

Lecture 2 SOAC

Numerical approximation to the time derivative:

1. Centred (*leap-frog*) scheme
2. Multi-step schemes: *Matsuno* and *Heun* schemes

Exercise 1

Linear advection equation: analytical solution

Numerical approximation of the linear advection equation:

Truncation error due to numerical diffusion and numerical dispersion.

Introduction to Exercise 2

Recap. from lecture 1

Inertial oscillation

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$$\frac{\partial u(t)}{\partial t} = fv(t)$$

$$\frac{\partial v(t)}{\partial t} = -fu(t)$$

Numerical approximation: Euler-forward scheme

time-step

$$\frac{u(t + \Delta t) - u(t)}{\Delta t} = fv(t)$$

$$\frac{v(t + \Delta t) - v(t)}{\Delta t} = -fu(t)$$

Error: “first order” (linear) in Δt

Can we improve on this?

Centred time-difference scheme

Taylor series:

Forward: $u(t + \Delta t) = u(t) + \Delta t \frac{\partial u}{\partial t}(t) + \frac{\Delta t^2}{2} \frac{\partial^2 u}{\partial t^2}(t) + \frac{\Delta t^3}{6} \frac{\partial^3 u}{\partial t^3}(t) + O(\Delta t^4)$

Backward: $u(t - \Delta t) = u(t) - \Delta t \frac{\partial u}{\partial t}(t) + \frac{\Delta t^2}{2} \frac{\partial^2 u}{\partial t^2}(t) - \frac{\Delta t^3}{6} \frac{\partial^3 u}{\partial t^3}(t) + O(\Delta t^4)$

Centred time-difference scheme

Taylor series:

$$u(t + \Delta t) = u(t) + \Delta t \frac{\partial u}{\partial t}(t) + \frac{\Delta t^2}{2} \frac{\partial^2 u}{\partial t^2}(t) + \frac{\Delta t^3}{6} \frac{\partial^3 u}{\partial t^3}(t) + O(\Delta t^4)$$

$$u(t - \Delta t) = u(t) - \Delta t \frac{\partial u}{\partial t}(t) + \frac{\Delta t^2}{2} \frac{\partial^2 u}{\partial t^2}(t) - \frac{\Delta t^3}{6} \frac{\partial^3 u}{\partial t^3}(t) + O(\Delta t^4)$$

Subtract:

$$u(t + \Delta t) - u(t - \Delta t) = 2\Delta t \frac{\partial u}{\partial t}(t) + \frac{\Delta t^3}{3} \frac{\partial^3 u}{\partial t^3}(t) + O(\Delta t^4) \longrightarrow$$

divide by $2\Delta t$

$$\longrightarrow \frac{u(t + \Delta t) - u(t - \Delta t)}{2\Delta t} = \frac{\partial u}{\partial t}(t) + \frac{\Delta t^2}{6} \frac{\partial^3 u}{\partial t^3}(t) + O(\Delta t^3)$$

Centred finite difference
approximation to time-derivative

Error: “second order” in Δt

Centred time-difference scheme

$$\frac{u(t + \Delta t) - u(t - \Delta t)}{2\Delta t} = \frac{\partial u}{\partial t}(t) + \frac{\Delta t^2}{6} \frac{\partial^3 u}{\partial t^3}(t) + O(\Delta t^3)$$

Centred finite difference

Error: “second order” in Δt

This scheme is also called “**leap-frog**” scheme.
Initialise this scheme with one Euler-forward step.

Drawback: scheme is unreliable because odd and even time steps are decoupled.

In practice the following type of multi-step time-stepping scheme is frequently used

Multi-step schemes

Equation: $\frac{\partial u}{\partial t} = F(t, u(t))$

Predictor step 1: $u_{n+1}^* - u_n = \Delta t F_n$  n : time-index

u_{n+1}^* represents the *first* guess of u_{n+1}

Corrector Step 2: $u_{n+1} - u_n = \Delta t (\alpha F_n + \beta F_{n+1}^*)$

$$\alpha + \beta = 1$$

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$$\alpha + \beta = 1$$

Matsuno scheme: $\beta = 1$ (“semi-implicit”)

Taroh Matsuno



Taroh Matsuno (1934-) is a Japanese theoretical meteorologist

https://www.af-info.or.jp/better_future/html/vol_V/2013/Dr_Matsuno/2013a_Matsuno1.html#7⁴⁰

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Predictor step 1: $u_{n+1}^* - u_n = \Delta t F_n$ $\swarrow$ n : time-index

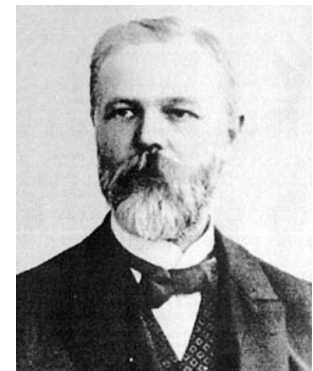
u_{n+1}^* represents the *first* guess of u_{n+1}

Corrector Step 2: $u_{n+1} - u_n = \Delta t (\alpha F_n + \beta F_{n+1}^*)$

$$\alpha + \beta = 1$$

Heun scheme: $\alpha = 1/2$

Karl Heun



Karl Heun (1859-1929) is a German mathematician

Which scheme, do you expect, performs best: “leap-frog”, “Matsuno” or “Heun”?

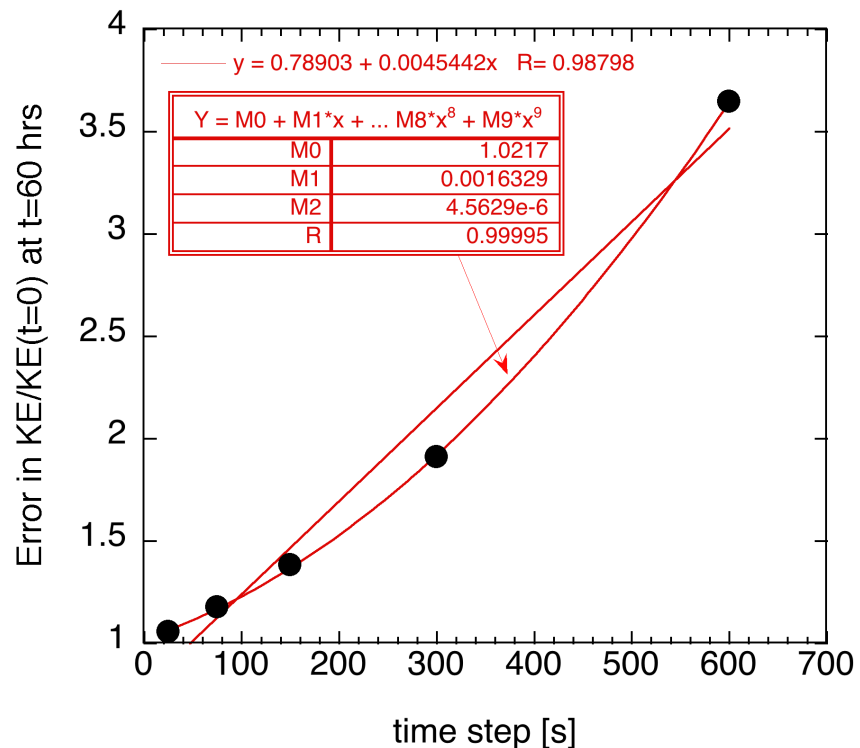
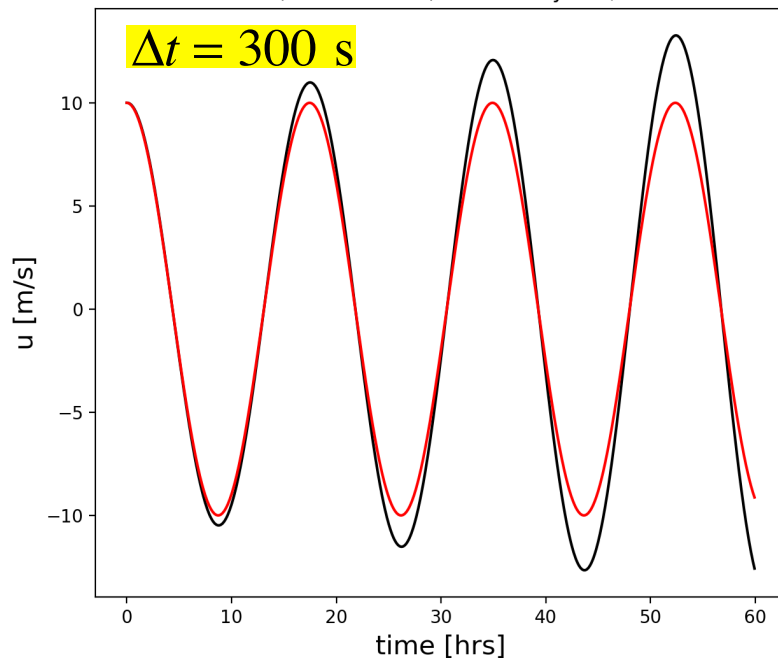
Exercise 1

Exercise 1: Repeat the analysis of the numerical accuracy of slides 29-31 (lecture 1), but now for the leap-frog scheme, Matsuno’s scheme and Heun’s scheme.

Deadline hand in exercises 1: Thursday 16 September 2021

Lecture 1:

Inertial oscillation (Euler forward) - red: analytical; black: numerical



Reference: Roger K. Smith and Wolfgang Ulrich, 2008: **Lectures on Numerical Meteorology**.

<https://www.meteo.physik.uni-muenchen.de/~roger/manuskripte/NumericalMeteorology.pdf> .

Advection equation

Canonical equation of geophysical fluid dynamics:

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + fv$$

pressure

$$\frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x} - \frac{1}{\rho} \frac{\partial p}{\partial x} + fv$$

density

Horizontal velocity perpendicular to u

Advection equation:

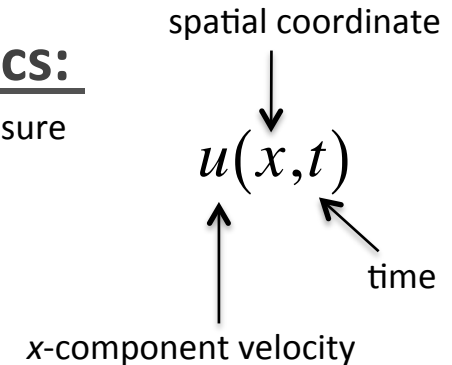
$$\frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x}$$

Advection of “C”:

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

Advection of the concentration, C , of a passive scalar

(for simplicity this equation can be linearised: next slide...)



Linear advection equation: analytical solution

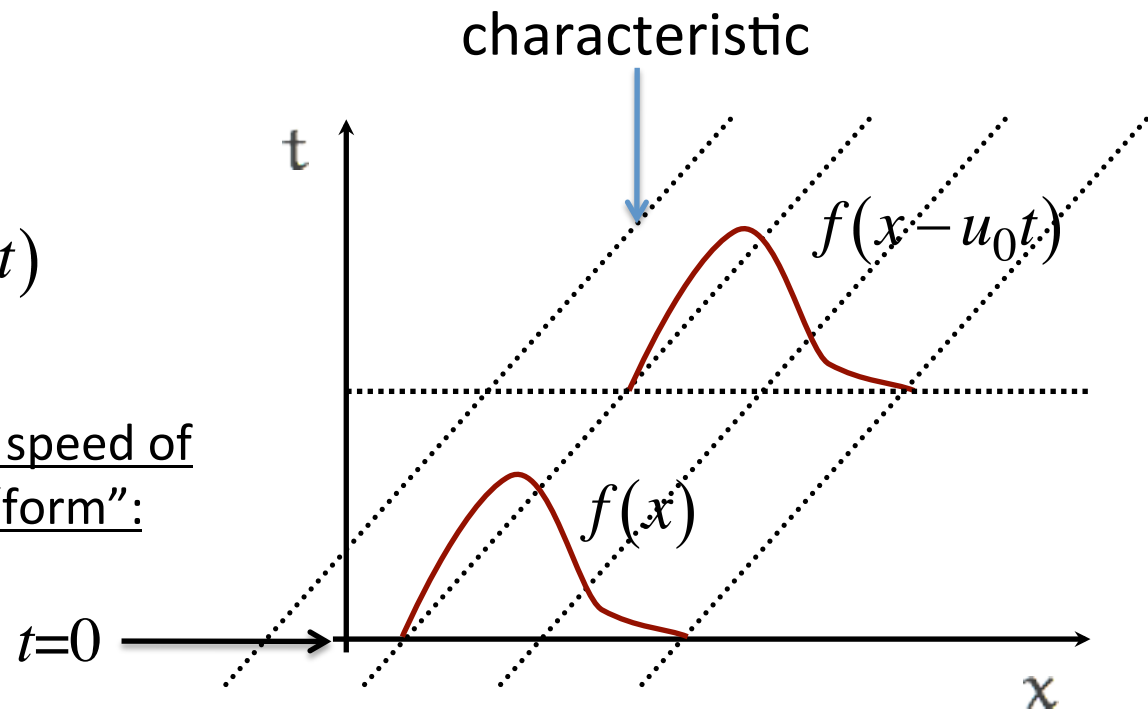
Linear advection (advection of C with a constant velocity, u_0)

$$\frac{\partial C}{\partial t} + u_0 \frac{\partial C}{\partial x} = 0$$

Solution:

$$C(x, t) = f(x - u_0 t)$$

Propagation at constant speed of
a signal without loss of “form”:



Numerical solution of the advection equation

$$\frac{\partial C}{\partial t} + u_0 \frac{\partial C}{\partial x} = 0$$



Taylor series approximation to *time & spatial* derivative yields:

$$\rightarrow \frac{\partial C(x,t)}{\partial t} = \frac{C(x,t+\Delta t) - C(x,t)}{\Delta t} - \frac{\Delta t}{2} \frac{\partial^2 C(x,t)}{\partial t^2} - \frac{\Delta t^2}{6} \frac{\partial^3 C(x,t)}{\partial t^3} + O(\Delta t^3)$$

$$\rightarrow \frac{\partial C(x,t)}{\partial x} = \frac{C(x+\Delta x,t) - C(x,t)}{\Delta x} - \frac{\Delta x}{2} \frac{\partial^2 C(x,t)}{\partial x^2} - \frac{\Delta x^2}{6} \frac{\partial^3 C(x,t)}{\partial x^3} + O(\Delta x^3)$$

Numerical solution of the advection equation

$$\frac{\partial C}{\partial t} + u_0 \frac{\partial C}{\partial x} = 0$$

Taylor series approximation to *time & spatial* derivative yields:

$$\rightarrow \frac{\partial C(x,t)}{\partial t} = \frac{C(x,t+\Delta t) - C(x,t)}{\Delta t} - \frac{\Delta t}{2} \frac{\partial^2 C(x,t)}{\partial t^2} - \frac{\Delta t^2}{6} \frac{\partial^3 C(x,t)}{\partial t^3} + O(\Delta t^3)$$

$$\rightarrow \frac{\partial C(x,t)}{\partial x} = \frac{C(x+\Delta x,t) - C(x,t)}{\Delta x} - \frac{\Delta x}{2} \frac{\partial^2 C(x,t)}{\partial x^2} - \frac{\Delta x^2}{6} \frac{\partial^3 C(x,t)}{\partial x^3} + O(\Delta x^3)$$

Multiply second equation by u_0 and add the two equations:

$$\begin{aligned} \frac{\partial C}{\partial t} + u_0 \frac{\partial C}{\partial x} &= \frac{C(x,t+\Delta t) - C(x,t)}{\Delta t} + u_0 \frac{C(x+\Delta x,t) - C(x,t)}{\Delta x} \\ &\quad - \frac{\Delta t}{2} \frac{\partial^2 C(x,t)}{\partial t^2} - \frac{\Delta t^2}{6} \frac{\partial^3 C(x,t)}{\partial t^3} - \frac{u_0 \Delta x}{2} \frac{\partial^2 C(x,t)}{\partial x^2} - \frac{u_0 \Delta x^2}{6} \frac{\partial^3 C(x,t)}{\partial x^3} + \dots \end{aligned}$$

Repeat equation on previous slide:

$$\frac{\partial C}{\partial t} + u_0 \frac{\partial C}{\partial x} = \frac{C(x, t + \Delta t) - C(x, t)}{\Delta t} + u_0 \frac{C(x + \Delta x, t) - C(x, t)}{\Delta x}$$

$$- \frac{\Delta t}{2} \frac{\partial^2 C(x, t)}{\partial t^2} - \frac{\Delta t^2}{6} \frac{\partial^3 C(x, t)}{\partial t^3} - \frac{u_0 \Delta x}{2} \frac{\partial^2 C(x, t)}{\partial x^2} - \frac{u_0 \Delta x^2}{6} \frac{\partial^3 C(x, t)}{\partial x^3} + \dots$$

Re-arrange terms:

$$\frac{C(x, t + \Delta t) - C(x, t)}{\Delta t} + u_0 \frac{C(x + \Delta x, t) - C(x, t)}{\Delta x} - \frac{\partial C}{\partial t} - u_0 \frac{\partial C}{\partial x} =$$

$$\frac{\Delta t}{2} \frac{\partial^2 C(x, t)}{\partial t^2} + \frac{\Delta t^2}{6} \frac{\partial^3 C(x, t)}{\partial t^3} + \frac{u_0 \Delta x}{2} \frac{\partial^2 C(x, t)}{\partial x^2} + \frac{u_0 \Delta x^2}{6} \frac{\partial^3 C(x, t)}{\partial x^3} + \dots$$

Repeat equation on previous slide:

$$\frac{C(x, t + \Delta t) - C(x, t)}{\Delta t} + u_0 \frac{C(x + \Delta x, t) - C(x, t)}{\Delta x} - \frac{\partial C}{\partial t} - u_0 \frac{\partial C}{\partial x} =$$

$$\frac{\Delta t}{2} \frac{\partial^2 C(x, t)}{\partial t^2} + \frac{\Delta t^2}{6} \frac{\partial^3 C(x, t)}{\partial t^3} + \frac{u_0 \Delta x}{2} \frac{\partial^2 C(x, t)}{\partial x^2} + \frac{u_0 \Delta x^2}{6} \frac{\partial^3 C(x, t)}{\partial x^3} + \dots$$

$$\begin{aligned} \xrightarrow{\text{red}} \frac{\partial^2 C}{\partial t^2} &= -u_0 \frac{\partial}{\partial t} \frac{\partial C}{\partial x} = -u_0 \frac{\partial}{\partial x} \frac{\partial C}{\partial t} = u_0^2 \frac{\partial^2 C}{\partial x^2} & \longrightarrow & \boxed{\frac{\partial^2 C}{\partial t^2} = u_0^2 \frac{\partial^2 C}{\partial x^2}} \longrightarrow \\ \xrightarrow{\text{blue}} \frac{\partial^3 C}{\partial t^3} &= -u_0 \frac{\partial^2}{\partial t^2} \frac{\partial C}{\partial x} = -u_0 \frac{\partial}{\partial x} \frac{\partial^2 C}{\partial t^2} = u_0^3 \frac{\partial^3 C}{\partial x^3} & \longrightarrow & \boxed{\frac{\partial^3 C}{\partial t^3} = -u_0^3 \frac{\partial^3 C}{\partial x^3}} \longrightarrow \end{aligned}$$

Now: eliminate the time derivatives on the r.h.s. (the error) next slide:

Repeat equation on previous slide:

$$\frac{C(x, t + \Delta t) - C(x, t)}{\Delta t} + u_0 \frac{C(x + \Delta x, t) - C(x, t)}{\Delta x} - \frac{\partial C}{\partial t} - u_0 \frac{\partial C}{\partial x} =$$

$$\frac{\Delta t}{2} \frac{\partial^2 C(x, t)}{\partial t^2} + \frac{\Delta t^2}{6} \frac{\partial^3 C(x, t)}{\partial t^3} + \frac{u_0 \Delta x}{2} \frac{\partial^2 C(x, t)}{\partial x^2} + \frac{u_0 \Delta x^2}{6} \frac{\partial^3 C(x, t)}{\partial x^3} + \dots$$



$$\frac{\partial^2 C}{\partial t^2} = u_0^2 \frac{\partial^2 C}{\partial x^2}$$

$$\frac{\partial^3 C}{\partial t^3} = -u_0^3 \frac{\partial^3 C}{\partial x^3}$$

Eliminate time-derivative:

$$\frac{C(x, t + \Delta t) - C(x, t)}{\Delta t} + u_0 \frac{C(x + \Delta x, t) - C(x, t)}{\Delta x} - \frac{\partial C}{\partial t} - u_0 \frac{\partial C}{\partial x} =$$

$$+ \frac{\Delta t}{2} u_0^2 \frac{\partial^2 C(x, t)}{\partial x^2} - \frac{\Delta t^2}{6} u_0^3 \frac{\partial^3 C(x, t)}{\partial x^3} + \frac{u_0 \Delta x}{2} \frac{\partial^2 C(x, t)}{\partial x^2} + \frac{u_0 \Delta x^2}{6} \frac{\partial^3 C(x, t)}{\partial x^3} + \dots$$



Repeat equation on previous slide:

$$\begin{aligned} & \frac{C(x, t + \Delta t) - C(x, t)}{\Delta t} + u_0 \frac{C(x + \Delta x, t) - C(x, t)}{\Delta x} - \frac{\partial C}{\partial t} - u_0 \frac{\partial C}{\partial x} = \\ & + \frac{\Delta t}{2} u_0^2 \frac{\partial^2 C(x, t)}{\partial x^2} - \frac{\Delta t^2}{6} u_0^3 \frac{\partial^3 C(x, t)}{\partial x^3} + \frac{u_0 \Delta x}{2} \frac{\partial^2 C(x, t)}{\partial x^2} + \frac{u_0 \Delta x^2}{6} \frac{\partial^3 C(x, t)}{\partial x^3} + \dots \end{aligned}$$



$$\begin{aligned} & \frac{C(x, t + \Delta t) - C(x, t)}{\Delta t} + u_0 \frac{C(x + \Delta x, t) - C(x, t)}{\Delta x} - \frac{\partial C}{\partial t} - u_0 \frac{\partial C}{\partial x} = \\ & \frac{u_0 \Delta x}{2} \left(1 + \frac{u_0 \Delta t}{\Delta x} \right) \frac{\partial^2 C(x, t)}{\partial x^2} + \frac{u_0 \Delta x^2}{6} \left(1 - \frac{u_0^2 \Delta t^2}{\Delta x^2} \right) \frac{\partial^3 C(x, t)}{\partial x^3} + \dots \end{aligned}$$

“Right hand side” of this equation, which should be zero, represents the **truncation error** of the numerical approximation to the terms on the left hand side of the linear advection equation

Truncation error due to *numerical diffusion* and *numerical dispersion*

Repeat equation on previous slide:

Euler forward in time

downwind in space if $u_0 > 0$

$$\frac{C(x, t + \Delta t) - C(x, t)}{\Delta t} + u_0 \frac{C(x + \Delta x, t) - C(x, t)}{\Delta x} - \frac{\partial C}{\partial t} - u_0 \frac{\partial C}{\partial x} =$$
$$\frac{u_0 \Delta x}{2} \left(1 + \frac{u_0 \Delta t}{\Delta x} \right) \frac{\partial^2 C(x, t)}{\partial x^2} + \frac{u_0 \Delta x^2}{6} \left(1 - \frac{u_0^2 \Delta t^2}{\Delta x^2} \right) \frac{\partial^3 C(x, t)}{\partial x^3} + \dots$$

“numerical diffusion”

“numerical dispersion”

Truncation error has both a *diffusive effect* and a *dispersive effect*

You will see this in **exercise 2** !

But you will also see in the next lecture that
the downwind scheme is **numerically unstable and therefore useless**

Numerical diffusion

First error-term on right hand side:

$$\frac{u_0 \Delta x}{2} \left(1 + \frac{u_0 \Delta t}{\Delta x} \right) \frac{\partial^2 C(x,t)}{\partial x^2}$$

“numerical diffusion”

small for small Δx and small Δt

$$\frac{u_0 \Delta x}{2} \left(1 + \frac{u_0 \Delta t}{\Delta x} \right) \equiv \frac{u_0 \Delta x}{2} (1 + \sigma)$$

non-dimensional parameter

represents “numerical diffusion coefficient”.

The next lecture (4) will demonstrate that $\sigma \equiv u_0 \Delta t / \Delta x$ also determines the “numerical stability” of the numerical solution of the advection equation.

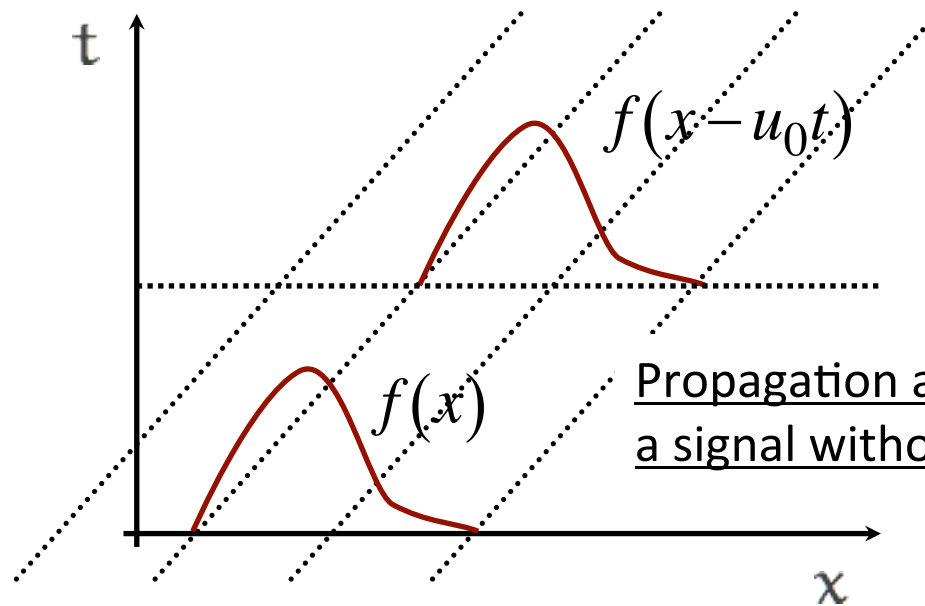
Analytical solution - linear advection equation

Linear advection equation

$$\frac{\partial C}{\partial t} + u_0 \frac{\partial C}{\partial x} = 0$$

Initial condition: $C(x,0) = f(x)$

Solution: $C(x,t) = f(x - u_0 t)$



Exercise 2: “Molenkamp test”*

Solve $\frac{\partial C}{\partial t} + u_0 \frac{\partial C}{\partial x} = 0$ for an idealized situation

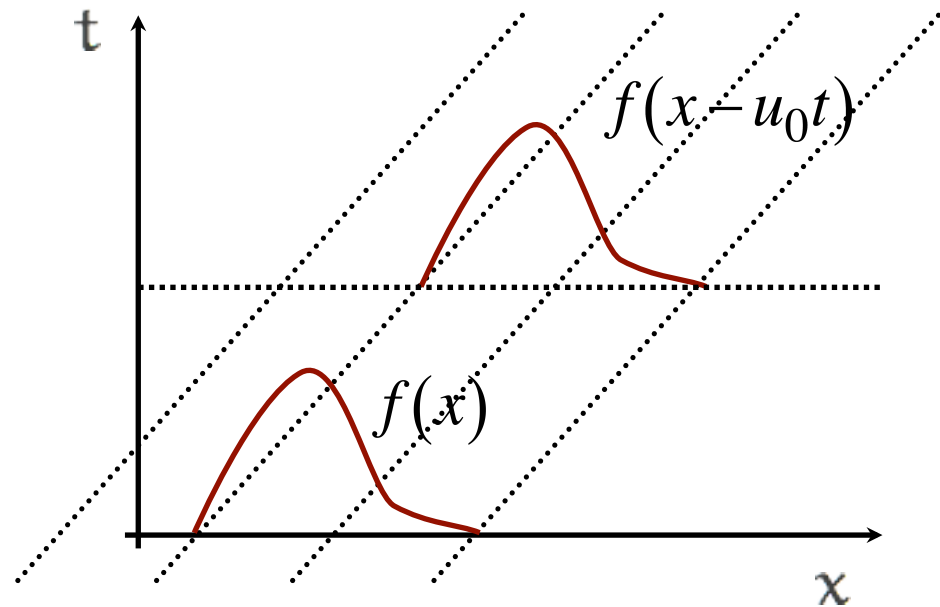
The domain of solution of this equation is $L=2500$ km wide and is periodic. Let us divide this domain into grid cells of equal size, $\Delta x=25$ km. The index of the corresponding gridpoints, j , runs from 0 to $j=100$. The concentration, C , at $t=0$ is prescribed as follows.

$C = C_0$ if $1125 \text{ km} \leq x \leq 1375 \text{ km}$

and

$C = 0$ if $x < 1125 \text{ km}$ and $x > 1375 \text{ km}$

Let $u_0 = 10 \text{ m/s}$



* C. Molenkamp, 1968: **J.Appl. Meteorol.**, 7, 160-167.

Exercise 2: “Molenkamp test”

Perform this simulation using **three different numerical schemes**.

You will discover that some schemes exhibit numerical diffusion and others exhibit numerical dispersion, or both. This exercise is called the “Molenkamp-test” (Molenkamp, 1968). A copy of the Molenkamp’s paper is provided.

- (1) Euler forward in time and upwind in space
- (2) “Lax-Wendroff” scheme (**lecture 3**)
- (3) The spectral method (**lecture 3**)

If “first-order upwind”:
$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + u_0 \frac{C_j^n - C_{j-1}^n}{\Delta x} = 0 \quad \boxed{u_0 > 0}$$

The Lax-Wendroff and spectral methods are explained in **lecture 3**.

Deadline exercises 2: Thursday 7 October 2021