Conservation Laws and Finite-Volume Methods

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Conservation Laws

A fundamental modelling principle for physical systems is the conservation of a given quantity Q:

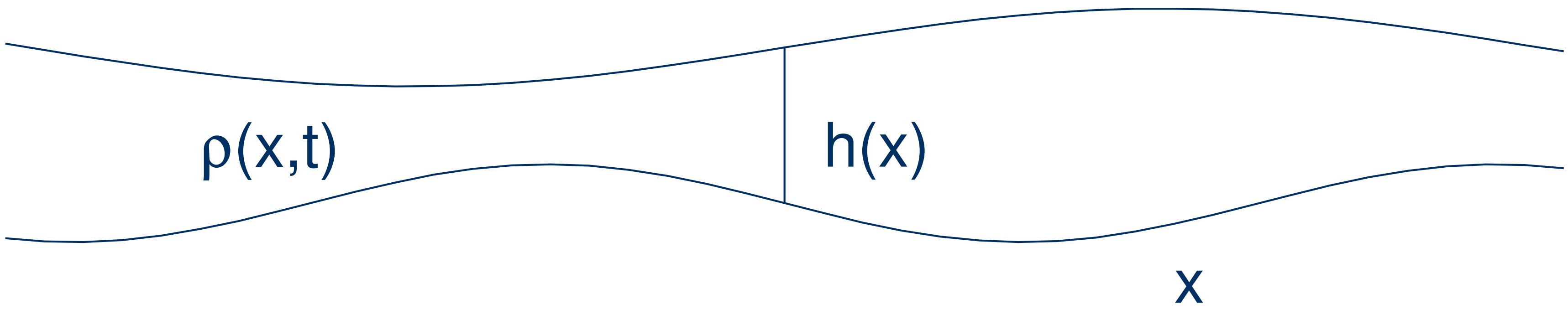
$$\begin{pmatrix}\text{change of } Q \\ \text{volume } \Omega\end{pmatrix} = \begin{pmatrix}\text{flux } F \text{ over the} \\ \text{boundary of } \Omega\end{pmatrix}$$

Examples of conserved quantities:

- mass
- momentum
- energy

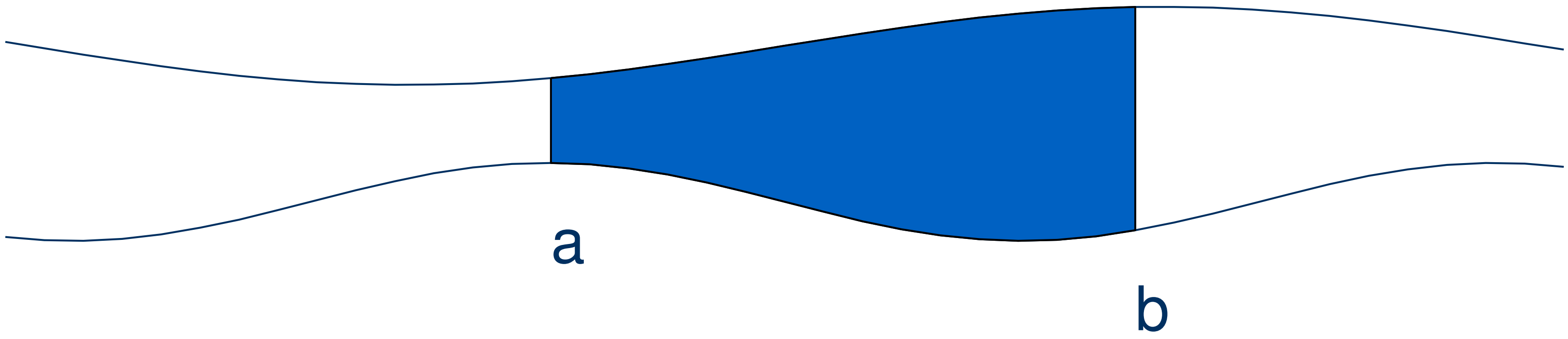
Conservation laws are basic building blocks when studying the behaviour of fluids.

A Motiviation Example: Pipe Flow



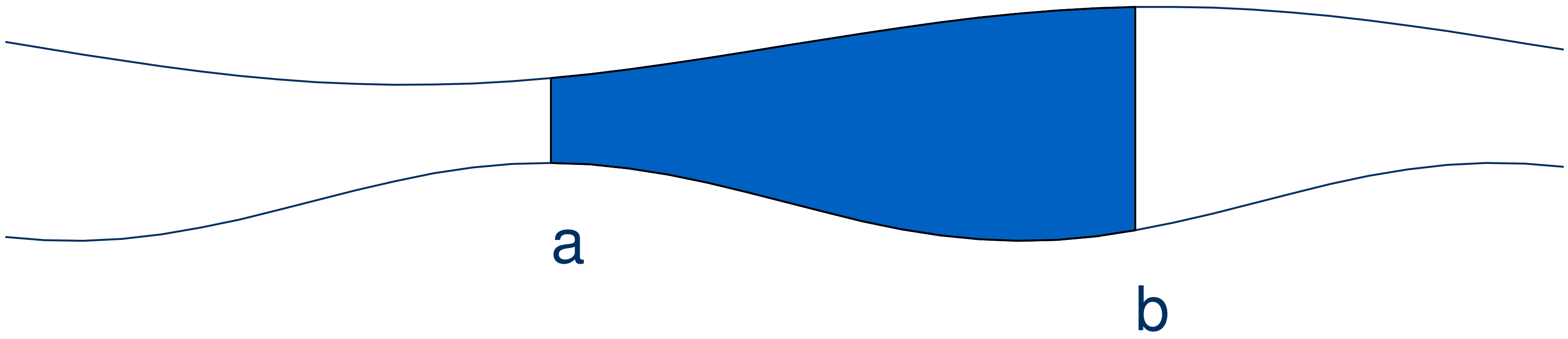
- Consider a one-dimensional pipe parametrised with the variable x
- At every point x, the pipe has a cross-section $h(x)$
- The pipe is filled with a fluid of density $\rho(x,t)$ (which is constant in the cross-sectional direction).

Pipe Flow: Derivation of Conservation Law



- Let us now consider a section of the pipe $x \in [a, b]$
- Assume that the fluid flows with a velocity $u(x, t)$ (which we for the moment assume is positive so that all fluid flows in the positive x-direction)
- Assume that no fluid is created or destroyed at any point inside the section

Derivation of Conservation Law, cont'd



Conservation law:

$$\begin{pmatrix}\text{time rate of change of fluid} \\ \text{inside the section}[a,b]\end{pmatrix} = \begin{pmatrix}\text{flow } \textit{into} \text{ the pipe} \\ \text{at } x = a\end{pmatrix} - \begin{pmatrix}\text{flow } \textit{out of} \text{ the pipe} \\ \text{at } x = b\end{pmatrix}$$

Mathematically, an equation on integral form:

$$\frac{d}{dt}\int_a^b \rho(x,t)h(x)\,dx = \big[\rho(a,t)u(a,t)h(a)\big] - \big[\rho(b,t)u(b,t)h(b)\big]$$

Derivation of Conservation Law, cont'd

Let us rewrite the conservation law:

$$\frac{d}{dt}\int_a^b \rho(x,t)h(x)\,dx = \big[\rho(a,t)u(a,t)h(a)\big] - \big[\rho(b,t)u(b,t)h(b)\big]$$

$$= -\int_a^b \frac{\partial}{\partial x}\big[\rho(x,t)u(x,t)h(x)\big]\,dx$$

Now, since the section $[a,b]$ does not move in time:

$$\int_a^b \Big(\frac{\partial}{\partial t}\big[\rho(x,t)h(x)\big] + \frac{\partial}{\partial x}\big[\rho(x,t)u(x,t)h(x)\big]\Big)\,dx = 0$$

If the equation holds for all a, b and the integrand is continuous, then:

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x}(\rho u h) = 0$$

Closure of the Model

Our model so far:

$$\frac{\partial}{\partial t}\big(\rho h\big) + \frac{\partial}{\partial x}\big(\rho u h\big) = 0$$

To close the model, we must specify

- the velocity: $u(x,t) = f\big(x,t,\rho\big)$,
- the initial data: $\rho(x,0) = \rho_0(x)$
- and some boundary data, e.g, a given value at the inflow and outflow boundaries

$$\rho(x_1,t) = \rho_1(t), \qquad \rho(x_2,t) = \rho_2(t)$$

or a given inflow value and free outflow

$$\rho(x_1,t) = \rho_1(t), \qquad \partial_x \rho(x_2,t) = 0$$

Example: Advection Equation

In the case where $h(x) \equiv 1$ and $u(x,t)$ does not depend on the unknown ρ, the conservation law reduces to the *linear advection equation*

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0, \qquad \rho(x,0) = \rho_0(x)$$

This equation is hyperbolic and describes the passive advection of a quantity ρ within a given velocity field u.

Let us now consider a particularly simple example, for which $u(x,t) \equiv c > 0$, i.e.,

$$\frac{\partial \rho}{\partial t} + c\frac{\partial \rho}{\partial x} = 0, \qquad \rho(x,0) = \rho_0(x)$$

Solving the Advection Equation

To solve the advection equation, we perform a change of variables

$$\tau = t, \qquad \xi = x - ct$$

Using the chain rule:

$$\frac{\partial}{\partial t} = \frac{\partial \tau}{\partial t}\frac{\partial}{\partial \tau} + \frac{\partial \xi}{\partial t}\frac{\partial}{\partial \xi} = \frac{\partial}{\partial \tau} - c\frac{\partial}{\partial \xi}$$

$$\frac{\partial}{\partial x} = \frac{\partial \tau}{\partial x}\frac{\partial}{\partial \tau} + \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi} = \frac{\partial}{\partial \xi}$$

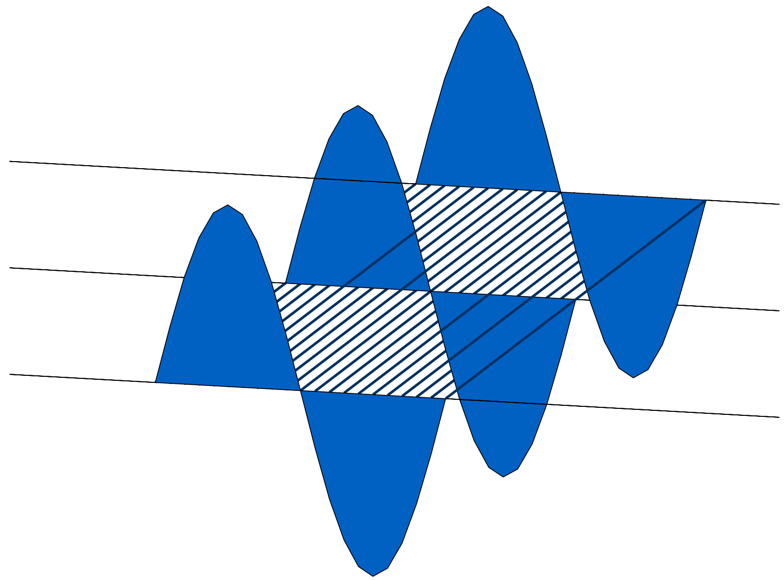
Hence:

$$0 = \frac{\partial \rho}{\partial t} + c\frac{\partial \rho}{\partial x} = \left(\frac{\partial \rho}{\partial \tau} - c\frac{\partial \rho}{\partial \xi}\right) + c\frac{\partial \rho}{\partial \xi} = \frac{\partial \rho}{\partial \tau}$$

Solving the Advection Equation, cont'd

This is easy to solve:

$$\frac{\partial \rho}{\partial \tau} = 0 \quad \Longrightarrow \quad \rho = \rho(\xi)$$



From the initial condition:

$$\begin{aligned} \rho(x,t) &= \rho(\xi) = \rho(\xi, \tau = 0) \\ &= \rho_0(\xi) = \rho_0(x - ct) \end{aligned}$$

In other words, the profile of the solution is shifted in the positive x-direction with time, but the shape does not change

The lines $x - ct = constant$ are called the *characteristics* of the equation. If we know the solution $\rho(x,t)$ at one point on a characteristic, we also know it at all other points on the same characteristic.

What About Discontinuous Data?

Well, the integral equation is still valid:

$$\frac{d}{dt}\int_a^b \rho(x,t)h(x)\,dx = \big[\rho(a,t)u(a,t)h(a)\big] - \big[\rho(b,t)u(b,t)h(b)\big]$$

However, we cannot derive a PDE as above. Instead we define a so-called *weak* solution that satisfies

$$\int_0^\infty \int_{-\infty}^\infty \Big(\frac{\partial\phi}{\partial t}(\rho h) + \frac{\partial\phi}{\partial x}(\rho u h)\Big)\,dxdt = 0,$$

for a sufficiently smooth function $\phi(x,t)$

Example: Burgers' Equation

Assume now that the velocity $u = \frac{1}{2}\rho$. This gives Burgers' equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\Big(\frac{1}{2}\rho^2\Big) = 0$$

Burgers' equation is a simple *nonlinear* equation is often used as a model for the momentum equations in fluid mechanics

The Method of Characteristics

In order to use our previous method of characteristics, we rewrite the equation as

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

Now we can introduce a change of variables as above

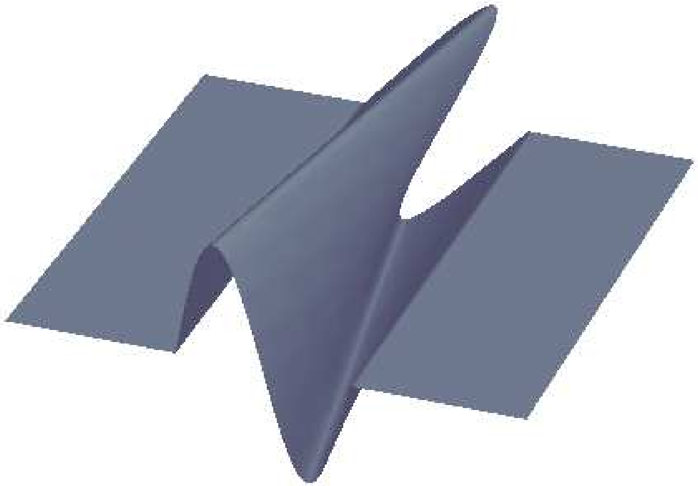
$$\tau = t, \qquad \xi = x - \rho t$$

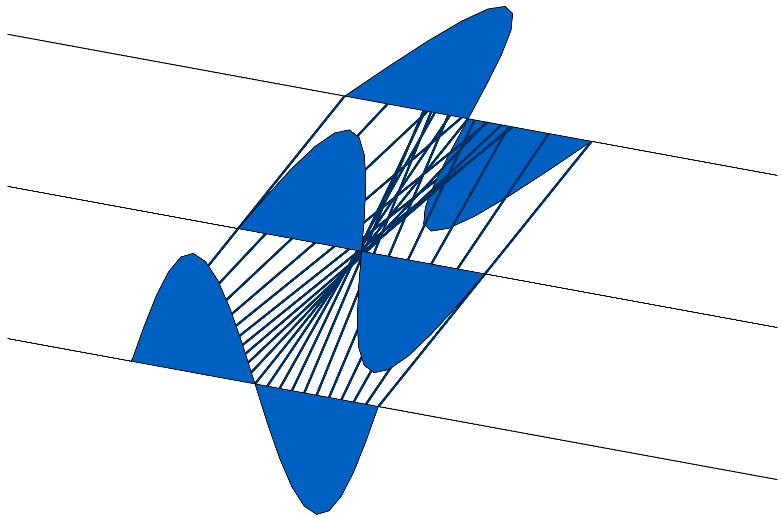
which gives

$$\frac{\partial \rho}{\partial \tau} = 0, \qquad \rho(\xi) = \rho_0(\xi)$$

The Method of Characteristics, cont'd

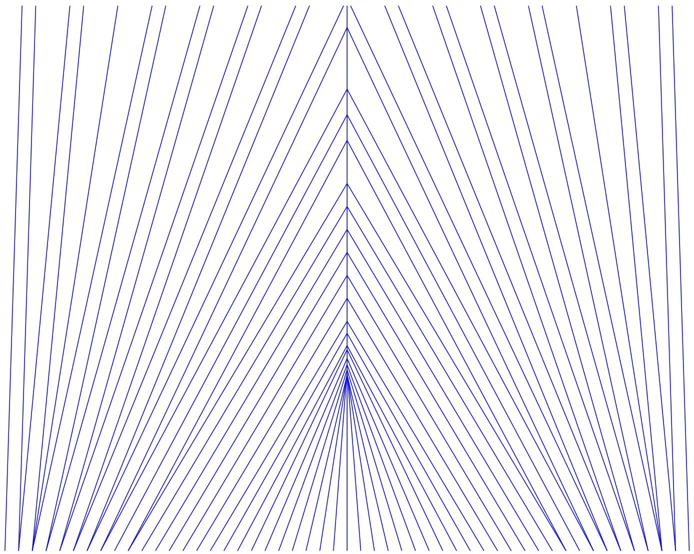
Problem: the characteristics depend on the solution
$\longrightarrow$ triple-valued solutions reminiscent of 'breaking waves'.
This is clearly not mathematically valid

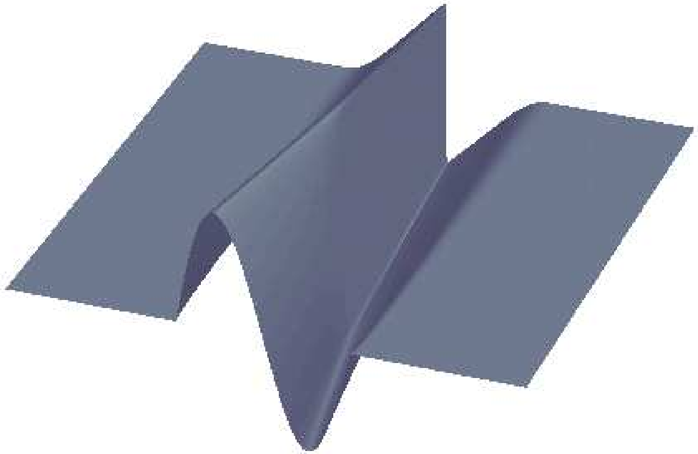




Burgers Equation: Correct Solution

The correct solution forms a discontinuity (a so-called shock) where the characteristics meet





Shocks and Other Discontinuities

Observation: The method of characteristics failed to give mathematically feasible solutions.

Solution: use our definition of weak solutions

$$\int_0^\infty \int_{-\infty}^\infty \Big(\frac{\partial \phi}{\partial t}\rho + \frac{\partial \phi}{\partial x} f(\rho)\, dxdt = 0,$$

Introduce shock waves that are propagating discontinuities that satisfies

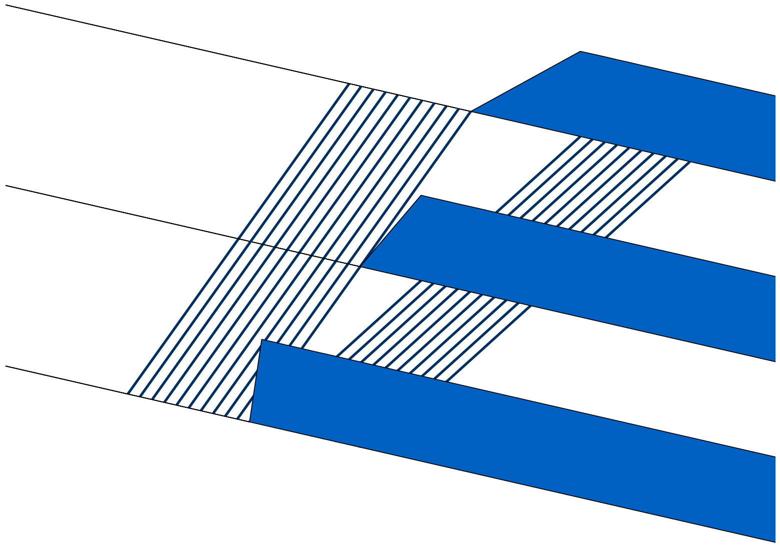
$$\frac{dx}{dt} = \frac{f(\rho_L) - f(\rho_R)}{\rho_L - \rho_R}$$

where ρ_L and ρ_R are the left and right values, respectively.

The Method of Characteristics, revisited

Consider now initial data of the form

$$\rho_0(x) = \begin{cases} 0, & x < 0 \\ 1, & x > 0 \end{cases}$$

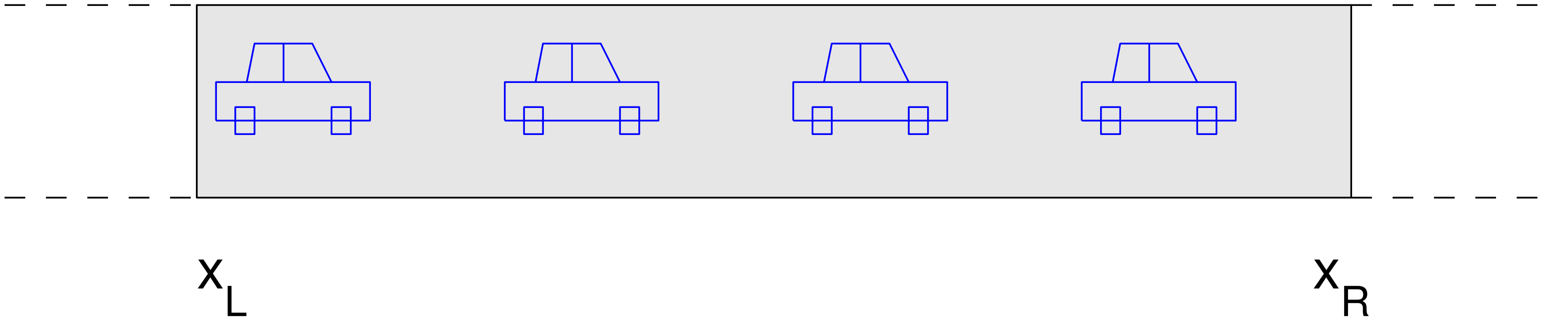


How do we fill the missing part?
Use a piecewise linear wave?

Generally: several weak solutions are possible!

We need extra conditions to determine correct solution (e.g., by incorporating viscosity, which has been neglected in the model, and study the vanishing viscosity limit).

Example: A Traffic Model



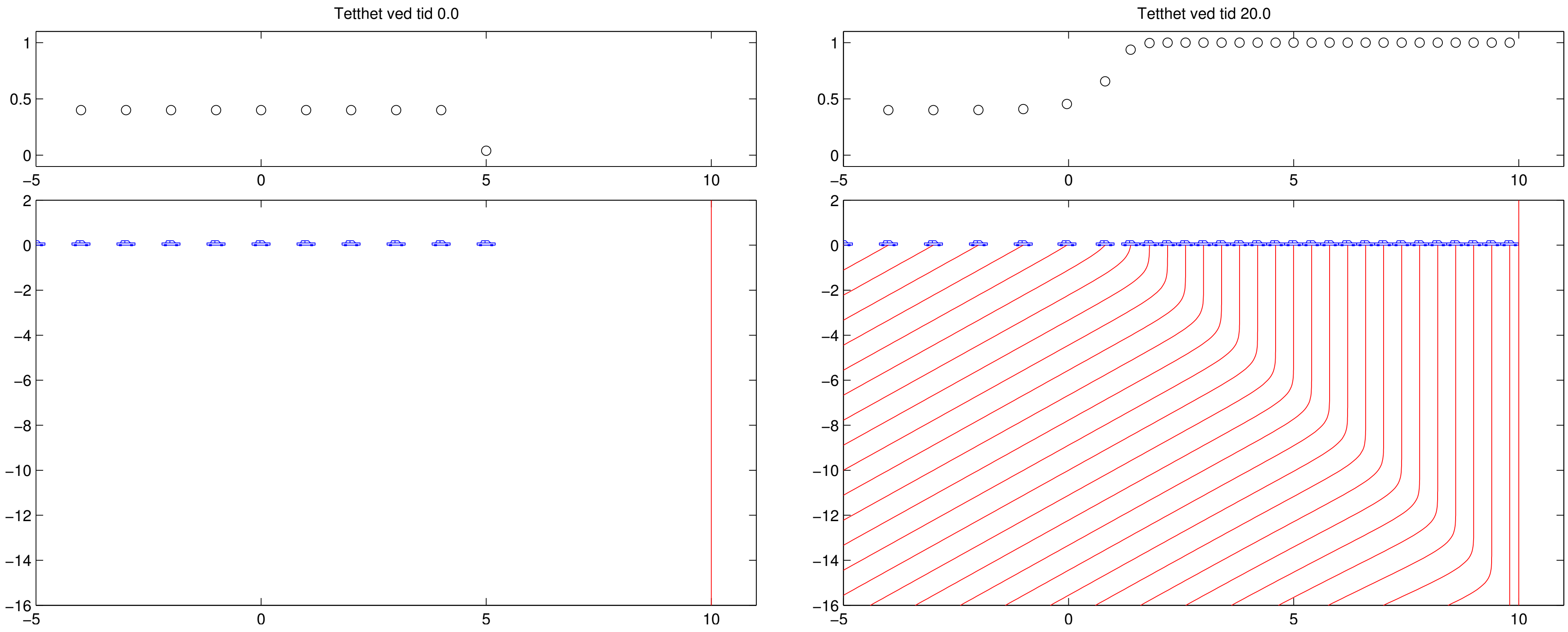
- Density of cars: ρ
- Velocity of each car: $u(\rho) = \rho_m - \rho$
- Conservation of 'mass':

$$\big[\rho(t+\Delta t) - \rho(t)\big](x_L - x_R) = \Delta t\big[\rho_L u(\rho_L) - \rho_r u_R(\rho_R)\big]$$

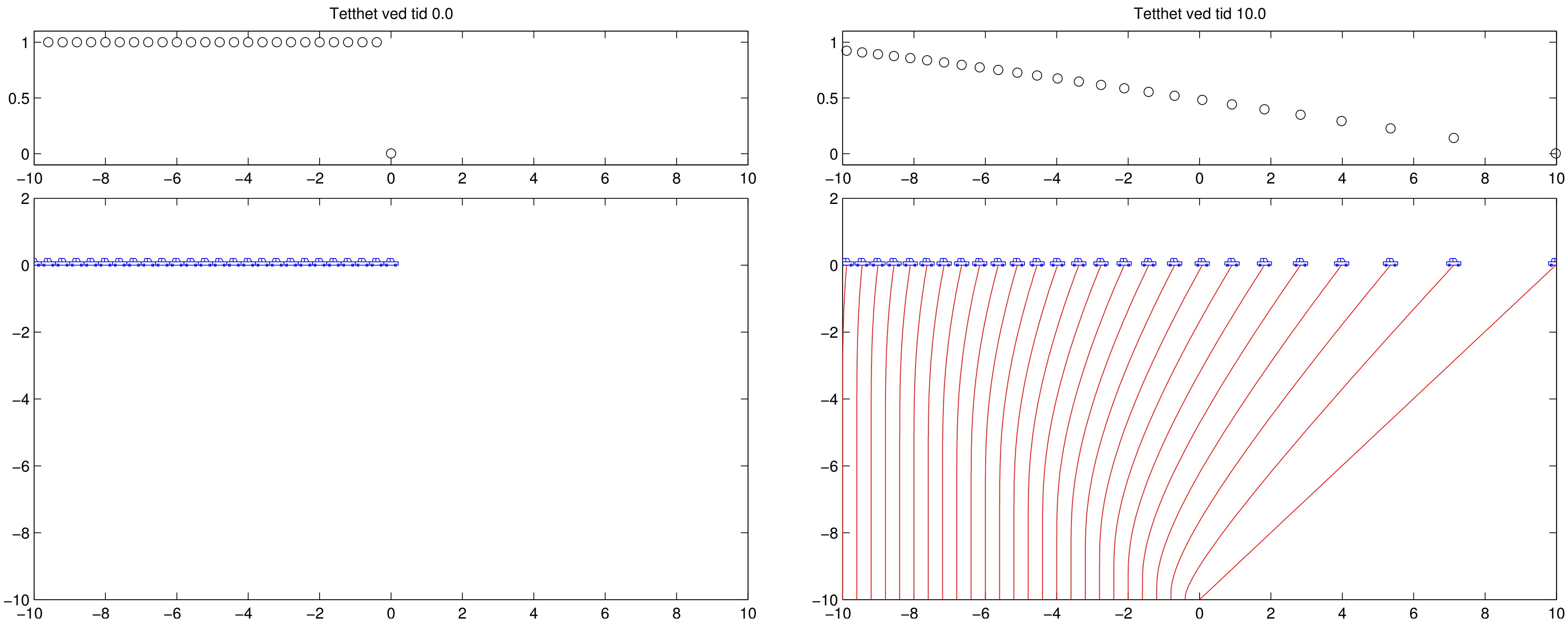
- In the limit, $x_R \to x_L$, $\Delta t \to 0$

$$\rho_t + f(\rho)_x = 0, \qquad f(\rho) = \rho u(\rho) = \rho(\rho_m - \rho)$$

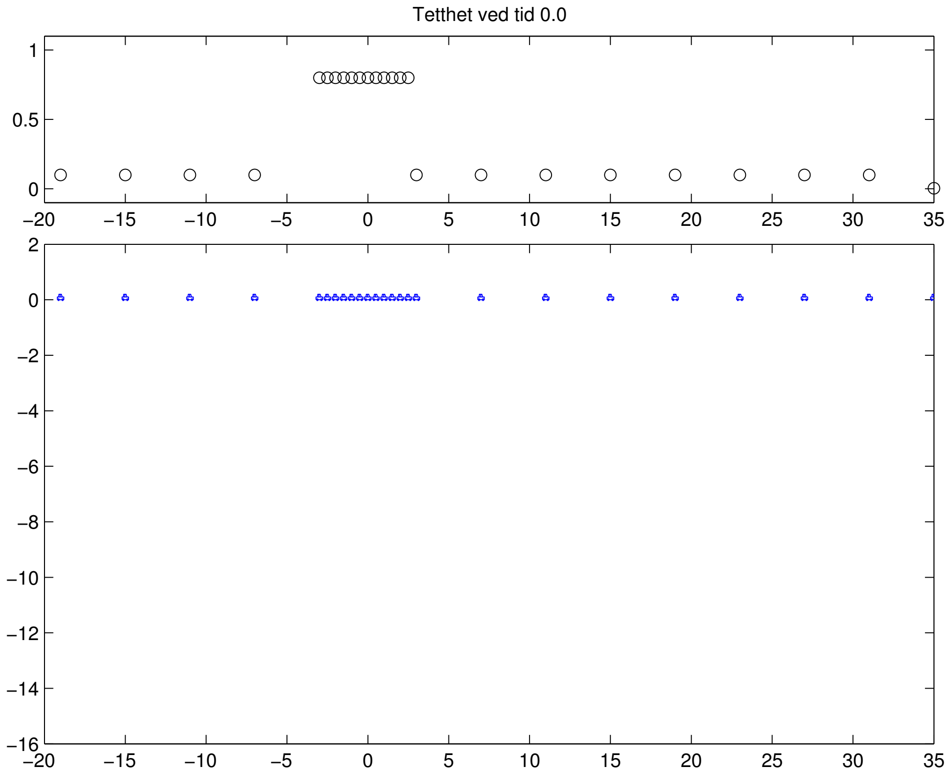
The Traffic Light Turns Red

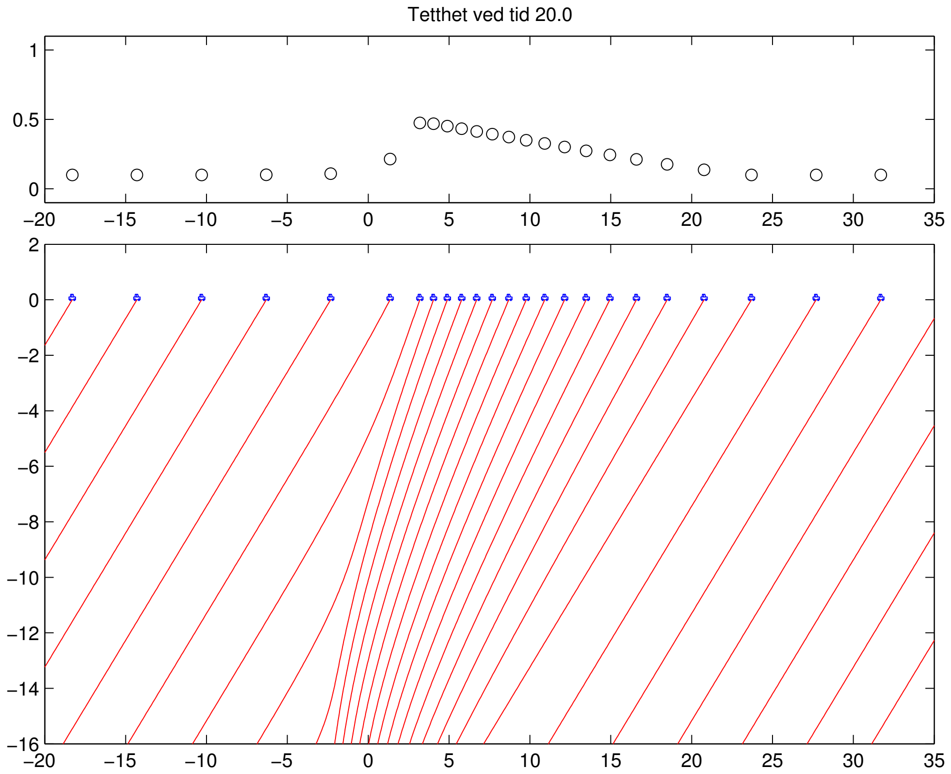


The Traffic Light Turns Green



A Local Congestion in the Traffic





Linear Systems of Conservation Laws

Consider the linear system

$$U_t + AU_x = 0, \qquad U(x,0) = U_0(x)$$

Hyperbolicity means that A is diagonalisable with real eigenvalues λ_i:

$$A = R\Lambda R^{-1}, \qquad \Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_m)$$

where each column r_i of R is a right eigenvector of A

Now, premultiply the conservation law by R^{-1} and define $V = R^{-1}U$. Then

$$\partial_t V + \Lambda \partial_x V = 0$$

Thus, we have a set of scalar equations $\partial_t v_i + \lambda_i \partial_x v_i = 0$

Linear Systems of Conservation Laws, cont'd

Each scalar equation is solved by

$$v_i(x,t) = v_i^0(x - \lambda_i t)$$

Now the solution is given as a superposition of m simple waves

$$U(x,t) = \sum_{i=0}^{m} v_i^0(x - \lambda_i t) r_i$$

Nonlinear systems:

$$Q_t + F(Q)_x = 0$$

We can rewrite

$$Q_t + A(Q)Q_x = 0, \qquad A(Q) = \frac{dF}{dQ}$$

Although we cannot repeat the analysis from the linear case, we observe that eigenvalues and eigenvectors must have some importance for the local solution.

The Shallow Water Model

The model is a *nonlinear* system of conservation laws:

$$\begin{bmatrix} h \\ hu \end{bmatrix}_t + \begin{bmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \end{bmatrix}_x = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Here h is water depth, g is acceleration of gravity, and (u, v) the water velocity.

As opposed to our previous wave model (the linear wave equation), this model accounts for water height and allows for bores, hydraulic jumps, 'breaking waves', etc.

(Modelling passive advection of pollution particles: $q_t + (qu)_x = 0$)

The Euler Equations for Gas Dynamics

This is the canonical example of a conservation law. Here in two spatial dimensions:

$$\begin{bmatrix} \rho \\ \rho u \\ \rho v \\ E \end{bmatrix}_t + \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ u(E+p) \end{bmatrix}_x + \begin{bmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ v(E+p) \end{bmatrix}_y = 0.$$

Here ρ denotes density, u and v velocity in x- and y- directions, p pressure, and E is the total energy (kinetic plus internal energy) given by

$$E = \rho(u^2 + v^2)/2 + p/(\gamma - 1)$$

We will return to the Euler and the shallow-water equations later

Finite-Volume Methods

Previously we have used finite-differences to make *pointwise* approximations to PDEs.

We now take another approach. Let us revisit the linear advection equation:

$$\frac{d}{dt}\int_a^b \rho(x,t)\,dx = c\rho(a,t) - c\rho(b,t)$$

Let us now divide the section $[a,b]$ into grid-cells $[x_{i-1/2}, x_{i+1/2}]$ such that $x_{M-1/2} = a$ and $x_{N+1/2} = b$ for some integers N, M.

Now define the cell-averages

$$\rho_i(t) = \frac{1}{x_{i+1/2} - x_{i-1/2}}\int_{x_{i-1/2}}^{x_{i+1/2}} \rho(x,t)\,dx$$

Finite-Volume Methods, cont'd

By imposing the conservation law on each grid-cell, we obtain

$$\frac{d}{dt}\rho_i(t)\Delta x_i = c\rho(x_{i-1/2}, t) - c\rho(x_{i+1/2}, t)$$

The grid-cells $[x_{i-1/2}, x_{i+1/2}]$ are referred to as *finite volumes*; hence the name of the method.

Two points remain:

- How do we solve the ODEs for the cell-averages $\rho_i(t)$?
- And given cell-averages ρ_i: how do we evaluate the *point-values* $\rho(x_{i\pm1/2})$ at the cell-edges?

Finite-Volume Methodcont'd

The first question has a simple answer: we use a standard ODE solver, e.g., forward Euler:

$$\frac{(\rho_i^{n+1} - \rho_i^n)}{r_i} = c\rho(x_{i-1/2}, n\Delta t) - c\rho(x_{i+1/2}, n\Delta t)$$

where $r_i = \Delta t / \Delta x_i$

The second question is a bit more complicated and consists of two parts:

- *reconstruction* of point-values from cell-averages
- and evaluation of edge-fluxes

Finite-Volume Methods: Reconstruction

In the finite-volume method, our discrete quantities are the cell-averages ρ_i defined over the grid-cells $[x_{i-1/2}, x_{i+1/2}]$.

To define point-values, we must *assume a functional form* for the unknown solution $\rho(x,t)$.

Obvious idea: use a piecewise polynomial inside each finite volume.

Simplest solution: piecewise constant,

$$\rho(x,t) = \rho_i(t), \text{ for } x \in [x_{i-1/2}, x_{i+1/2}]$$

More advanced methods: higher-order reconstruction based upon piecwise polynomial (or rational function) interpolation of cell-averages.

Finite-Volume Methods: Flux-Evaluation

Problem: our piecewise constant approximation gives two candidate values for $\rho(x_{i+1/2})$:

- $\rho(x^-_{i+1/2})$ obtained from the grid-cell $[x_{i-1/2}, x_{i+1/2}]$ to the left of the cell edge
- $\rho(x^+_{i+1/2})$ obtained from the grid-cell $[x_{i+1/2}, x_{i+3/2}]$ to the right of the cell edge

Question: which one should we choose?

Answer: this depends upon the equation, and different choices gives different numerical methods!
Here: since $c > 0$, the solution shifts from left to right as time increases. Hence, we should use the *upwind* value $\rho(x^-_{i+1/2}) = \rho_i$

Our First Finite-Volume Method ...

Summing up, we have obtained:

$$\rho_i^{n+1} = \rho_i^n - c r_i \big[\rho_i^n - \rho_{i-1}^n\big]$$

This is called the first-order upwind method and is stable under the CLF conditions

$$c \max_i r_i = c \max_i \frac{\Delta t}{\Delta x_i} \leq 1.$$

If $c < 0$, we can derive an analogous method

$$\rho_i^{n+1} = \rho_i^n - c r_i \big[\rho_{i+1}^n - \rho_i^n\big]$$

Linear systems: upwind in each characteristic component v_i

A Conservative Method

Since conservation was the fundamental modelling principle, our numerical methods should obey the same principle

To see that the method is conservative: summing over all i gives a telescoping sum for the fluxes:

$$\sum_{i=M}^{N} \rho_i^{n+1} \Delta x_i = \sum_{i=M}^{N} \rho_i^{n} \Delta x_i - c\Delta t \big[\rho_N^n - \rho_M^n\big],$$

where $\rho_M = \rho(a)$ and $\rho_N = \rho(b)$

Generalisation to Nonlinear Equations

Let us now consider a general nonlinear equation

$$\rho_t + f(\rho)_x = \rho_t + f'(\rho)\rho_x = 0$$

The finite-volume scheme then reads

$$\frac{(\rho_i^{n+1} - \rho_i^n)}{r_i} = f\big(\rho(x_{i-1/2}, n\Delta t)\big) - f\big(\rho(x_{i+1/2}, n\Delta t)\big)$$

Point-values at cell edges from piecewise constant reconstruction $\longrightarrow$ two candidate values:

$$\rho(x_{i+1/2}, n\Delta_t) = \rho_i^n \quad \text{or} \quad \rho(x_{i+1/2}, n\Delta t) = \rho_{i+1}^n$$

In other words, the scheme reads:

$$\frac{(\rho_i^{n+1} - \rho_i^n)}{r_i} = F\big(\rho_{i-1}^n, \rho_i^n\big) - F\big(\rho_i^n, \rho_{i+1}^n\big)$$

Generalisation to Nonlinear Equation, cont'd

Repeating the argument from the linear case:

$$F(\rho_i^n, \rho_{i+1}^n) = \begin{cases} f(\rho_i^n), & f'(\rho) > 0 \quad \forall\rho, \\ f(\rho_{i+1}^n), & f'(\rho) < 0 \quad \forall\rho, \\ ?? & \text{otherwise} \end{cases}$$

Generally: must solve local (Riemann) problems of the form

$$\rho_t + f(\rho)_x = 0, \qquad \rho(x,0) = \begin{cases} \rho_i, & x < 0, \\ \rho_{i+1}, & x > 0 \end{cases}$$

This has a similarity solution $\rho(x,t) = v(x/t)$. If we know $v(\zeta)$, then $F(\rho_i, \rho_{i+1}) = f\big(v(0)\big) \longrightarrow$ Godunov schemes, which are generalisations of the upwind scheme for nonlinear equations

Another Approach

Rather than using the Godunov flux, we can try the simple choice

$$F(\rho_i^n, \rho_{i+1}^n) = \tfrac{1}{2}\big[f\big(\rho_i^n\big) + f\big(\rho_{i+1}^n\big)\big]$$

This gives a centred scheme

$$\frac{(\rho_i^{n+1} - \rho_i^n)}{r_i} = f\big(\rho_{i-1}^n\big) - f\big(\rho_{i+1}^n\big)$$

which is notoriously unstable.

Remedy: stabilize by adding artificial diffusion, $(\Delta x^2/\Delta t)\partial_x^2\rho$, discretized by standard finite-differences $\longrightarrow$ the centred Lax–Friedrichs scheme

$$\rho_i^{n+1} = \frac{1}{2}\Big(\rho_{i+1}^n + \rho_{i-1}^n\Big) + \tfrac{1}{2}r_i\Big[f\big(\rho_{i+1}^n\big) - f\big(\rho_{i-1}^n\big)\Big].$$

Higher Order

The upwind and the Lax–Friedrichs schemes are first order.
To obtain higher order, we can solve the ODEs

$$\frac{d}{dt}\rho_i(t)\Delta x_i = f\big(\rho(x_{i-1/2},t)\big) - f\big(\rho(x_{i+1/2},t)\big)$$

by the modfied Euler method

$$\frac{(\rho_i^{n+1}-\rho_i^n)}{r_i} = f\Big(\rho\big(x_{i-1/2},(n+\tfrac{1}{2})\Delta t\big)\Big) - f\Big(\rho\big(x_{i+1/2},(n+\tfrac{1}{2})\Delta t\big)\Big)$$

The point-values $\rho\big(x_{i\pm1/2},(n+\frac{1}{2})\Delta t\big)$ can be obtained from the Lax–Friedrichs scheme on a grid with half the grid size $\longrightarrow$ the second-order Lax–Wendroff's method

$$\begin{aligned}
\rho_{i+1/2}^{n+1/2} &= \tfrac{1}{2}\big(\rho_i^n + \rho_{i+1}^n\big) - \tfrac{1}{2}r_i\big[f(\rho_{i+1}^n) - f(\rho_i^n)\big],\\
\rho_i^{n+1} &= \rho_i - r_i\big[f(\rho_{i+1/2}^{n+1/2}) - f(\rho_{i-1/2}^{n+1/2})\big].
\end{aligned}$$

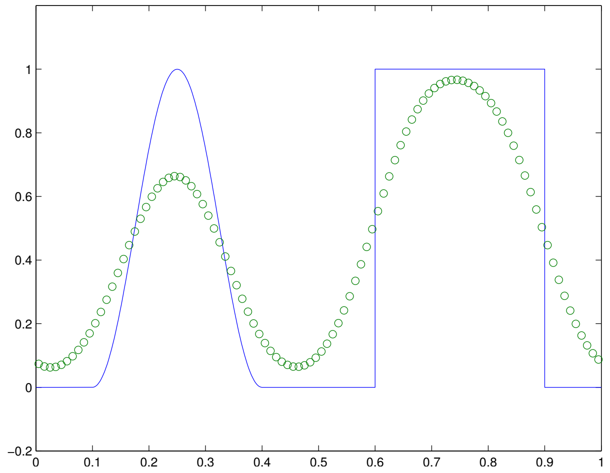
Numerical Examples

Consider a linear advection equation with periodic boundaries

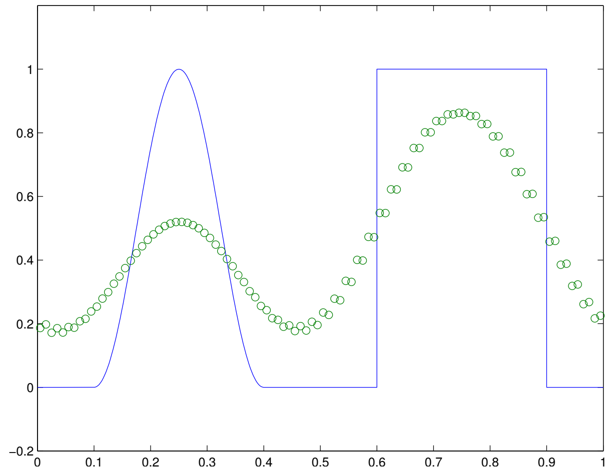
$$u_t + u_x = 0, \qquad u(x,0) = u_0(x), \qquad u(0,t) = u(1,t).$$

As initial data $u_0(x)$ we choose a combination of a smooth squared cosine wave and a double step function.

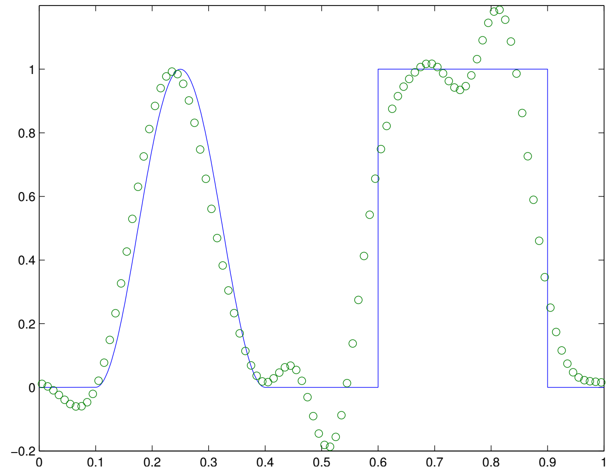
upwind



Lax–Friedrichs



Lax–Wendroff

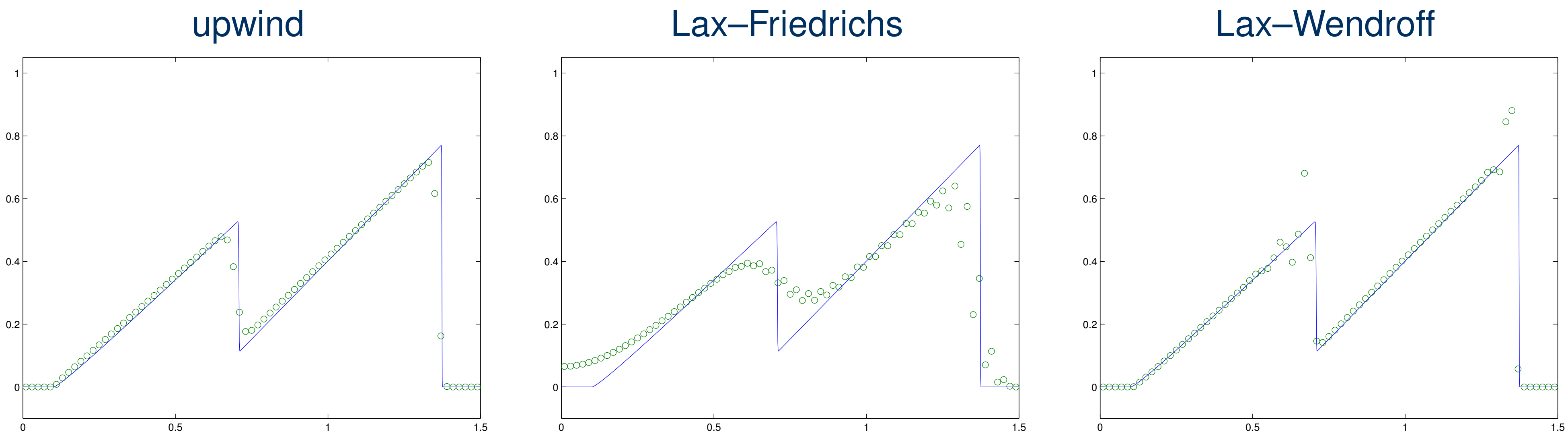


Numerical Examples, cont'd

Consider a Burgers' equation with periodic boundaries

$$u_t + u_x = 0, \qquad u(x,0) = u_0(x), \qquad u(0,t) = u(1.5,t).$$

As initial data $u_0(x)$ we choose a combination of a smooth squared cosine wave and a double step function.



Finite Volumes vs. Finite Differences

Observation: for the linear advection equation, the upwind method can be obtained directly in a finite-difference setting with forward differences in time and backward differences in space. Similarly for other methods and other equations.

Question: so, what is the difference?

Short answer: the interpretations are different!

Longer answer: the generalisations to higher-order, higher-dimesions, complex grids, etc are different...

Moreover, to add to the confusion: it is customary conservative finite-difference methods for finite-volume methods

Two Spatial Dimensions

The Lax–Friedrichs scheme on a Cartesian grid

$$
\begin{aligned}
\rho_{ij}^{n+1} = & \frac{1}{4}\Big(\rho_{i+1,j}^{n} + \rho_{i-1,j}^{n} + \rho_{i,j+1}^{n} + \rho_{i,j-1}^{n}\Big) \\
& - \frac{1}{2}r\Big[f\big(\rho_{i+1,j}^{n}\big) - f\big(\rho_{i-1,j}^{n}\big)\Big] - \frac{1}{2}r\Big[g\big(\rho_{i,j+1}^{n}\big) - g\big(\rho_{i,j-1}^{n}\big)\Big]
\end{aligned}
$$

The extensions for the upwind scheme and Lax–Wendroff are similar.

Using the finite-volume approach, the extension to more complex grids are rather straightforward. This is one major advantage of finite volumes versus finite differences.

High-Resolution Schemes

The schemes we have introduced so far suffer from the following drawbacks:

- they have low (formal) spatial accuracy (order one or two)
- first-order schemes smear discontinuitites
- second-order schemes create spurious oscillations

Remedy: Introduction of modern *high-resolution schemes*

> A high-resolution scheme delivers high-order resolution in smooth parts and avoids the creation of spurious oscillations near discontinuities

Today there are a lot of high-resolution schemes available: flux-limiter schemes, slope-limiter schemes, wave-propagation, (W)ENO schemes, discontinuous Galerkin,... However, these schemes are outside the scope of this course.