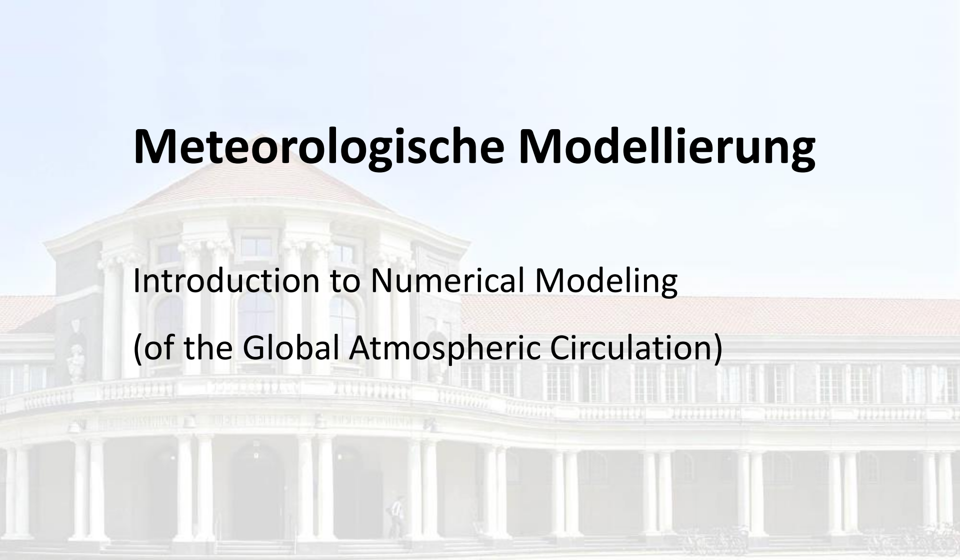


Meteorologische Modellierung

Introduction to Numerical Modeling

(of the Global Atmospheric Circulation)

Frank Lunkeit

Outline

0. Introduction: Where/what is the problem and basics
1. The (linear) evolution (decay) equation (discretization in time)
2. One-dimensional linear advection (discretization in time and space)
3. One-dimensional linear diffusion and one-dimensional linear transport equation
4. Nonlinear advection and 1d nonlinear transport equation (Burgers-equation)
5. More dimensions (grids)
6. Design of an atmospheric general circulation model (AGCM)

(7. An example: qg barotropic channel (weather prediction)) next semester

References

D. R. Durran: Numerical Methods for Wave Equations in Geophysical Fluid Dynamic, Springer 1999, ISBN:0-387-98376-7.

G.J. Holtiner & R.T. Williams: Numerical Prediction and Dynamic Meteorology, Second Edition, John Wiley & Sons 1980, ISBN: 0-471-05971-4.

D. Randall: An Introduction to Atmospheric Modeling, http://kiwi.atmos.colostate.edu/group/dave/at604.html

Introduction to Numerical Modeling

0. Introduction: The Problem and Basics

The Problem

Nonlinear (quasi-linear) coupled partial differential equations (without a known analytic solution)

Example: Two dimensional flow

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} - v\frac{\partial u}{\partial y} + fv - \frac{1}{\rho}\frac{\partial P}{\partial x} + F_x(u,v,T,..)$$

Eq. of motion

$$\frac{\partial v}{\partial t} = -u\frac{\partial v}{\partial x} - v\frac{\partial v}{\partial y} - fu - \frac{1}{\rho}\frac{\partial P}{\partial y} + F_y(u,v,T,...)$$

Eq. of motion

$$\frac{\partial \rho}{\partial t} = -u\frac{\partial \rho}{\partial x} - v\frac{\partial \rho}{\partial y} - \rho\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)$$

Continuity eq.

$$\frac{\partial \theta}{\partial t} = -u\frac{\partial \theta}{\partial x} - v\frac{\partial \theta}{\partial y} + F_\theta(u,v,T,...)$$

First law of thermodynamics

$$P = \rho RT$$

Eq. of state

$$\theta = T\left(\frac{P_0}{P}\right)^{R/c_p}$$

Pot. temperature

The Problem

Example: First law (1-d, p=const.,…)

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x} + K\frac{\partial^2 T}{\partial x^2} + F(T,u,...)$$

local change with time	advection	diffusion	other forcing
first derivative in time	first derivative in space	Second derivative in space	?

Numerical Solution of (Partial) Differential Equations

From theory (the equations) to the numerics:

a) continuous functions	-> discrete values
b) differential (integral) equations	-> algebraic equations

Tasks:

a) choice of the discretization

b) calculation (representation) of the derivatives

Approaches (Algorithms):

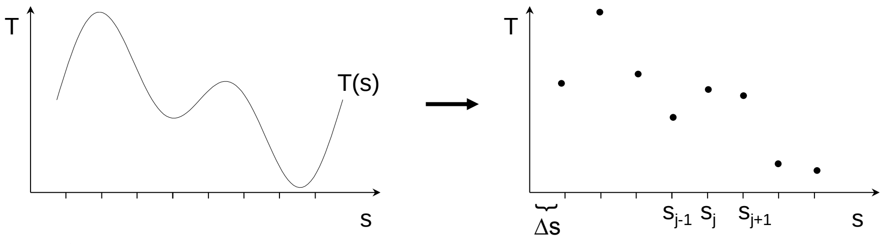
- grid point methods (finite differences)
- series expansion (spectral method and finite elements)

Evaluation of a method:

- consistency, accuracy, convergence and stability

Example: The Grid Point Method

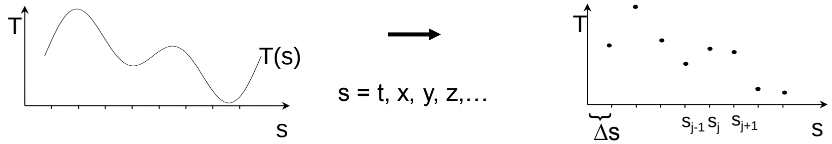
a) continuous function -> discrete values



s = t, x, y, z,…

Δs defines the **resolution**

Example: The Grid Point Method



s = t, x, y, z,…

b) derivatives -> finite differences (e.g. from Taylor-expansion)

$$1)\quad T(s+\Delta s) = T(s) + \frac{dT}{ds}|_s\ \Delta s + ...$$

$$2)\quad T(s-\Delta s) = T(s) - \frac{dT}{ds}|_s\ \Delta s + ...$$

$$\text{from 1)} \Rightarrow \frac{dT}{ds} = \frac{T(s_{j+1}) - T(s_j)}{\Delta s}[+ ...$$

Forward differences

$$\text{from 2)} \Rightarrow \frac{dT}{ds} = \frac{T(s_j) - T(s_{j-1})}{\Delta s}[+ ...$$

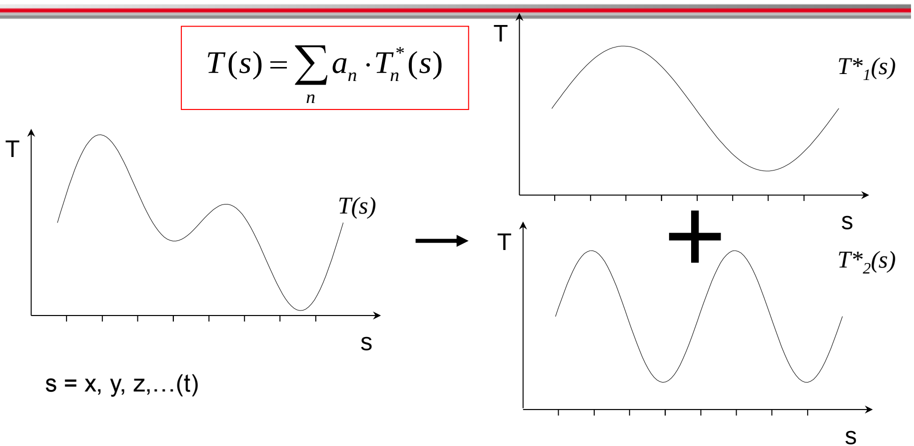
Backward differences

$$\text{from 1)} - 2) \Rightarrow \frac{dT}{ds} = \frac{T(s_{j+1}) - T(s_{j-1})}{2\Delta s}[+ ...$$

Central differences

Example: Series Expansion -The Spectral Method

$$T(s) = \sum_n a_n \cdot T_n^*(s)$$



s = x, y, z,…(t)

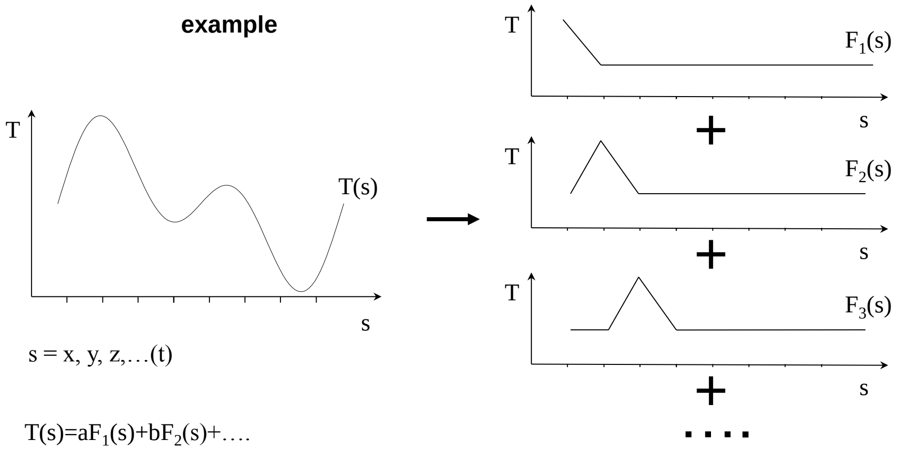
T^*_n differentiable orthogonal (Basis-) functions (Fourier-series; Legendre Polynomials). The **resolution** is given by the number of modes ***n***

derivatives -> analytical derivatives of the basis-functions

$$\frac{dT}{ds} = \sum_n a_n \cdot \frac{dT_n^*}{ds}$$

Example: Series Expansion –Finite Elements

example



s = x, y, z,…(t)

$T(s)=aF_1(s)+bF_2(s)+\ldots.$

$F_1,F_2,\ldots$ arbitrary function which is only locally non zero

Derivatives -> depending on the function

Evaluation: Consistency

The discretization must converge to the differential: $\lim_{\Delta s\to 0}\left\|\frac{\Delta T}{\Delta s}\right\|=\frac{dT}{ds}$

Example: forward difference: $\frac{\Delta T}{\Delta s}=\frac{T(s+\Delta s)-T(s)}{\Delta s}$

Consistency from Taylor-expansion:

$$T(s+\Delta s)=T(s)+\frac{dT}{ds}\Delta s+\frac{d^2T}{ds^2}\frac{(\Delta s)^2}{2}+\ldots$$

$$\Rightarrow\frac{T(s+\Delta s)-T(s)}{\Delta s}=\frac{dT}{ds}+\frac{d^2T}{ds^2}\frac{\Delta s}{2}+\ldots$$

$$\Rightarrow\lim_{\Delta s\to 0}\left(\frac{T(s+\Delta s)-T(s)}{\Delta s}\right)=\lim_{\Delta s\to 0}\left(\frac{dT}{ds}+\frac{d^2T}{ds^2}\frac{\Delta s}{2}+\ldots\right)=\frac{dT}{ds}$$

Evaluation: Accuracy

Accuracy: Smallest power of Δs in the deviation from the truth

a: Accuracy (order of accuracy) of the discretization

Example: forward differences
$$\frac{\Delta T}{\Delta s}=\frac{T(s+\Delta s)-T(s)}{\Delta s}$$

Taylor-expansion
$$T(s+\Delta s)=T(s)+\frac{dT}{ds}\Delta s+\frac{d^2T}{ds^2}\frac{(\Delta s)^2}{2}+\dots$$
$$\Rightarrow\frac{T(s+\Delta s)-T(s)}{\Delta s}=\frac{dT}{ds}+\frac{d^2T}{ds^2}\frac{\Delta s}{2}+\dots$$
$$\Rightarrow\frac{\Delta T}{\Delta s}=\frac{dT}{ds}+O(\Delta s)$$

=> forward differences are of first order accuracy

b (mostly): Accuracy (order of accuracy) of the scheme

Considering the whole equation, i.e. including the ‚right hand side‘ (see, e.g., Section ‘Evolution (decay) equation’)

Evaluation: Convergence

Convergence: Convergence of the **error** to 0 for small Δs:

$$\lim_{\Delta s\to 0}\left\|T(t)-T_A(t)\right\|=0$$

Error: Deviation of the numerical solution (T) from the truth (analytical solution; T_A)

Error measure (Norm) $\|\ \|$

Examples

a) Euclidean (quadratic) Norm: $\|\Theta\|_2=\left(\sum_{j=1}^{N}|\Theta_j|^2\right)^{1/2}$

b) Maximum Norm: $\|\Theta\|_\infty=\max_{1\le j\le N}|\Theta_j|$

Evaluation: Stability

(most important for practical use)

Stability: A scheme is stable if the difference between the numerical and the analytical solution is bounded: $\|T(t)-T_A(t)\| < C(t) \quad \forall\, t$

or: A scheme is unstable if the numerical and the analytical solutions diverge with time: $\|T(t)-T_A(t)\| \xrightarrow[t\to\infty]{} \infty$

If $T_A(t)$ is bounded:

$\|T(t)\| < C(t) \quad \forall\, t$ stable

$\|T(t)\| \xrightarrow[t\to\infty]{} \infty$ unstable

Stability may depend on Δs

Stability analyses: various methods (e.g.):

Direct (heuristic),

Energy Method and Von Neumann Method (see advection equation)

Interrelation (Lax Equivalence Theorem):
‚For a consistent scheme stability is a necessary and sufficient condition for convergence‘.

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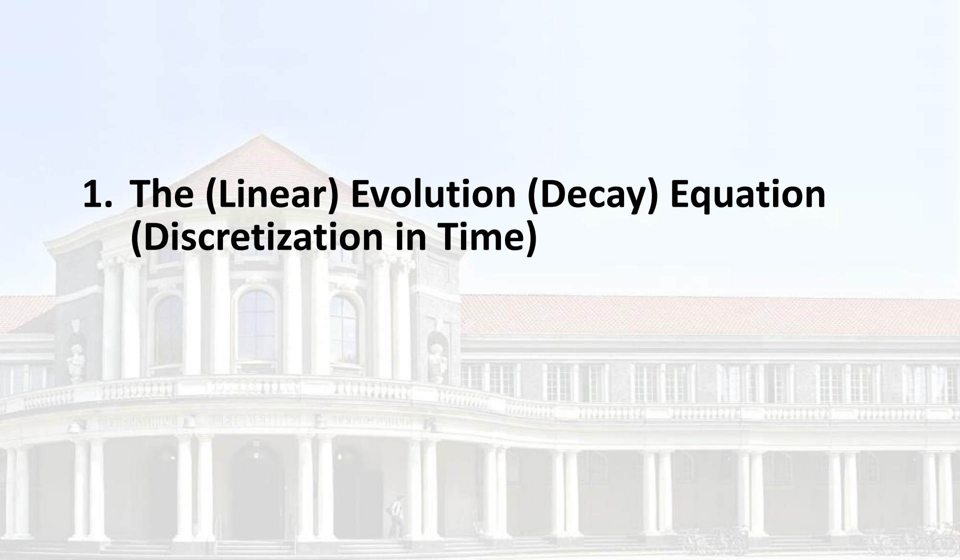
0. Introduction: The Problem and Basics

Summary:

- Reason to do numerics: No analytic solution of the problem
- Methods: Grid point method, spectral method, finite elements (,…)
- Finite Differences: forward, backward, central
- Evaluation: consistency, accuracy, convergence and stability

Introduction to Numerical Modeling



1. The (Linear) Evolution (Decay) Equation (Discretization in Time)

The (Linear) Evolution (Decay) Equation

equation:

$$\frac{\partial T}{\partial t} = -aT + F$$

note: with a imaginary, i.e. $a=ib$, und complex T, $T=T_R+iT_I$ an oscillation equation results: e.g. inertial oscillation:

$$1)\,\frac{\partial u}{\partial t} = fv,\quad 2)\,\frac{\partial v}{\partial t} = -fu \qquad \text{with}\quad \upsilon = u + iv \;\Rightarrow\; 3)\,\frac{\partial \upsilon}{\partial t} = -if\upsilon$$

$$\text{since}\quad \mathrm{Re}(3) = 1);\quad \mathrm{Im}(3) = 2)$$

Analytical Solution

equation: $$\frac{\partial T}{\partial t} = -aT + F$$

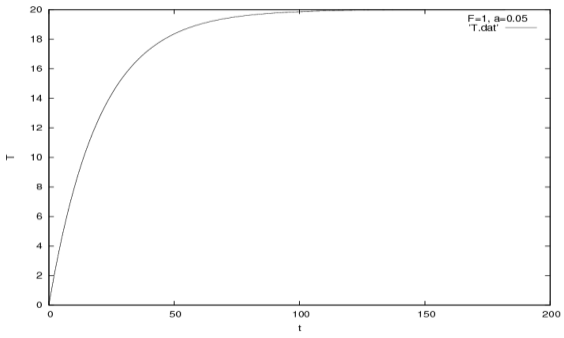
solution: $$T(t) = \Delta T \exp(-at) + \frac{F}{a}$$

Describes the exponential decay of an initial perturbation $\Delta T = T_0 - F/a$ (T_0=initial value) to the stationary solution F/a. *time scale:* $1/a$

initial value problem (T_0 needed; eq. is first order in time)

example:

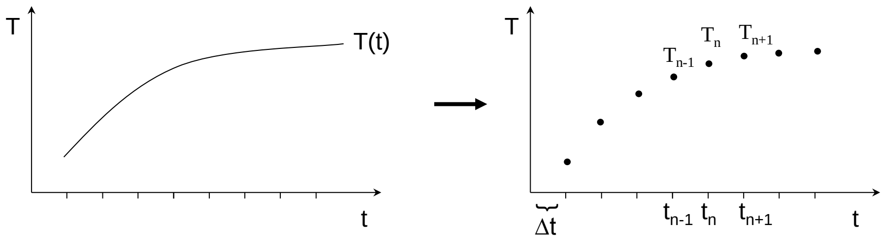
$T_0=0, F=1, a=0.05$



Numerical Solution

$$\frac{\partial T}{\partial t} = -aT + F$$

a) Discretization in time: $t \rightarrow t_0 + n\,\Delta t$ (Δt: **timestep**; n: integer)

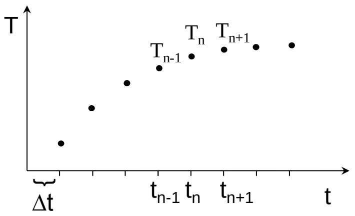


(continuous) (discrete)

timestep Δt must be chosen adequately (physically meaningful)!

Numerical Solution

$$\frac{\partial T}{\partial t} = -aT + F$$



b) Derivatives -> finite Differences

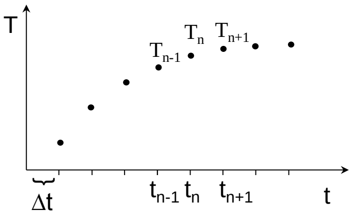
Backward differences $\frac{\partial T}{\partial t} = \frac{T_n - T_{n-1}}{\Delta t}$ Improper since *T(t)* known and *T(t+Δt)* needed

Forward differences $\frac{\partial T}{\partial t} = \frac{T_{n+1} - T_n}{\Delta t}$ Two level scheme (Einschritt-Verfahren)

Centered differences $\frac{\partial T}{\partial t} = \frac{T_{n+1} - T_{n-1}}{2\Delta t}$ Three level scheme (Zweischritt-Verfahren)

Numerical Solution

$$\frac{\partial T}{\partial t} = -aT + F$$



c) dealing with the ‚right hand side‘ (the tangent)

general: equation $\frac{\partial T}{\partial t} = f(T);$ discretization (two level) $\frac{T_{n+1} - T_n}{\Delta t} = f(T)$

Choice of T in *f(T)*:

$\frac{T_{n+1} - T_n}{\Delta t} = f(T_n)$ **Explicit (Euler)**

$\frac{T_{n+1} - T_n}{\Delta t} = f(T_{n+1})$ **Implicit**

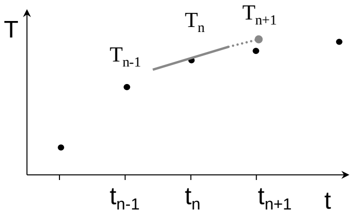
$\frac{T_{n+1} - T_n}{\Delta t} = f_{nl}(T_n) + f_{lin}(T_{n+1})$ **Semi-implicit**

(f_{nl}=nonlinear part; f_{lin}=linear part)

Explicit (Euler)

Discretization: $$\frac{T_{n+1}-T_n}{\Delta t}=f(T_n)\Rightarrow T_{n+1}=T_n+\Delta t\cdot f(T_n)$$

Tangent (gradient) at t_n , i.e. computed from T_n

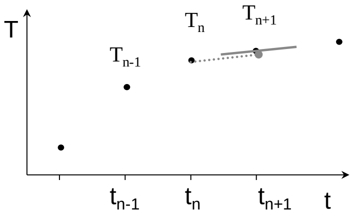


evolution (decay) equation: $$T_{n+1}=T_n-\Delta t\cdot(a\cdot T_n-F)$$

Implicit

Discretization: $$\frac{T_{n+1}-T_n}{\Delta t}=f(T_{n+1})\Rightarrow T_{n+1}=T_n+\Delta t\cdot f(T_{n+1})$$

Tangent (gradient) at t_{n+1} , i.e. computed from T_{n+1} but used at t_n.



A re-arrangement of the equation is necessary to obtain T_{n+1}!

evolution (decay) equation: $$\frac{T_{n+1}-T_n}{\Delta t}=-a\cdot T_{n+1}+F\Rightarrow T_{n+1}=\frac{T_n+\Delta t\cdot F}{1+\Delta t\cdot a}$$

Two Level Scheme: Explicit (Euler)

$$\frac{T_{n+1}-T_n}{\Delta t} = -aT_n + F \Rightarrow T_{n+1} = T_n - \Delta t \cdot (a \cdot T_n - F)$$

Consistency ($\frac{\partial T}{\partial t} = \lim\limits_{\Delta t \to 0} \left\| \frac{\Delta T}{\Delta t} \right\|$) **?** **Yes,** from Taylor-expansion:

$$T(t+\Delta t) = T(t) + \frac{\partial T}{\partial t}\Delta t + \frac{\partial^2 T}{\partial t^2}\frac{\Delta t^2}{2} + \ldots \Rightarrow \frac{T_{n+1}-T_n}{\Delta t} = \frac{\partial T}{\partial t} + \frac{\partial^2 T}{\partial t^2}\frac{\Delta t}{2} + \ldots$$

$$\Rightarrow \lim_{\Delta t \to 0}\left(\frac{T_{n+1}-T_n}{\Delta t}\right) = \lim_{\Delta t \to 0}\left(\frac{\partial T}{\partial t} + \frac{\partial^2 T}{\partial t^2}\frac{\Delta t}{2} + \ldots\right) = \frac{\partial T}{\partial t}$$

Accuracy (order) of the discretization: first order (Error goes with Δt)

Two Level Scheme: Explicit (Euler)

$$\frac{T_{n+1}-T_n}{\Delta t} = -aT_n + F \Rightarrow T_{n+1} = T_n - \Delta t \cdot (a \cdot T_n - F)$$

Accuracy (order) of the scheme? (here with $F=0$)

Ansatz: insert the analytic solution

$$\frac{T_A(t+\Delta t) - T_A(t)}{\Delta t} = -a \cdot T_A(t) + Err$$

Taylor-expansion:

$$T_A(t+\Delta t) = T_A(t) + \sum_{n=1}^{\infty} \frac{(\Delta t)^n}{n!}\frac{\partial^n T_A}{\partial t^n}$$

Insert the Taylor-expansion:

$$Err = \frac{T_A(t) + \sum_{n=1}^{\infty} \frac{(\Delta t)^n}{n!}\frac{\partial^n T}{\partial t^n} - T_A(t)}{\Delta t} + a \cdot T_A(t)$$

Since $-aT_A(t) = \frac{\partial T_A}{\partial t}$

$$\Rightarrow Err = \sum_{n=1}^{\infty} \frac{(\Delta t)^n}{(n+1)!}\frac{\partial^{n+1} T}{\partial t^{n+1}}$$

$$\boxed{\text{=> Err= O(1)}}$$

Two Level Scheme: Explicit (Euler)

$$\frac{T_{n+1}-T_n}{\Delta t} = -aT_n + F \Rightarrow T_{n+1} = T_n - \Delta t \cdot (a \cdot T_n - F)$$

Stability $\left\| T(t) - T_A(t) \right\| \underset{t\to\infty}{\rightarrow} \infty$ **?**

(F=0) analytically: $T_A(t) = \Delta T \exp(-at) \Rightarrow T_A(t_0 + n\Delta t) = \Delta T \exp(-an\Delta t)) \quad \Delta T = T(t_0)$

numerically: $T(t_0 + \Delta t) = \Delta T(1 - a\Delta t) \Rightarrow T(t_0 + n\Delta t) = \Delta T(1 - a\Delta t)^n$

=> Amplitude increases/diminishes with factor $A = (1 - a\Delta t)^n$

=> for $a \cdot \Delta t > 2 \Rightarrow |A| > 1 \Rightarrow \left\| T(t) - T_A(t) \right\| \underset{t\to\infty}{\rightarrow} \infty$ **(unstable)**

for $a \cdot \Delta t \le 2 \Rightarrow |A| \le 1 \Rightarrow \left\| T(t) - T_A(t) \right\|_{t\to\infty}$ bounded **(stable)**

but for $1 < a \cdot \Delta t \le 2 \quad (A < -1)$ +/- jumps

=> choice of Δ*t such that* $\boxed{\Delta t \le 1/a}$!

Convergence $(\lim_{\Delta t\to 0} \left\| T(t) - T_A(t) \right\| = 0)$ **?** **Yes** (from Lax equivalence theorem)

Note: $(1 - a\Delta t)^n \approx (1 - an\Delta t) = \exp(-an\Delta t) + O(\Delta t^2)$

Two Level Scheme: Implicit

$$\frac{T_{n+1}-T_n}{\Delta t} = -a \cdot T_{n+1} + F \Rightarrow T_{n+1} = \frac{T_n + \Delta t \cdot F}{1 + \Delta t \cdot a}$$

Consistency? **yes**, like explicit

Accuracy (Order)? First order scheme (i.e. error grows with Δ*t*)

Stability?

with *F=0*: $T(t + \Delta t) = \frac{T(t)}{(1 + a\Delta t)} \Rightarrow T(t + n\Delta t) = \frac{T(t)}{(1 + a\Delta t)^n}$

=> Amplitude diminishes with factor $A = \frac{1}{(1 + a\Delta t)^n}$

=> $\left\| T(t) - T_A(t) \right\| < C(t) \forall t$ For all Δ*t, since A* < 1

=> **implicit always stable**

but Δ*t* >*1/a* not appropriate to the problem!

Convergence? Yes

Two Level Scheme: Crank-Nicolson

$$\frac{T_{n+1}-T_n}{\Delta t}=-a\cdot(g\cdot T_n+(1-g)\cdot T_{n+1})+F$$

(g = 1 : explicit; g = 0 : implicit)

Consistency? **yes**, like explicit und implicit

Accuracy (Order)? (with $F=0$)

Insert analytical solution: $\frac{T_A(t+\Delta t)-T_A(t)}{\Delta t}=-a\cdot[g\cdot T_A(t)+(1-g)\cdot T_A(t+\Delta t)]+Err$

Taylor-expansion: $T_A(t+\Delta t)=T_A(t)+\sum_{n=1}^{\infty}\frac{(\Delta t)^n}{n!}\frac{\partial^n T_A}{\partial t^n}$

Insert Taylor-expansion: $Err=\frac{T_A(t)+\sum_{n=1}^{\infty}\frac{(\Delta t)^n}{n!}\frac{\partial^n T}{\partial t^n}-T_A(t)}{\Delta t}+a[gT_A(t)+(1-g)(T_A(t)+\sum_{n=1}^{\infty}\frac{(\Delta t)^n}{n!}\frac{\partial^n T}{\partial t^n})]$

$\Rightarrow Err=\sum_{n=1}^{\infty}\frac{(\Delta t)^n}{n!}\frac{\partial^{n+1}T}{\partial t^{n+1}}\underbrace{(g-\frac{1}{n+1})}_{=0 \text{ for } n=1 \text{ and } g=0.5}$ => for g= 1,0 (ex., im.): Err= O(1); **for** $\boxed{\mathbf{g=0.5: Err=O(2)}}$)

Two Level Scheme: Crank-Nicolson

$$\frac{T_{n+1}-T_n}{\Delta t}=-a\cdot(g\cdot T_n+(1-g)\cdot T_{n+1})+F$$

Stability?

with $F=0$: $T(t+\Delta t)=T(t)-a\cdot\Delta t\cdot(g\cdot T(t)+(1-g)\cdot T(t+\Delta t))$

$$\Rightarrow T(t+\Delta t)=T(t)\frac{(1-ga\Delta t)}{(1+(1-g)a\Delta t)}\Rightarrow T(t+n\Delta t)=T(t)\left[\frac{(1-ga\Delta t)}{(1+(1-g)a\Delta t)}\right]^n$$

=> Amplitude changes with factor $A=\left[\frac{(1-ga\Delta t)}{(1+(1-g)a\Delta t)}\right]^n$

=> $\|T(t)-T_A(t)\|<C(t)\forall t$ For all Δt, |A| < 1 (denominator > numerator)

=> $\boxed{\text{always stable } \textbf{(for } g \textbf{ <1)}}$

but: $\Delta t > 1/a$ not appropriate to the problem

=> Convergence

Two Level Scheme: 4th order Runge-Kutta

General equation: $\frac{dT}{dt} = f(T,t)$

Runge-Kutta (4th order): $T(t+\Delta t) = T(t) + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4)$

$$\text{with} \quad K_1 = \Delta t \cdot f(T(t),t)$$

$$K_2 = \Delta t \cdot f(T(t) + \frac{K_1}{2}, t + \frac{\Delta t}{2})$$

$$K_3 = \Delta t \cdot f(T(t) + \frac{K_2}{2}, t + \frac{\Delta t}{2})$$

$$K_4 = \Delta t \cdot f(T(t) + K_3, t + \Delta t)$$

Order: $Err = O(\Delta t^4)$

Decay equation: $f(T,t) = -a \cdot T + F = f(T)$ (not explicitly dependent on t)

Stability: Stable for $|1 - a\Delta t + \frac{a^2 \Delta t^2}{2} - \frac{a^3 \Delta t^3}{6} + \frac{a^4 \Delta t^4}{24}| \leq 1$

Two level scheme: 4th order Runge-Kutta

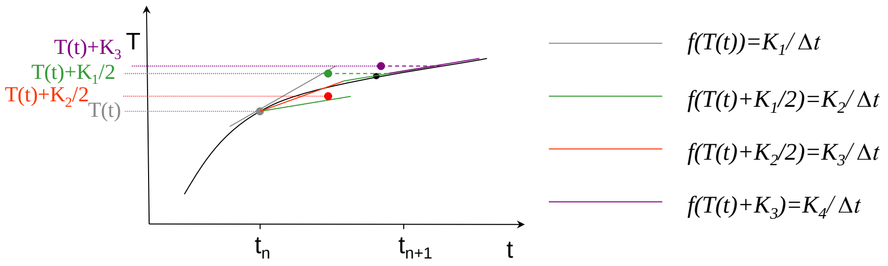
$T(t+\Delta t) = T(t) + \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4)$

$K_1 = \Delta t \cdot f(T(t),t), K_2 = \Delta t \cdot f(T(t) + \frac{K_1}{2}, t + \frac{\Delta t}{2})$

$K_3 = \Delta t \cdot f(T(t) + \frac{K_2}{2}, t + \frac{\Delta t}{2}), K_4 = \Delta t \cdot f(T(t) + K_3, t + \Delta t)$

Idea: Average of tangents for different T ($T(t)$, $T(t)+K_1/2$, $T(t)+K_2/2$, $T(t)+K_3$)

with ‚artificial' base points $T(t)+K_i$



Expensive since $f(T)$ needs to be computed 4 times

Three Level Schemes

General: three level schemes do not only consider time *t* und *t*+Δ*t* but also time *t*-Δ*t*.
e.g. From Taylor-expansion:

$$T(t+\Delta t)=T(t)+\frac{dT}{dt}|_t\,\Delta t+\frac{d^2T}{dt^2}|_t\,\frac{\Delta t^2}{2}+\frac{d^3T}{dt^3}|_t\,\frac{\Delta t^3}{6}+\ldots$$

$$T(t-\Delta t)=T(t)-\frac{dT}{dt}|_t\,\Delta t+\frac{d^2T}{dt^2}|_t\,\frac{\Delta t^2}{2}-\frac{d^3T}{dt^3}|_t\,\frac{\Delta t^3}{6}+\ldots$$

$$\Rightarrow \boxed{\frac{dT}{dt}=\frac{T(t+\Delta t)-T(t-\Delta t)}{2\Delta t}+\frac{d^3T}{dt^3}|_t\,\frac{\Delta t^2}{6}+\ldots}$$

=> Discretization is **consistent, 2nd Order (*Err*=*O*(Δ*t*²))**

Decay equation:

$$\boxed{\frac{T(t+\Delta t)-T(t-\Delta t)}{2\Delta t}=-a\cdot T(t)+F}$$

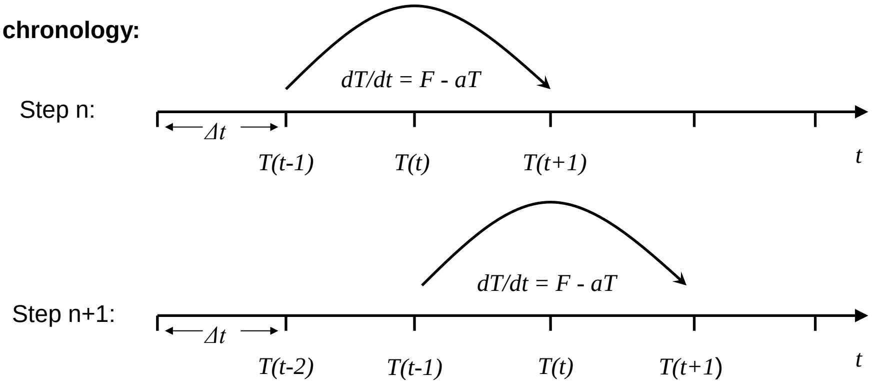
Leap frog

Leap Frog

$$\frac{T(t+\Delta t)-T(t-\Delta t)}{2\Delta t}=-a\cdot T(t)+F\Rightarrow T(t+\Delta t)=T(t-\Delta t)+2\Delta t(-a\cdot T(t)+F)$$

i.e. evaluation of the gradient at *t* for step *T(t-Δt)-> T(t+Δt)*

chronology:



Two time levels are needed (*t-1* and *t*)!

Leap Frog

$$\frac{T(t+\Delta t)-T(t-\Delta t)}{2\Delta t}=-a\cdot T(t)+F\Rightarrow T(t+\Delta t)=T(t-\Delta t)+2\Delta t(-a\cdot T(t)+F)$$

Stability (Computational Mode)?

$$(\text{with F}=0:)\qquad T^{n+1}=T^{n-1}-2\Delta t\cdot a\cdot T^{n}$$

Assumption: T changes each time step by factor λ

$$T^{n+1}=\lambda\cdot T^{n}=\lambda^{2}\cdot T^{n-1}$$

$$\Rightarrow\lambda^{2}\cdot T^{n-1}=T^{n-1}-2\Delta t\cdot a\cdot\lambda\cdot T^{n-1}$$

i.e. two solutions:

$$\lambda_{1,2}=-a\Delta t\pm\left(a^{2}\Delta t^{2}+1\right)^{1/2}$$

For Δt ->0 : $\lambda_1=1$ (physical since correct); $\lambda_2=-1$ (unphysical)

For $\Delta t > 0$: *physical mode* $0 < \lambda_1 < 1$ *(attenuation)*
computational Mode $\lambda_2 < -1$ i.e. **oscillating instability**!

Leap Frog not suited for damped (dissipative) systems!

Leap Frog: Unstable Computational Mode

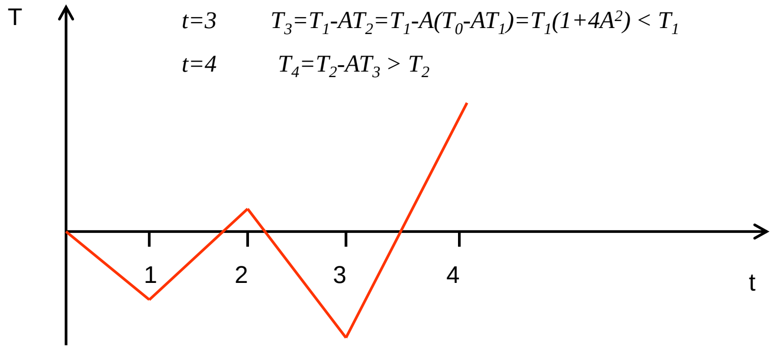
$$T_{t+1}=T_{t-1}-2\Delta taT_{t}=T_{t-1}-AT_{t}$$

Leap-Frog initialization $T_0=0$; $T_1<0$

$t=2$ $T_2=T_0-AT_1= 0-AT_1 > 0$

$t=3$ $T_3=T_1-AT_2=T_1-A(T_0-AT_1)=T_1(1+4A^2) < T_1$

$t=4$ $T_4=T_2-AT_3 > T_2$



Three Level Scheme: Adams-Bashforth(2)

$$\frac{T(t+\Delta t)-T(t)}{\Delta t}=-\frac{a}{2}\cdot(3T(t)-T(t-\Delta t))+F$$

gradient by averaging gradient from $T(t)$ and gradient from ‚extrapolated' $T'(t+\Delta t)$ $(=T(t)+(T(t)-T(t-\Delta t)))$

consistent and 2nd order (*Err=O(*Δt^2*)*)

stability (computational mode)?

$$(\text{with F}=0:)\qquad T^{n+1}=T^n-\frac{\Delta t\cdot a}{2}\cdot(3T^n-T^{n-1})=T^n(1-\frac{3\Delta t\cdot a}{2})+T^{n-1}\frac{\Delta t\cdot a}{2}$$

$$T^{n+1}=\lambda\cdot T^n=\lambda^2\cdot T^{n-1}\qquad\Rightarrow\lambda^2-\lambda(1-\frac{3\Delta t\cdot a}{2})=\frac{\Delta t\cdot a}{2}$$

i.e. two solutions:

$$\lambda_{1,2}=\frac{(1-\frac{3a\Delta t}{2})}{2}\pm\left(\frac{a\ \Delta t}{2}+\frac{(1-\frac{3a\Delta t}{2})^2}{4}\right)^{1/2}$$

for $\Delta t \rightarrow 0$: $\lambda_1=1$ (physical, correct solution); $\lambda_2=0$ (unphysical)

for $\Delta t > 0$: *physical mode* $0 < \lambda_1 < 1$ *(damped)*
computational mode $0 < \lambda_2 < 1$ (damped) => stability!

The (Linear) Evolution (Decay) Equation

Summary:

- Decay (linear evolution) equation: first order in time, initial value
- Schemes: implicit, explicit, semi-implicit, two-level, three-level
- Specific schemes: Euler, Crank-Nicolson, Runge-Kutta, Leapfrog, Adams-Bashford
- Computational mode
- Leapfrog unstable for dissipative systems!

Introduction to Numerical Modeling

2. One-Dimensional Linear Advection (Discretization in Time and Space)

The Linear 1-d Advection Equation

equation: $$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x}$$ u=const.

hyperbolic, first order in time and space: initial and boundary conditions needed

---

$$a\frac{\partial^2 T}{\partial t^2} + b\frac{\partial^2 T}{\partial t \partial x} + c\frac{\partial^2 T}{\partial x^2} + d\frac{\partial T}{\partial t} + e\frac{\partial T}{\partial x} + f = 0$$

hyperbolic: $b^2\text{-}4ac > 0$

parabolic: $b^2\text{-}4ac = 0$

elliptic: $b^2\text{-}4ac < 0$

---

analytical solution: $$T(x,t) = f(x-ut)$$ with any function f

example: $$T(x,t) = \sum_k T_k \exp(ik(x-ut))$$

Superposition of waves with wave number k and phase velocity u

Numerical Solution: Spectral Method

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x}$$

Idea: transformation of T into new basis functions which are differentiable orthogonal functions of x => derivations in space can be calculated analytically.

Example: Fourier-series $T(t,x) = \sum_{k=-N}^{N} T_k(t)\exp(ikx)$

$T_k(t)$ = time dependent (complex) Fourier coeff.; N = considered modes (resolution)

(N<< ∞ => T might not be perfectly represented)

Insert into advection equation: => $\sum_{k=-N}^{N}\frac{\partial T_k(t)}{\partial t}\exp(ikx) = -u\sum_{k=-N}^{N} ikT_k(t)\exp(ikx)$

=> $2N+1$ uncoupled ordinary differential equations $\boxed{\frac{\partial T_k}{\partial t} = -iukT_k}$

Spectral Method

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x} \quad \rightarrow \quad \frac{\partial T_k}{\partial t} = -iukT_k$$

$\frac{\partial T_k}{\partial t} = -iukT_k$ Similar to the evolution (decay) equation but with imaginary *a=iuk and complex T (oscillation equation)*

Analytical solution: $T_k = T_k^0\exp(-iukt)$

=> complete solution of the advection eq: $T = \sum_k T_k^0\exp(ik(x-ut))$ (as expected)

=> local: oscillation, global: non dispersive waves with phase velocity u

Spectral Method: Explicit

$$\frac{\partial T}{\partial t}=-u\frac{\partial T}{\partial x} \qquad \rightarrow \qquad \frac{\partial T_k}{\partial t}=-iukT_k$$

Numerical solution: Analog to evolution (decay) eq. but: different characteristics

example: explicit (Euler) $\frac{\partial T}{\partial t}=-iukT \quad \rightarrow \quad \frac{T(t+\Delta t)-T(t)}{\Delta t}=-iukT(t)$ (one wave k only, index k omitted)

Stability?

$$\frac{T(t+\Delta t)-T(t)}{\Delta t}=-iukT(t)$$

$$\Rightarrow T(t+\Delta t)=T(t)(1-iuk\Delta t)=T(t)A\exp(i\phi)$$

$$\text{with } \; A=\left|(1-iuk\Delta t)\right|=\sqrt{1+(uk\Delta t)^2}$$

$$\text{and } \phi=\arctan(-uk\Delta t)\approx -uk\Delta t+\frac{(uk\Delta t)^3}{3}=-uk\Delta t(1-\frac{(uk\Delta t)^2}{3})$$

$$\Rightarrow \text{a) Amplitude increases with A} = \sqrt{1+(uk\Delta t)^2}\approx 1+\frac{(uk\Delta t)^2}{2}>1$$

always unstable

$$\text{b) Phase error } \frac{\phi_N}{\phi_A}\approx 1-\frac{(uk\Delta t)^2}{3} \text{ since } \phi_A(\mathit{analytically})=-uk\Delta t$$

slower and *k*-dependent, i.e. **numerical dispersion**

Spectral Method: Implicit

$$\frac{\partial T}{\partial t}=-u\frac{\partial T}{\partial x} \qquad \rightarrow \qquad \frac{\partial T_k}{\partial t}=-iukT_k$$

example: implicit $\frac{\partial T}{\partial t}=-iukT \quad \rightarrow \quad \frac{T(t+\Delta t)-T(t)}{\Delta t}=-iukT(t+\Delta t)$

Stability? $\frac{T(t+\Delta t)-T(t)}{\Delta t}=-iukT(t+\Delta t)$

$$\Rightarrow T(t+\Delta t)=\frac{T(t)}{(1+iuk\Delta t)}=T(t)A\exp(i\phi)$$

$$\text{with } \; A=\sqrt{\frac{1}{1+(uk\Delta t)^2}}$$

$$\text{and } \phi=\arctan(-uk\Delta t)\approx -uk\Delta t+\frac{(uk\Delta t)^3}{3}=-uk\Delta t(1-\frac{(uk\Delta t)^2}{3})$$

$$\Rightarrow \text{a) Amplitude decreases}$$

always stable but k-dependent damping, i.e. **numerical diffusion**

$$\text{b) Phase error } \frac{\phi_N}{\phi_A}\approx 1-\frac{(uk\Delta t)^2}{3} \text{ since } \phi_A(\mathit{analytically})=-uk\Delta t$$

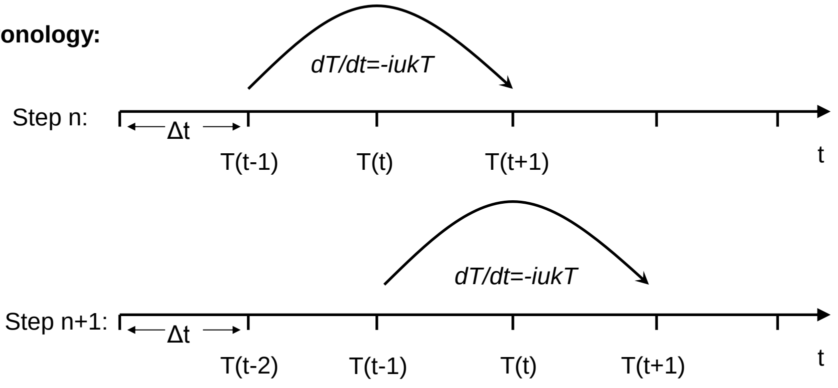
slower and *k*-dependent, i.e. **numerical dispersion**

Spectral Method: Leap Frog

Leap frog: $$\frac{\partial T}{\partial t} = -iukT \quad \rightarrow \quad \frac{T_{n+1}-T_{n-1}}{2\Delta t} = -iukT_n$$

Recall:

chronology:



Spectral Method: Leap Frog

Leap frog: $$\frac{\partial T}{\partial t} = -iukT \quad \rightarrow \quad \frac{T_{n+1}-T_{n-1}}{2\Delta t} = -iukT_n$$

Stability?

$$\frac{T(t+\Delta t)-T(t-\Delta t)}{2\Delta t} = -iukT(t) \Rightarrow T(t+\Delta t) = T(t-\Delta t) - 2iuk\Delta t T(t)$$

$$\text{with } T(t+\Delta t) = \lambda \cdot T(t) \Rightarrow \lambda^2 - 2iuk\Delta t - 1 = 0 \Rightarrow \lambda = iuk\Delta t \pm \sqrt{1-(uk\Delta t)^2}$$

$\Rightarrow$ a) $\boxed{\text{Two solutions}}$ (physical(+) and 'computational' (-) mode)

b) with $(uk\Delta t)^2 < 1 \Rightarrow |\lambda| = 1$ $\boxed{\text{(both modes neutral)}}$

c) phase error : $\frac{1}{uk\Delta t}\arctan\left(\frac{\pm uk\Delta t}{\sqrt{1-(uk\Delta t)^2}}\right) \approx \pm\left(1+\frac{(uk\Delta t)^2}{6}\right)$ $\boxed{\text{(faster)}}$

(computational (-) mode 180° out of phase)

Leapfrog appropriate (but numerical dispersion); computational mode bothers

Leap Frog: Computational Mode

equation: $\frac{\partial T}{\partial t} = -iukT$ with k=0 (advection of the zonal mean) $\Rightarrow \frac{\partial T}{\partial t} = 0$

$$\Rightarrow \text{a) (Leap frog)} \quad \frac{T(t+\Delta t) - T(t-\Delta t)}{2\Delta t} = 0 \Rightarrow T(t+\Delta t) = T(t-\Delta t)$$

$$\text{b) (amplitude change } \lambda\text{)} \; \lambda = iuk\Delta t \pm \sqrt{1-(uk\Delta t)^2} = \pm 1$$

initial condition: $T(t=0)=T_0$ $\overset{\text{a)}}{\Rightarrow} T(2\Delta t) = T(4\Delta t) = T(6\Delta t) = \ldots = T_0$ even Δt correct

problem: $T(\Delta t)$ needed but unknown (in most cases computed with Euler).

let $T(\Delta t)=T_0+E$ (E=small error) $\Rightarrow$ complete solution: $T(n\Delta t) = (T_0 + \frac{E}{2}) - (-1)^n \frac{E}{2}$

$$\Rightarrow \text{a) physical mode } (\lambda = 1): (T_0 + \frac{E}{2})$$

$$\text{b) computational mode } (\lambda = \text{-}1): \frac{E}{2}$$

the computational mode is determined by the initialization error (E) only

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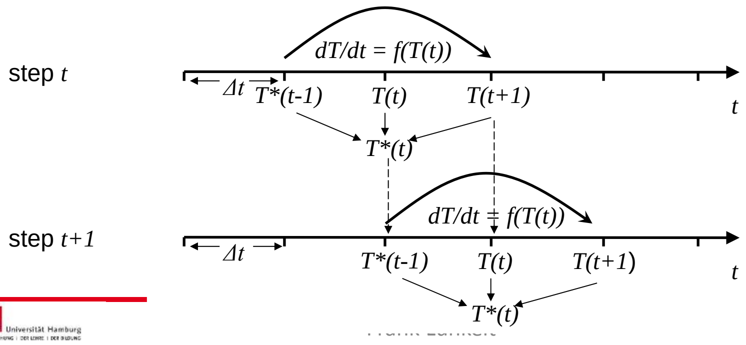
Leap Frog: Robert-Asselin Filter

Modification of the leap frog scheme:

Computation of $T(t)$ (or $T(t-\Delta t)$) by weighted averages of $T(t+\Delta t)$, $T(t)$ and $T(t-\Delta t)$

Calculation role:
1. $T(t+\Delta t) = T^*(t-\Delta t) + 2\Delta t \cdot f(T(t))$
2. $T^*(t) = T(t) + \gamma(T^*(t-\Delta t) - 2T(t) + T(t+\Delta t))$ $(\gamma = \textit{filter const.})$
3. $T^*(t) \rightarrow T^*(t-\Delta t)$; $T(t+\Delta t) \rightarrow T(t)$



Leap Frog with Robert-Asselin Filter

Stability?

a) $T_{t+1} = T^*_{t-1} - i2\Delta tukT_t$

b) $T^*_t = T_t + \gamma(T^*_{t-1} - 2T_t + T_{t+1})$

$$\frac{\partial T}{\partial t} = -iukT$$

T_{t+1} from a) insert into b)
(plus rearrange):

$$T_{t+1} = T^*_{t-1} - i2\Delta tukT_t$$
$$T^*_t = T_t(1 - 2\gamma - i2\gamma\Delta tuk) + 2\gamma T_{t-1}$$

Matrix-formulation:

$$\underset{\text{new}}{\begin{pmatrix} T_{t+1} \\ T^*_t \end{pmatrix}} = \underset{\text{transition-matrix}}{\begin{pmatrix} -i2\Delta tuk & 1 \\ 1 - 2\gamma - i2\gamma\Delta tuk & 2\gamma \end{pmatrix}} \underset{\text{old}}{\begin{pmatrix} T_t \\ T^*_{t-1} \end{pmatrix}} \quad \underset{\text{Eigenvalue problem}}{\equiv \mathrm{A} \cdot X = \lambda \cdot X}$$

Eigenvalues λ_i from

$$\begin{pmatrix} -i2\Delta tuk - \lambda & 1 \\ 1 - 2\gamma - i2\gamma\Delta tuk & 2\gamma - \lambda \end{pmatrix} = 0 \Rightarrow \begin{array}{l} \lambda_1 = -(iuk\Delta t - \gamma) + \left((1-\gamma)^2 - (uk\Delta t)^2\right)^{1/2} \\ \lambda_2 = -(iuk\Delta t - \gamma) - \left((1-\gamma)^2 - (uk\Delta t)^2\right)^{1/2} \end{array}$$

- For $(uk\Delta t)^2 < (1-\gamma)^2$ the scheme is always stable!
- For $\Delta t \to 0$: $\lambda_1 = 1$ (physical, neutral); $\lambda_2 = 2\gamma - 1$ (computational, damped)
- For $\Delta t > 0$: $|\lambda_2| < |\lambda_1| < 1$, i.e. both modes damped, stronger for computational
- Damping k dependent (larger k stronger damp.): **Numerical diffusion**
- **Numerical dispersion** (k dependent phase error)

Grid Point Method: Finite Differences

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x}$$

Discretization in space and time, i.e. space and time derivatives are approximated by differences.

Two level schemes (explicit):

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x} \rightarrow \frac{T^{n+1}_j - T^n_j}{\Delta t} = -u\frac{T^n_{j+1} - T^n_{j-1}}{2\Delta x}$$

centered differences

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x} \rightarrow \frac{T^{n+1}_j - T^n_j}{\Delta t} = -u\frac{T^n_{j+1} - T^n_j}{\Delta x}$$

downstream (u>0)

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x} \rightarrow \frac{T^{n+1}_j - T^n_j}{\Delta t} = -u\frac{T^n_j - T^n_{j-1}}{\Delta x}$$

upstream (u>0)

n = time; j = space

Finite Differences

Two level scheme (Einschritt-Verfahren): accuracy and order

a) centered differences:

$$\frac{T(x,t+\Delta t)-T(x,t)}{\Delta t}=-u\frac{T(x+\Delta x,t)-T(x-\Delta x,t)}{2\Delta x}+Err$$

$$\Rightarrow\frac{T(x,t)+\sum\frac{(\Delta t)^n}{n!}\frac{\partial^n T}{\partial t^n}-T(x,t)}{\Delta t}=-u\frac{T(x,t)+\sum\frac{(\Delta x)^n}{n!}\frac{\partial^n T}{\partial x^n}-T(x,t)-\sum(-1)^n\frac{(\Delta x)^n}{n!}\frac{\partial^n T}{\partial x^n}}{2\Delta x}+Err$$

$$\Rightarrow Err=\frac{\sum\frac{(\Delta t)^n}{n!}\frac{\partial^n T}{\partial t^n}}{\Delta t}+u\frac{\sum\frac{(\Delta x)^n}{n!}\frac{\partial^n T}{\partial x^n}-\sum(-1)^n\frac{(\Delta x)^n}{n!}\frac{\partial^n T}{\partial x^n}}{2\Delta x}$$

$$\Rightarrow Err=\cancel{\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}}+\sum_{n=2}\frac{(\Delta t)^{n-1}}{n!}\frac{\partial^n T}{\partial t^n}+u(\sum_{n=2}\frac{(\Delta x)^{n-1}}{n!}\frac{\partial^n T}{\partial x^n}-\sum_{n=2}(-1)^n\frac{(\Delta x)^{n-1}}{n!}\frac{\partial^n T}{\partial x^n})=\boxed{O(\Delta t)+O(\Delta x^2)}$$

2nd order in Δx

1st order in Δ t

Finite Differences

Two level scheme: accuracy and order

b) Downsteam:

$$\frac{T(x,t+\Delta t)-T(x,t)}{\Delta t}=-u\frac{T(x+\Delta x,t)-T(x,t)}{\Delta x}+Err$$

$$\Rightarrow\frac{T(x,t)+\sum\frac{(\Delta t)^n}{n!}\frac{\partial^n T}{\partial t^n}-T(x,t)}{\Delta t}=-u\frac{T(x,t)+\sum\frac{(\Delta x)^n}{n!}\frac{\partial^n T}{\partial x^n}-T(x,t)}{\Delta x}+Err$$

$$\Rightarrow Err=\cancel{\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}}+\sum_{n=2}\frac{(\Delta t)^{n-1}}{n!}\frac{\partial^n T}{\partial t^n}+u\sum_{n=2}\frac{(\Delta x)^{n-1}}{n!}\frac{\partial^n T}{\partial x^n}=\boxed{O(\Delta t)+O(\Delta x)}$$

1st order in Δx and Δ t

c) Upsteam:

$$\frac{T(x,t+\Delta t)-T(x,t)}{\Delta t}=-u\frac{T(x,t)-T(x-\Delta x,t)}{\Delta x}+Err$$

$$\Rightarrow\frac{T(x,t)+\sum\frac{(\Delta t)^n}{n!}\frac{\partial^n T}{\partial t^n}-T(x,t)}{\Delta t}=-u\frac{T(x,t)-T(x,t)-\sum(-1)^n\frac{(\Delta x)^n}{n!}\frac{\partial^n T}{\partial x^n}}{\Delta x}+Err$$

$$\Rightarrow Err=\cancel{\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}}+\sum_{n=2}\frac{(\Delta t)^{n-1}}{n!}\frac{\partial^n T}{\partial t^n}+u\sum_{n=2}(-1)^n\frac{(\Delta x)^{n-1}}{n!}\frac{\partial^n T}{\partial x^n}=\boxed{O(\Delta t)+O(\Delta x)}$$

1st order in Δx and Δ t

Finite Differences: Stability

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x}$$

Two level scheme: **Stability**

a) centered differences: $$\frac{T_j^{n+1}-T_j^n}{\Delta t} = -u\frac{T_{j+1}^n - T_{j-1}^n}{2\Delta x} \Rightarrow T_j^{n+1} = T_j^n - \frac{u\Delta t}{2\Delta x}(T_{j+1}^n - T_{j-1}^n) \quad (1)$$

1. Energy Method

general: take a (scalar) quadratic norm for the total ‚energy' (E) in the space state of the system and show that E remains bounded with time.

Advantage: applicable also for non linear problems.   Disadvantage: definition of *E* needed

Here: $E = \sum_j (T_j)^2$

square (1) and sum up: $$\sum_j (T_j^{n+1})^2 = \sum_j (T_j^n - \mu(T_{j+1}^n - T_{j-1}^n))^2 \qquad \mu = \frac{u\Delta t}{2\Delta x}$$
$$= \sum_j (T_j^n)^2 - 2\mu T_j^n (T_{j+1}^n - T_{j-1}^n) + \mu^2 (T_{j+1}^n - T_{j-1}^n)^2$$

cyclic boundary conditions: $$\Rightarrow \sum_j (T_j^{n+1})^2 = \sum_j (T_j^n)^2 + 2\mu^2((T_j^n)^2 - (T_{j-1}^n T_{j+1}^n))$$

Schwarz'sche inequality: $$\Rightarrow \sum_j (T_j^{n+1})^2 \geq \sum_j (T_j^n)^2 \quad \forall \mu$$

$$\sum_j (T_{j-1}^n T_{j+1}^n)^2 \leq \sum_j (T_j^n)^2$$

=> unstable

Finite Differences: Stability

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x}$$

Two level scheme: **Stability**

a) centered differences: $$\frac{T_j^{n+1}-T_j^n}{\Delta t} = -u\frac{T_{j+1}^n - T_{j-1}^n}{2\Delta x} \Rightarrow T_j^{n+1} = T_j^n - \frac{u\Delta t}{2\Delta x}(T_{j+1}^n - T_{j-1}^n) \quad (1)$$

2. Von Neumann Method

General: Linearize the problem. Replace dependence in space by Fourier expansion (analytical). Investigate the ‚amplification factor' A of one time step ($T^{n+1}=AT^n$). The scheme is stable if $|A|\leq 1$.

Advantage: Relatively easy. Disadvantage: Linearization

Here: already linear, Fourier-expansion: $T_j(t) = \sum_k T_k(t)e^{ikj\Delta x}$ linear -> only one k to consider

Insert into (1): $$\Rightarrow AT^n e^{ikj\Delta x} = T^n e^{ikj\Delta x} - \mu T^n (e^{ik(j+1)\Delta x} - e^{ik(j-1)\Delta x}) \qquad \mu = \frac{u\Delta t}{\Delta x}$$
$$\Rightarrow A = 1 - \mu(e^{ik\Delta x} - e^{-ik\Delta x}) = 1 - i\mu\sin(k\Delta x)$$
$$\Rightarrow A = |A|e^{i\varphi} \text{ with } |A| = (1+\mu^2\sin^2(k\Delta x))^{1/2} \quad \varphi = \arctan(-\mu\sin(k\Delta x))$$

Numerical solution (k): $$T_k(t+\Delta t) = |A|T_k(t)e^{i\varphi}$$

=>

1. Amplification factor |A| > 1 => unstable

2. Phase error since $\varphi \neq -uk\Delta t$ (=analytical solution)

Finite Differences: Stability

Two level scheme: **Stability analysis**

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x}$$

b) Downstream: $\frac{T_j^{n+1} - T_j^n}{\Delta t} = -u\frac{T_{j+1}^n - T_j^n}{\Delta x} \quad \Rightarrow T_j^{n+1} = T_j^n - u\Delta t\frac{T_{j+1}^n - T_j^n}{\Delta x}$ (1)

Von Neumann method ($T_j(t) = \sum_k T_k(t) e^{ikj\Delta x}$; investigate $T^{n+1} = AT^n$)

Insert into (1): $\Rightarrow AT^n e^{ikj\Delta x} = T^n e^{ikj\Delta x} - \mu T^n (e^{ik(j+1)\Delta x} - e^{ikj\Delta x})$ $\quad \mu = \frac{u\Delta t}{\Delta x}$

$$\Rightarrow A = 1 - \mu(e^{ik\Delta x} - 1) = 1 + \mu(1 - \cos(k\Delta x)) - i\mu\sin(k\Delta x)$$

$$\Rightarrow A = |A| e^{i\varphi}$$

with $|A| = (1 + 2\mu(1 - \cos(k\Delta x))(1 - \mu))^{1/2} \quad \varphi = \arctan\left(-\frac{\mu\sin(k\Delta x)}{1 + \mu(1 - \cos(k\Delta x))}\right)$

Numerical solution (k): $T_k(t + \Delta t) = |A| T_k(t) e^{i\varphi}$

=>

1. amplification factor |A| > 1 => unstable

2. Phase error since $\varphi \neq -uk\Delta t$ (=analytical solution)

Finite Differences: Stability

Two level scheme: **Stability analysis**

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x}$$

c) Upstream: $\frac{T_j^{n+1} - T_j^n}{\Delta t} = -u\frac{T_j^n - T_{j-1}^n}{\Delta x} \quad \Rightarrow T_j^{n+1} = T_j^n - u\Delta t\frac{T_j^n - T_{j-1}^n}{\Delta x}$ (1)

Von Neumann method ($T_j(t) = \sum_k T_k(t) e^{ikj\Delta x}$; investigate $T^{n+1} = AT^n$)

Insert into (1): $\Rightarrow AT^n e^{ikj\Delta x} = T^n e^{ikj\Delta x} - \mu T^n (e^{ikj\Delta x} - e^{ik(j-1)\Delta x})$ $\quad \mu = \frac{u\Delta t}{\Delta x}$

$$\Rightarrow A = 1 - \mu(1 - e^{-ik\Delta x}) = 1 - \mu(1 - \cos(k\Delta x)) - i\mu\sin(k\Delta x)$$

$$\Rightarrow A = |A| e^{i\varphi}$$

with $|A| = (1 - 2\mu(1 - \cos(k\Delta x))(1 - \mu))^{1/2} \quad \varphi = \arctan\left(-\frac{\mu\sin(k\Delta x)}{1 - \mu(1 - \cos(k\Delta x))}\right)$

Stable for $|A| \leq 1 \Rightarrow 1 - 2\mu(1 - \cos(k\Delta x))(1 - \mu) \leq 1 \Rightarrow 1 - 2\mu((1 - \mu) \leq 1$ since $(1 - \cos(k\Delta x)) > 0$

$$\Rightarrow 2\mu(1 - \mu) \geq 0 \Rightarrow 0 \leq \mu \leq 1$$

=> Upstream stable for $0 \leq \frac{u\Delta t}{\Delta x} \leq 1$ Courant-Friedrich-Levy criterion

$\frac{u\Delta t}{\Delta x}$ = Courant-number

Finite Differences: Upstream

One level scheme: **Upstream** $T_j^{n+1} = T_j^n - u\Delta t \frac{T_j^n - T_{j-1}^n}{\Delta x}$ with $u > 0$

Numerical solution (one wave k): $T_k(t+\Delta t) = |A| T_k(t) e^{i\varphi}$

with $|A| = (1 - 2\mu(1-\cos(k\Delta x))(1-\mu))^{1/2}$ $\varphi = \arctan\left(-\frac{\mu \sin(k\Delta x)}{1-\mu(1-\cos(k\Delta x))}\right)$ $\mu = \frac{u\Delta t}{\Delta x}$

For small Δx: $|A| = (1 - 2\mu(1-\cos(k\Delta x))(1-\mu))^{1/2} \approx (1 - \mu k^2 \Delta x^2 (1-\mu))^{1/2}$

$$\approx 1 - \frac{\mu k^2 \Delta x^2 (1-\mu)}{2} \approx 1 - (1-\mu)\left[\frac{uk^2 \Delta x \Delta t}{2} + \dots\right]$$

$$\varphi = \arctan\left(-\frac{\mu \sin(k\Delta x)}{1-\mu(1-\cos(k\Delta x))}\right)$$

Error

$$\approx -\mu k \Delta x\left(1 - \frac{k^2\Delta x^2}{6} - \frac{\mu^2 k^2 \Delta x^2}{3} + \dots\right) = -uk\Delta t\left(1 \boxed{- \frac{k^2\Delta x^2}{6} - \left(\frac{u\Delta t}{\Delta x}\right)^2 \frac{\mu k^2 \Delta x^2}{3} + \dots}\right)$$

- $|A|<1$ => **Numerical diffusion** (for $\mu<1$; stronger damping for larger k; $O(\mu\Delta x^2)$)
- Phase error k-dependent => **Numerical dispersion** (slower; $O(\Delta x^2)$)

Finite Differences: Leap Frog

Three level scheme: Leapfrog $\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x} \rightarrow \frac{T_j^{n+1} - T_j^{n-1}}{2\Delta t} = -u\frac{T_{j+1}^n - T_{j-1}^n}{2\Delta x}$

Stability: Von Neumann method ($T_j(t) = \sum_k T_k(t) e^{ikj\Delta x}$; investigate $T^{n+1} = AT^n$)

$$T_j^{n+1} = T_j^{n-1} - \mu(T_{j+1}^n - T_{j-1}^n) \qquad \mu = \frac{u\Delta t}{\Delta x}$$

$$\Rightarrow A^2 T^{n-1} e^{ikj\Delta x} = T^{n-1} e^{ikj\Delta x} - \mu A (T^{n-1} e^{ik(j+1)\Delta x} - T^{n-1} e^{ik(j-1)\Delta x})$$

$$\Rightarrow A^2 = 1 - A\mu(e^{ik\Delta x} - e^{-ik\Delta x})$$

$$\Rightarrow A^2 + 2iA\mu \sin(k\Delta x) = 1$$

$$\Rightarrow A = -i\mu \sin(k\Delta x) \pm \sqrt{1-\mu^2 \sin^2(k\Delta x)} = |A| e^{i\varphi}$$

+ = physical mode

$$\text{with } |A| = 1 \quad \text{for } \mu^2 = \left(\frac{u\Delta t}{\Delta x}\right)^2 \le 1$$

$$\text{and } \varphi = -\arctan\left(\frac{\pm \mu \sin(k\Delta x)}{\sqrt{1-\mu^2\sin^2(k\Delta x)}}\right) \approx -uk\Delta t + \left[\mu \frac{k^3 \Delta x^3}{6} - \mu^3 k^3 \Delta x^3 + \dots\right]$$

- Stable (**neutral**; |A| = 1) for (uΔt/Δx)^2 ≤ 1 (Courant-Friedrich-Levy criterion)
- Phase error => **Numerical dispersion**
- Computational Mode (-) => Robert-Asselin Filter

(Semi-) Lagrange Method

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x}$$

Idea: During advection the property (here T) of a particle/volume remains constant:

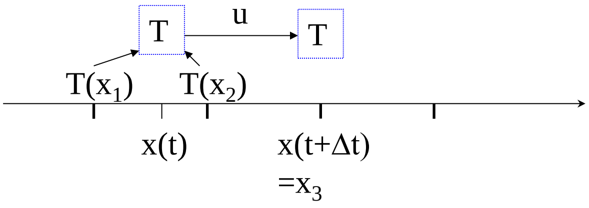
$$\frac{dT}{dt} = 0$$

=> New T distribution from parcel re-distribution by advection

Explicit: New parcel positions from velocities $x^{n+1} = x(t+\Delta t) = x + u \cdot \Delta t$

Implicit: Old parcel positions from velocities $x^{n} = x(t) = x - u \cdot \Delta t$

T typically at fixed grid => interpolation (**Semi**-Lagrange) =>diffusion



One-Dimensional Linear Advection

Summary

- Numerical methods: Spectral, finite differences and semi-Lagrange
- Stability analysis: Energy method, Von Neumann method
- Numerical diffusion: Amplitude damping (wave number dependent)
- Numerical dispersion: Error in phase velocity (wave number dependent)
- Important parameter: Courant-number (uΔt/Δx)
- Courant-Friedrich-Levy criterion

Introduction to Numerical Modeling

3. One-Dimensional Linear Diffusion and One-Dimensional Linear Transport Equation

The (Linear) Diffusion Equation (Heat Equation)

equation (one dimensional):

$$\frac{\partial T}{\partial t} = K \frac{\partial^2 T}{\partial x^2}$$

(parabolic, first order in time,
second order in space)

K=const.= Diffusion coeff.

Initial and boundary values needed

an analytic solution:

damped wave (wave number k):

$$T(x,t) = T_0 \exp(ikx) \exp(-Kk^2 t)$$

Exponential decay of the amplitude dependent on k^2

(the shorter the faster)

Numerical Solution: Spectral Method

$$\frac{\partial T}{\partial t} = K\frac{\partial^2 T}{\partial x^2}$$

T as Fourier-series: $$T(t,x) = \sum_{k=-N}^{N} T_k(t)\exp(ikx)$$

Insert => $$\sum_{k=-N}^{N} \frac{\partial T_k(t)}{\partial t}\exp(ikx) = -K\sum_{k=-N}^{N} k^2 T_k(t)\exp(ikx)$$

=> $2N$ uncoupled ordinary differential equations $$\boxed{\frac{\partial T_k}{\partial t} = -Kk^2 T_k}$$

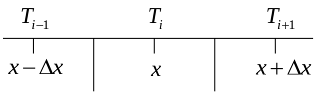
Numerical solution similar to decay equation

Grid Point Method: Finite Differences

$$\frac{\partial T}{\partial t} = K\frac{\partial^2 T}{\partial x^2}$$

Discretization for second derivative in space: $\frac{\partial^2 T}{\partial x^2}$

a) from discretization of $\frac{\partial T}{\partial x}$



$$\frac{\partial T}{\partial x} \rightarrow \frac{T_i - T_{i-1}}{\Delta x} \qquad \frac{\partial T}{\partial x} \rightarrow \frac{T_{i+1} - T_i}{\Delta x}$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial T}{\partial x}\right)$$

$$\Rightarrow \frac{\partial^2 T}{\partial x^2} \rightarrow \frac{T(x+\Delta x)+T(x-\Delta x)-2T(x)}{\Delta x^2} = \frac{T_{j+1}+T_{j-1}-2T_j}{\Delta x^2}$$

b) from Taylor expansion

$$T(x+\Delta x) = T(x) + \Delta x\frac{\partial T}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 T}{\partial x^2} + \ldots$$

$$T(x-\Delta x) = T(x) - \Delta x\frac{\partial T}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 T}{\partial x^2} - \ldots$$

$$\Rightarrow \frac{\partial^2 T}{\partial x^2} = \frac{T(x+\Delta x)+T(x-\Delta x)-2T(x)}{\Delta x^2} + O(\Delta x^2)$$

Finite Differences

$$\frac{\partial T}{\partial t} = K\frac{\partial^2 T}{\partial x^2}$$

Possible discretizations (two level schemes)

with $\frac{\partial^2 T}{\partial x^2} \rightarrow \frac{T_{j+1}+T_{j-1}-2T_j}{\Delta x^2}$

a) Explicit (forward in time centered in space; FTCS): $\boxed{\frac{T_j^{n+1}-T_j^n}{\Delta t} = K\frac{T_{j+1}^n+T_{j-1}^n-2T_j^n}{\Delta x^2}}$

b) Implicit: $\frac{T_j^{n+1}-T_j^n}{\Delta t} = K\frac{T_{j+1}^{n+1}+T_{j-1}^{n+1}-2T_j^{n+1}}{\Delta x^2}$

c) Crank-Nicolson: $\frac{T_j^{n+1}-T_j^n}{\Delta t} = gK\frac{T_{j+1}^{n+1}+T_{j-1}^{n+1}-2T_j^{n+1}}{\Delta x^2}+(1-g)K\frac{T_{j+1}^n+T_{j-1}^n-2T_j^n}{\Delta x^2}$

Note: Leap frog is unstable

Finite Differences

Forward in Time Centered in Space; FTCS

Accuracy/order:

$$\frac{T(x,t+\Delta t)-T(x,t)}{\Delta t} = K\frac{T(x+\Delta x,t)+T(x-\Delta x,t)-2T(x,t)}{\Delta x^2}+Err$$

$$\Rightarrow \frac{\sum\frac{\Delta t^n}{n!}\frac{\partial^n T}{\partial t^n}}{\Delta t} = K\frac{\sum\frac{\Delta x^n}{n!}\frac{\partial^n T}{\partial x^n}+\sum(-1)^n\frac{\Delta x^n}{n!}\frac{\partial^n T}{\partial x^n}}{\Delta x^2}+Err \Rightarrow Err = O(\Delta t,\Delta x^2)$$

Stability: Von Neumann method ($T_j(t) = \sum_k T_k(t)e^{ikj\Delta x}$ and $T^{n+1}=AT^n$)

$$\Rightarrow AT^n = T^n(1+\frac{K\Delta t}{\Delta x^2}(e^{ik\Delta x}+e^{-ik\Delta x}-2)) \Rightarrow A = 1+\frac{2K\Delta t}{\Delta x^2}(\cos(k\Delta x)-1) = 1-\frac{4K\Delta t}{\Delta x^2}\sin^2(\frac{k\Delta x}{2})$$

=> stable for $|A| \le 1 \quad \Rightarrow \boxed{\frac{4K\Delta t}{\Delta x^2} \le 1}$

For small Δx: $T^{n+1} = T^n(1-\frac{4K\Delta t}{\Delta x^2}(\frac{k\Delta x}{2})^2) = T^n(1-Kk^2\Delta t)$ convergence

analytical: $T^{n+1} = T^n\exp(-Kk^2\Delta t) = T^n(1-Kk^2\Delta t+...)$

The (Linear) Transport Equation (Advection and Diffusion)

equation (one dimensional): $$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x} + K\frac{\partial^2 T}{\partial x^2}$$

(2nd order parabolic)

An analytical solution: damped traveling wave

$$T(x,t) = T_0 \exp(ik(x-ut))\exp(-Kk^2 t)$$

Finite Differences

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x} + K\frac{\partial^2 T}{\partial x^2}$$

Previous knowledge: FTCS improper for advection; Leap frog improper for diffusion

=> mixed scheme:

$$\frac{T_j^{n+1} - T_j^{n-1}}{2\Delta t} = \boxed{-u\frac{T_{j+1}^n - T_{j-1}^n}{2\Delta x}} + \boxed{K\frac{T_{j+1}^{n-1} + T_{j-1}^{n-1} - 2T_j^{n-1}}{\Delta x^2}}$$

Leap frog für Advektion FTCS für Diffusion

More general:

Time splitting method:

Partitioning of tendencies and different numerical treatments

Climate models (ECHAM, PlaSim): Adiabatic part (leap frog) und diabatic parts (Euler or impl.)

Finite Differences

Time splitting (Leap frog und FTCS)

$$\frac{T_j^{n+1}-T_j^{n-1}}{2\Delta t}=-u\frac{T_{j+1}^{n}-T_{j-1}^{n}}{2\Delta x}+K\frac{T_{j+1}^{n-1}+T_{j-1}^{n-1}-2T_j^{n-1}}{\Delta x^2} \qquad (1)$$

Stability (Von Neumann method) $\left(T_j(t)=\sum_k T_k(t)e^{ikj\Delta x}\right.$ and $\left.T^{n+1}=AT^n\right)$

(1) $\Rightarrow T^{n+1}=T^{n-1}-\mu T^n\left(e^{ik\Delta x}-e^{-ik\Delta x}\right)+\frac{2K\Delta t}{\Delta x^2}T^{n-1}\left(e^{ik\Delta x}+e^{-ik\Delta x}-2\right)$ $\qquad \mu=\frac{u\Delta t}{\Delta x}$

$$\Rightarrow A^2=-i2A\mu\sin(k\Delta x)+1-\frac{4K\Delta t}{\Delta x^2}(1-\cos(k\Delta x))$$

$$\Rightarrow A=-i\mu\sin(k\Delta x)\pm\sqrt{1-\frac{4K\Delta t}{\Delta x^2}(1-\cos(k\Delta x))-\mu^2\sin^2(k\Delta x)}=|A|e^{i\varphi}$$

(+=physical)

i.e. **stable for** $\Delta t\le-\frac{4K}{u^2}+\sqrt{\left(\frac{\Delta x}{u}\right)^2+\left(\frac{4K}{u^2}\right)^2}$ or $\Delta t\le\frac{\Delta x^2}{4K+\sqrt{(4K)^2+(u\Delta x)^2}}$

with $|A|=\left(1-\frac{4K\Delta t}{\Delta x^2}(1-\cos(k\Delta x))\right)^{1/2}=1-Kk^2\Delta t+\ldots\le1$ (i.e. analytical +…)

$$\varphi=-\arctan\frac{\mu\sin k\Delta x}{\sqrt{1-\frac{4K\Delta t}{\Delta x^2}(1-\cos(k\Delta x)-\mu^2\sin^2 k\Delta x}}\approx-uk\Delta t\left(1-\frac{1}{6}(k\Delta x)^2\left(1-\mu^2-6\frac{K\Delta t}{\Delta x^2}\right)\right)$$

dependent on K

1-d Linear Diffusion
and 1-d Linear Transport Equation

Summary

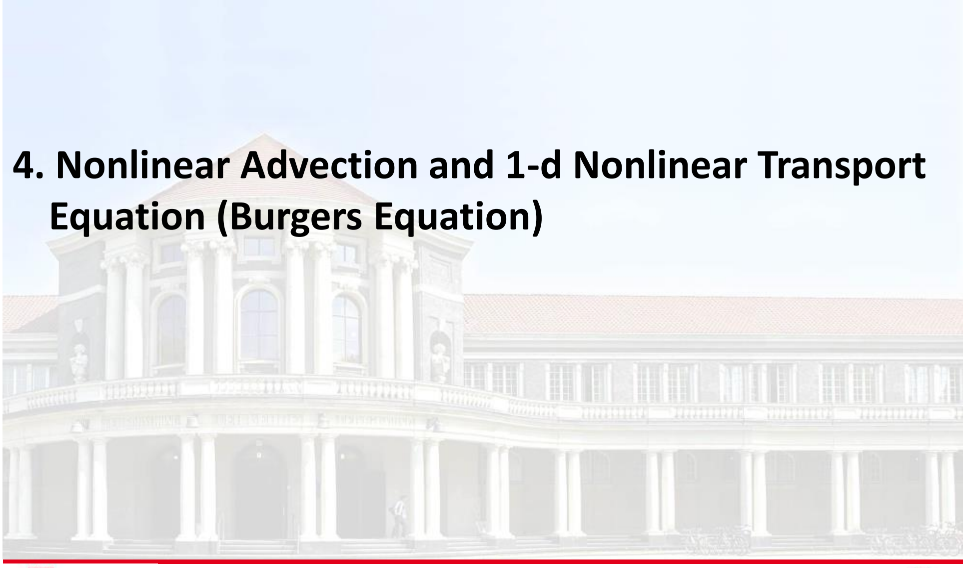
a) Diffusion equation (heat equation)

- Spectral: like decay equation
- Grid point: FTCS

b) Transport equation

- Time spitting method

Introduction to Numerical Modeling



4. Nonlinear Advection and 1-d Nonlinear Transport Equation (Burgers Equation)

The Nonlinear Advection Equation (Inviscid Burgers Equation)

equation (one dimensional): $\frac{du}{dt} = \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0 \Leftrightarrow \frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial u^2}{\partial x} = 0$

Solution: $u(x,t) = f(x-ut)$ with any function f

Like linear advection, but f depends on u itself (implicit equation)

Solvable (for practical use) in few special cases only.

---

e.g. Platzmann 1964, Tellus:

Initial condition: $u(x,t=0) = -\sin(x)$

Solution: $u(x,t) = \sum_{k=1}^{\infty} \tilde{u}_s(k,t)\sin(kx)$ with $\tilde{u}_s(k,t) = -2\frac{I_k(kt)}{kt}$

$I_k(kt)$ = first kind Bessel function

A ‚formal' (geometrical) solution can be constructed by using the method of characteristics

The Method of Characteristics

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

Lagrangian perspective: discussing the paths of individual parcels (points)

(paths = characteristics)

from $\frac{du}{dt} = 0$ => velocity of individual parcel is constant in time

=> parcels are moving on a straight lines: $x = u(x_0, t = 0)t + x_0$

=> characteristics are straight lines with slope $u(x_0,t=0)$

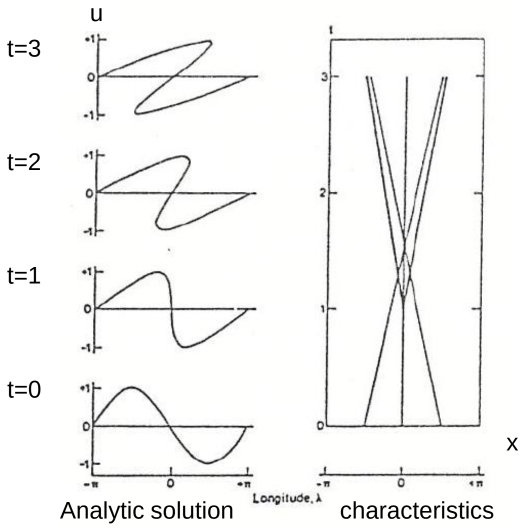
if $u(x_0,t=0)$ varies in space: characteristics cross at a certain time t_c

=> a) discontinuities (shock waves) are formed

=> b) after t_c one parcel can have more than one location (unphysical!)

=> physical solutions only possible up to $t=t_c$

Characteristics of Platzmanns Solution



After: Platzmann, G.W., 1964: An exact integral of complete spectral equations for unsteady one-dimensional flow. Tellus, 16, 422-431.

The Nonlinear Advection Equation

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

The nonlinear term:

Example: $u(x,t)=\sum_k u_k(t)\sin(kx)$ $\qquad k=\frac{2\pi n}{L}$

Sine-series (waves) with time dependent amplitudes

Non linear term after inserting sine-series:

$$\begin{aligned}u\frac{\partial u}{\partial x} &= \sum_{k_1} u_{k_1}(t)\sin(k_1x)\sum_{k_2} k_2u_{k_2}(t)\cos(k_2x)\\ &= \sum_{k_1}\sum_{k_2} k_2u_{k_1}(t)u_{k_2}(t)\sin(k_1x)\cos(k_2x)\\ &= \sum_{k_1}\sum_{k_2} k_2u_{k_1}(t)u_{k_2}(t)(\sin[(k_1+k_2)x]+\sin[(k_1-k_2)x])\end{aligned}$$

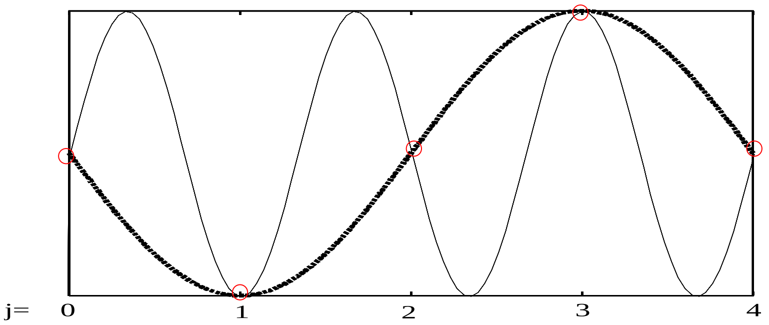
The non linear wave-wave interaction of the waves k_1 and k_2 forces waves with wave number k_1+k_2 and k_1-k_2.

=> Energy/momentum is redistributed within the wave spectrum

Grid Point Method: Aliasing

Problem: With a finite number of grid points (e.g. *0-M*) waves with wave numbers *k > M/2* get erroneously interpreted (as *M-k*)

Example: M=4; k=3 => ‚false‘ wave with k‘=1



Aliasing: Consequence for Energy

Example: let $u(x,t=0)=u_0\sin(kx)\Rightarrow\frac{\partial u}{\partial x}=ku_0\cos(kx)$ $\qquad x=0-2\pi$

=> kin. Energy: $E_0=\frac{u_0^2}{2}\int\limits_0^{2\pi}\sin^2(kx)dx=\frac{u_0^2}{2}\pi$

Energy change: $\frac{\partial E}{\partial t}=\int\limits_0^{2\pi}\frac{1}{2}\frac{\partial u^2}{\partial t}dx=\int\limits_0^{2\pi}u\frac{\partial u}{\partial t}dx=\int\limits_0^{2\pi}u\left(-u\frac{\partial u}{\partial x}\right)dx$

$$\text{with}\left(-u\frac{\partial u}{\partial x}\right)=-ku_0^2\sin(kx)\cos(kx)=-\frac{k}{2}u_0^2\sin(2kx)$$

$$\Rightarrow\frac{\partial E}{\partial t}=-\frac{ku_0^3}{2}\int\limits_0^{2\pi}\sin(kx)\sin(2kx)dx=0$$

=> analytically the total energy is conserved

But With resolution M=3k

$$\Rightarrow\sin(2kx)\xrightarrow{\mathit{Aliasing}}-\sin(kx)\Rightarrow\frac{\partial E}{\partial t}=\frac{ku_0^3}{2}\int\limits_0^{2\pi}\sin(kx)\sin(kx)dx=\frac{ku_0^3\pi}{2}$$

=> Energy increase (due to aliasing from limited resolution)

Nonlinear Instability

- At each time level short waves (k_1+k_2) may be forced which (potentially) are not resolved and, therefore, erroneously interpreted.
- This leads to unrealistic increase of wave amplitudes (i.e. energy), in particular in the short wave part of the spectrum, and finally to a ‘blow up’ of the numerical solution.
- This mechanism is, in principal, independent of the time step length or the grid size.
- Nonlinear instability

Nonlinear Instability

Solutions

- Artificial elimination of short waves
- Diffusive schemes (e.g. upstream)
- Explicit diffusion
- Appropriate discretization of non linear terms

Discretization of the Nonlinear Term

Analytically:

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} \Rightarrow u\frac{\partial u}{\partial t} = -u^2\frac{\partial u}{\partial x} \Rightarrow \frac{1}{2}\frac{\partial u^2}{\partial t} = -\frac{1}{3}\frac{\partial u^3}{\partial x} \Rightarrow \int_x \frac{1}{2}\frac{\partial u^2}{\partial t}dx = 0$$

i.e. total energy (~u²) is conserved

If this would also be the case numerically => no non linear instability

Solution: Discretization of the non linear term

1st try: $\left(u\frac{\partial u}{\partial x}\right)_i \rightarrow u_i\frac{u_{i+1}-u_{i-1}}{2\Delta x}$

$$\frac{\partial E}{\partial t} = \int u\frac{\partial u}{\partial t}dx = \int u\left(-u\frac{\partial u}{\partial t}\right)dx \rightarrow -\sum_j u_j^2\frac{u_{j+1}-u_{j-1}}{2} = -\frac{1}{2}\sum_j u_j^2u_{j+1} - u_j^2u_{j-1} \neq 0$$

Not appropriate

example: 3 Points, cyclic boundary conditions:

$$= -\frac{1}{2}\left(u_1^2u_2 - u_1^2u_3 + u_2^2u_3 - u_2^2u_1 + u_3^2u_1 - u_3^2u_2\right) \neq 0$$

Discretization of the Nonlinear Term

2nd try: $$\left(u\frac{\partial u}{\partial x}\right)_j \rightarrow \frac{u_{j+1}u_{j+2}-u_{j-1}u_{j-2}}{6\Delta x}=\frac{1}{3}\left[\frac{u_j(u_{j+1}-u_{j-1})}{2\Delta x}+\frac{u_{j+1}(u_{j+2}-u_j)}{2\Delta x}+\frac{u_{j-1}(u_j-u_{j-2})}{2\Delta x}\right]$$

$$\Rightarrow \frac{\partial E}{\partial t}\rightarrow -\frac{1}{6\Delta x}\sum_j u_j\left(u_{j+1}u_{j+2}-u_{j-1}u_{j-2}\right)=0$$

appropriate

example: 3 points, cyclic boundary conditions

$$=-\frac{1}{6}\left(u_1u_2u_3-u_1u_3u_2+u_2u_3u_1-u_2u_1u_3+u_3u_1u_2-u_3u_2u_1\right)=0$$

3rd try: $$\left(u\frac{\partial u}{\partial x}\right)_j \rightarrow \left(\frac{u_{j+1}+u_j+u_{j-1}}{3}\right)\left(\frac{u_{j+1}-u_{j-1}}{2\Delta x}\right)=\frac{1}{6\Delta x}\left[u_{j+1}^2+u_ju_{j+1}-u_ju_{j-1}-u_{j-1}^2\right]$$

$$\Rightarrow \frac{\partial E}{\partial t}\rightarrow -\frac{1}{6\Delta x}\sum_j u_j\left[u_{j+1}^2+u_ju_{j+1}-u_ju_{j-1}-u_{j-1}^2\right]=0$$

appropriate

But: Still transfere of energy into ‚wrong‘ waves (unphysical)

Finite Differences

options

Two level Euler: $$\frac{\partial u}{\partial t}=-u\frac{\partial u}{\partial x}\rightarrow\frac{u_i^{n+1}-u_i^n}{\Delta t}=-\frac{u_{i+1}^n u_{i+2}^n-u_{i-1}^n u_{i-2}^n}{6\Delta x}$$

Three level Leap frog: $$\frac{\partial u}{\partial t}=-u\frac{\partial u}{\partial x}\rightarrow\frac{u_i^{n+1}-u_i^{n-1}}{2\Delta t}=-\frac{u_{i+1}^n u_{i+2}^n-u_{i-1}^n u_{i-2}^n}{6\Delta x}$$

Caution: a) slightly unstable due to t-discretization

b) linear instability may occur => mind the CFL criterion

Spectral Method

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

Ansatz: transformation of u into new basis functions which are differentiable orthogonal functions of x, e.g. Fourier-series: $u(x,t) = \sum_{k=-N}^{N} u_k(t)\exp(ikx)$

=> left hand side: $\frac{\partial u}{\partial t} = \sum_{k=-N}^{N} \frac{\partial u_k}{\partial t}\exp(ikx)$

=> right hand side:

$$\begin{aligned} -u\frac{\partial u}{\partial x} &= -\sum_{k_1} u_{k_1}\exp(ik_1x)\sum_{k_2} ik_2u_{k_2}\exp(ik_2x) \\ &= -\sum_{k_1}\sum_{k_2} ik_2u_{k_1}u_{k_2}\exp(i(k_1+k_2)x) \\ &= \sum_{k=-2N}^{2N} F_k\exp(ikx) \end{aligned}$$

Since contributions to wavenumbers $-2N$ to $2N$ are obtained

with $k=k_1+k_2$ and $F_k = -i\sum_{l=L_1}^{L_2}(k-l)u_lu_{k-l}$ (interaction coefficients)

$L_1=max(-N,k-N)$; $L_2=min(N,k+N)$, i.e. $L_1=k-N$, $L_2=N$ for $k \geq 0$, and $L_1=-N$, $L_2=k+N$ for $k < 0$

Spectral Method

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} \rightarrow \sum_{k=-N}^{N}\frac{\partial u_k}{\partial t}\exp(ikx) = \sum_{k=-2N}^{2N} F_k\exp(ikx) \quad \text{with} \quad F_k = -i\sum_{l=L_1}^{L_2}(k-l)u_lu_{k-l}$$

$L_1=max(-N,k-N)$; $L_2=min(N,k+N)$

with $$\sum_{k=-2N}^{2N} F_k\exp(ikx) = \sum_{k=-N}^{N} F_k\exp(ikx) + \sum_{N<|k|\leq 2N} F_k\exp(ikx)$$

resolved waves

unresolved waves

Neglecting the unresolved waves leads to $2N$ **coupled ordinary differential equations (ODE's)**:

$$\boxed{\frac{\partial u_k}{\partial t} = F_k = -i\sum_{l=L_1}^{L_2}(k-l)u_lu_{k-l}}$$

$L_1=max(-N,k-N)$; $L_2=min(N,k+N)$

$-N \leq k \leq N$

To be solved using common methods

Cut off: no aliasing but not conserving moments higher than u^2

The Spectral Transform Method

spectral method versus finite differences:

spectral: exact spatial derivatives but numerical effort goes with N^2

finite differences: numerical effort goes with N but spatial derivatives not exact

Improvement by combination: **The spectral transform method**

Idea: compute derivatives (and linear terms) in spectral space and non linear term on corresponding grid (≥ 3N+1 grid points to avoid aliasing). The effort goes with $N \ln(N)$ (using a fast fourier transform (fft)).

Non linear advection: $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0 \rightarrow \frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial u^2}{\partial x} = 0$

Step 1: transform u into grid point domain (inverse Fourier transformation (via fft))

Step 2: compute u^2 on grid points

Step 3: transform u^2 into spectral space (via fft)

Step 4: compute the x-derivative of u^2 in spectral space, and do the time stepping

Step 1: ….

The (Viscid) Burgers Equation: Advection and Diffusion

equation (one dimension): $$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = K\frac{\partial^2 u}{\partial x^2}$$

Various applications to describe processes in science and technology in a ‚simple' way (e.g. road traffic) and important test bed for numerical schemes.

(formal) analytic solution using Cole-Hopf transformation: $u = -\frac{2K}{z}\frac{\partial z}{\partial x} = -2K\frac{\partial \ln z}{\partial x}$

$$\Rightarrow \frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial u^2}{\partial x} = K\frac{\partial^2 u}{\partial x^2}$$

$$\Rightarrow 2K\frac{\partial}{\partial x}\frac{\partial \ln z}{\partial t} + 2K^2\frac{\partial}{\partial x}\left(\frac{\partial \ln z}{\partial x}\right)^2 = -2K^2\frac{\partial}{\partial x}\frac{\partial^2 \ln z}{\partial x^2}$$

$$\Rightarrow \frac{\partial z}{\partial t} = K\frac{\partial^2 z}{\partial x^2}$$ Linear heat equation

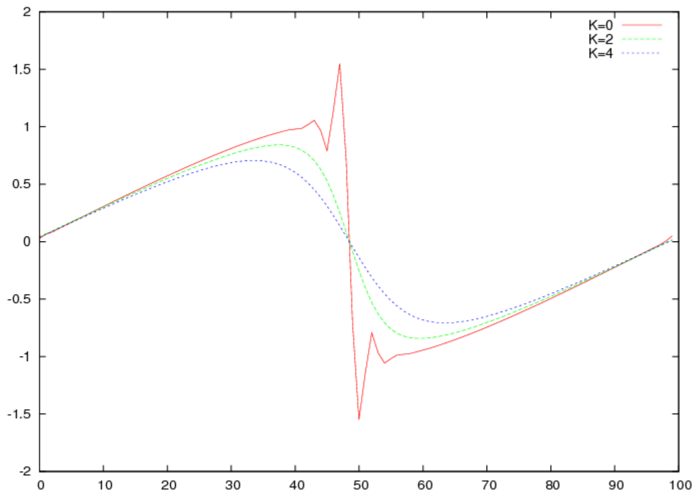
=>

$$u = \frac{\int_{-\infty}^{\infty}\frac{x-\xi}{t}\exp(-\frac{G(\xi;x,t)}{2K})d\xi}{\int_{-\infty}^{\infty}\exp(-\frac{G(\xi;x,t)}{2K})d\xi}$$

$$G(\xi;x,t) = \int_0^{\xi} u_0(\eta)d\eta + \frac{(x-\xi)^2}{2t}$$

Numerical Solution: Spectral or finite differences with the known schemes. In most cases by using time splitting (separating advection and diffusion)

Numerical Solution of Burgers Equation using different *K*



Nonlinear Advection and 1-d Nonlinear Transport Equation (Burgers Equation)

Summary

- Viscid and inviscid Burgers equation
- Aliasing
- Non linear instability
- Energy conserving discretization
- Spectral transform method

Introduction to Numerical Modeling

5. More Dimensions (Grids)

Three Dimensions with Scalar and Vector Fields

Problem: not only one dimension and variable but three (x,y,z) dimensions and various (coupled) variables (scalars and vectors).

typically: Scalars (temperature, height, vorticity, divergence, etc.) and 3d flow (u,v,w)

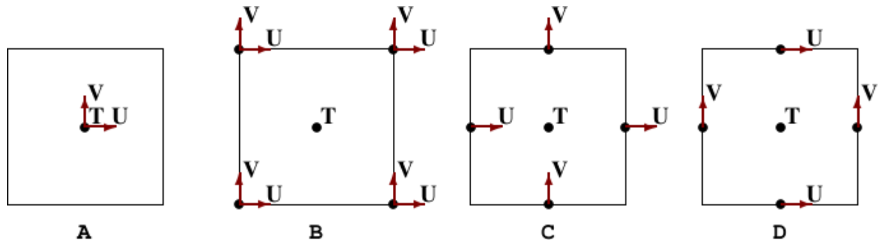
Numerics:

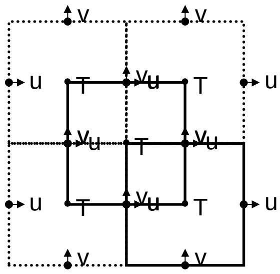
Grid point models: discretization using staggered grids (e.g. scalars shifted compared to vectors).

(Semi-) Spectral models: (non linear terms) and parameterizations on corresponding (Gaussian) grids with staggering in the vertical.

Grids

Horizontal: **‚classical' grids according to Arakawa (T=scalar, (u,v)=flow)**

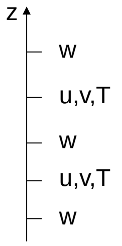




E = two shifted C-grids

Grids

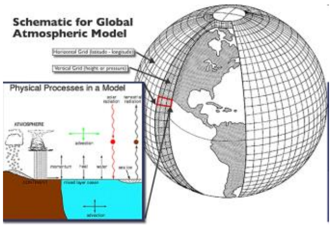
Vertical: **staggered**



w vertically staggered to all other variables (u,v,T), horizontally at T or u or v grid points

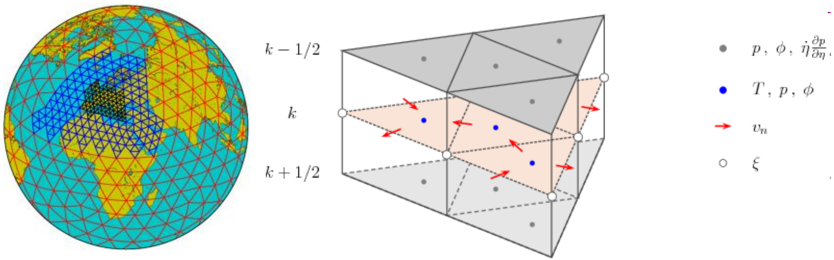
Grids

Global grids



‚classical': lon-lat grid

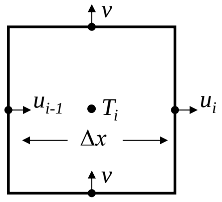
New: Icosahedron



Grids: Discretizations

Staggered grid: Discretization using appropriate averaging:

Example: Advection (x-direction) on C-grid:

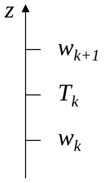


$$\left(u\frac{\partial T}{\partial x}\right)_i \rightarrow \frac{1}{2}\left(u_{i-1}\frac{T_i-T_{i-1}}{\Delta x}+u_i\frac{T_{i+1}-T_i}{\Delta x}\right)$$

or (better)

$$\left(u\frac{\partial T}{\partial x}\right)_i \rightarrow \frac{1}{2}(u_i+u_{i+1})\frac{T_{i+1}-T_{i-1}}{2\Delta x}$$

Vertical advection:



$$\left(w\frac{\partial T}{\partial z}\right)_k \rightarrow \frac{1}{2}\left(w_k\frac{T_k-T_{k-1}}{\Delta z}+w_{k+1}\frac{T_{k+1}-T_k}{\Delta z}\right)$$

or

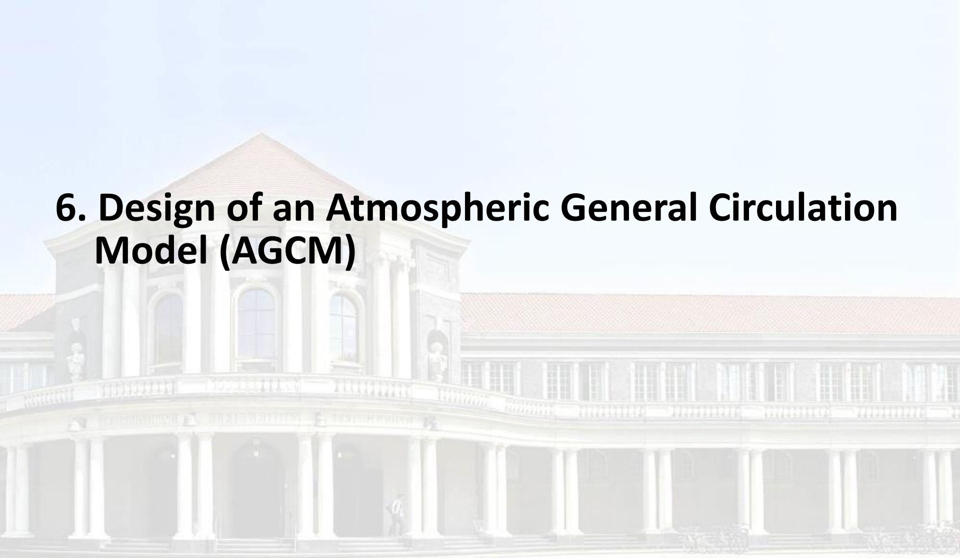
$$\left(w\frac{\partial T}{\partial z}\right)_k \rightarrow \frac{1}{2}(w_k+w_{k+1})\frac{T_{k+1}-T_{k-1}}{2\Delta z}$$

More Dimensions (Grids)

Summary

- Grids after Arakawa (A,B,C,D,E)
- Staggered grid
- Lon-lat- und icosahedral-grids

Introduction to Numerical Modeling



6. Design of an Atmospheric General Circulation Model (AGCM)

An Atmospheric General Circulation Model (AGCM)

Processes:

Adiabatic: moist atmospheric fluid dynamics

Diabatic: forcing (sources) and dissipation (sinks)

Variables:

prognostic (dynamic) variables

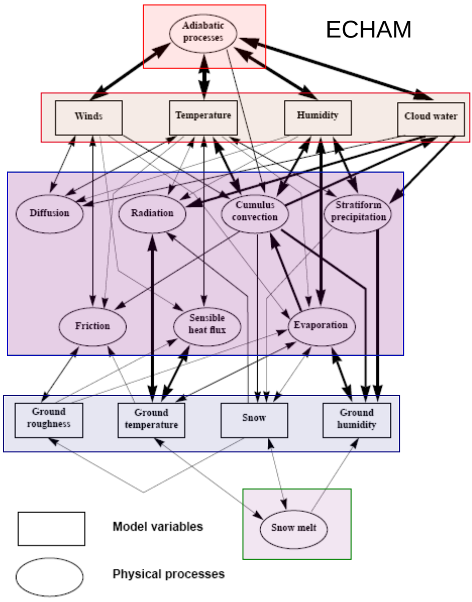
boundary conditions (partially prognostic)

Representation (equations):

Adiabatic: resolved scales; based on fundamental laws (approximated; e.g. primitive eq.)

Diabatic: unresolved scales; parametrerized, i.e. linked to the prognostic variables (resolved scales)

ECHAM



An Atmospheric General Circulation Model (AGCM)

Numerics

Representation and discretization:

Horizontal: spectral transform method (Legendre polynomials) or grid point (finite diff.); semi-Lagrangian tracer transport (q)

Vertical: staggered grid (z-, p-, σ- and/or θ-system (mostly mixed: p (top) and σ (ground))

Time: time splitting method; adiabatic: mostly leapfrog with Asselin filter; semi-implicit (divergence eq.); diabatic: explicit or implicit (e.g. diffusion)

Resolution:

Horizontal: about 10-500km

Vertical: about 20-100 levels; 0-30/100km

Time: some minutes

An Atmospheric General Circulation Model (AGCM)

Numerics

Input: Initial fields (or restart files) and boundary conditions

Output: Prognostic variables, deduced parameters, history (restart files)

Work flow:

1 Initialization: read boundary conditions (z_0, albedo, SST, ice, etc.)
Set initial conditions (e.g. normal mode initialization for NWP, start date for climate) or read history (restart files)

2 Time stepping: a) update boundary conditions (e.g. radiation, SST)
b) compute adiabatic and diabatic tendencies
c) update prognostic variables
d) write output
a) …

3 Termination: write history (restart files) for continuation

Design of an Atmospheric General Circulation Model (AGCM)

Summary

- Time splitting method (adiabatic/diabatic)
- Resolved and unresolved processes -> parameterizations
- Prognostic and diagnostic variables
- Boundary an initial conditions