t = 0, \quad (12.3.53a)$$

$$\lambda \sin \omega_r \Delta t = \frac{\alpha}{2} \mp \frac{1}{2} \sqrt{\alpha^2 - 4}. \quad (12.3.53b)$$

Now, summing the squares of the above two equations

$$|\lambda| = \frac{\alpha}{2} \mp \frac{1}{2} \sqrt{\alpha^2 - 4} \quad \text{if } \alpha^2 > 4. \quad (12.3.54)$$

*Claim: This scheme is unstable when  $\alpha^2 > 4$ .*

To prove this, we only need to find a counter example of  $|\lambda| > 1$ .

For example, we may assume  $\alpha = 2 + \varepsilon$ , where  $\varepsilon$  is a small positive number. Substituting  $\alpha$  into the positive root of Eq. (12.3.54) gives

$$|\lambda| = 1 + \frac{\varepsilon}{2} \mp \frac{1}{2} \sqrt{4\varepsilon + \varepsilon^2}. \quad (12.3.55)$$

Since either root is possible, we may look at the solution with positive root,

$$|\lambda| = 1 + \frac{\varepsilon}{2} + \frac{1}{2} \sqrt{4\varepsilon + \varepsilon^2}. \quad (12.3.56)$$



This gives  $|\lambda| > 1$ . Therefore, *the scheme of leapfrog in time and centered in space is linearly unstable when  $\alpha^2 > 4$ .*

Note that  $\alpha = 2C \sin k\Delta x$ .

*Thus, the stability is retained only when  $\alpha^2 \leq 4$ .* Based on the definition of  $\alpha$  for Eq. (12.3.50), it requires

$$C^2 \sin^2 k\Delta x \leq 1. \quad (12.3.57)$$

Since the maximum value of the sine square function is 1, the above equation is satisfied when

$$|C| \leq 1. \quad (12.3.58)$$

In fact, the CFL criterion is not only a necessary condition, but also a sufficient condition, for the linear stability for the scheme of leapfrog in time and second-order centered in space.

➤ *Phase characteristics of the leapfrog in time and second-order centered in space scheme*

Divide (12.3.52b) by (12.3.52a),

$$\left\{ \lambda \cos \omega_r \Delta t = \pm \frac{1}{2} \sqrt{4 - \alpha^2} \quad (12.3.52a) \right\} \quad \left\{ \lambda \sin \omega_r \Delta t = \frac{\alpha}{2} \quad (12.3.52b) \right\}$$

$$\omega_r \Delta t = \tan^{-1} \left( \frac{\pm \alpha}{\sqrt{4 - \alpha^2}} \right). \quad (12.3.59)$$

This gives the computational phase speeds,

$$\tilde{c}_p = \frac{\omega_r}{k} = \frac{\pm 1}{k \Delta t} \tan^{-1} \left( \frac{\alpha}{\sqrt{4 - \alpha^2}} \right). \quad (12.3.60)$$

The *phase error* can then be obtained,

$$\frac{\tilde{c}_p}{c} = \frac{\pm 1}{kc \Delta t} \tan^{-1} \left( \frac{\alpha}{\sqrt{4 - \alpha^2}} \right). \quad (12.3.61)$$

For  $c > 0$ , Eq. (12.3.60) has two solutions, one propagating to the right ( $\tilde{c}_p > 0$ ) and the other propagating to the left ( $\tilde{c}_p < 0$ ).

The first solution represents the physical mode, while the second solution represents the computational mode, which is purely generated by the numerical scheme. This causes the so-called *time-splitting problem*.

This scheme also induces computational dispersion since the computational phase speed is a function of wave number ( $k$ ). In summary, the scheme of leapfrog in time and second-order centered in space is able to preserve the

amplitude when  $\alpha^2 \leq 4$ , but can generate errors due to the *computational wave dispersion*.

Figure 12.6 shows examples of the amplitude and phase errors produced by applying this scheme and the forward in time and upstream in space scheme to the advection equation and comparing the numerical solutions with the analytical solution.

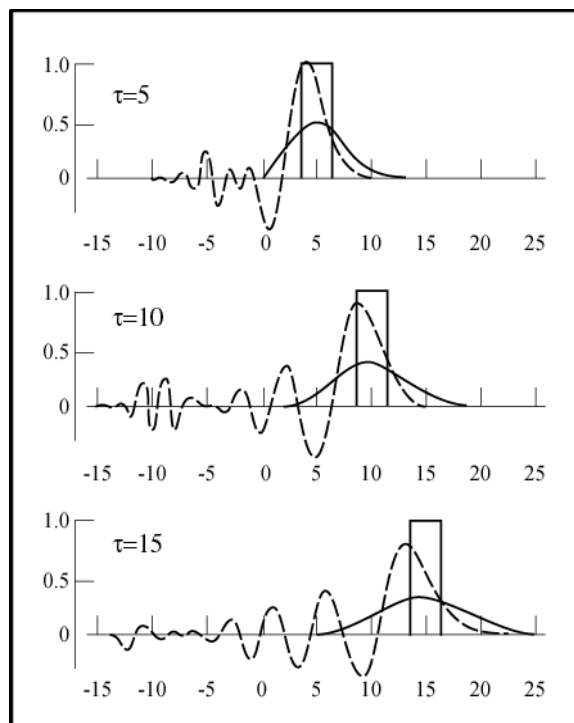


Fig. 12.6: An example of computational damping and dispersion. Comparison of the analytical solution (thin solid curve) and numerical solutions of applying the leapfrog in time and second-order centered in space scheme (dashed curve) and the forward in time and upstream in space scheme (heavy solid curve) to the advection equation with an initial rectangular wave. Three nondimensional times are shown. (Adapted after Wurtele, 1961)

The scheme of leapfrog in time and second-order centered in space is able to preserve the amplitude of the initial rectangular

wave much better than the scheme of forward in time and upstream in space.

However, it produces a severe computational dispersion than the scheme of forward in time and upstream in space.

In addition to the second-order centered in space, a higher-order accuracy scheme in the space difference may be derived.

For example, consider the following Taylor series expansions for  $f(x + \Delta x)$  and  $f(x - \Delta x)$ ,

$$f(x + \Delta x) = f(x) + f'(x)\Delta x + f''(x)\frac{\Delta x^2}{2!} + f'''(x)\frac{\Delta x^3}{3!} + \dots \quad (12.3.62)$$

$$f(x - \Delta x) = f(x) - f'(x)\Delta x + f''(x)\frac{\Delta x^2}{2!} - f'''(x)\frac{\Delta x^3}{3!} + \dots \quad (12.3.63)$$

Subtracting (12.3.63) from (12.3.62) leads to

$$f(x + \Delta x) - f(x - \Delta x) = 2f'(x)\Delta x + \frac{1}{3}f'''(x)\Delta x^3 + \dots \quad (12.3.64)$$

Now, consider the following Taylor series expansions for  $f(x + 2\Delta x)$  and  $f(x - 2\Delta x)$ ,

$$f(x + 2\Delta x) = f(x) + 2f'(x)\Delta x + f''(x)\frac{4\Delta x^2}{2!} + f'''(x)\frac{8\Delta x^3}{3!} + \dots \quad (12.3.65)$$

$$f(x-2\Delta x) = f(x) - 2f'(x)\Delta x + f''(x)\frac{4\Delta x^2}{2!} - f'''(x)\frac{8\Delta x^3}{3!} + \dots \quad (12.3.66)$$

Subtracting (12.3.66) from (12.3.65) leads to

$$f(x+2\Delta x) - f(x-2\Delta x) = 4f'(x)\Delta x + \frac{8}{3}f'''(x)\Delta x^3 + \dots \quad (12.3.67)$$

Eliminating  $f'''(x)$  terms from Eqs. (12.3.64) to (12.3.67) yields

$$f'(x) = \frac{8[f(x+\Delta x) - f(x-\Delta x)] - [f(x+2\Delta x) - f(x-2\Delta x)]}{12\Delta x} + O(\Delta x^4)$$

(12.3.68)

This scheme has a *fourth-order centered difference* for the approximation of  $f'(x)$ .

Notice that the boundary points may be approximated by adjacent interior points. For example,  $f'(x)$  at the left boundary can be approximated by  $f(x+\Delta x)$ ,  $f(x+2\Delta x)$ ,  $f(x+3\Delta x)$ , and  $f(x+4\Delta x)$ . It can be shown that Eq. (12.3.68) can be obtained by extrapolation for the value  $2\Delta x/3$  of the quotients of  $f'(x)$  from (12.3.66) and (12.3.67).

Now apply the fourth-order-centered difference to the advective equation with the leapfrog in time,

$$\frac{u_i^{\tau+1} - u_i^{\tau-1}}{2\Delta t} + c \left( \frac{8(u_{i+1}^\tau - u_{i-1}^\tau) - (u_{i+2}^\tau - u_{i-2}^\tau)}{12\Delta x} \right) = 0. \quad (12.3.69)$$

The above equation may be rearranged to be

$$u_i^{\tau+1} = u_i^{\tau-1} - \frac{C}{6} [8(u_{i+1}^\tau - u_{i-1}^\tau) - (u_{i+2}^\tau - u_{i-2}^\tau)], \quad (12.3.70)$$

where  $C$  is the *Courant number*, as defined earlier.

It can be shown that

$$\frac{\tilde{c}_p}{c} = \frac{4 \sin k\Delta x}{3 k\Delta x} - \frac{1 \sin 2k\Delta x}{3 2k\Delta x}. \quad (12.3.71)$$

for the fourth-order centered difference. Compared with that of the second-order centered in space scheme

$$\frac{\tilde{c}_p}{c} = \frac{\sin k\Delta x}{k\Delta x}, \quad (12.3.72)$$

we have

$$\tilde{c}_p = c \left[ 1 - \frac{4}{5!} (k\Delta x)^2 + \dots \right] \quad \text{for 4th-order scheme,} \quad (12.3.73)$$

$$\tilde{c}_p = c \left[ 1 - \frac{1}{3!} (k\Delta x)^2 + \dots \right] \quad \text{for 2nd-order scheme.} \quad (12.3.74)$$

**Thus, both schemes are dispersive.** However, the phase speed error has been much reduced for longer waves (smaller  $k$ ) by using the 4th-order scheme.

The computational phase speeds associated with the 2nd-order and 4th-order centered difference schemes are shown in Fig. 12.7.

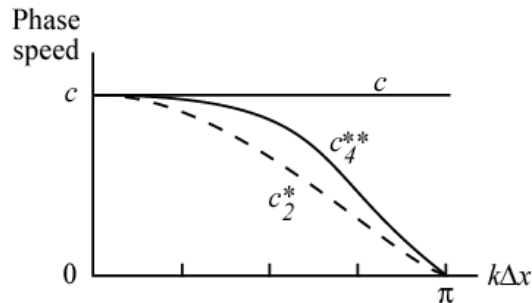


Fig. 12.7: The computational phase speeds associated with the 2nd-order and 4th-order centered difference schemes. (Adapted after Mesinger and Arakawa, 1976)

This figure indicates that

- (a) Very significant increase in accuracy of the phase speed for large-scale and mesoscale waves, and
- (b) More computational dispersion for shorter waves is associated with the 4th-order scheme since the slope of  $c_4$  is larger than  $c_2$ .

Because of the decrease in the phase speed error of the longer waves, the use of 4th-order centered difference in space scheme for the advection equation has brought significant improvements in operational numerical forecasting in both barotropic and baroclinic models.

### ***(b) Adams-Bashforth Scheme***

Eq. (12.3.45) is approximated by

$$u^{\tau+1} = u^{\tau} + \Delta t \left( \frac{3}{2} F(u^{\tau}) - \frac{1}{2} F(u^{\tau-1}) \right). \quad (12.3.47)$$

*Advantages:* It does not generate *time splitting* as that produced by the *leapfrog scheme*, or the *numerical diffusion* produced by the upstream difference.

Lilly (1965) reviewed eight schemes adopted in atmospheric models then and found that the Adams-Bashforth scheme is the best in considering the simplicity, efficiency, and accuracy together.

Baer and Simons (1970) found that the nonlinear advection terms and energy components might have large errors.

### 3.4 Implicit schemes

➤ With the finite difference schemes proposed as above, the advection term is evaluated at time step  $\tau$ . In this way, the variable at time step  $\tau+1$  can be predicted explicitly by those at time step  $\tau$ . Thus, these schemes are called *explicit schemes*.

However, the CFL stability criterion imposes a severe restriction on the time interval with a resultant increase in computational time.



- This restriction may be relaxed by evaluating the advection term at time step  $\tau + 1$ . For example, let us consider the *Euler implicit method* (e.g. see Tannehill et al., 1997)

$$\frac{u_i^{\tau+1} - u_i^\tau}{\Delta t} + c \left( \frac{u_{i+1}^{\tau+1} - u_{i-1}^{\tau+1}}{2\Delta x} \right) = 0. \quad (12.4.1)$$

In the above approximation, the forward difference is applied to the time derivative, while the 2nd-order-centered difference is applied to the spatial derivative at time step  $\tau + 1$ . In order to solve  $u$  at time step  $\tau + 1$ , we move all of them to the left-hand side

$$-\frac{C}{2}u_{i-1}^{\tau+1} + u_i^{\tau+1} + \frac{C}{2}u_{i+1}^{\tau+1} = u_i^\tau, \quad i = 1, 2, 3, \dots, N-1. \quad (12.4.2)$$

Thus, one cannot solve the equation for a general point,  $u_i^{\tau+1}$ , alone. Instead, we have to solve the system of algebraic equations, as shown in Fig. 12.8, simultaneously.

$$\begin{pmatrix} 1 & \frac{C}{2} & 0 & \cdots & \cdots & \cdots & 0 \\ -\frac{C}{2} & 1 & \frac{C}{2} & 0 & \cdots & \cdots & 0 \\ 0 & -\frac{C}{2} & 1 & \frac{C}{2} & \cdots & \cdots & 0 \\ 0 & 0 & -\frac{C}{2} & 1 & \frac{C}{2} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & -\frac{C}{2} & 1 & \frac{C}{2} & 0 \\ 0 & 0 & 0 & \cdots & \cdots & -\frac{C}{2} & 1 & \frac{C}{2} \\ 0 & 0 & 0 & \cdots & \cdots & \cdots & -\frac{C}{2} & 1 \end{pmatrix} \begin{pmatrix} u_1^{\tau+1} \\ u_2^{\tau+1} \\ u_3^{\tau+1} \\ u_4^{\tau+1} \\ \vdots \\ u_{N-3}^{\tau+1} \\ u_{N-2}^{\tau+1} \\ u_{N-1}^{\tau+1} \end{pmatrix} = \begin{pmatrix} u_1^\tau \\ u_2^\tau \\ u_3^\tau \\ u_4^\tau \\ \vdots \\ u_{N-3}^\tau \\ u_{N-2}^\tau \\ u_{N-1}^\tau \end{pmatrix}$$

Fig. 12.8: The system of algebraic equations of (12.4.2) for Euler implicit method with boundary conditions,

$$u(0, t) = u_1^{\tau+1} = 0 \text{ and } u((N-1)\Delta x, t) = u_N^{\tau+1} = 0.$$

- In general, one can introduce a weighing factor  $\alpha$  and replace (12.4.2) by

$$-\frac{\alpha C}{2} u_{i-1}^{\tau+1} + u_i^{\tau+1} + \frac{\alpha C}{2} u_{i+1}^{\tau+1} = \frac{(1-\alpha)C}{2} u_{i-1}^{\tau} + u_i^{\tau} - \frac{(1-\alpha)C}{2} u_{i+1}^{\tau}, \quad i = 1, 2, 3, \dots, N-1. \quad (12.4.3)$$

If  $\alpha = 0$ , the above formula reduces to the complete **explicit scheme**, i.e. the forward in time and centered in space scheme, Eq. (12.3.6).

If  $\alpha = 1$ , the **Euler implicit scheme**, (12.4.2) is recovered.

- To find out the **computational stability**, we substitute Eq. (12.3.8) into Eq. (12.4.2) to obtain

$$|\lambda| = \frac{1}{\sqrt{1 + C^2 \sin^2 k\Delta x}}. \quad (12.4.4)$$

- The above equation indicates that *the implicit Euler scheme is unconditionally stable* since the right-hand side is always less than 1.

- In general, the use of an implicit scheme permits larger time steps than the explicit form without causing linear instability.
- To invert the matrix, either direct or iterative methods can be applied. The **direct methods** include the **Gaussian elimination method, LU decomposition, etc.** The **iterative methods** include the **Jacobi method, Gauss-Seidel method, relaxation method, etc.** Discussions on the direct and iterative methods of inverting a matrix can be found in numerical analysis textbooks.
- Sometimes, a **semi-implicit scheme** is adopted, in which those terms in the equations of motion that are primarily responsible for the propagation of gravity waves are treated fully implicitly, while other terms are treated explicitly (e.g., Kwizak and Robert, 1971).
- One simple semi-implicit scheme has been adopted in modeling the geophysical fluid flow is the **trapezoidal semi-implicit scheme**. For example, the linear horizontal shallow water momentum equation in  $x$ -direction, i.e. Eq. (4.4.21),

$$\frac{\partial u'}{\partial t} + U \frac{\partial u'}{\partial x} + g \frac{\partial h'}{\partial x} = 0,$$

may be discretized by the trapezoidal semi-implicit scheme as

$$\left( \frac{u_i^{\tau+1} - u_i^\tau}{\Delta t} \right) + U \left( \frac{u_{i+1}^\tau - u_{i-1}^\tau}{2\Delta x} \right) + \frac{g}{2} \left[ \left( \frac{h_{i+1}^\tau - h_{i-1}^\tau}{2\Delta x} \right) + \left( \frac{h_{i+1}^{\tau+1} - h_{i-1}^{\tau+1}}{2\Delta x} \right) \right] = 0. \quad (12.4.5)$$

The primes have been ignored in the above equation.

Notice that the advection term is treated in explicit manner and the spatial derivative is centered at  $\tau + 1/2$  time step by averaging values at time steps  $\tau$  and  $\tau + 1$ . It also can be shown that *the trapezoidal implicit scheme is unconditionally stable* (Mesinger and Arakawa, 1976).

- The disadvantage of this scheme is that it has a serious phase error not only for short waves as in the leapfrog time difference scheme, but also for relatively large Courant number (Haltiner and Williams, 1980).

### 3.5 Semi-Lagrangian Methods

- Ideally, the advection equation may be integrated by following the fluid particles in a Lagrangian manner ( $Du/Dt$ ), so that one does not have to discretize the local

rate of change ( $\partial u / \partial t$ ) and advection terms (e.g.,  $u \partial u / \partial x$ ) separately.

In fact, Fjortoft (1952) has proposed a graphical method for solving the barotropic vorticity equation using a single time step of 24h by following a set of fluid particles, or say by taking a *Lagrangian approach*.

Welander (1955) pointed out that in general a set of fluid particles, which are initially distributed regularly at the initial time will soon become greatly deformed, and are thus rendered unsuitable for numerical integration.

To avoid the above difficulty, Wiin-Nielson (1959) then introduced a *semi-Lagrangian* (occasionally referred to as *quasi-Lagrangian*) *approach*.

In a *semi-Lagrangian approach*, a set of particles which arrive at a regular set of grid points are traced backward over a single time interval to their *departure points*. The values of the dynamical quantities at the departure points are obtained by interpolation from neighboring grid points where their values are known.

Notice that in this semi-Lagrangian method, the set of fluid particles in question changes at each time step,

which is different from the Lagrangian method, such as that used by Fjortoft (1952).

Robert (1981) showed that the use of the *semi-Lagrangian semi-implicit scheme* offers significant advantages over the purely Eulerian approach for NWP. For detailed reviews, the readers are referred to Bates and McDonald (1982) and Staniforth and Côté' (1991).

[Reading Assignment] To demonstrate the *semi-Lagrangian method*, we may consider the one-dimensional nonlinear advection equation in the form of total derivative,

$$\frac{D\psi}{Dt} = 0, \quad \frac{D}{Dt} \equiv \frac{\partial}{\partial t} + u \frac{\partial}{\partial x}, \quad (12.5.1)$$

where  $\psi$  is any variable under consideration.

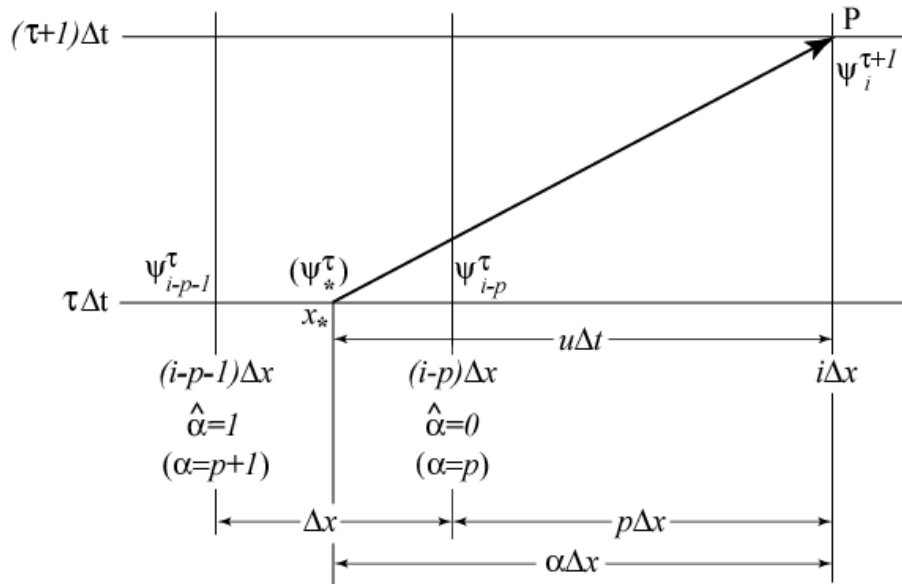


Fig. 12.9: A schematic of semi-Lagrangian method.

Integrating over the trajectory of a fluid particle that arrives at a grid point  $i\Delta x$  and at time  $(\tau+1)\Delta t$ , denoted as P in Fig. 12.9, we have

$$\psi_i^{\tau+1} = \psi_*^{\tau}, \quad (12.5.2)$$

where  $\psi_*^{\tau}$  is the value of  $\psi$  at the departure point of the particle at time  $\tau\Delta t$ .

Note that  $\psi_*^{\tau}$  is obtained by polynomial interpolation from the neighboring grid points.

The stability and accuracy of the scheme depends on the interpolation method used.

For example, we may consider the linear interpolation from the surrounding grid points  $(i-p)$  and  $(i-p-1)$  for  $\psi_*^\tau$ ,

$$\frac{\psi_{i-p}^\tau - \psi_*^\tau}{u\Delta t - p\Delta x} = \frac{\psi_{i-p}^\tau - \psi_{i-p-1}^\tau}{\Delta x}, \quad (12.5.3)$$

where  $u$  is the advection velocity as represented in Eq. (12.5.1). The above equation may be rearranged to be

$$\psi_*^\tau = \psi_{i-p}^\tau - \left( \frac{u\Delta t}{\Delta x} - p \right) (\psi_{i-p}^\tau - \psi_{i-p-1}^\tau). \quad (12.5.4)$$

or

$$\psi_*^\tau = \psi_{i-p}^\tau - \hat{\alpha} (\psi_{i-p}^\tau - \psi_{i-p-1}^\tau), \quad (12.5.5)$$

where

$$\hat{\alpha} = \alpha - p, \quad \alpha = u\Delta t / \Delta x. \quad (12.5.6)$$

Therefore, from (12.5.2) we have

$$\psi_i^{\tau+1} = \psi_{i-p}^\tau - \hat{\alpha} (\psi_{i-p}^\tau - \psi_{i-p-1}^\tau). \quad (12.5.7)$$

According to Eq. (12.5.6) and Fig. (12.9),  $\hat{\alpha}$  is the fractional part and  $p$  is the integral part after advection of a non-dimensional distance  $u\Delta t / \Delta x$ .



- **To examine whether the semi-Lagrangian method is computationally stable or not**, we may again assume a wave-like solution,

$$\psi_i^\tau = \hat{\psi} e^{-i\omega_r \tau \Delta t} e^{ikn\Delta x} \lambda^\tau. \quad (12.5.8)$$

Substituting it into Eq. (12.5.7) yields

$$\lambda^2 = 1 - 2\hat{\alpha}(1 - \hat{\alpha})(1 - \cos k\Delta x), \quad \lambda \equiv e^{\omega_i \Delta t}. \quad (12.5.9)$$

Thus, in order to have a computationally stable solution ( $|\lambda| \leq 1$ ), we require

$$0 \leq \hat{\alpha} \leq 1. \quad (12.5.10)$$

{Note that  $\hat{\alpha} = \alpha - p$ ,  $\alpha = u\Delta t / \Delta x$ . (12.5.6) and Fig. 12.9. }

That is, the departure points must lie within the interpolation interval ( $i-p-1, i-p$ ). However, the choice of departure is just based on this. **Therefore, the semi-Lagrangian scheme is unconditionally stable.**

- The *semi-implicit method* may be incorporated into the integration by considering the other terms (Robert 1982), such as the pressure gradient force term in the momentum equation, as time averages along the trajectory, while the total time derivative is evaluated by

either leapfrog, forward or other time difference schemes.

To elucidate this, let us consider the following Boussinesq, horizontal momentum equation,

$$\frac{Du}{Dt} - fv + \frac{1}{\rho_o} \frac{\partial p}{\partial x} = 0. \quad (12.5.11)$$

The total derivative of the above equation may be approximated by the scheme of forward in time,

$$\frac{Du}{Dt} = \frac{u(x, t + \Delta t) - u(x - a, t)}{\Delta t}, \quad (12.5.12)$$

where

$$a = u(x - a, t)\Delta t. \quad (12.5.13)$$

The above equation can be solved by using an iterative method to obtain the upstream displacement or the departure point,  $a$ .

We may apply the semi-implicit approximation to the other terms on the left hand side of Eq. (12.5.11)

$$\psi_{av}^t = \frac{\psi(x, t + \Delta t) + \psi(x - a, t)}{2} \quad (12.5.12)$$

where the subscript  $av$  denotes the time average.

Then, the horizontal momentum equation can be approximated by the *semi-implicit semi-Lagrangian scheme*,

$$\frac{u(x, t + \Delta t) - u(x - a, t)}{\Delta t} - fv_{av}^t + \left( \frac{1}{\rho_o} \frac{\partial p}{\partial x} \right)_{av}^t = 0, \quad (12.5.15)$$

The above equation may also be rewritten as

$$\left( [u]_x^{t+\Delta t} - [u]_{x-a}^t \right) - \frac{f\Delta t}{2} \left( [v]_x^{t+\Delta t} + [v]_{x-a}^t \right) + \frac{\Delta t}{2\rho_o} \left( \left[ \frac{\partial p}{\partial x} \right]_x^{t+\Delta t} + \left[ \frac{\partial p}{\partial x} \right]_{x-a}^t \right) = 0. \quad (12.5.16)$$

Moving all terms at time  $t + \Delta t$  to the left-hand side gives the following form of the *semi-implicit semi-Lagrangian method*,

$$[u]_x^{t+\Delta t} - \frac{f\Delta t}{2} [v]_x^{t+\Delta t} + \frac{\Delta t}{2\rho_o} \left[ \frac{\partial p}{\partial x} \right]_x^{t+\Delta t} = [u]_{x-a}^t + \frac{f\Delta t}{2} [v]_{x-a}^t - \frac{\Delta t}{2\rho_o} \left[ \frac{\partial p}{\partial x} \right]_{x-a}^t. \quad (12.5.17)$$

This will form a set of linear algebraic equations, which can be written in a matrix form. Thus, a method for inverting the matrix, such as the Gaussian elimination method or the Gauss-Seidel method, is needed to obtain the solution for time step  $t + \Delta t$ .

Notice that the advantage of the semi-implicit semi-Lagrangian scheme is that it is unconditionally stable, so that a relatively large time step can be used. The disadvantage of this scheme is that the iterative method for finding the departure points and the method for inverting the matrix is time consuming.

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## Appendices

### Appendix 12.1: Formulas for Finite Difference Approximations of Derivatives

(Modified from Gerald and Wheatley 1984)

#### Formulas for the first derivatives:

$$f'(x) = \frac{f(x + \Delta x) - f(x)}{\Delta x} + O(\Delta x), \quad (\text{forward difference})$$

$$f'(x) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x} + O(\Delta x^2), \quad (2^{\text{nd}}\text{-order centered difference})$$

$$f'(x) = \frac{-f(x + 2\Delta x) + 4f(x + \Delta x) - 3f(x)}{2\Delta x} + O(\Delta x^2),$$

$$f'(x) = \frac{-f(x + 2\Delta x) + 8f(x + \Delta x) - 8f(x - \Delta x) + f(x - 2\Delta x)}{12\Delta x} + O(\Delta x^4). \quad (4^{\text{th}}\text{-order centered difference})$$

#### Formulas for the second derivatives:

$$f''(x) = \frac{f(x + 2\Delta x) - 2f(x + \Delta x) + f(x)}{\Delta x^2} + O(\Delta x), \quad (\text{forward difference})$$

$$f''(x) = \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} + O(\Delta x^2), \quad (2^{\text{nd}}\text{-order centered difference})$$

$$f''(x) = \frac{-f(x + 3\Delta x) + 4f(x + 2\Delta x) - 5f(x + \Delta x) + 2f(x)}{\Delta x^2} + O(\Delta x^2),$$

$$f''(x) = \frac{-f(x + 2\Delta x) + 16f(x + \Delta x) - 30f(x) + 16f(x - \Delta x) - f(x - 2\Delta x)}{12\Delta x^2} + O(\Delta x^4). \quad (4^{\text{th}}\text{-order centered difference})$$

#### Formulas for the third derivatives:

$$f'''(x) = \frac{f(x + 3\Delta x) - 3f(x + 2\Delta x) + 3f(x + \Delta x) - f(x)}{\Delta x^3} + O(\Delta x),$$

$$f'''(x) = \frac{f(x + 2\Delta x) - 2f(x + \Delta x) + 2f(x - \Delta x) - f(x - 2\Delta x)}{2\Delta x^3} + O(\Delta x^2).$$

(averaged differences)

#### Formulas for the fourth derivatives:

$$f^{iv}(x) = \frac{f(x + 4\Delta x) - 4f(x + 3\Delta x) + 6f(x + 2\Delta x) - 4f(x + \Delta x) + f(x)}{\Delta x^4} + O(\Delta x),$$

$$f^{iv}(x) = \frac{f(x + 2\Delta x) - 4f(x + \Delta x) + 6f(x) - 4f(x - \Delta x) + f(x - 2\Delta x)}{\Delta x^4} + O(\Delta x^2).$$

(centered difference)

