Meteorology

Lecture 11

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Properties of numerical methods

The following criteria are crucial to the performance of a numerical algorithm:

1. Consistency: The discretization of a PDE should become exact as the mesh size tends to zero (truncation error should vanish)

2. Stability: Numerical errors which are generated during the solution of discretized equations should not be magnified

3. Convergence: The numerical solution should approach the exact solution of the PDE and converge to it as the mesh size tends to zero

4. Conservation: Underlying conservation laws should be respected at the discrete level (artificial sources/sinks are to be avoided)

5. Boundedness: Quantities like densities, temperatures, concentrations etc. should remain nonnegative and free of spurious wiggles

These properties must be verified for each (component of the) numerical scheme

Effects of the numerical approximations

This section focusses on the important subject of how the numerical methods that are employed to integrate the equations can affect the model solution in various ways.

The discussion of truncation error shows how the derivatives in the equations are incorrectly estimated by finite-difference approximations.

Truncation error

Because the equations that govern atmospheric processes are differential equations, with derivatives in most of the terms, approximating the continuous space and time derivatives with finite-difference expressions represents a considerable potential source of error in the modeling process.

The following polynomial is called *Taylor's series*, where *f* is any meteorological variable in the derivative terms of basic Equations, and the series can be written for any independent variable:

$$f(x) = f(a) + (x-a)\frac{\partial f(a)}{\partial x} + \frac{(x-a)^2}{2!}\frac{\partial^2 f(a)}{\partial x^2} + \frac{(x-a)^3}{3!}\frac{\partial^3 f(a)}{\partial x^3} + \cdots + \frac{(x-a)^n}{n!}\frac{\partial^n f(a)}{\partial x^n} + R(n,x)$$

It states that the value of a function, *f*, at any point, *x*, can be approximated by using the known value and derivatives at point *a*.

In the case of an infinite series, the expression would be exact.

For a series truncated at *n* terms, there is a residual, *R*, that defines the error.

The truncation error will be defined here for three finite-difference approximations to the derivative: two-point, three-point, and five-point formulae.

For a two-point approximation, let $x = a + \Delta x$ in top Eq. , truncate the series by dropping second-order and higher terms, and solve for the derivative, to obtain the following:

$$\frac{\partial f(a)}{\partial x} = \frac{f(a+\Delta x) - f(a)}{\Delta x}$$

$$\frac{\partial f(a)}{\partial x} = \frac{f(a+\Delta x) - f(a)}{\Delta x}$$

This is called the forward-in-space differencing formula, which has first-order accuracy because second-order and higher terms in Taylor's series were dropped.

An analogous backward-in-space formula results from letting x = a - Δx

A three-point differencing scheme can be obtained by writing Taylor's series as

$$f(a+\Delta x) = f(a) + \Delta x\frac{\partial f(a)}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 f(a)}{\partial x^2} + \frac{(\Delta x)^3}{3!}\frac{\partial^3 f(a)}{\partial x^3} + \cdots$$

and

$$f(a-\Delta x) = f(a) - \Delta x\frac{\partial f(a)}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 f(a)}{\partial x^2} - \frac{(\Delta x)^3}{3!}\frac{\partial^3 f(a)}{\partial x^3} + \cdots$$

Subtracting the two series produces

$$f(a+\Delta x) - f(a-\Delta x) = 2\Delta x\frac{\partial f(a)}{\partial x} + \frac{2(\Delta x)^3}{3!}\frac{\partial^3 f(a)}{\partial x^3} + \cdots$$

Solving for $\frac{\partial f(a)}{\partial x}$ provides

$$\frac{\partial f(a)}{\partial x} = \frac{f(a+\Delta x) - f(a-\Delta x)}{2\Delta x} - \frac{(\Delta x)^2}{3!}\frac{\partial^3 f(a)}{\partial x^3} + \cdots$$

Truncating this equation after the first term on the right produces the following approximation, which we say has second-order accuracy because we ignore the third-order and higher terms in the series.

This is called a three-point approximation to the derivative because it spans points $x-\Delta x$, x , and $x+\Delta x$

$$\frac{\partial f(a)}{\partial x} = \frac{f(a+\Delta x) - f(a-\Delta x)}{2\Delta x}$$

One way of calculating the effect of truncating the series on the accuracy of the derivative is to compare the value of the derivative from this approximation with the exact value.

Let $f = A\cos kx$, Where $k=2\pi/L$ and and L is the wavelength

$$\frac{\partial f}{\partial x} = -kA\sin kx,$$

where the approximation is

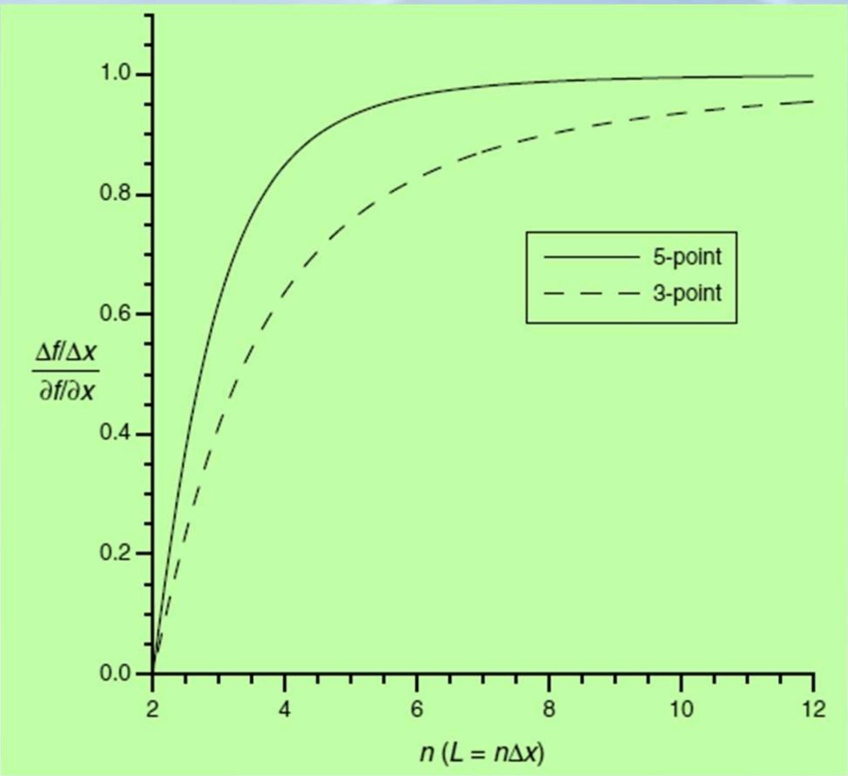
$$\frac{\Delta f}{\Delta x} = \frac{A\cos k(x+\Delta x) - A\cos k(x-\Delta x)}{2\Delta x}$$

Using trigonometric identities it can be shown that

$$\frac{\frac{\Delta f}{\Delta x}}{\frac{\partial f}{\partial x}} = \frac{\sin k\Delta x}{k\Delta x},$$

where, as $\Delta x/L \to 0$, $k\Delta x \to 0$ and $\sin k\Delta x \to k\Delta x$.

That is, as the argument of the sine function approaches zero, so does the function itself, and the ratio approaches unity.



$$\sin\alpha\sin\beta = \frac{1}{2}\left[\cos(\alpha-\beta)-\cos(\alpha+\beta)\right]$$

Taylor's series can also be used to estimate the truncation error for a five-point approximations to the derivative. For example, add Eqs. In page 13 and solve for the second derivative to obtain

$$\frac{\partial^2 f(a)}{\partial x^2} = \frac{f(a+\Delta x) + f(a-\Delta x) - 2f(a)}{(\Delta x)^2} + \cdots$$

A third derivative can then be defined as

$$\frac{\partial^3 f(a)}{\partial x^3} = \frac{\dfrac{\partial^2 f(a+\Delta x)}{\partial x^2} - \dfrac{\partial^2 f(a-\Delta x)}{\partial x^2}}{2\Delta x}$$

Using the above expression for the second derivative,

$$\frac{\partial^3 f(a)}{\partial x^3} = \frac{\dfrac{f(a+2\Delta x) + f(a) - 2f(a+\Delta x)}{(\Delta x)^2} - \dfrac{f(a) + f(a-2\Delta x) - 2f(a-\Delta x)}{(\Delta x)^2}}{2\Delta x},$$

and simplifying yields

$$\frac{\partial^3 f(a)}{\partial x^3} = \frac{f(a+2\Delta x) - f(a-2\Delta x) - 2f(a+\Delta x) + 2f(a-\Delta x)}{2(\Delta x)^3}$$

Substituting this expression for the third derivative into Eq.

$$\frac{\partial f(a)}{\partial x} = \frac{f(a+\Delta x) - f(a-\Delta x)}{2\Delta x} - \frac{(\Delta x)^2}{3!}\frac{\partial^3 f(a)}{\partial x^3} + \cdots$$

and simplifying produces the following expression, which is a five-point approximation to the derivative:

$$\frac{\partial f(a)}{\partial x} = \frac{1}{2\Delta x}\left[\frac{4}{3}(f(a+\Delta x) - f(a-\Delta x)) - \frac{1}{6}(f(a+2\Delta x) - f(a-2\Delta x))\right]$$

Linear stability, and damping properties

The term *stability* in the context of atmospheric modeling is related to whether the amplitudes of waves in the numerical solution to Eqs. 2.1–2.7, or some other equation set that is the basis for a model, grow exponentially for numerical (i.e., nonphysical) reasons, quickly causing floating-point-overflow conditions that halt the integration of the equations.

Each term in Eqs. 2.1–2.7 contributes to the stability of the numerical solution of its respective equation, but the advection terms are often the most problematic.

It is fortunate that the condition for stability of the linear advection equation is about the same as that of the nonlinear advection equation, allowing us to analytically calculate a useful stability criterion with the linear term.

Linear stability of an advection term

The following linear equation will be used as the basis for our analysis of the stability of the advection equation.

Assume that h is a meteorological variable such as the height of a pressure surface or the depth of a shallow fluid,

and that U is a mean wind speed.

This notation indicates that the terms apply at grid point j on the x axis and at time step

$$\left.\frac{\partial h}{\partial t}\right|_j^{\tau} = -U\left.\frac{\partial h}{\partial x}\right|_j^{\tau}$$

Assume harmonic solutions to this equation of the following form, $h = \hat{h}e^{i(kx - \omega t)}$,

$$k = 2\pi / L \quad , \quad \omega = Uk$$

Now assume that ω is complex $\omega + \omega_R = i\omega_I$

The implication of this can be seen by substitution into Eq. $h = \hat{h}e^{i(kx-\omega t)}$,

$$h = \hat{h}e^{\omega_I t}e^{i(kx-\omega_R t)}$$

The assumption of a complex frequency has allowed for a wave-amplitude variation with time,

positive ω_I is associated with exponential wave growth as time (t) increases,

negative ω_I is associated with wave damping

$\omega_I = 0$ means that the amplitude remains constant at $\hat{h}$

The value of ω_I will determine which of these situations prevails, where wave growth is associated with an unstable model solution.

The second exponential defines the phase of the wave in the x direction.

For instructional purposes, we will first analyze the stability of the advection equation using forward differencing for the time derivative and backward differencing for the space derivative.

The finite-difference expression is

$$\frac{h_j^{\tau+1} - h_j^{\tau}}{\Delta t} = -U\frac{h_j^{\tau} - h_{j-1}^{\tau}}{\Delta x},$$

or

$$h_j^{\tau+1} - h_j^{\tau} = -\frac{U\Delta t}{\Delta x}(h_j^{\tau} - h_{j-1}^{\tau}),$$

Where τ is the time-step number and j is the grid-point number.

Expressing the assumed form of the solution in Eq. $h = \hat{h}e^{\omega_I t}e^{i(kx - \omega_R t)}$

in finite-difference form by letting $x = j\Delta x$ and $t = \tau\Delta t$

produces

$$h_j^{\tau} = \hat{h}e^{\omega_I \tau\Delta t}e^{i(kj\Delta x - \omega_R \tau\Delta t)}$$

Substitute this form of the solution into the finite-difference expression Eq.

$$h_j^{\tau+1} - h_j^{\tau} = -\frac{U\Delta t}{\Delta x}(h_j^{\tau} - h_{j-1}^{\tau}),$$

producing

$$e^{\omega_I \Delta t} e^{-i\omega_R \Delta t} - 1 = -\frac{U\Delta t}{\Delta x}[1 - e^{ik\Delta x}]$$

Using Euler's relations

$$e^{ix} = \cos x + i\sin x$$

$$e^{-ix} = \cos x - i\sin x$$

$$e^{\omega_I \Delta t}(\cos\omega_R \Delta t - i\sin\omega_R \Delta t) = 1 + \frac{U\Delta t}{\Delta x}(\cos k\Delta x - 1 + i\sin k\Delta x)$$

In order to obtain information about whether the solution damps or amplifies, the complex equation is separated into its real and imaginary parts:

$$e^{\omega_I \Delta t}\cos\omega_R \Delta t = 1 + \frac{U\Delta t}{\Delta x}(\cos k\Delta x - 1),$$

$$e^{\omega_I \Delta t}\sin\omega_R \Delta t = -\frac{U\Delta t}{\Delta x}\sin k\Delta x.$$

Squaring both sides of each equation and adding them eliminates the real part of the frequency, leaving

$$e^{\omega_I \Delta t} = \sqrt{1 + 2\left(\frac{U\Delta t}{\Delta x}\right)(\cos k\Delta x - 1)\left(1 - \frac{U\Delta t}{\Delta x}\right)}. \quad *$$

Recall that Eq. shows that the value of this exponential in the assumed form of the model solution controls whether the solution increases or decreases in amplitude with increasing time. That is

$$e^{\omega_I t} = e^{\omega_I \tau \Delta t} = \left(e^{\omega_I \Delta t}\right)^{\tau},$$

so the value of the solution amplifies or damps exponentially as the time-step value τ increases with the model integration.

For this particular combination of space and time differencing schemes, Eq. * shows the dependence of the exponential on wavelength and the ratio $\frac{U\Delta t}{\Delta x}$.

Figure indicates that the model solution damps exponentially with time for $\frac{U\Delta t}{\Delta x} < 1$

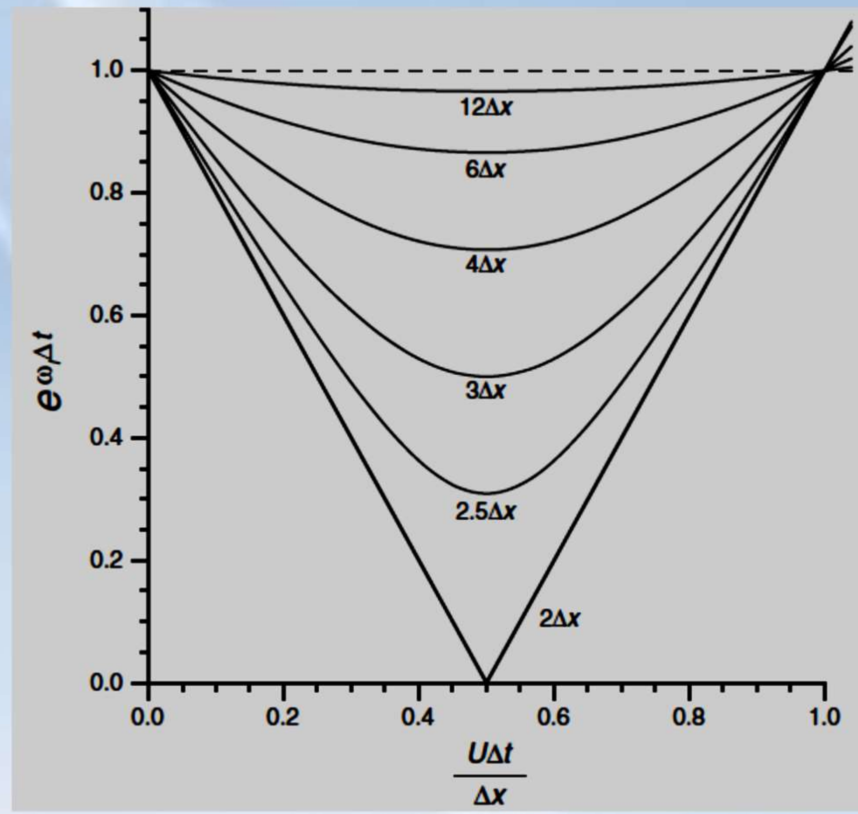
it does not change amplitude when this ratio is unity, and it amplifies exponentially for ratios greater than unity.

Shorter wavelengths are damped more severely than are longer wavelengths.

Thus, the stability criterion for this differencing scheme is $\frac{U\Delta t}{\Delta x} \leq 1$

The ratio $\frac{U\Delta t}{\Delta x}$ is the previously defined CFL condition.

It is also called the *Courant number*, and is described in Courant *et al*. (1928).



Fractional amplification or damping each time step, of different wavelengths for the forward-in-time, backward-inspace linear advection equation, as a function of the Courant number.

Dimensionless Number

The Courant-Friedrichs-Lewy number or CFL number, or Courant number $\frac{U \Delta t}{\Delta x} \leq 1$

It is the ratio of two velocities $\frac{U}{\Delta x / \Delta t}$

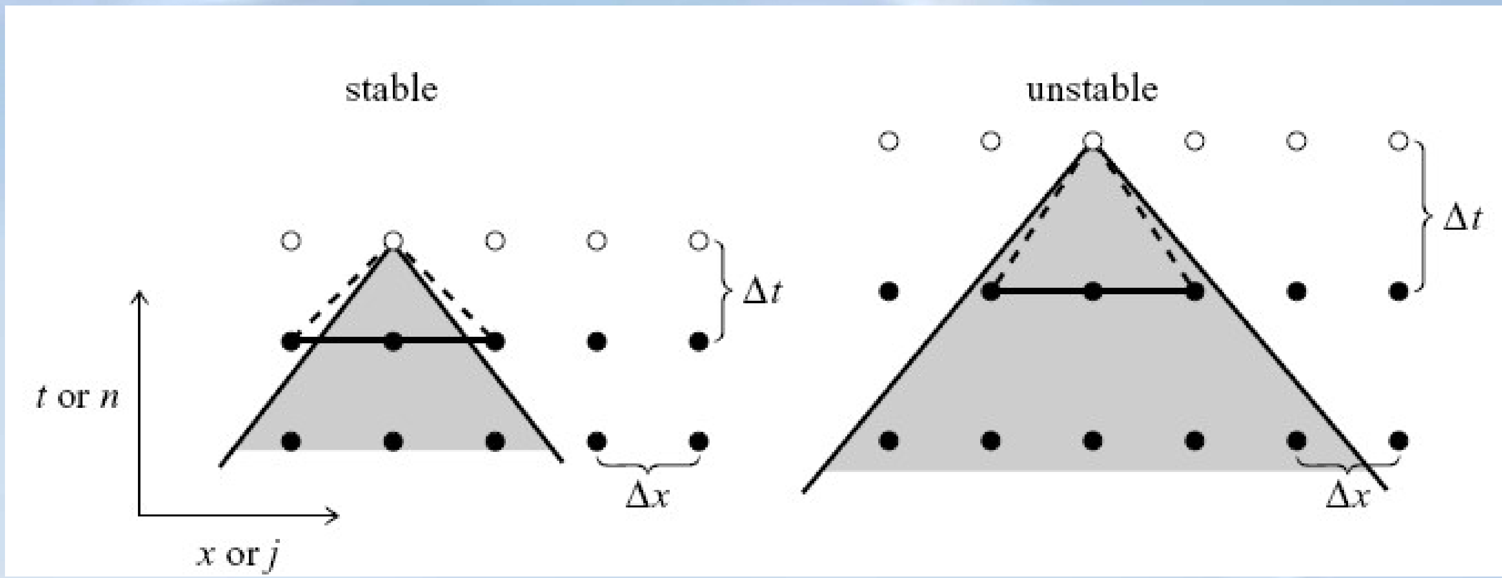
U is a mean wind speed or speed of PDE

$\Delta x / \Delta t$ speed of mesh

Famous stability condition in numerical mathematics
Valid for many physical applications

The Courant criterion, the smallest grid increment and the largest velocity determine the (global or local) time step of the simulation.

CFL-condition



Value at a certain point depends on information within some area (shaded) as defined by the PDE. (say advection speed v, wave velocity or speed of light.)

These physical points of dependency must be inside the computational used grid points for a stable method.

Thus, given the chosen grid increment, and the largest wave speed that is likely to exist anywhere on the grid during the forecast (U), the time step required for stability is chosen.

Note that such selective damping of short waves that are poorly resolved on a grid is sometimes considered to be an advantageous property of a differencing scheme.

A similar procedure can be used to analyze the stability criterion for the forward-in-time, centered-in-space advection equation

$$\frac{h_j^{\tau+1} - h_j^{\tau}}{\Delta t} = -U\frac{(h_{j+1}^{\tau} - h_{j-1}^{\tau})}{2\Delta x},$$

obtaining

$$e^{\omega_I \Delta t} = \sqrt{1 + \left(\frac{U\Delta t}{\Delta x}\right)^2 \sin^2 k\Delta x}$$

The only time step that will allow the exponential to be less than or equal to unity, and guarantee a stable solution, is zero.

Thus, this differencing scheme is absolutely unstable.

stability of the three-point

Now consider the stability of the three-point centered-in-space, centered-in-time, linear advection equation:

$$\frac{h_j^{\tau+1} - h_j^{\tau-1}}{2\Delta t} = -U\frac{(h_{j+1}^{\tau} - h_{j-1}^{\tau})}{2\Delta x}$$

From the assumed form of the solution in Eq. $h_j^{\tau} = \hat{h}e^{\omega_I \tau \Delta t} e^{i(kj\Delta x - \omega_R \tau \Delta t)}$ it is easy to obtain

$$h_{j+\beta}^{\tau} = e^{i\beta k \Delta x} h_j^{\tau}$$

and

$$h_j^{\tau+\upsilon} = e^{\omega_I \upsilon \Delta t} e^{-i\omega_R \upsilon \Delta t} h_j^{\tau}$$

$$h_j^{\tau+1} = h_j^{\tau-1} - \frac{U\Delta t}{\Delta x}(2i\sin k\Delta x)h_j^{\tau}$$

Defining $\alpha = (2U\Delta t/\Delta x)\sin k\Delta x$ produces

$h_j^{\tau+1} = h_j^{\tau-1} - i\alpha h_j^{\tau}$ and $h_j^{\tau+2} = h_j^{\tau} - i\alpha h_j^{\tau+1}$

$$h_j^{\tau+2} = (1-\alpha^2)h_j^{\tau} - i\alpha h_j^{\tau-1}$$

$$\begin{bmatrix} h_j^{\tau+1} \\ h_j^{\tau+2} \end{bmatrix} = \begin{bmatrix} 1 & -i\alpha \\ -i\alpha & 1-\alpha^2 \end{bmatrix} \begin{bmatrix} h_j^{\tau-1} \\ h_j^{\tau} \end{bmatrix}$$

$$h_j^{\tau+2} = \lambda h_j^{\tau},$$

where $\lambda = e^{2\omega_I \Delta t} e^{-i2\omega_R \Delta t}$

$$h_j^{\tau+1} = \lambda h_j^{\tau-1}$$

$$0 = (1-\lambda)h^{\tau-1} - i\alpha h_j^{\tau}$$

$$0 = (1-\alpha^2-\lambda)h_j^{\tau} - i\alpha h^{\tau-1}$$

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1-\lambda & -i\alpha \\ -i\alpha & 1-\alpha^2-\lambda \end{bmatrix} \begin{bmatrix} h^{\tau-1} \\ h_j^{\tau} \end{bmatrix}$$

$$\begin{vmatrix} 1-\lambda & -i\alpha \\ -i\alpha & 1-\alpha^2-\lambda \end{vmatrix} = 0$$

$$\lambda^2 + (\alpha^2 - 2)\lambda + 1 = 0.$$

$$\lambda = 1 - \frac{\alpha^2}{2} \pm \frac{\alpha}{2}\sqrt{\alpha^2 - 4}$$

$$|\lambda| = \left|1 - \frac{\alpha^2}{2} \pm \frac{\alpha}{2}\sqrt{\alpha^2 - 4}\right|$$

$$|\lambda| = \sqrt{|\lambda_R|^2 + |\lambda_I|^2}$$

Substituting the definition for a into the stability requirement leads to

$$\frac{U\Delta t}{\Delta x}\sin k\Delta x \le 1 ,$$

and because the sine can equal unity, the stability requirement is

$$\frac{U\Delta t}{\Delta x} \le 1$$

The stability requirement for the five-point

Using a similar approach, it can be shown that the stability requirement for the five-point centered-in-space (see Eq.),

$$\frac{\partial f(a)}{\partial x} = \frac{1}{2\Delta x}\left[\frac{4}{3}(f(a+\Delta x) - f(a-\Delta x)) - \frac{1}{6}(f(a+2\Delta x) - f(a-2\Delta x))\right]$$

and centered-in-time, linear advection equation

$$\frac{h_j^{\tau+1} - h_j^{\tau-1}}{2\Delta t} = -U\frac{\frac{4}{3}(h_{j+1}^{\tau} - h_{j-1}^{\tau}) - \frac{1}{6}(h_{j+2}^{\tau} - h_{j-2}^{\tau})}{2\Delta x}$$

$$U\Delta t/\Delta x \le 0.73 .$$

Advection-Diffusion Equation

For incompressible flow with constant viscosity, the momentum equation in the Navier–Stokes equations can be written in Cartesian coordinates.

The advective term here is nonlinear and requires special care in numerical calculation.

The diffusive term smoothes out the velocity profile and provides a stabilizing effect in numerical computations.

The pressure gradient term represents forcing on a fluid element induced by the spatial variation in pressure.

External forcing includes gravitational, electromagnetic, or fictitious forces (due to non-inertial reference frames).

Hence we in general consider a simplified model without the pressure gradient and external forcing terms in one dimension,

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2},$$

which is known as the *Burgers' equation*

We can further consider the linear approximation of the above equation with constant advective speed $c\ (\geq 0)$ and diffusivity $a\ (\geq 0)$ to obtain the linear advection-diffusion equation.

$$\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = a\frac{\partial^2 f}{\partial x^2}$$

When each of the terms is removed from the advection-diffusion equation, the resulting equations have different characteristic properties.

When we set $a = 0$, we obtain the advection equation

$$\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = 0,$$

which is hyperbolic. When we set $c = 0$, we have the diffusion equation

$$\frac{\partial f}{\partial t} = a\frac{\partial^2 f}{\partial x^2},$$

which is parabolic.

Finally, if $\partial f/\partial t = 0$, we find the steady advection-diffusion equation

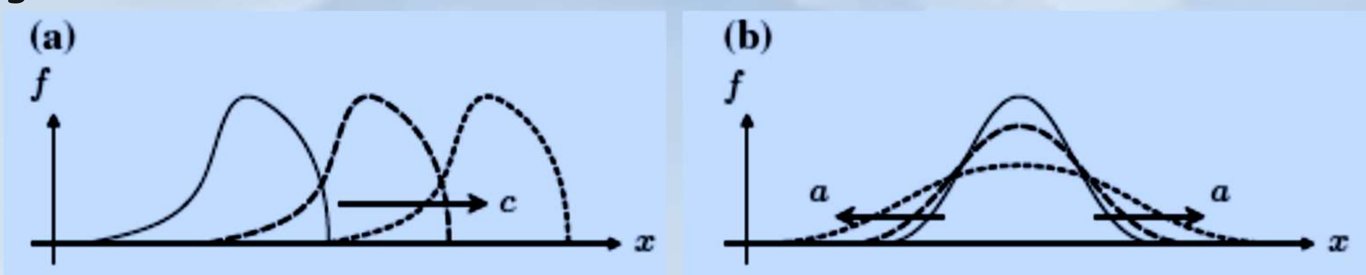
$$c\frac{\partial f}{\partial x} = a\frac{\partial^2 f}{\partial x^2},$$

which is elliptic.

In other words, the advective-diffusion equation as well as the Navier–Stokes equations consist of the combination of these three types of partial differential equations. Properties from one of the models may become more dominant than the others depending on the flow condition.

Solutions for one-dimensional constant coefficient advection and diffusion equations are presented in Fig.

$$\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = 0,$$



$$\frac{\partial f}{\partial t} = a\frac{\partial^2 f}{\partial x^2},$$

Behavior of the solutions to the advection and diffusion equations.
a Advection. **b** Diffusion

Solutions for one-dimensional constant coefficient advection and diffusion equations are presented in Fig. Since $f(x, t) = f(x - ct, 0)$ satisfies the advection equatio. we observe that the solution keeps the initial profile while translating in the x-direction with speed c.

For the diffusion equation, Eq.the solution decreases $(\partial f/\partial t < 0)$ where the solution profile is convex $(\partial^2 f/\partial x^2 < 0)$ and increases $(\partial f/\partial t > 0)$ where the profile is concave $(\partial^2 f/\partial x^2 > 0)$, smoothing out the solution profile over time.