An Introduction to Numerical Methods

For Weather Prediction

by

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Based on lectures given by Mariano Hortal

What do we want to achieve?

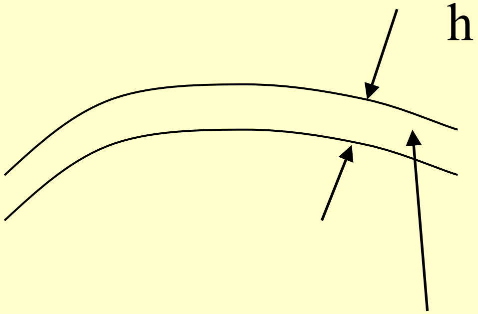
- Warm-up session
- Objectives
  - Get a general feel for some numerical problems
  - Get an understanding of simple methods
- Unfortunately no time for an exercise session
- Do not expect to be an expert in numerical mathematics afterwards
- Come in my office if you have question which you do not want to ask publically

Shallow water equations in 1 dimension

$$\left\{\begin{aligned} \frac{\partial u}{\partial t} &= -u\frac{\partial u}{\partial x} - g\frac{\partial h}{\partial x} + \frac{\partial}{\partial x}\left(K\frac{\partial u}{\partial x}\right) \\ \frac{\partial h}{\partial t} &= -u\frac{\partial h}{\partial x} - h\frac{\partial u}{\partial x} + \frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right) \end{aligned}\right.$$

advection adjustement diffusion

Non linear equations



Velocity is equal
in layers vertical
direction (shallow)

u … velocity along x direction

h … absolute height

g … acceleration due to gravity

K …diffusion coefficient

Linearization

$u=U_0+u'$ → Const. + perturb. in the x-comp. of velocity

$h=H+h'$ Const. + perturb. in the height of the free surface

↑

Small perturbations

Substitute and drop products of perturbations

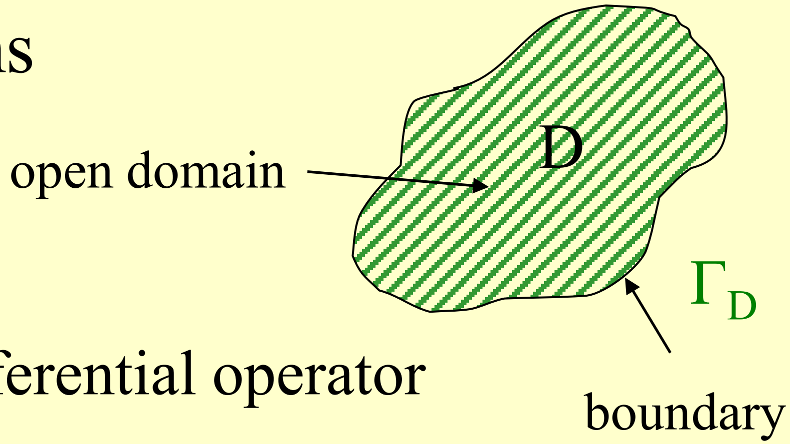
$$\begin{cases} \frac{\partial}{\partial t}u' = -U_0 \frac{\partial}{\partial x}u' - g\frac{\partial}{\partial x}h' + K\frac{\partial^2}{\partial x^2}u' \\ \frac{\partial}{\partial t}h' = -U_0 \frac{\partial}{\partial x}h' - H\frac{\partial}{\partial x}u' + K\frac{\partial^2}{\partial x^2}h' \end{cases}$$

Classification of PDE’s

- Boundary value problems

$\underline{x} \in$

$\underline{x} \in$

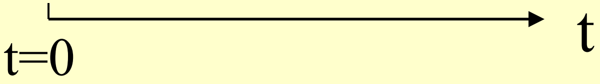


f, g: known function; L, B: differential operator

φ: unknown function of $\underline{x}$

- Initial value problems (most important to us)

φ: unknown function of t



Classification of PDE’s (II)

- Initial and boundary value problems

$$\left\{ \begin{array}{l} \\ \\ \Gamma \end{array} \right.$$

- Eigenvalue problems

$$L(\varphi =$$

φ: unknown eigenfunction
λ: eigenvalue of operator L

Existence and uniqueness of solutions

$$\frac{dy}{dt} = f(t, y) \quad ; \quad y(t_0)=y_0$$ (initial value problem)

- Does it have a solution?
- Does it have only one solution?
- Do we care?

If it has one and only one solution it is called a well posed problem

Picard’s Theorem

Let f and $\frac{\partial f}{\partial y}$ be continuous in the rectangle

$$R:\begin{cases} t_0 \le t \le t_0 + a \\ |y - y_0| \le b \end{cases}$$

then, the initial-value problem

$$\begin{cases} \frac{dy}{dt} = f(t, y) \\ y(t_0) = y_0 \end{cases}$$

Has a unique solution y(t)
on the interval $t_0 \le t \le t_0 + a$

Finding the solution (not analytical)
Numerical methods (finite dimensions)

Discretization

- Finite differences
- Spectral
- Finite elements

$$f(x) \sim f(x_j),\ j = \ldots\ldots N$$

$$f(x) \sim \sum_{j=1}^{M} f_j \omega_j(x)$$

Transform the continuous differential equation into a system of ordinary algebraic equations where the unknowns are the numbers f_j

The Lax-Richtmeyer theorem

- Convergence

  Discretized solution ---------> continuous solution

  discretization finer and finer

- Consistency

  Discretized equation ---------> continuous equation

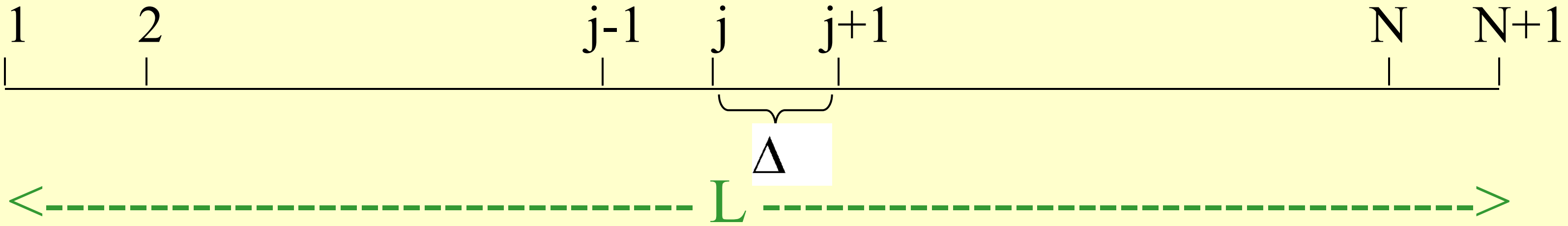
- Stability

  Discretized solution bounded

- **Lax-Richtmeyer theorem**

> **If a discretization scheme is consistent and stable then it is convergent, and vice versa**

Finite Differences - Introduction



$$\phi \quad \square \quad = \quad +$$

Taylor series expansion:

$$\phi_{j+} = \quad + \quad \Delta \quad + \frac{1}{2!} \quad \Delta \quad + \frac{1}{3!} \quad \Delta \quad +$$

$$\phi_{j-} = \quad - \quad \Delta \quad + \frac{1}{2!} \quad \Delta \quad - \frac{1}{3!} \quad \Delta \quad +$$

Finite differences approximations

$$\phi_j = \frac{\phi \quad -}{\Delta} \quad + \qquad\qquad E_1 = -\frac{1}{2!}\;{}_j\,\Delta - \frac{1}{3!}\;{}_j(\quad)^2 +$$

forward approximation

Consistent if $\phi_j, \phi_j,$ ... are bounded

$$\phi_j = \frac{\phi \quad -}{\Delta} \quad + \qquad\qquad E_2 = \frac{1}{2!}\;{}_j\,\Delta - \frac{1}{3!}\;{}_j(\quad)^2 +$$

backward approximation

adding both

$$\phi_j = \frac{\phi \quad -}{2\Delta} \quad + \qquad\qquad E = -\frac{1}{3!}\;{}_j(\Delta)^2 +$$

centered differences

Consistent if $\phi_j,$ ... are bounded

Finite differences approximations (2)

Also

$$\phi_j = \frac{4}{3}\left[\qquad\right]\qquad\left[\qquad\right]$$

fourth order approximation to the first derivative

Using the Taylor expansion again we can easily get the second derivative:

$$\phi_j = \frac{\phi \quad - \quad +}{(\Delta} + \Delta$$

second order approximation of the second derivative

The linear advection equation

$$\boxed{\frac{\partial \varphi}{\partial t} + U_0 \frac{\partial \varphi}{\partial x} = 0}$$

+ initial and boundary conditions

We start with a guess: $\varphi(x,t) = X(x) \cdot T(t)$

Substituting we get: $\frac{U_0}{X}\frac{dX}{dx} = -\frac{1}{T}\frac{dT}{dt} = C \equiv U_0 \lambda$

$$\left.\begin{aligned} \frac{dX}{dx} &= \lambda X \\ \frac{dT}{dt} &= -U_0 \lambda T \end{aligned}\right\}$$

Eigenvalue problems for $\frac{d}{dx}$ *and* $\frac{d}{dt}$

$$\left.\begin{aligned} X &= X_0 e^{\lambda x} \\ T &= T_0 e^{-U_0 \lambda t} \end{aligned}\right\}$$

With periodic B.C. λ can only have certain (imaginary) values where k is the wave number $\lambda \equiv ik$

The general solution is a linear combination of several wave numbers

The linear advection equation (2)

The analytic solution is then:

$$\varphi(x,t) = X_0 T_0 e^{\lambda(x-U_0 t)} \equiv \varphi_0 e^{\lambda(x-U_0 t)} = f(x-U_0 t)$$

↓

Propagating with speed U_0 → No dispersion

For a single wave of wave number k the frequency is $\omega = kU_0$

Energy: $$E(t) \equiv \frac{1}{2}\int_0^L \varphi^2 \, dx$$

For periodic B.C.: $$\frac{\partial E}{\partial t} = \frac{-U_0}{2}\int_0^L \frac{\partial \varphi^2}{\partial x} dx = \frac{-U_0}{2}\left[\varphi^2\right]_0^L = 0$$

Space discretization

$$\left(\frac{\partial \varphi}{\partial\ }\right)_j \approx \frac{\varphi_{j+1} - \varphi_{j-1}}{2\Delta}$$

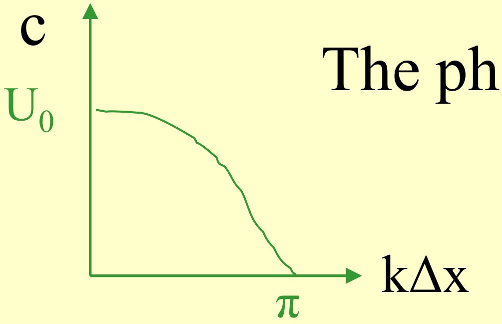
centered second-order approximation

$$\frac{\partial \varphi_j}{\partial} = -U_0 \frac{\varphi_{j+1} - \varphi_{j-1}}{2\Delta} \equiv \frac{d\varphi_j}{dt}$$

Try: $\phi_j(\ ) = \Phi(\ )\ \Delta$

results in $\frac{d\Phi}{dt} + ikU_0 \frac{\sin(k\Delta x)}{k\Delta x}\Phi = \ )$

whose solution is $\Phi = \Phi_0 e^{-ikct}$ with $c(k) = {}_0\frac{\sin(k\Delta}{k\Delta}$



The phase speed c depends on k ➡ dispersion

kΔx= π ---> λ=2Δx ==> c=0

Group velocity

$$c_g = \frac{d\omega}{dk} \qquad \begin{cases} c_g = \dfrac{d(kU_0)}{dk} = U_0 \\[2ex] c_g^* = \dfrac{d(kc)}{dk} = U_0 \cos(k\Delta x) \end{cases}$$

Continuous equation

Discretized equation

↓

$=-U_0$ for $k\Delta x=\pi$

Approximating the space operator introduces dispersion

Time discretization

In addition to our 2nd order centered approx. for the space derivative we use a 1st order forward approx. for the time derivative:

$$\left(\quad \right)_n \quad - \quad = - \quad \frac{-}{\Delta}$$

$$\phi_j^{\;+} = \;_j - \Delta \;_0 \frac{\phi \quad -}{2\Delta}$$

Try $\varphi_j^{\,n} = \varphi_0 e^{-\omega\;\Delta} e^{ikj\Delta}$

Substituting we get $e^{-\;\Delta} = - \frac{\Delta}{\Delta}\;\Delta$

Courant-Friedrich-Levy number

ω=a+ib

- If b>0, φ_j^n increases exponentially with time (unstable)
- If b<0, φ_j^n decreases exponentially with time (damped)
- If b=0, φ_j^n maintains its amplitude with time (neutral)

Also another dispersion is introduced, as we have approximated the operator ∂/ ∂t

Three time level scheme (leapfrog)

$$\varphi_j^{n+} = \rho_j^{n-} - \chi(\rho^n_{j+} - \rho^n_{j-})$$

This scheme is centered (second order accurate) in both space and time

Try a solution of the form

exponential

$$\varphi_j^n = \rho_0 \cdot \lambda_k^n \cdot e^{ikj\Delta}$$

If $|\lambda_k| > 1$ solution unstable
if $|\lambda_k| = 1$ solution neutral
if $|\lambda_k| < 1$ solution damped

Substituting $\lambda_k - \quad p_k - = \qquad \equiv - \qquad \Delta$

$$\lambda_k = p \pm \sqrt{1 - p^2}$$

$$\lambda_k = ip + \sqrt{1 - p^2} - - - - - - - >$$ physical mode

$\Delta x \rightarrow 0$
$\Delta t \rightarrow 0$

$$\lambda_k = ip - \sqrt{1 - p^2} - - - - - - - > -$$ computational mode

Stability analysis

Energy method

We have defined $E(t) = \frac{1}{2}\int_0^L \varphi \ dx$; $\frac{\partial E}{\partial t} = -\frac{U_0}{2}\int_0^L \frac{\partial \varphi^2}{\partial x} dx = -\frac{U_0}{2}\varphi^2]_0^L = 0$

For periodic boundary conditions

We have discretized *t* and
hence the discretized analog of *E(t)* is E^n

$$E^n = \frac{1}{2}\sum_{j=1}^{N} (\varphi_j^n)^2 \Delta x$$

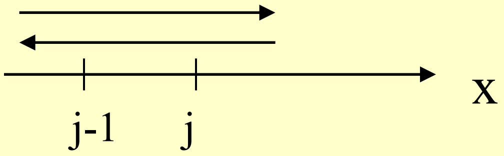
$$\boldsymbol{\varphi}^n_{N+1} \equiv \boldsymbol{\varphi}^n_1$$

If $E^n = const$, $\varphi \underset{t\to}{\not\longrightarrow}$ than the scheme is stable

Example of the energy method

$$\frac{\varphi_j^{n+1}-\varphi_j^{n}}{\Delta t} = -U_0\,\frac{\varphi_j^{n}-\varphi_{j-1}^{n}}{\Delta x}$$

upwind if $U_0>0$
downwind if $U_0<0$



$$(\phi_j^{n+1})^2-(\phi_j^{n})^2=-\alpha(\phi_j^{n+1}+\phi_j^{n})(\phi_j^{n}-\phi_{j-1}^{n}) \qquad \boxed{\alpha = U_0\frac{\Delta t}{\Delta x}}$$

$$\sum_j \qquad (\varphi_j^{n+1})^2-(\varphi_j^{n})^2=-\alpha\{(\varphi_j^{n})^2-(\varphi_{j-1}^{n})^2\}-\alpha(1-\alpha)(\varphi_j^{n}-\varphi_{j-1}^{n})^2$$

$$E^{n+1}-E^{n}=-\alpha(1-\alpha)\underbrace{\sum_{j=1}^{N}(\varphi_j^{n}-\varphi_{j-1}^{n})^2\,\Delta x}_{>0}$$

$E^{n+1}=E^{n}$ if
- $\alpha=0 \Rightarrow U_0=0$ → no motion
- $\alpha=1$ → $\Delta t=\Delta x/U_0$

$E^{n+1}>E^{n}$ → unstable

$E^{n+1}<E^{n}$ if
- $\alpha>0 \Rightarrow U_0>0$ → upwind
- $\alpha<1$ → $U_0\,\Delta t/\Delta x<1$ CFL cond.

damped

Von Neumann method

Consider a single wave $\varphi(x_j, t_n) = c_k \lambda_k e^{ikx_j}$

if $|\lambda_k| < 1$ the scheme is damping for this wave number *k*

if $|\lambda_k| = 1$ $\forall k$ the scheme is neutral

if $|\lambda_k| > 1$ for some value of *k*, the scheme is unstable

alternatively $\varphi(x_j, t_n) = c_k e^{-\omega \Delta} e^{ikx_j}$

if $\mathrm{Im}(\omega) > 0 \longrightarrow$ scheme unstable

if $\mathrm{Im}(\omega) = 0 \longrightarrow$ scheme neutral

if $\mathrm{Im}(\omega) < 0 \longrightarrow$ scheme damping

$V_f = \omega / k$

$v_g = \partial\omega / \partial k$

Stability of some schemes

- Forward in time, centered in space (FTCS) scheme

$$\frac{\varphi_j^{+1} - \rho_j}{\Delta} = - /_0 \frac{\varphi_{j+1} - \rho_{j-1}}{2\Delta}$$ using Von Neumann, we find

$$\lambda_k = - \quad (\quad \Delta \quad) \quad |\ _k| \geq \quad \forall$$ → scheme unstable

- Upwind or downwind

$$\frac{\varphi_j^{+1} - \rho_j}{\Delta} = - /_0 \frac{\varphi_j - \rho_{j-1}}{\Delta}$$

→ upwind if $U_0 > 0$

→ downwind if $U_0 < 0$

Using Von Neumann, we find

$$\lambda_k = - \quad - \quad (\quad) \quad |\ _k| = + \quad (\quad - \quad) \underbrace{- \quad \wedge}_{>}$$

$\alpha(\alpha-1) > 0$ → unstable $\begin{cases} \alpha < 0 & \text{downwind} \\ \alpha > 1 & \text{CFL limit} \end{cases}$

$-1/4 < \alpha(\alpha-1) < 0 \Rightarrow 0 \leq \alpha \leq 1$ → stable damped scheme

Stability of some schemes (cont)

- Leapfrog $$\frac{\varphi_j^{+1} - \varphi_j^{-1}}{2\Delta} = -U_0 \frac{\varphi_{j+1} - \varphi_{j-1}}{2\Delta}$$

Using von Neumann we find $|\alpha|\leq 1$ as stability condition

As a reminder α is the Courant-Friedrich-Levy number:

$$\alpha = {}_0\frac{\Delta}{\Delta}$$

Stability of some schemes (cont)

- Lax Wendroff scheme

From a Taylor expansion in *t* we get:

$$\varphi(x,t+\Delta t) \approx \varphi(x,t) + \Delta t \frac{\partial \varphi}{\partial t} + \frac{1}{2!}(\Delta t)^2 \frac{\partial^2 \varphi}{\partial t^2}$$

Substitution the advection equation we:

$$\varphi(x,t+\Delta t) \approx \varphi(x,t) - U_0 \Delta t \frac{\partial \varphi}{\partial x} + \frac{1}{2!}(\Delta t)^2 U_0^2 \frac{\partial^2 \varphi}{\partial x^2}$$

Discretization:

$$\varphi_j^{n+1} = \varphi_j^n - \frac{\alpha}{2}(\varphi_{j+1}^n - \varphi_{j-1}^n) + \frac{\alpha^2}{2}(\varphi_{j+1}^n - 2\varphi_j^n + \varphi_{j-1}^n)$$

Applying Von Neumann we can find that $|\alpha| \leq 1$ -----> stable

Stability of some schemes (cont)

- Implicit centered scheme

We replace the space derivation by the average value of the centred space derivation at time level *n*-1 and *n*+1

$$\frac{\phi_{j}^{+} - \quad {}_{j}}{\Delta} = - \left(\quad - \quad \quad - \quad \right)$$

using von Neumann

$$\lambda = \frac{1 - i\alpha \quad \mathrm{in}(\; k\Delta x)}{1 + i\alpha \quad \mathrm{in}(\; k\Delta x)} \rightarrow |\lambda| =$$

Always neutral, however an expensive implicit equation needs to get solved

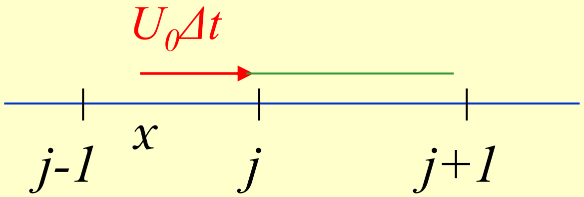
$$\frac{c}{U_0} = \frac{\omega}{\tan(\omega)}$$

Dispersion worse than leapfrog

“Intuitive” look at stability

If the information for the future time step “comes from” inside the interval used for the computation of the space derivative, the scheme is stable. Otherwise it is unstable

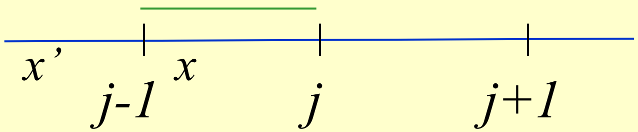
Downwind scheme (unstable)



x, x’ … point where the information comes from $(x_j - U_0\Delta t)$

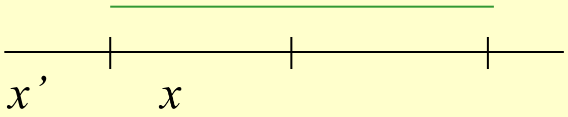
— Interval used for the computation of ∂φ/∂x

Upwind scheme (conditionally stable)



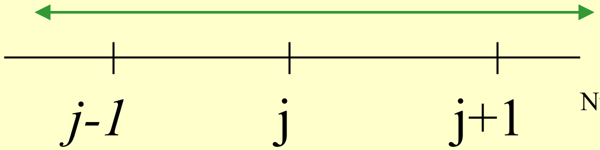
x if $\alpha < 1$
x’ if $\alpha > 1$

Leapfrog (conditionally stable)



CFL number ==> fraction of Δx traveled in Δt seconds

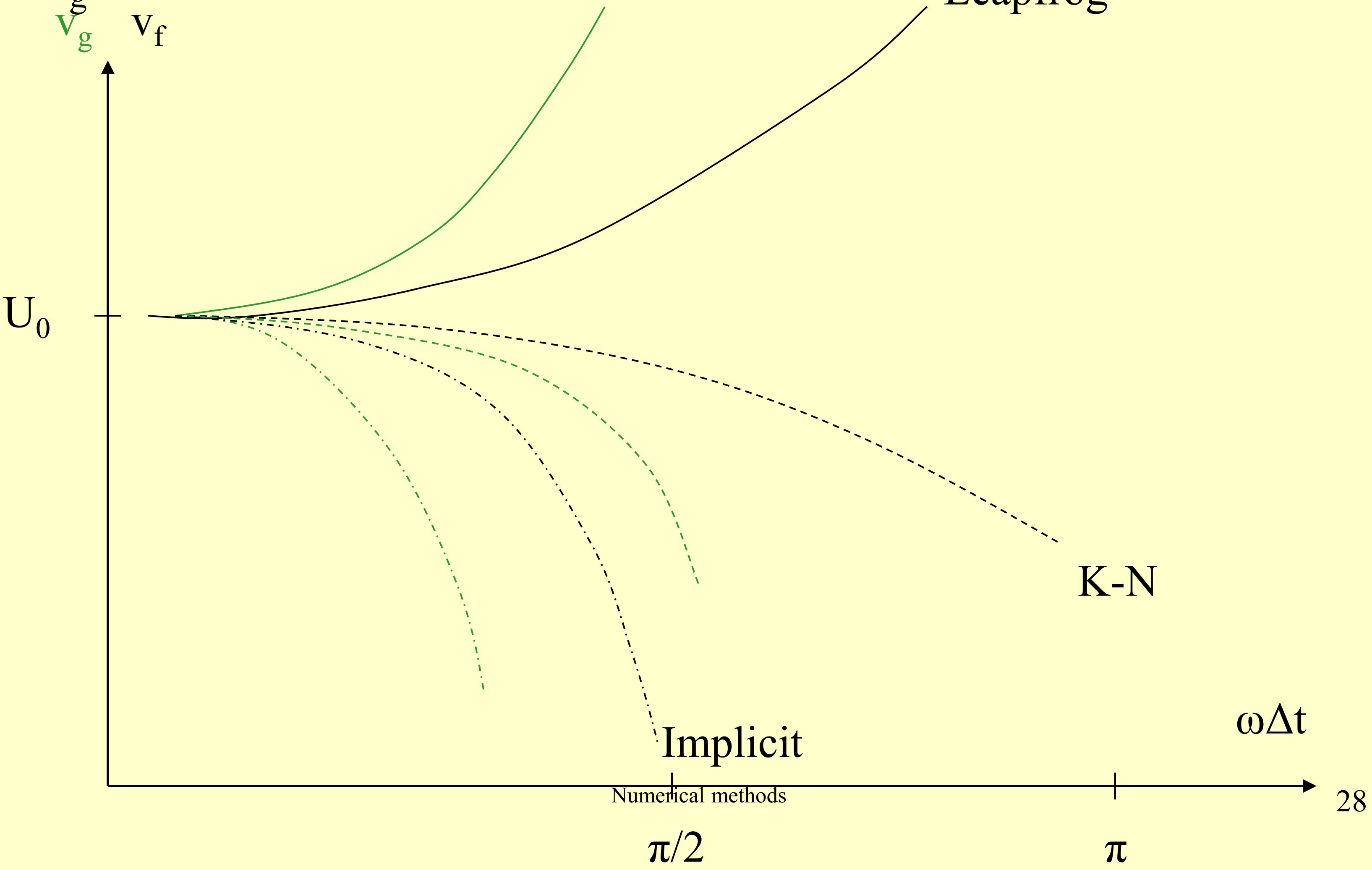
Implicit (unconditionally stable)



Dispersion and group velocity

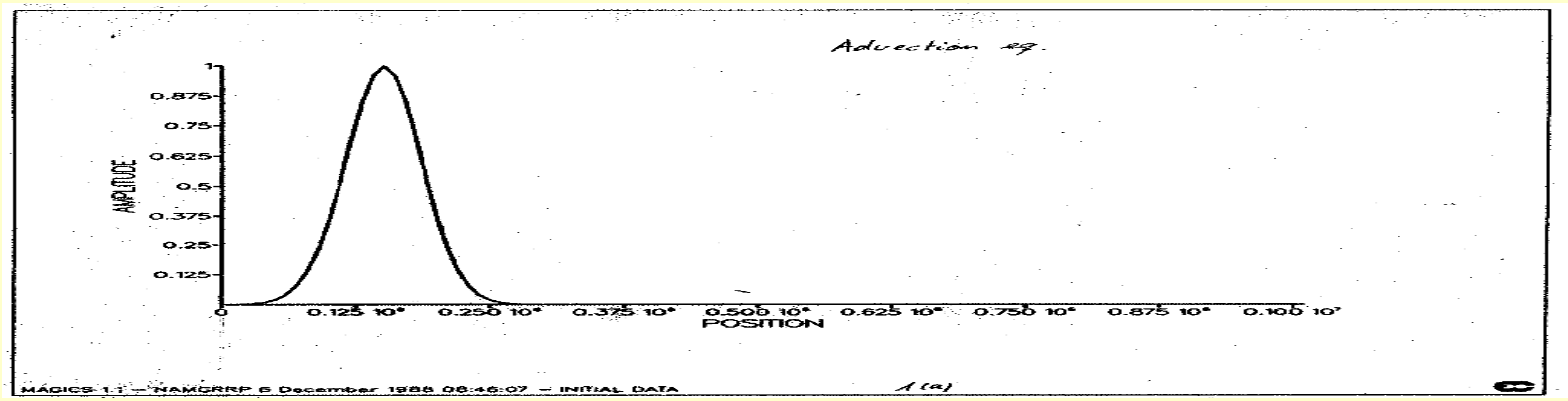
$v_f = \omega/k$

$v_g = \partial\omega/\partial k$



Effect of dispersion

Initial



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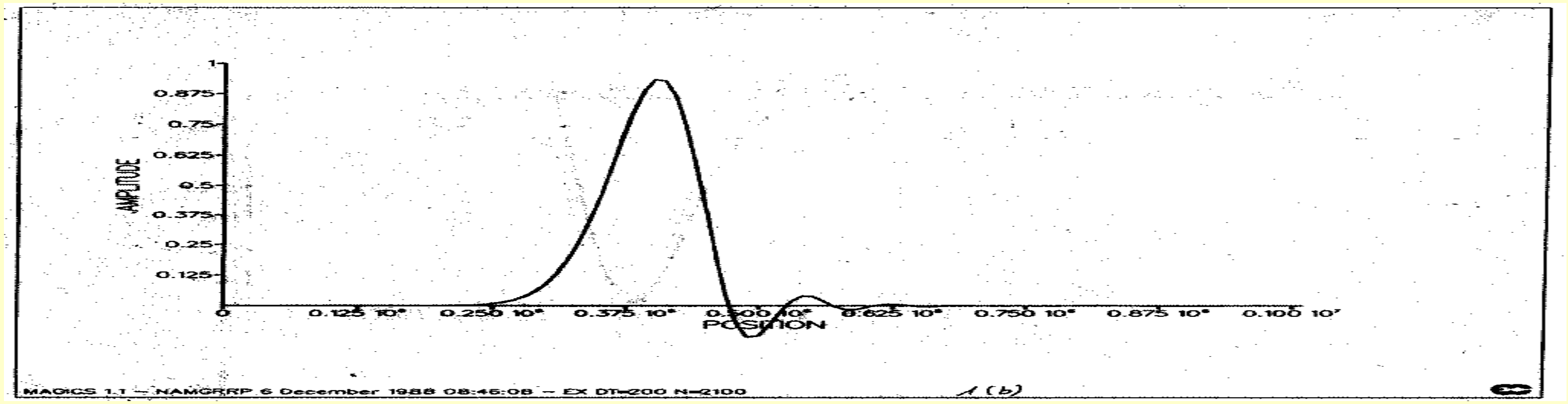
1(a)

Leapfrog



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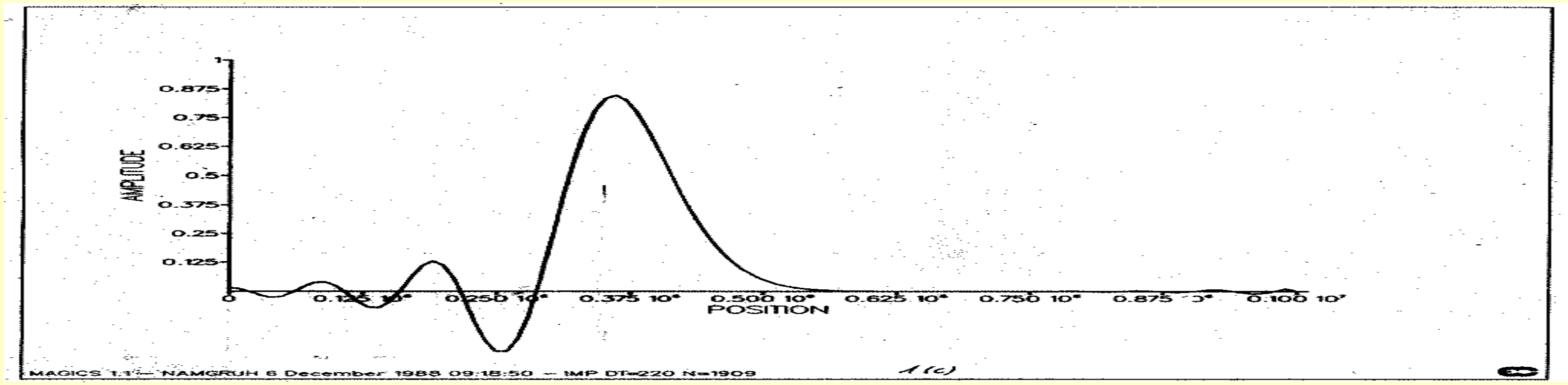
1(b)

implicit



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1(c)

Two-dimensional advection equation

$$\frac{\partial \rho}{\partial t} + U_0 \frac{\partial \rho}{\partial x} + V_0 \frac{\partial \rho}{\partial y} = 0$$

Using von Neumann, assuming a solution of the form $\varphi = \rho \ \lambda \ e^{i(kx+ \ y)}$

we obtain $\lambda = \Delta t \left[\frac{U_0 \sin(k\Delta x)}{\Delta x} + \frac{V_0 \sin(l\Delta y)}{\Delta y} \right]$

using $\vec{V} = (U_0, V_0) = (R\cos\theta, R\sin\theta)$

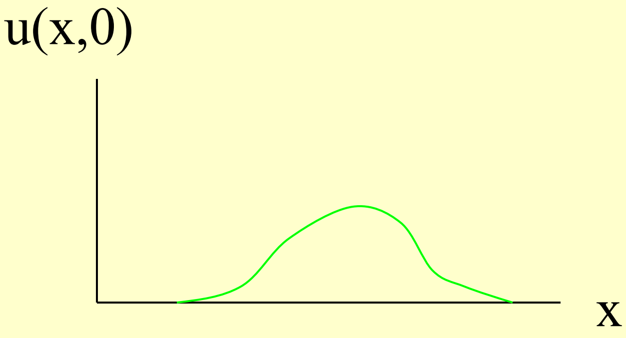
we obtain, for |λ| ≤ 1 the condition

where Δs= Δx= Δy $\Delta \ \leq \frac{\Delta}{R\sqrt{2}}$

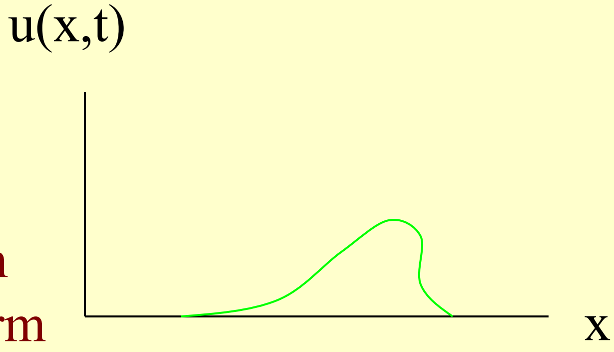
This is more restrictive than in one dimension by a factor $\sqrt{2}$

Non linear advection equation
Continuous form

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$



Change in shape even for the continuous form



One Fourier component $u_k e^{ikx}$ no longer moving with constant speed but interacting with other components

Fourier decomposition valid at each individual time but it changes amplitude with time

$$u = \sum_k u_k(t) e^{-i\omega t} e^{ikx}$$

No analytical solution!

Energy conservation

Define again: $E = \frac{1}{2}\int_0^L u^2\,dx$

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} \Rightarrow u\frac{\partial u}{\partial t} \equiv \frac{1}{2}\frac{\partial u^2}{\partial t} = -u^2\frac{\partial u}{\partial x} \Rightarrow \underline{\underline{\frac{\partial E}{\partial t}}} = -\int u^2\frac{\partial u}{\partial x}\,dx = f(u)\Big|_0^L = 0$$

periodic B.C.

Discretization in space

First attempt: $u\frac{\partial}{\partial} \rightarrow \frac{-}{\Delta} \rightarrow \frac{\partial}{\partial} = -\frac{-}{\Delta}$

$$\frac{\partial}{\partial}\sum_j \qquad \partial \qquad \sum$$

Second attempt: $\frac{\partial \quad_j}{\partial} = -\underbrace{\quad + \quad + \quad}_{\sim u_j}\frac{-}{\Delta}$

averaging

terms joined by arrows cancel from consecutive j's

$$\frac{\partial}{\partial} = -\sum_j \frac{}{6} \qquad - \qquad =$$

Aliassing

Aliasing occurs when the non-linear interactions in the advection term produce a wave which is too short to be represented on the grid.

Consider the product $A \equiv \xi(x) \dfrac{d\eta(x)}{dx}$

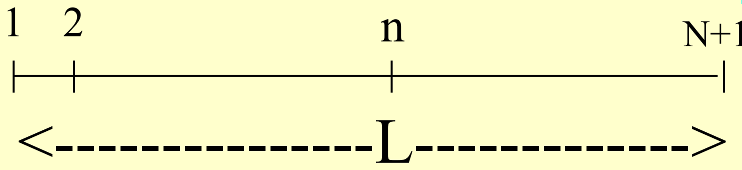
$\xi(x) = \sum_k \xi_k \sin(kx)$ $\quad \eta(x) = \sum_k \eta_k \sin(kx)$ $\quad$ in the interval 0≤x ≤2π

$$A = \sum_{k_1}\sum_{k_2} {}_1\, \eta_{k_2} \sin(k_1 x)\, k_2 \cos(k_2 x) =$$

$$\sum_{k_1}\sum_{k_2} {}_1\, \eta_{k_2} k_2 \{\sin[(\underline{k_1 + k_2})x] + \sin[(\underline{k_1 - k_2})x]\} \frac{1}{2}$$

Minimum wavelength $\quad \lambda_m = \Delta \quad \rightarrow \quad {}_M = \dfrac{L}{\lambda_m} = N$

Maximum wave number representable with the discretized grid

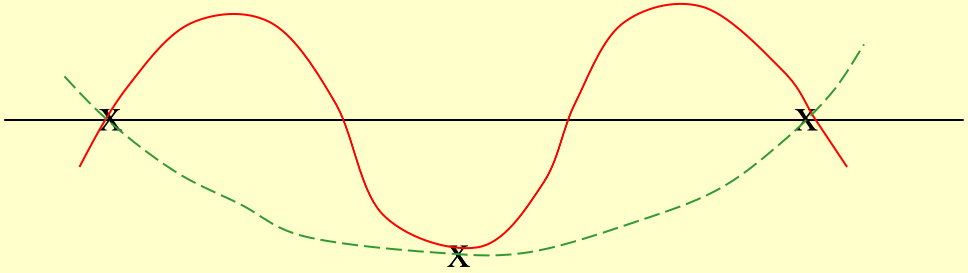


Aliassing (cont.)

Trigonometrical manipulations lead to: $\sin(kx_j)=-\sin[(2k_M-k)x_j]$

Therefore, it is not possible to distinguish wave numbers k and $(2k_M-k)$ on the grid.

wave number k ⇔ wave number $2k_M$-k



Non-linear instability

If k_1+k_2 is misrepresented as k_1 there is positive feedback, which causes instability

$$k_1 = 2k_M - (k_1+k_2) \text{ ----------> } 2k_1=2k_M-k_2$$

$$2k_M \geq 2k_1 \geq k_M$$

$$2\Delta x \leq \lambda_1 \leq 4\Delta x$$

These wavelengths keep storing energy and total energy is not conserved

We can remove energy from the smallest wavelengths by

- Fourier filtering
- Smoothing
- Diffusion
- Use some other discretization (e.g. semi-Lagrangian)