- Consistency and Accuracy

- Stability

- Convergence

Consistency

- A discretization scheme is called "consistent" if the truncation error goes to zero as the grid size becomes smaller. With reduced grid size (both time and space co-ordinates), the "original PDE" is recovered for a consistent scheme

- **Consistency** is also a property of the discretization scheme: e.g.

    - truncation errors are proportional to $\Delta x/\Delta t$ (inconsistent scheme)

    - can be investigated by looking at the modified equation

The MODIFIED EQUATION is obtained by substituting the expression for the finite difference approximations, including the error terms, into the finite difference equation. For a CONSISTENT finite difference approximation the error terms go to zero as $h \to 0$ and $\Delta t \to 0$.

The modified equation can often be used to infer the nature of the error of the finite difference scheme. More about that later.

Consistency

- Consider advection diffusion equation in 1D. Find the modified equation.

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

- Consider forward Euler in time and central differencing in space

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U\frac{f_{j+1}^n - f_{j-1}^n}{2h} = D\frac{f_{j+1}^n - 2f_j^n + f_{j-1}^n}{h^2}$$

- Discrepancy between the two can be found by deriving a modified equation

Consistency

- Expand the terms using Taylor series

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} = \frac{\partial f(t)}{\partial t} + \frac{\partial^2 f(t)}{\partial t^2}\frac{\Delta t}{2} + \cdots$$

$$\frac{f_{j+1}^n - f_{j-1}^n}{2h} = \frac{\partial f(x)}{\partial x} + \frac{\partial^3 f(x)}{\partial x^3}\frac{h^2}{6} + \cdots$$

$$\frac{f_{j+1}^n - 2f_j^n + f_{j-1}^n}{h^2} = \frac{\partial^2 f(x)}{\partial x^2} + \frac{\partial^4 f(x)}{\partial x^4}\frac{h^2}{12} + \cdots$$

- Substitute into the finite difference approximation

Consistency

- Results in

$$\underbrace{\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} - D\frac{\partial^2 f}{\partial x^2}}_{\text{Original Equation}} = \underbrace{-\frac{\partial^2 f(t)}{\partial t^2}\frac{\Delta t}{2} - U\frac{\partial^3 f(x)}{\partial x^3}\frac{h^2}{6} + D\frac{\partial^4 f(x)}{\partial x^4}\frac{h^2}{12} + \cdots}_{\text{Error terms}}$$

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} - D\frac{\partial^2 f}{\partial x^2} = O(\Delta t, h^2)$$

In this case, the error goes to zero as $h \to 0$ and $\Delta t \to 0$, so the approximation is said to be CONSISTENT

Consistency

- Although most finite difference approximations are consistent, simple, naive modifications can lead to inconsistency!

- Dufort-Frankel Scheme

Solve the diffusion equation

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

Using the Leapfrog time integration method and standard finite-difference approximation for the spatial derivative gives:

$$\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} = \frac{D}{h^2}\left[f_{j+1}^n - 2f_j^n + f_{j-1}^n\right]$$

Leapfrog method

Consistency

Solve the diffusion equation

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

Using the Leapfrog time integration method and standard finite-difference approximation for the spatial derivative gives:

$$\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} = \frac{D}{h^2}\left[f_{j+1}^n - 2f_j^n + f_{j-1}^n\right]$$

Leapfrog method

- Formally second order in space and time
- Explicit!
- But, unconditionally unstable.

Consistency

- Slightly modify the scheme

$$\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} = \frac{D}{h^2}\left[f_{j+1}^n - 2f_j^n + f_{j-1}^n\right]$$

Replace by: $f_j^n = \frac{1}{2}\left(f_j^{n+1} + f_j^{n-1}\right)$

- How does this modification change the order of accuracy of the scheme?

$$f_j^{n+1} = f_j^{n-1} + 2\frac{\Delta t\, D}{h^2}\left(f_{j+1}^n - f_j^{n+1} - f_j^{n-1} + f_{j-1}^n\right).$$

- Can show that this is unconditionally stable!

Consistency

- But, let's look at the modified equation

$$\frac{\partial f}{\partial t} - D\frac{\partial^2 f}{\partial x^2} = -\frac{\Delta t^2}{6}\frac{\partial^3 f}{\partial t^3} + \frac{Dh^2}{12}\frac{\partial^4 f}{\partial x^4} - \frac{D\Delta t^2}{h^2}\frac{\partial^2 f}{\partial t^2} - \frac{D\Delta t^4}{12h^2}\frac{\partial^4 f}{\partial x^4} + \cdots$$

- **Inconsistent as we do not recover the original PDE as h and Δt tend to 0.**

- **It is thus critical to examine the consistency of the scheme. Even small/innocent changes to original method can lead to inconsistent methods.**

Accuracy

- Both finite difference and finite volume methods yield an algebraic set of equations in the format $\mathbf{A}\underline{x} = \underline{b}$ which needs to be solved using some martix inversion technique

- **Order of accuracy**

    - in Finite Difference scheme is based on the Taylor Series truncation

    - in Finite Volume it is based on the profile assumption

    - Order of accuracy is based on the “power of the grid size” in the leading-order truncation term. It is simply the property of the discretization scheme

    - when more than one method of discretization is involved, the order of accuracy is given by the “lowest order” representation of a term.

Stability

- **Property of the path to solution**

- **Appears in two places**

    - **Stability of iterative schemes**

        - An iterative scheme is called unstable if it fails to produce solution to the discrete set of equations

        - Depends on the characteristics of the coefficient matrix, errors per iteration may either be damped or grow

    - **Stability of numerical scheme for unsteady problems**

        - a scheme used for time-depended problems is “unstable” if the solution grows unbounded

        - “**unconditionally unstable**” (for any parameters of grid size and time-steps solution grows unbounded)

        - “**conditionally stable**” (solution is stable for a specific set of grid sizes and times steps)

        - “**unconditionally stable**” (solution stable for any parameters)

        - von-Neumann **Linear** stability analysis (gives some indications even for non-linear problems)

Stability of Iterative Methods

- **Scarborough Criterion** to obtain converged solution of an iterative scheme

For the finite-difference approximation of the type

$$a_P \phi_P = \sum a_{\mathrm{nbr}} \phi_{\mathrm{nbr}} + b_P$$

A sufficient condition for convergence is :

$$\frac{\sum |a_{\mathrm{nbr}}|}{|a_P|} \begin{cases} \leq 1 & \text{for all equations} \\ < 1 & \text{for at least one equation} \end{cases}$$

Coefficient Matrix Must be Diagonally Dominant

Scarborough for Point-Jacobi

- **Starting with iteration k=0 and some initial guess**

$$a_P \phi_P^{(k+1)} = \sum_{\text{nbr}} a_{\text{nbr}} \phi_{\text{nbr}}^{(k)} + b_P \qquad => \qquad \phi_P^{(k+1)} = \frac{\sum a_{\text{nbr}} \phi_{\text{nbr}}^{(k)} + b_P}{a_P}$$

Example

$$\begin{aligned} T_1 &= 0.4 T_2 + 0.2 \\ T_2 &= T_1 + 1 \end{aligned}$$

$$\begin{aligned} T_1^{(k+1)} &= 0.4 T_2^{(k)} + 0.2 \\ T_2^{(k+1)} &= T_1^{(k)} + 1 \end{aligned}$$

Scarborough Satisfied?

Iteration #	0	1	2	3	4	5	6	7
T_1	0	0.2	0.6	0.68	0.84	0.872	0.936	
T_2	0	1	1.2	1.6	1.68	1.84	1.872	

Scarborough for Gauss-Seidel

$$a_P \phi_P = \sum a_{\mathrm{nbr}} \phi_{\mathrm{nbr}} + b_P$$

Example (same as before, but equations rearranged)

$$\begin{aligned} T_1 &= T_2 - 1 \\ T_2 &= 2.5 T_1 - 0.5 \end{aligned}$$

Scarborough Satisfied?

Iteration #	0	1	2	3	4	5	6	7
T_1	0	-1	-4	-11.5	-30.25	..		
T_2	0	-3	-10.5	-29.25	-76.13	..		

Formal Stability Analysis

• Generally a formal stability analysis of a non-linear differential equation is highly involved and not practical. Instead, we use a simplified model problem that is "linearized" and **study the linear stability** of that problem. For small perturbations, this analysis predicts the stability limits fairly accurately.

• What is involved in a stability analysis?

- we look at the behavior of the system when it is subject to a small perturbation (typically periodic in nature)

- if the solution to the perturbation remains bounded, we have a stable (at least condiotinally stable) scheme. If it grows unbounded it is unstable.

- A **linear advection-diffusion** equation is a good model problem for generalized conservation laws

Von-Neumann Stability Analysis

- Model problem

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

- Consider forward in time and central in space

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U\frac{f_{j+1}^n - f_{j-1}^n}{2h} = D\frac{f_{j+1}^n - 2f_j^n + f_{j-1}^n}{h^2}$$

- Look at evolution of a small perturbation in the form of a wave written in Fourier series

$$f_j^n = \varepsilon_j^n$$

$$\varepsilon_j^n = \varepsilon^n(x_j) = \sum_{k=-\infty}^{\infty} \varepsilon_k^n e^{ikx_j}$$

Superscript “n” is not raised to

Von-Neumann Stability Analysis

• Evolution of perturbation is governed by

$$\frac{\varepsilon_j^{n+1}-\varepsilon_j^n}{\Delta t}+U\frac{\varepsilon_{j+1}^n-\varepsilon_{j-1}^n}{2h}=D\frac{\varepsilon_{j+1}^n-2\varepsilon_j^n+\varepsilon_{j-1}^n}{h^2}$$

Substitute above

• Errors at different nodes

$$\varepsilon_j^n=\varepsilon^n e^{ikx_j}$$

$$\varepsilon_{j+1}^n=\varepsilon^n e^{ikx_{j+1}}=\varepsilon^n e^{ik(x_j+h)}=\varepsilon^n e^{ikx_j}e^{ikh}$$

$$\varepsilon_{j-1}^n=\varepsilon^n e^{ikx_{j-1}}=\varepsilon^n e^{ik(x_j-h)}=\varepsilon^n e^{ikx_j}e^{-ikh}$$

Recall:

$$e^{ikx}=\cos kx+i\sin kx$$

Von-Neumann Stability Analysis

- Evolution of perturbation is governed by

$$\frac{\varepsilon^{n+1}\cancel{e^{ikx_j}} - \varepsilon^{n}\cancel{e^{ikx_j}}}{\Delta t} + U\frac{\varepsilon^{n}}{2h}\left(e^{ikh}\cancel{e^{ikx_j}} - e^{-ikh}\cancel{e^{ikx_j}}\right) =$$

$$D\frac{\varepsilon^{n}}{h^{2}}\left(e^{ikh}\cancel{e^{ikx_j}} - 2\cancel{e^{ikx_j}} + e^{-ikh}\cancel{e^{ikx_j}}\right)$$

- Dividing by error at time n

$$\frac{\varepsilon^{n+1}}{\varepsilon^{n}} = 1 - \frac{U\Delta t}{2h}\left(e^{ikh} - e^{-ikh}\right) + \frac{D\Delta t}{h^{2}}\left(e^{ikh} - 2 + e^{-ikh}\right)$$

Amplification factor

Von-Neumann Stability Analysis

- Amplification factor

amplification factor

$$\frac{\varepsilon^{n+1}}{\varepsilon^{n}} = 1 - \frac{U\Delta t}{2h}\left(e^{ikh} - e^{-ikh}\right) + \frac{D\Delta t}{h^2}\left(e^{ikh} - 2 + e^{-ikh}\right)$$

$$= 1 - \frac{U\Delta t}{h} i \sin kh + \frac{D\Delta t}{h^2} 2(\cos kh - 1)$$

$$= 1 - 4\frac{D\Delta t}{h^2}\sin^2 k\frac{h}{2} - i\frac{U\Delta t}{h}\sin kh$$

- Stability Criterion

$$\left|\frac{\varepsilon^{n+1}}{\varepsilon^{n}}\right| \le 1$$

$$e^{ikh} + e^{-ikh} = 2\cos kh; \quad e^{ikh} - e^{-ikh} = i2\sin kh; \quad 2\sin^2\theta = 1 - \cos 2\theta$$

Von-Neumann Stability Analysis

- Pure diffusion (U=0)

$$\frac{\varepsilon^{n+1}}{\varepsilon^{n}} = 1 - 4\frac{D\Delta t}{h^2}\sin^2 k\frac{h}{2}$$

$$\sin^2() \le 1$$

$$-1 \le 1 - 4\frac{D\Delta t}{h^2} \le 1$$

$$\frac{D\Delta t}{h^2} \le \frac{1}{2}$$

Von-Neumann Stability Analysis

- Pure Advection (D=0)

$$\frac{\varepsilon^{n+1}}{\varepsilon^{n}} = 1 - i\frac{U\Delta t}{h}\sin kh$$

Absolute value is always larger than 1!

Unconditionally unstable in the limit of zero diffusion

Von-Neumann Stability Analysis

- General advection diffusion (1D): Analysis involved but can show

$$\frac{\Delta t D}{h^2} \le \frac{1}{2} \quad \text{and} \quad \frac{U^2 \Delta t}{D} \le 2$$

$$\varepsilon_{i,j}^{n} = \varepsilon^{n} e^{i(kx_i + ly_j)}$$

- For 2D

$$\frac{D\Delta t}{h^2} \le \frac{1}{4} \quad \text{and} \quad \frac{(|U| + |V|)^2 \Delta t}{D} \le 4$$

- For 3D

$$\frac{D\Delta t}{h^2} \le \frac{1}{6} \quad \text{and} \quad \frac{(|U| + |V| + |W|)^2 \Delta t}{D} \le 8$$

Stability of Numerical Scheme

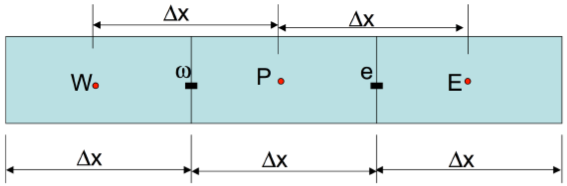
All numerical approaches lead to a set of simultaneous algebraic equations to be solved

$$a_P\phi_P = \sum a_{\text{nbr}}\phi_{\text{nbr}} + b_P$$

- value at P is influenced by immediate neighbors

$$\Gamma\frac{d^2\phi}{dx^2} + S = 0$$

$$\frac{2\Gamma_2}{(\Delta x)^2}\phi_2 = \frac{\Gamma_2}{(\Delta x)^2}\phi_1 + \frac{\Gamma_2}{(\Delta x)^2}\phi_3 + S_2$$



- If ϕ is temperature, and **let's assume there is no source (S = 0);** then temperature at P is influenced by temperature at E and W. Increase in temperature at W and E "should" increase temperature at "P". **This is possible in all cases, if the coefficients are "positive"** (or of same sign as a_p). Deviation from this may lead to unphysical or unstable behavior

Positivity of Coefficients

- General advection diffusion (1D): Analysis involved but can show

$$a_{\mathrm{P}}\phi_{\mathrm{P}} = \sum_{\mathrm{nbr}} a_{\mathrm{nbr}}\phi_{\mathrm{nbr}} + b_{\mathrm{P}}$$

$$f_j^{n+1} = (1 - 2\frac{\Delta t D}{h^2}) f_j^n + (\frac{D\Delta t}{h^2} - \frac{U\Delta t}{2h}) f_{j+1}^n + (\frac{D\Delta t}{h^2} + \frac{U\Delta t}{2h}) f_{j-1}^n$$

Neighbor in time

Convergence

- Used in two ways
  - **Convergence to mesh independent solution through mesh refinement study**
    - Can be measured by comparing the numerical solution to to true (exact) solution (if known)
    - Typically measured by comparing *the numerical solution on a certain grid resolution (in space and time) to the "finest" grid resolution* (assumed as true soln) for which solution is available (or obtained in a realistic time)
    - Rate of convergence is indicative of the accuracy of the discretization

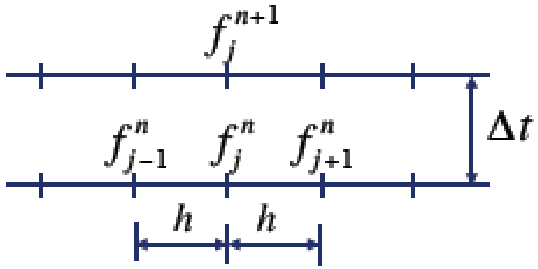
  - **Convergence of an iterative scheme used to invert the matrix A**
    - The iterative method convergences to a specified tolerance to obtain solution to the problem $\mathbf{A}\underline{x} = \underline{b}$
    - Rate of convergence related to the *magnitude of the eigenvalues of the inversion matrix (more on this later)*

Example: Error Quantification

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

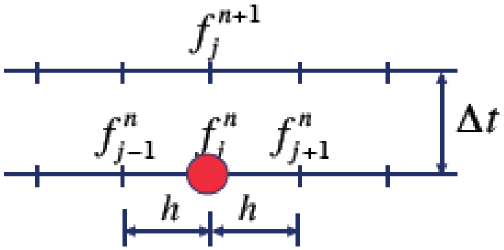
- Introduce notation for finite differencing

$$f_j^n = f(t, x_j)$$
$$f_j^{n+1} = f(t+\Delta t, x_j)$$
$$f_{j+1}^n = f(t, x_j + h)$$
$$f_{j-1}^n = f(t, x_j - h)$$



$$\left(\frac{\partial f}{\partial t}\right)_j^n + U\left(\frac{\partial f}{\partial x}\right)_j^n = D\left(\frac{\partial^2 f}{\partial x^2}\right)_j^n$$

- Evaluate the derivatives at a given point in the (x,t) domain i.e. *all terms in the equation should be computed at the same location*



Example: Error Quantification

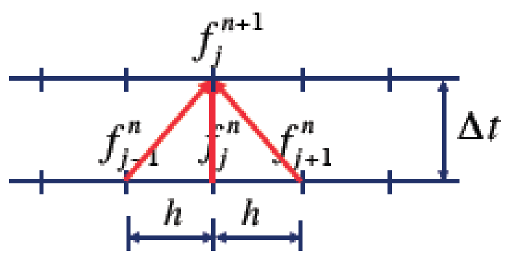
$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

gives

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U\frac{f_{j+1}^n - f_{j-1}^n}{2h} = D\frac{f_{j+1}^n - 2f_j^n + f_{j-1}^n}{h^2} + O(\Delta t, h^2)$$

Solving for the new value and dropping the error terms yields

$$f_j^{n+1} = f_j^n - \frac{U\Delta t}{2h}(f_{j+1}^n - f_{j-1}^n) + \frac{D\Delta t}{h^2}(f_{j+1}^n - 2f_j^n + f_{j-1}^n)$$



Example: Error Quantification

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = D\frac{\partial^2 f}{\partial x^2}$$

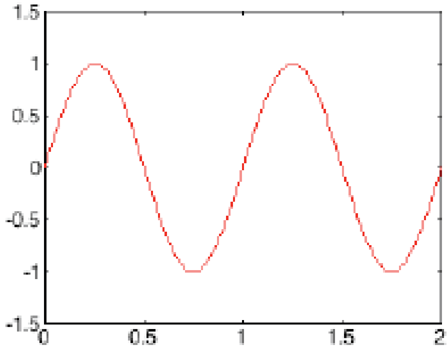
For initial conditions of the form:

$$f(x,t=0) = A\sin(2\pi kx)$$

It can be verified by direct substitution that the solution is given by:

$$f(x,t) = e^{-Dk^2 t}\sin(2\pi k(x-Ut))$$

which is a decaying traveling wave

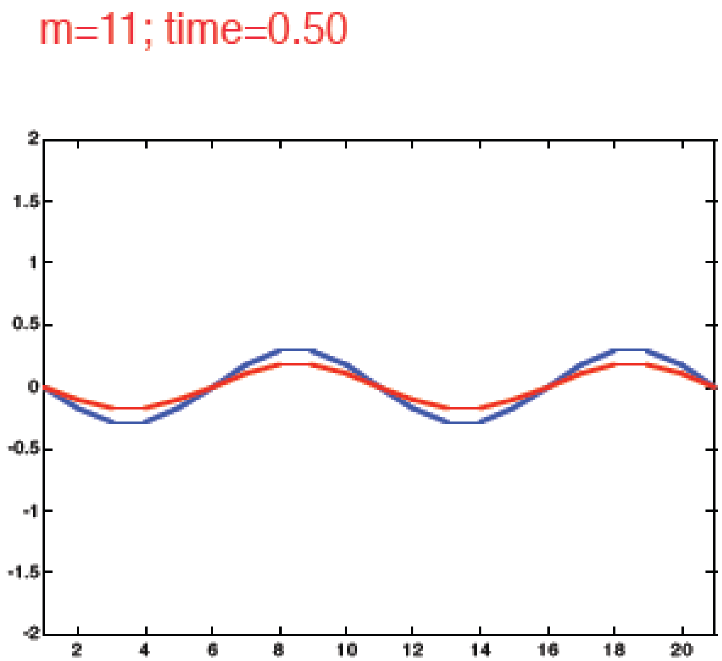


Example: Error Quantification

Evolution
for
U=1;
D=0.05;
k=1

N=21
Δt=0.05

Exact
Numerical

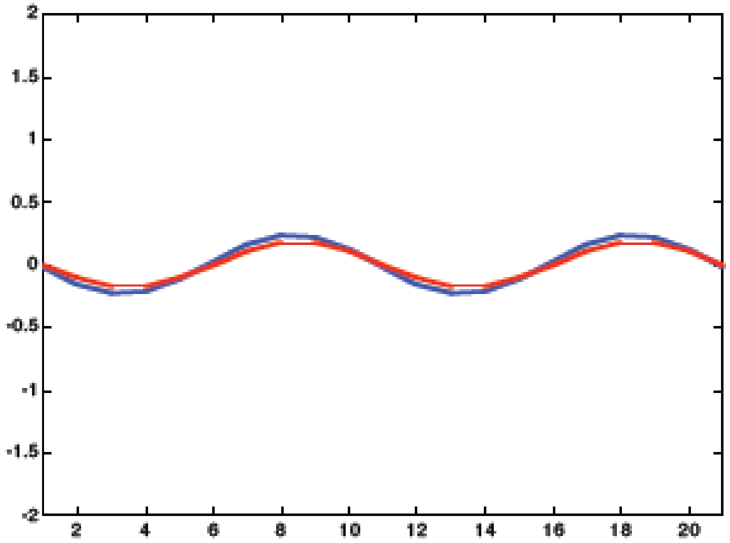


Example: Error Quantification

Repeat with a smaller time-step $\Delta t=0.025$

$N=21$

m=21; time=0.50



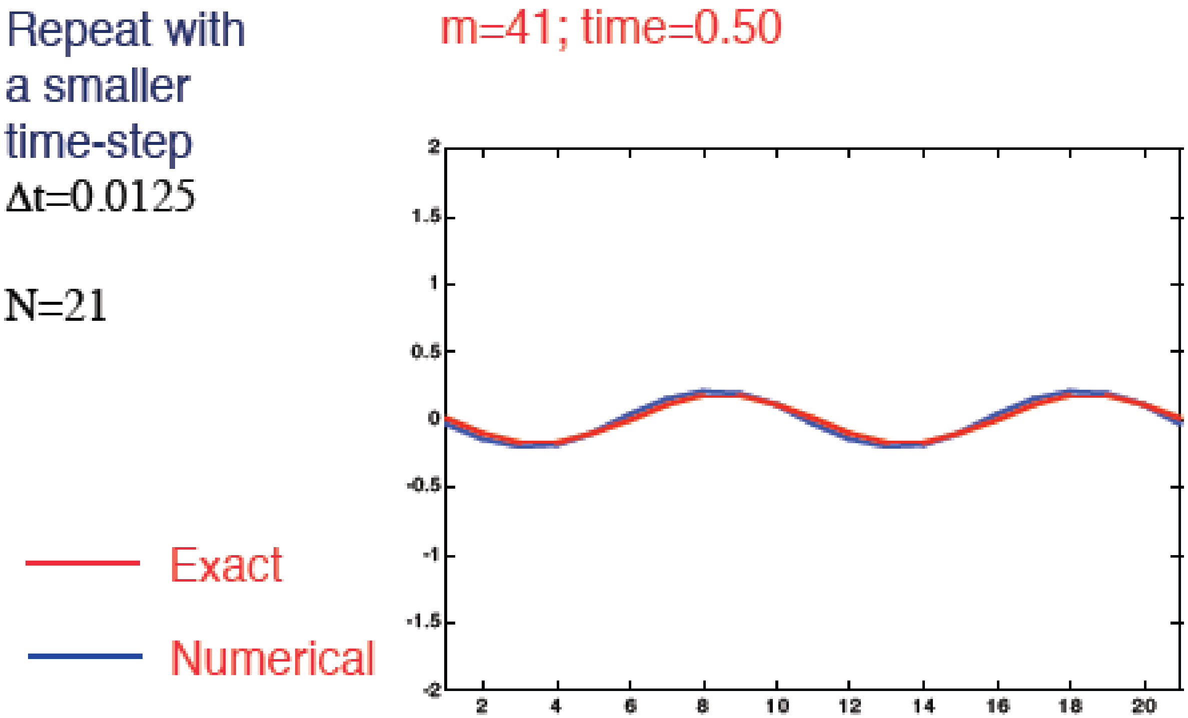
Exact

Numerical

Example: Error Quantification

Repeat with a smaller time-step Δt=0.0125

N=21

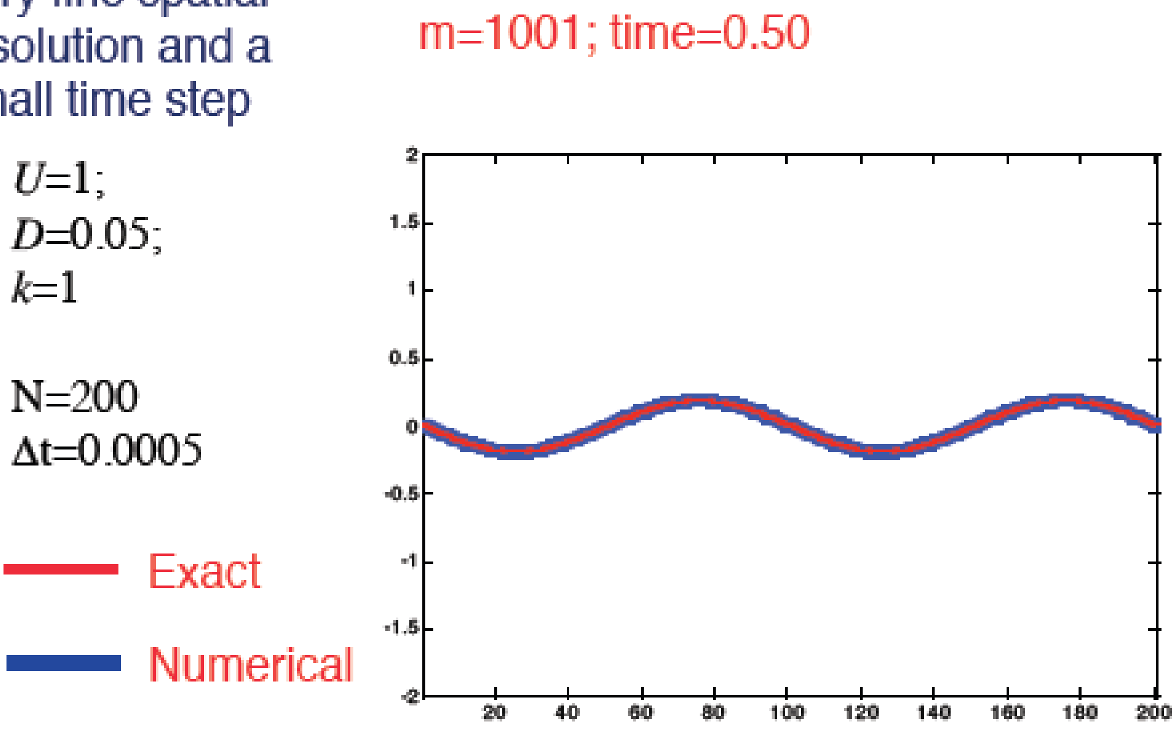


Example: Error Quantification

Very fine spatial resolution and a small time step

U=1;
D=0.05;
k=1

N=200
Δt=0.0005

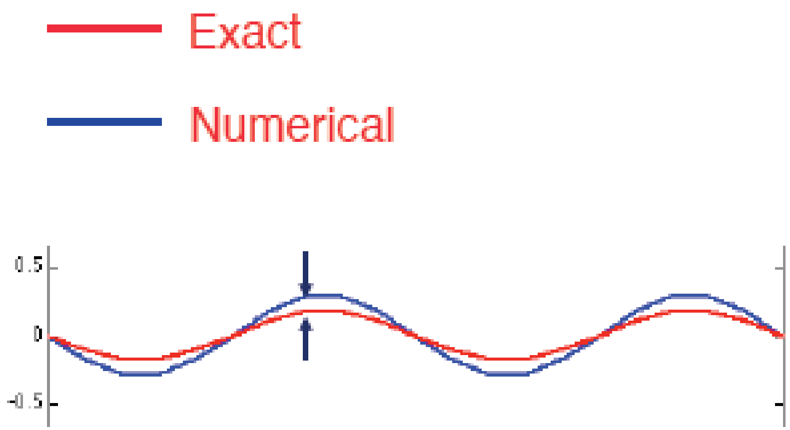


Example: Error Quantification

Examine the spatial accuracy by taking a very small time step, $\Delta t = 0.0005$ and vary the number of grid points, N, used to resolve the spatial direction.

The grid size is $h = L/N$ where $L = 1$ for our case

Example: Error Quantification



time=0.50

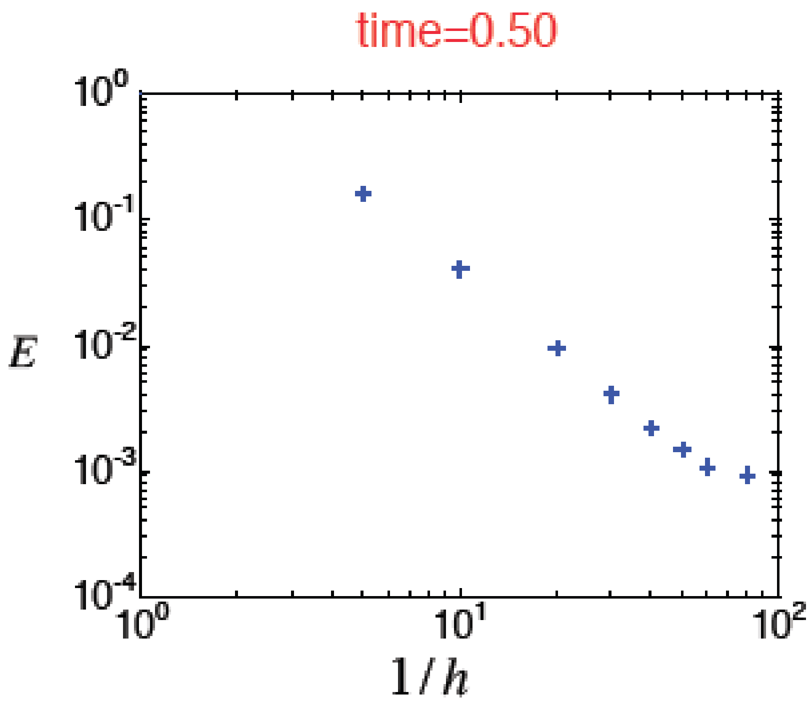
N=11;   E = 0.1633
N =21;   E = 0.0403
N =41;   E = 0.0096
N =61;   E = 0.0041
N =81;   E = 0.0022
N =101; E = 0.0015
N =121; E = 0.0011
N =161; E = 9.2600e-04

$$E = h\sqrt{\sum_{j=1}^{N}(f_j - f_{exact})^2}$$

Example: Error Quantification

Accuracy. Effect of spatial resolution

dt=0.0005
N=11 to N=161



Example: Error Quantification

If the error is of second order:

$$E = Ch^2 = C\left(\frac{1}{h}\right)^{-2}$$

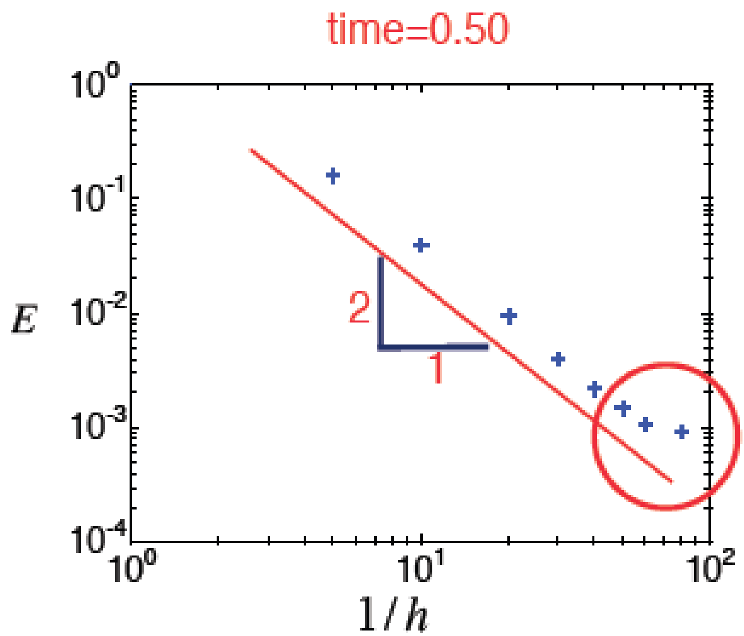
Taking the log:

$$\ln E = \ln\left(C\left(\frac{1}{h}\right)^{-2}\right) = \ln C - 2\ln\left(\frac{1}{h}\right)$$

Accuracy. Effect of spatial resolution

dt=0.0005

N=11 to N=161



Round off error

Convergence (Iterative Method)

All numerical methods lead to a discretized set of algebraic equations

$$\mathbf{A}\underline{\phi} = \underline{\mathrm{b}}$$

- **direct inversion of a matrix**

$$\underline{\phi} = \mathbf{A}^{-1}\underline{\mathrm{b}}$$

  - large storage (for N grid points must store NXN matrix)
  - direct inversion is order N^3 operation
  - For non-linear problems (or time-dependent problems), need inversion of matrix multiple times (every time-iteration)
  - Some smart implementations are sometimes feasible: Thomas Algorithm for tri-diagonal matrices

- **Iterative methods**
  - Solution can be obtained by order N operation! Use iterative methods
  - No need to store the entire matrix if it is a "sparse" matrix; take advantage of the banded nature

Convergence (Iterative Method)

For each point `P’ we have

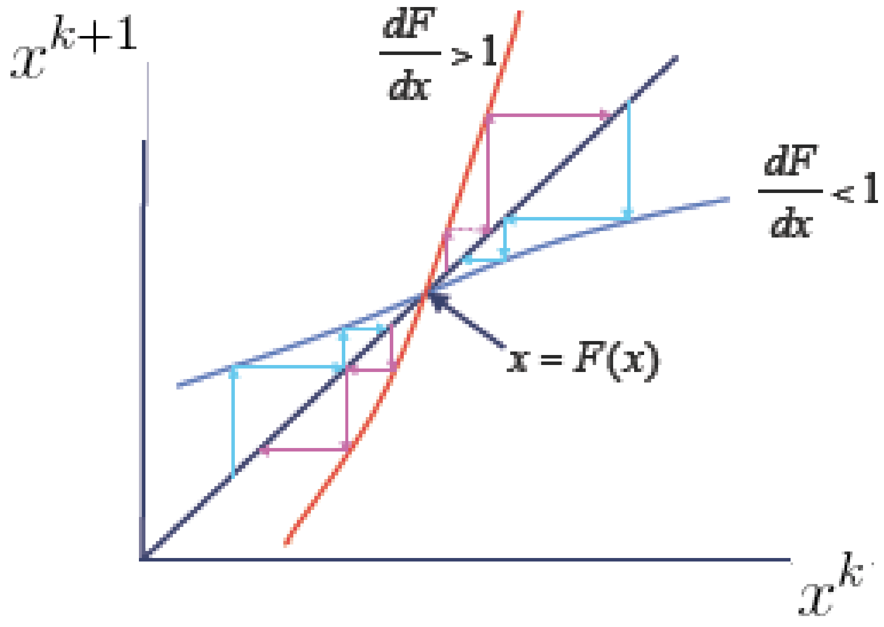
$$a_P \phi_P = \sum a_{\mathrm{nbr}} \phi_{\mathrm{nbr}} + b_P$$

- **Iterative methods**
    - Point-Jacobi
    - Gauss-Seidel
    - Successive Over Relaxation (SOR)
    - Conjugate Gradient (CG)
        - Preconditioned Conjugate Gradient (PCG)
        - Bi-Conjugate Gradient (BCG-STAB)
    - Multigrid Methods
    - Newton-Krylov methods

Concept Behind Iterative Scheme

$$x = F(x)$$

$$x^{k+1} = F(x^k)$$



Convergence Achieved When

$$x^{k+1} \approx x^k \quad \text{OR} \quad \left|\frac{x^{k+1}}{x^k} - 1\right| < \epsilon \quad \text{(small tolerance)}$$

Convergence possible only when $\dfrac{dF}{dx} < 1$

Concept Behind Iterative Scheme

One Dimensional Linear Problem:

$$x^{k+1} = ax^k + c; \qquad \text{For Convergence :} \quad |a| \leq 1$$

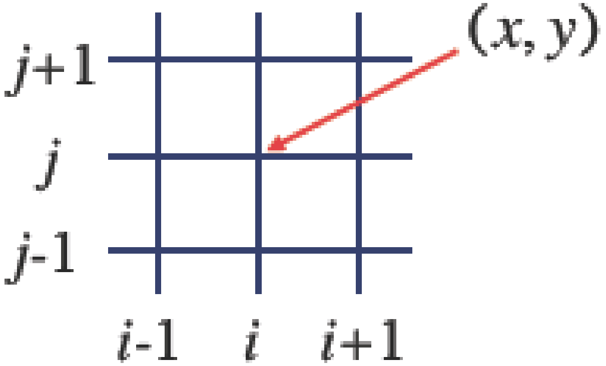
Multidimensional Linear Problem:

$$\underline{x}^{k+1} = \mathbf{M}\underline{x}^k + \underline{c}; \qquad \text{For Convergence?}$$

Spectral radius; maximum eigenvalue of the matrix

Iterative Scheme (Elliptical PDE)

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = S$$



Central differencing

$$\frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{\Delta x^2} + \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{\Delta y^2} = S_{i,j}$$

Let $\Delta x = \Delta y = h$

$$f_{i,j} = \frac{1}{4}\left[f_{i+1,j} + f_{i-1,j} + f_{i,j+1} + f_{i,j-1} - h^2 S_{i,j}\right]$$

Iterative Scheme (Elliptical PDE)

$$\text{Jacobi}: \quad f_{i,j}^{k+1} = \frac{1}{4}\left[f_{i+1,j}^{k} + f_{i-1,j}^{k} + f_{i,j+1}^{k} + f_{i,j-1}^{k} - h^2 S_{i,j}\right]$$

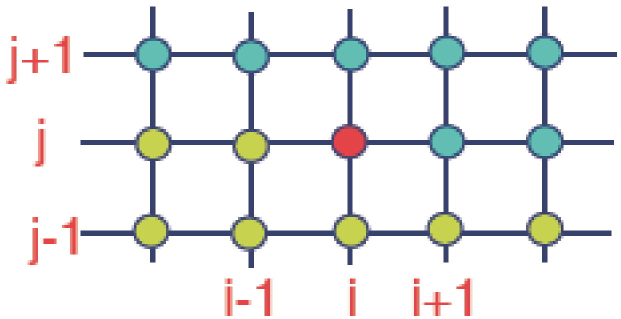
$$\text{Gauss} - \text{Seidel}: \quad f_{i,j}^{k+1} = \frac{1}{4}\left[f_{i+1,j}^{k} + f_{i-1,j}^{k+1} + f_{i,j+1}^{k} + f_{i,j-1}^{k+1} - h^2 S_{i,j}\right]$$

$$\text{SOR}: \quad f_{i,j}^{k+1} = \frac{\omega}{4}\left[f_{i+1,j}^{k} + f_{i-1,j}^{k+1} + f_{i,j+1}^{k} + f_{i,j-1}^{k+1} - h^2 S_{i,j}\right] + (1-\omega) f_{i,j}^{k}$$

$$\omega = 1: \quad \text{Gauss} - \text{Seidel}$$

$$1 < \omega < 2;$$

Gauss-Seidel




```
for j=1:m
for i=1:n
    iterate
end
end
```

$$\text{Gauss} - \text{Seidel}: \quad f_{i,j}^{k+1} = \frac{1}{4}\left[f_{i+1,j}^{k} + f_{i-1,j}^{k+1} + f_{i,j+1}^{k} + f_{i,j-1}^{k+1} - h^2 S_{i,j}\right]$$

- **Use the latest value of variable as soon as it is available**

- **for a left bottom to right top sweep, (i-1) and (j-1) values (yellow) are calculated when trying to solve for the (i,j) point (red point). Use the latest value**

- **programming wise, easier than the Point-Jacobi. For G-S, do not need to store the old values in an array for a simultaneous update at the end of iteration**

Iterative Schemes

At steady state, residual should be zero
(or smaller than a small tolerance value)

$$R_{i,j} = \frac{f_{i+1,j} + f_{i-1,j} + f_{i,j+1} + f_{i,j-1} - 4f_{i,j}}{h^2} - S_{i,j}$$

- **pointwise calculation of residual**
- **often simple criteria such as change from one iteration to next is used for convergence**

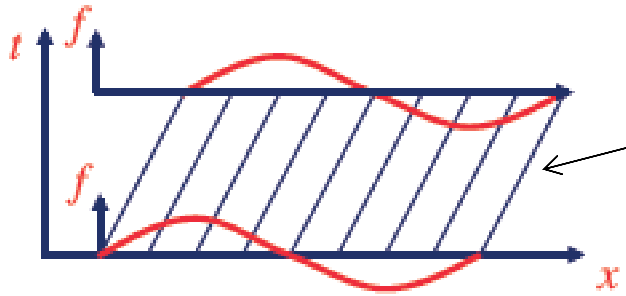
Hyperbolic Equation: Numerics

Hyperbolic Equation: Numerics

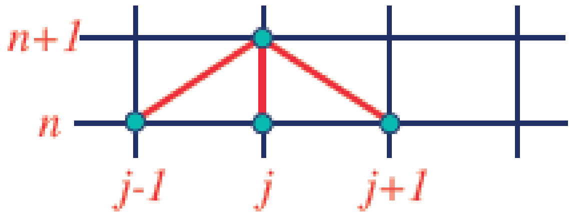
$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = 0$$

$$\frac{dx}{dt} = U; \quad \frac{df}{dt} = 0;$$

Characteristic lines in t-x plane



$$f_j^{n+1} = f_j^n - \frac{\Delta t}{2h}U(f_{j+1}^n - f_{j-1}^n)$$



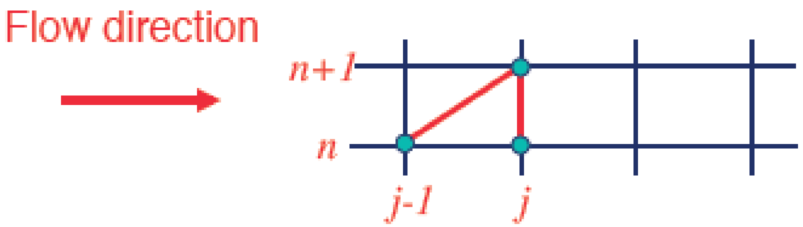
Naïve approach
Use von-Neumann analysis
To show unconditionally unstable

$$\frac{\varepsilon^{n+1}}{\varepsilon^n} = 1 - i\frac{U\Delta t}{2h}\sin kh$$

Hyperbolic Equation: Numerics

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

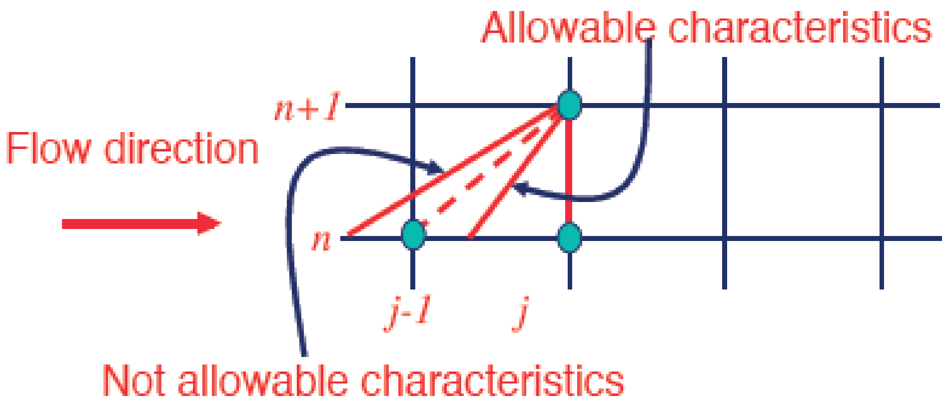
$$f_j^{n+1} = f_j^n - \frac{\Delta t}{h}U(f_j^n - f_{j-1}^n)$$



Upwind
Conditionally stable
The CFL (Courant Fredrichs Lewy number

$$\boxed{\frac{U\Delta t}{h} \le 1}$$

$$U\Delta t \le h$$



Signal has to travel
less than one grid
space in a time step

Modified Equation

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} + \frac{U}{h}(f_j^n - f_{j-1}^n) = 0$$

Convert the discrete equation, for say (x_j, t_n), into a continuous differential equation by using Taylor Series expansions around (x_j, t_n)

$$f_j^{n+1} = f_j^n + \frac{\partial f}{\partial t}\Delta t + \frac{\partial^2 f}{\partial t^2}\frac{\Delta t^2}{2} + \frac{\partial^3 f}{\partial t^3}\frac{\Delta t^3}{6} + \cdots$$

$$f_{j-1}^n = f_j^n - \frac{\partial f}{\partial x}h + \frac{\partial^2 f}{\partial x^2}\frac{h^2}{2} - \frac{\partial^3 f}{\partial x^3}\frac{h^3}{6} + \cdots$$

Modified Equation: Upwind

Substitute

$$\frac{1}{\Delta t}\left\{\left[\cancel{f_i^n}+\frac{\partial f}{\partial t}\Delta t+\frac{\partial^2 f}{\partial t^2}\frac{\Delta t^2}{2}+\frac{\partial^3 f}{\partial t^3}\frac{\Delta t^3}{6}+\cdots\right]-\cancel{f_i^n}\right\}$$

$$+\frac{U}{h}\left\{\cancel{f_i^n}-\left[\cancel{f_i^n}-\frac{\partial f}{\partial x}h+\frac{\partial^2 f}{\partial x^2}\frac{h^2}{2}-\frac{\partial^3 f}{\partial x^3}\frac{h^3}{6}+\cdots\right]\right\}=0$$

$$\frac{\partial f}{\partial t}+U\frac{\partial f}{\partial x}=-\frac{\Delta t}{2}f_{tt}+\frac{Uh}{2}f_{xx}-\frac{\Delta t^2}{6}f_{ttt}-\frac{Uh^2}{6}f_{xxx}+\cdots$$

First order in space and time

This is the modified equation

Consistency?

Modified Equation: Upwind

Express higher order time derivative terms into space derivative terms. Taking further derivatives in space and in time

$$f_{tt} + Uf_{xt} = -\frac{\Delta t}{2} f_{ttt} + \frac{Uh}{2} f_{xxt} - \frac{\Delta t^2}{6} f_{tttt} - \frac{Uh^2}{6} f_{xxxt} + \cdots$$

$$+ \quad -Uf_{tx} - U^2 f_{xx} = \frac{U\Delta t}{2} f_{ttx} - \frac{U^2 h}{2} f_{xxx} + \frac{U\Delta t^2}{6} f_{tttx} + \frac{U^2 h^2}{6} f_{xxxx} + \cdots$$

$$f_{tt} = U^2 f_{xx} + \Delta t\left(\frac{-f_{ttt}}{2} + \frac{U}{2} f_{ttx} + O(\Delta t)\right)$$

$$+\Delta x\left(\frac{U}{2} u_{xxt} - \frac{U^2}{2} u_{xxx} + O(h)\right)$$

Modified Equation: Upwind

$$f_{ttt} = -U^3 f_{xxx} + O(\Delta t, h)$$

$$f_{ttx} = U^2 f_{xxx} + O(\Delta t, h)$$

$$f_{xxt} = -U f_{xxx} + O(\Delta t, h)$$

Further simplified form

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = \frac{Uh}{2}(1-\lambda)f_{xx} - \frac{Uh^2}{6}\left(2\lambda^2 - 3\lambda + 1\right)f_{xxx} + O\left[h^3, h^2\Delta t, h\Delta t^2, \Delta t^3\right]$$

$$\lambda = \frac{U\Delta t}{h}$$

Modified Equation: Upwind

$$\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = \frac{Uh}{2}(1-\lambda)f_{xx} - \frac{Uh^2}{6}(2\lambda^2 - 3\lambda + 1)f_{xxx} + O\left[h^3, h^2\Delta t, h\Delta t^2, \Delta t^3\right]$$

$\lambda < 1$ implies that the coefficient ($Uh(1-\lambda)/2$) is positive

- Leading order truncation term has **diffusion-like** form

- Dissipative scheme

- The coefficient ($Uh(1-\lambda)/2$) if non-zero and positive, is called "**numerical viscosity**"

- Since upwind introduces numerical viscosity to advection equation, it can be used for flows with shocks. However, it is found that the discontinuities are smeared excessively owing the first-order accuracy of the scheme

Upwind Scheme

- An upwind scheme is conditionally stable

- It introduces **large amount of dissipation** (numerical or unphysical) that can overwhelm physical dissipation (if any)

- To reduce effect of the dissipation, very small grid sizes and small time-steps are needed (that can make the scheme prohibitively expensive)

- Upwind scheme provides **bounded solution** (i.e. overshoot and undershoot are avoided); a desirable trait for many scalar advection schemes

- Upwind scheme is conservative. Note that discontinuity is smeared, but the “conservation” of a scalar over the domain is maintained