Hyperbolic Systems (spring 2001)

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Introduction – motivation

Conservative form ideal MHD equations

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho\vec{v}\\ \frac{\rho v^2}{2}+\rho e+\frac{B^2}{2}\\ \vec{B}\end{bmatrix}+\nabla\cdot\begin{bmatrix}\rho\vec{v}\\ \rho\vec{v}\vec{v}+\left(p+\frac{B^2}{2}\right)\vec{I}-\vec{B}\vec{B}\\ \left(\frac{\rho v^2}{2}+\rho e+p\right)\vec{v}-(\vec{v}\times\vec{B})\times\vec{B}\\ \vec{v}\vec{B}-\vec{B}\vec{v}\end{bmatrix}=0$$

- MHD describes macroscopic behavior of many plasmas in space, laboratory, ...
- plasma $=$ ionized gas $\Rightarrow$ electromagnetic effects

theory

- eight complex equations: very 'old'
- MHD physics $\neq$ derive new equations

  $=$ find and understand solutions ($\sim$ general relativity)
- mathematical nature (complex!):

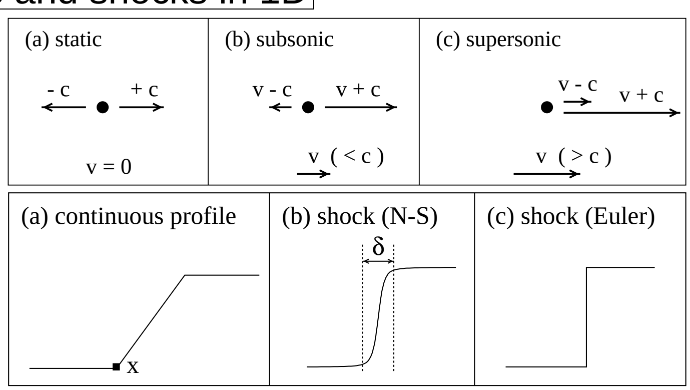
  - conservation law
  - hyperbolic $\Rightarrow$ waves

  three anisotropic waves (gasdynamics: one isotropic wave, sound wave)

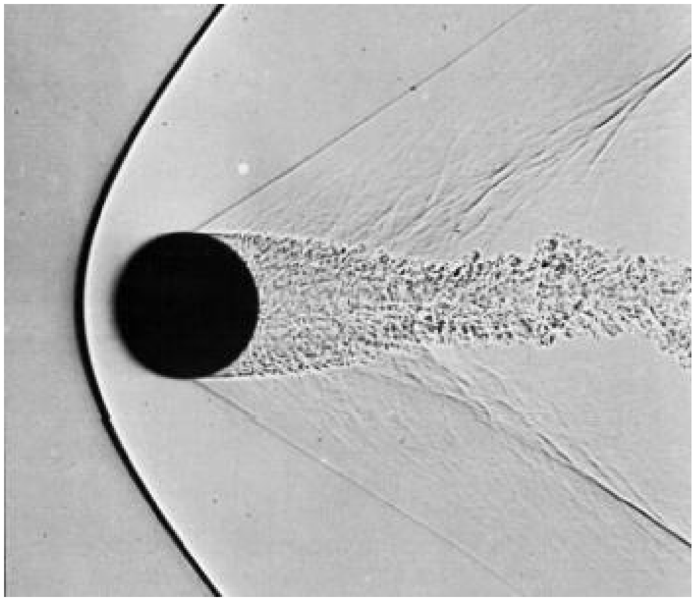
  - nonlinear $\Rightarrow$ waves can steepen into shocks (discontinuities)
- learn from simpler systems! (nonlinear hyperbolic conservation laws)

Shock phenomena

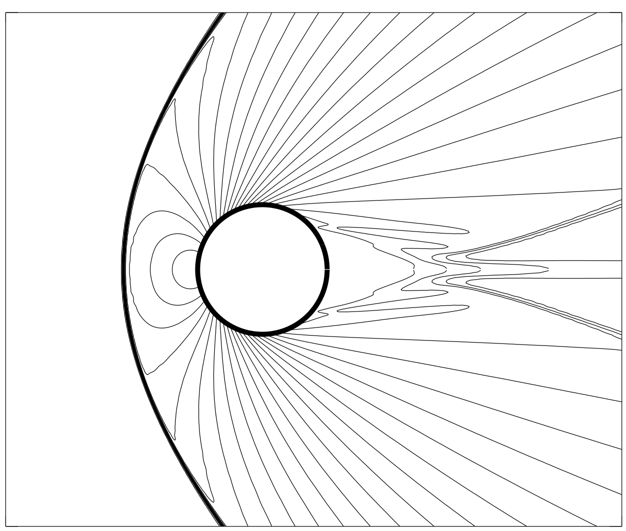
Sound waves and shocks in 1D



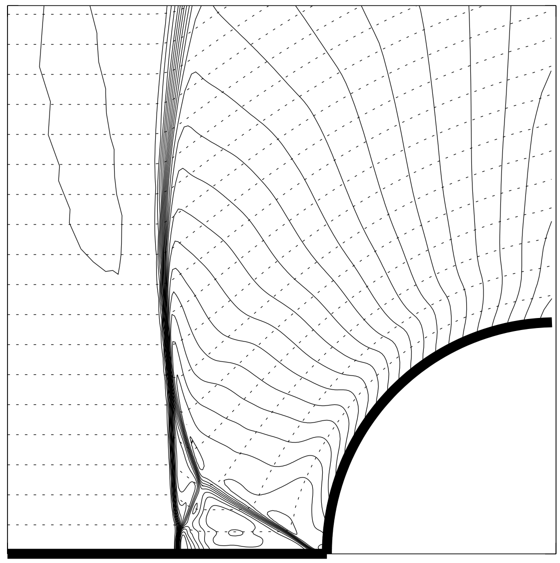
Supersonic airflow over sphere



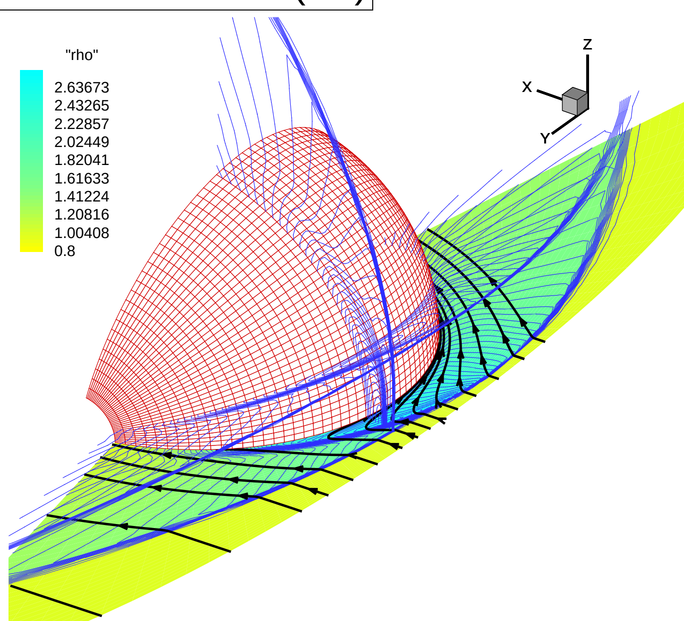
Numerical simulation of bow shock (gasdynamic)



MHD simulation of bow shock (2D)



MHD simulation of bow shock (3D)

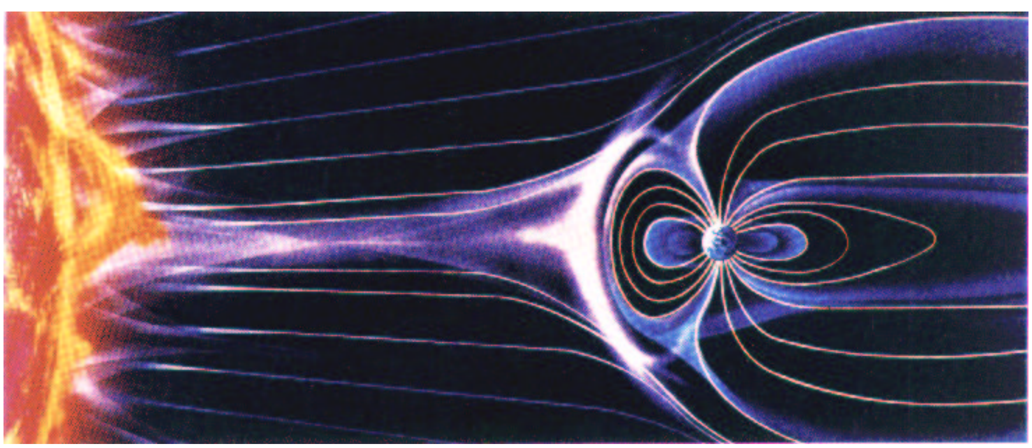


Numerical simulation techniques

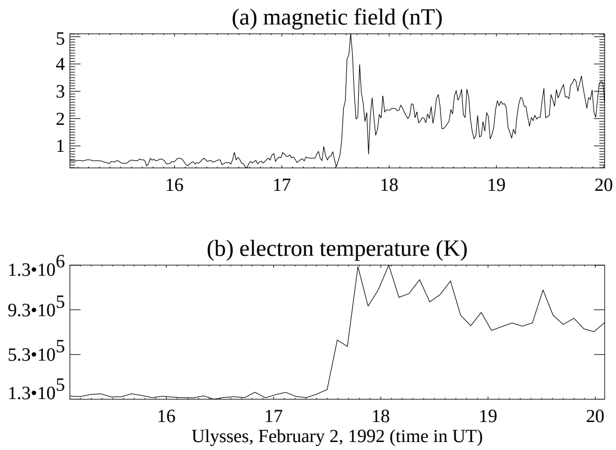
- nonlinear hyperbolic conservation law
- methods borrowed from Computational Fluid Dynamics (airplanes, ...)
- introduction to shock-capturing methods for MHD
- parallel computing using MPI

Applications

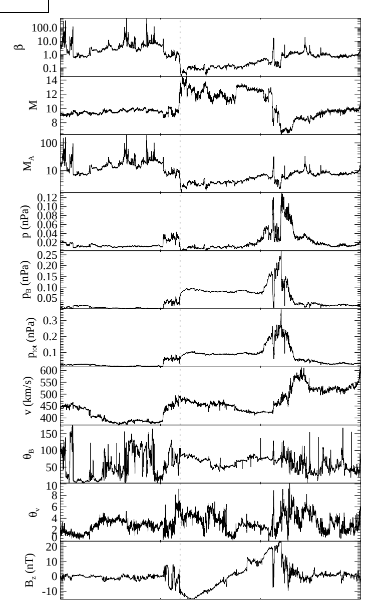
Earth's bow shock



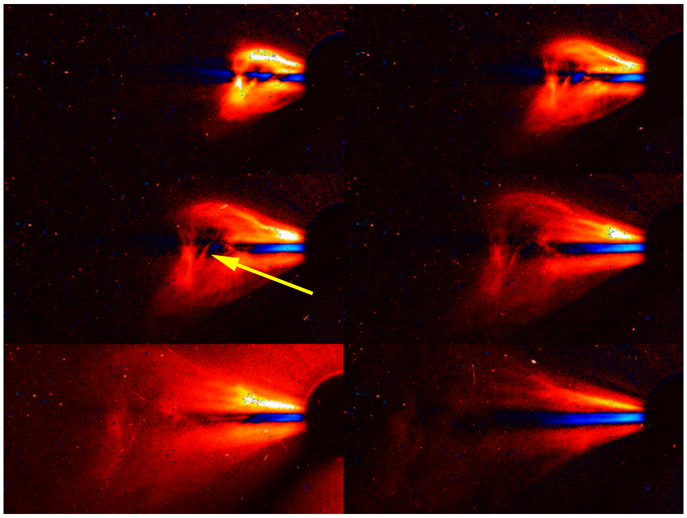
Jupiter's bow shock crossing



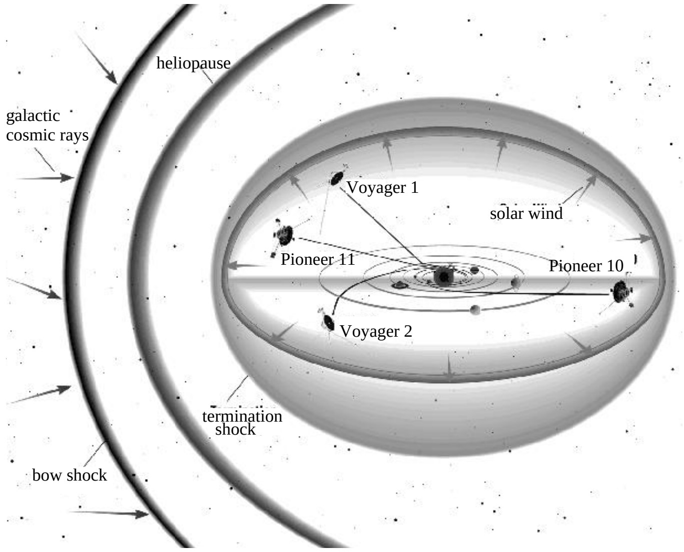
Magnetic cloud at Earth



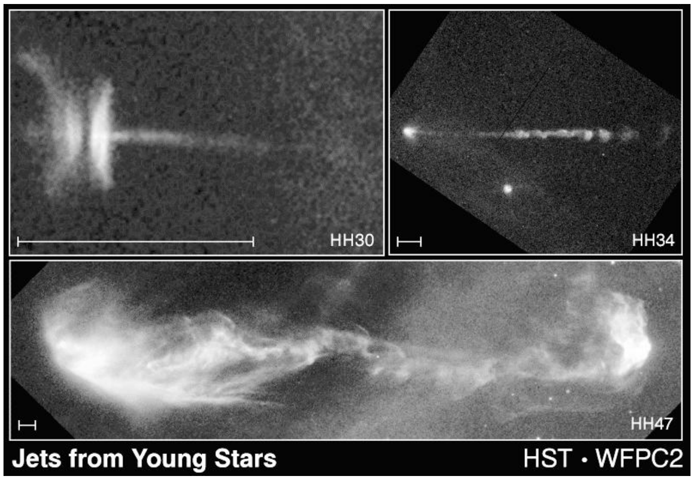
Solar Coronal Mass Ejections



Heliospheric bow shock



Astrophysical jets



Overview

1) Basic concepts of Hyperbolic Conservation Laws

2) Numerical simulation of flows with shocks

3) Derivation of the MHD equations

References

- introductory:

  - Leveque, Numerical methods for conservation laws, Birkhauser, 1992. (no MHD)

  - (also De Sterck, PhD thesis, 1999).

- general hyperbolic systems, advanced:

  - Courant and Hilbert, Methods of mathematical physics, vol. 2, Interscience, 1962.

  - Courant and Friedrichs, Supersonic flow and shock waves, Interscience, 1948.

  - Whitham, Linear and nonlinear waves, Wiley-Interscience, 1974.

- MHD:

  - Landau and Lifshitz, Electrodynamics of Continuous Media, Pergamon, 1984.

  - Jeffrey and Taniuti, Nonlinear wave propagation, Academic Press, 1964.

  - Anderson, Magnetohydrodynamic shock waves, MIT Press, 1963.

Basic concepts of Hyperbolic Conservation Laws

$$\boxed{\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0}$$

- general flow properties of $u(x,t)$ (nonlinear!)

  - continuous flow

  - flow with discontinuities

- hyperbolic $\Rightarrow$ waves

1.1 Conservation Laws: Introduction

1.2 Scalar Conservation Laws

1.3 Systems of Conservation Laws

1.1 Conservation Laws: Introduction

1.1.1 Conservation laws

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

- u is conserved variable (or rather, $\int u(x,t)dx$)
- $f(u)$ is the flux of u

Why is this equation called a 'conservation law'?

define $\overline{u}(t) = \int_{x_0}^{x_1} u(x,t)dx$ and $\overline{\overline{f}}(x) = \int_{t_0}^{t_1} f(u(x,t))dt$, then

$$\int\int \left(\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x}\right) dx\, dt = 0$$
$$\Downarrow$$
$$\int_{t_0}^{t_1} \frac{\partial \overline{u}(t)}{\partial t} dt + \int_{x_0}^{x_1} \frac{\partial \overline{\overline{f}}(x)}{\partial x} dx = 0$$
$$\Downarrow$$
$$\boxed{\overline{u}(t_1) - \overline{u}(t_0) + \overline{\overline{f}}(x_1) - \overline{\overline{f}}(x_0) = 0}$$

(fig)

$\Rightarrow \overline{u}(t) = \int u(x,t)dx$ conserved in time (if no flux through boundaries)

$\Rightarrow$ integral form of conservation law, also for discontinuous solutions: more general

1.1.2 A scalar example: the linear advection equation

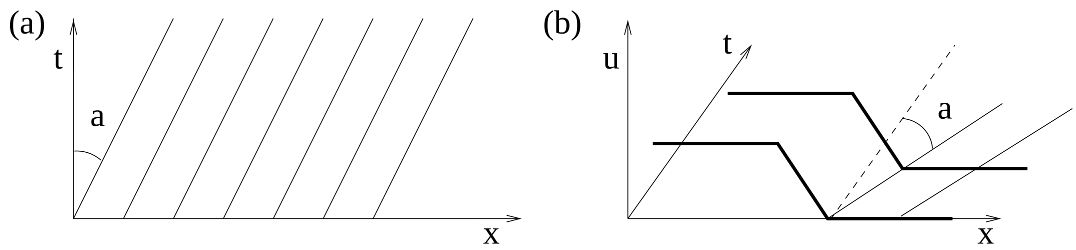
$$\boxed{\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0}$$

$$f(u) = a\,u \quad \Rightarrow \quad \frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

- general solution:

$$u(x,t) = u^*(y(x,t)) \text{ with } y = x - at$$
$$\frac{\partial u^*}{\partial y}\frac{\partial y}{\partial t} + a\,\frac{\partial u^*}{\partial y}\frac{\partial y}{\partial x} = 0$$
$$\frac{\partial u^*}{\partial y}(-a) + a\,\frac{\partial u^*}{\partial y}\,1 \equiv 0\,!$$

- linear advection of arbitrary profile $u^*(y)$: traveling wave



1.1.3 A system example: the Euler equations

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0 \quad \text{with } U(x,t) \in R^n$$

- Euler (dissipationless hydrodynamics or gasdynamics, compressible)

$$U = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_y \\ e \end{bmatrix} \qquad F(U) = \begin{bmatrix} \rho v_x \\ \rho v_x^2 + p \\ \rho v_x v_y \\ (e+p) v_x \end{bmatrix}$$

with $e = \dfrac{p}{\gamma - 1} + \dfrac{1}{2}\rho v^2$

- also MHD, shallow water, relativistic hydrodynamics, general relativity, ...

1.1.4 Generalization to 2D

$$\frac{\partial u}{\partial t} + \frac{\partial f_x(u)}{\partial x} + \frac{\partial f_y(u)}{\partial y} = 0 \qquad \text{with } u(x,y,t)$$

or

$$\boxed{\frac{\partial u}{\partial t} + \nabla \cdot \vec{f}(u) = 0} \qquad \text{with } \vec{f}(u) = (f_x(u), f_y(u))$$

define $\overline{u}(t) = \int\int u(x,y,t)dx\,dy$ and $\overline{\overline{\vec{f}}}(x,y) = \int_{t_0}^{t_1} \vec{f}(u(x,y,t))dt$, then

$$\overline{u}(t_1) - \overline{u}(t_0) + \int\int \nabla \cdot \overline{\overline{\vec{f}}}(x,y)dx\,dy = 0$$

$$\Downarrow$$

$$\boxed{\overline{u}(t_1) - \overline{u}(t_0) + \oint \overline{\overline{\vec{f}}}(x,y) \cdot \vec{n}dl = 0}$$

(fig)

1.1.5 The rest of this lecture

properties of (hyperbolic) conservation laws:

- continuous flow (characteristics, invariants, linear waves)
- flow with discontinuities (shocks, jump relations, Riemann problem)

1.2 Scalar Conservation Laws

- linear
- nonlinear
- nonconvex nonlinear

1.3 Systems of Conservation Laws

- linear system
- wave equation
- nonlinear 2×2 system
- Euler
- MHD

1.2 Scalar Conservation Laws

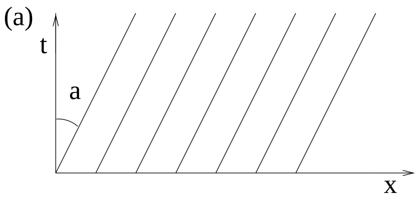
1.2.1 Linear advection equation

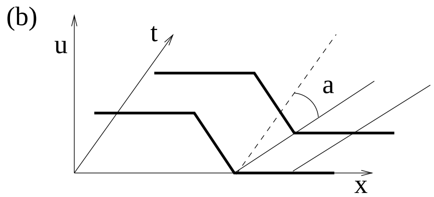
$$f(u) = a\,u \quad \Rightarrow \quad \frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

- general solution:

$$u(x,t) = u^*(y(x,t)) \text{ with } y = x - at$$

- linear advection of arbitrary profile $u^*(y)$, also discontinuous profile (integral form of conservation law) : traveling wave





Characteristics and Riemann Invariants

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

- consider curve $x(t)$ in xt-plane, how does u vary along curve?

$$\frac{\mathrm{d}u(x(t),t)}{\mathrm{d}t} = \frac{\partial u(x(t),t)}{\partial t} + \frac{\partial u(x(t),t)}{\partial x}\,\frac{\partial x(t)}{\partial t}$$

$$\frac{\mathrm{d}u(x(t),t)}{\mathrm{d}t} \equiv 0 \qquad \text{if} \qquad \frac{\partial x(t)}{\partial t} = a$$

- $\boxed{x(t) : \frac{\partial x(t)}{\partial t} = a}$ is called a **characteristic curve** (straight line!)

  slope of characteristic $\equiv$ characteristic speed = (advection) wave speed

- $\boxed{\frac{\mathrm{d}u(x(t),t)}{\mathrm{d}t} \equiv 0}$ along the characteristic $\Rightarrow$ u is a **Riemann Invariant** (RI)

1.2.2 Nonlinear scalar conservation laws

$$\boxed{\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0}$$

$$\frac{\partial u}{\partial t} + f'(u)\,\frac{\partial u}{\partial x} = 0 \qquad \text{with} \qquad f'(u) = \frac{\partial f(u)}{\partial u}$$

- example: (inviscid) Burgers equation

$$f(u) = \frac{u^2}{2}$$

$$f'(u) = u$$

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

Characteristics and Riemann Invariants (RIs)

$$\frac{\partial u}{\partial t} + f'(u)\,\frac{\partial u}{\partial x} = 0$$

- consider curve $x(t)$ in xt-plane, how does u vary along curve?

$$\frac{\mathrm{d}u(x(t),t)}{\mathrm{d}t} = \frac{\partial u(x(t),t)}{\partial t} + \frac{\partial u(x(t),t)}{\partial x}\,\frac{\partial x(t)}{\partial t}$$

$$\frac{\mathrm{d}u(x(t),t)}{\mathrm{d}t} \equiv 0 \qquad \text{if} \qquad \frac{\partial x(t)}{\partial t} = f'(u)$$

- $\boxed{x(t) : \frac{\partial x(t)}{\partial t} = f'(u)}$ is called a characteristic curve
- $\boxed{\frac{\mathrm{d}u(x(t),t)}{\mathrm{d}t} \equiv 0}$ along the characteristic $\Rightarrow$ u is a Riemann Invariant (RI)

- $x(t) : \dfrac{\partial x(t)}{\partial t} = f'(u)$ $\dfrac{\mathrm{d}u(x(t),t)}{\mathrm{d}t} \equiv 0$

$\Rightarrow$ u is advected along characteristic with slope $f'(u)$ $\Rightarrow$ $f'(u)$ is wave speed

$\Rightarrow$ slope of characteristic $\equiv$ characteristic speed = wave speed

$\Rightarrow$ characteristic is straight line !

- example:

  Burgers, $f(u) = u^2/2$, $f'(u) = u$

  slope between $u_l = 0$ and $u_r = 1$

  $f'(u_l) = 0$ and $f'(u_r) = 1$

$\Rightarrow$ expansion or rarefaction wave

- weak discontinuity $\equiv$ discontinuity in slope

  travels with characteristic speed

(fig)

Linear waves

$$\frac{\partial u}{\partial t} + f'(u)\,\frac{\partial u}{\partial x} = 0$$

- assume $u(x,t) = u_0 + u_1(x,t)$

  with u_0 constant background,

  $u_1(x,t)$ small perturbation

  $f'(u) = f'(u_0) + f''(u_0)\,u_1 + O(u_1^2)$

$$\Rightarrow \quad \frac{\partial u_1}{\partial t} + f'(u_0)\,\frac{\partial u_1}{\partial x} \approx 0$$

(fig)

linear advection equation for $u_1(x,t)$ with constant wave speed $f'(u_0)$!

profile u_1 is advected, wave speed (phase speed) is $f'(u_0)$

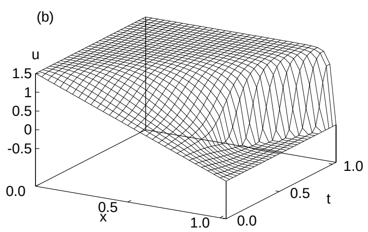
Steepening into shocks

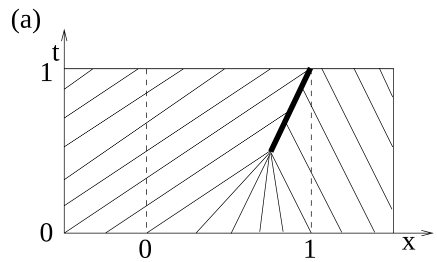
- Burgers, $f(u) = u^2/2$, $f'(u) = u$

  switch u_l and u_r, such that characteristics converge

  slope between $u_l = 1.5$ and $u_r = -0.5$

  $f'(u_l) = 1.5$ and $f'(u_r) = -0.5$





⇒ a shock wave is formed

shock wave = discontinuity in $u(x)$

characteristics enter into shock

shock propagates with constant speed, but how fast?

remark: for the (linear) advection equation the characteristics do not converge, so shocks cannot be formed through steepening

nonlinearity is necessary for shock formation!

Rankine-Hugoniot (RH) jump relations

- what is the shock speed s? $\Rightarrow$ use the integral form of the conservation law

$$\overline{u}(t_1) - \overline{u}(t_0) + \overline{\overline{f}}(x_1) - \overline{\overline{f}}(x_0) = 0$$

$$\Downarrow$$

$$-s\,\Delta t\,(u_r - u_l) + \Delta t\,(f(u_r) - f(u_l)) = 0$$

$$-s\,\Delta u + \Delta f = 0$$

$$s = \frac{\Delta f}{\Delta u} = \frac{f(u_r) - f(u_l)}{u_r - u_l}$$

(fig)

- linear advection: $s = a$
- Burgers: $s = \frac{u_r^2 - u_l^2}{2\,(u_r - u_l)} = \frac{u_r + u_l}{2}$

The Riemann problem

- Riemann problem $=$ how does initial discontinuity between two constant states u_l and u_r evolve in time?

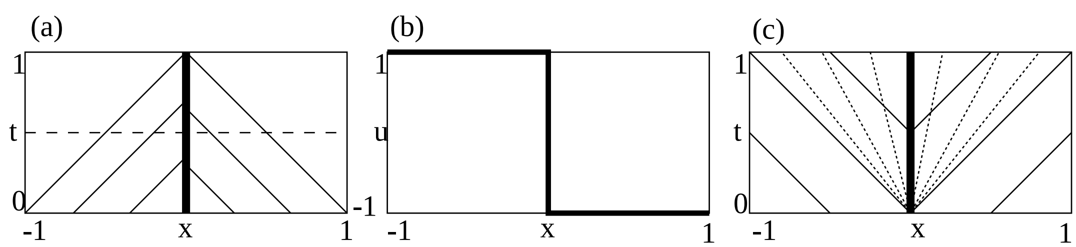
$\Rightarrow$ Burgers:

- $f'(u_l) > f'(u_r)$, characteristics converge

  $\Rightarrow$ shock with shock speed s from RH relation

- $f'(u_l) < f'(u_r)$, characteristics diverge

  $\Rightarrow$ (continuous) rarefaction wave



Instability of expansion shocks

- remark: the rarefaction case initially also satisfies the RH relation with shock speed s
- the characteristics would diverge from this shock : expansion shock
- BUT: this shock solution is intrinsically unstable

  - formation argument: cannot be formed from wave steepening

  - perturbation argument: 'infinitesimally' small or 'generic' perturbation makes the shock into a slope, which expands like the rarefaction wave

  (for a compressional wave, the slope resulting from perturbation would steepen again!)

- characteristics have to converge in a shock
- instability of expansion shocks is related to entropy (see Lecture 3)

Convexity of flux functions

- for Burgers: every Riemann problem results in either a shock or a rarefaction

  - this is true for all convex flux functions $f(u)$

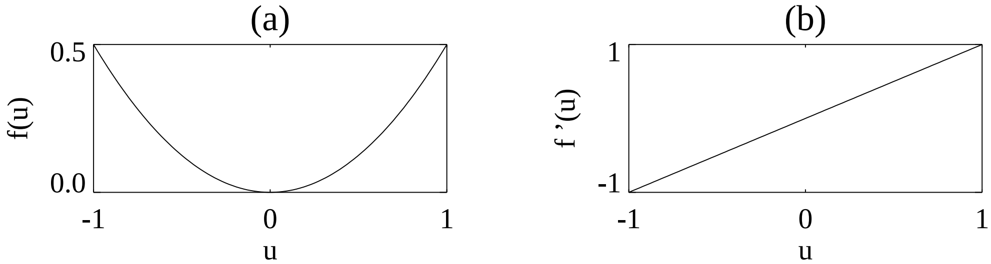
  - $f(u)$ is convex $\Leftrightarrow$ $f'(u)$ is monotone $\Leftrightarrow$ $f''(u)$ does not change sign

  - $f(u)$ is convex $\Rightarrow f'(u_l) > s > f'(u_r)$ when characteristics converge

  reason: $s = \dfrac{f(u_r) - f(u_l)}{u_r - u_l}$ and middle value theorem

  - Burgers is convex ($f(u) = u^2/2$)

- if $f(u)$ is non-convex: Riemann problems may have more complicated solutions than just a shock or a rarefaction



1.2.3 Nonconvex nonlinear scalar conservation laws

The Riemann problem

- example: $f(u) = \frac{u^3}{3}$, $f'(u) = 3\,u^2$

$\Rightarrow$ non-convex

Riemann problem: $u_l = 1$ and $u_r = -0.75$

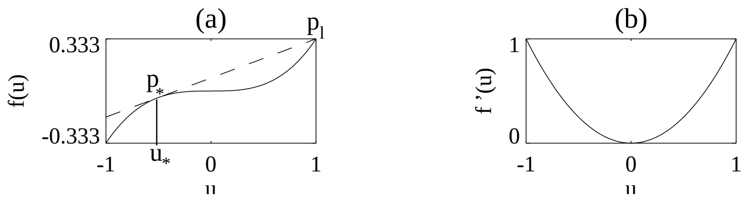
RH: $f'(u_l) > f'(u_r) > s = 37/168$

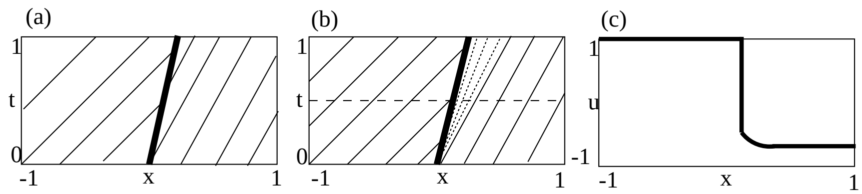
right characteristics diverge from shock : unstable

solution: rarefaction starting from right state until right characteristic becomes parallel to shock (with speed $\neq s$!)

condition: $f'(u^*) = s^* = \dfrac{f(u^*) - f(u_l)}{u^* - u_l}$

tangent hull construction





⇒ result: compound shock

- shock with attached rarefaction

- characteristic is parallel to shock where rarefaction is attached

- rarefaction is sonic where it is attached: shock speed = wave speed (characteristic speed)

⇒ Riemann problem (if one inflection point):

- $f'(u_l) > f'(u_r)$, characteristics converge

- if $f'(u_l) > s > f'(u_r)$: shock

- if $f'(u_l) > f'(u_r) > s$ or $s > f'(u_l) > f'(u_r)$: compound shock

- $f'(u_l) < f'(u_r)$, characteristics diverge

- (continuous) rarefaction wave

recapitulation: scalar conservation laws

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

- continous flow

$\Rightarrow$ $x(t) : \dfrac{\partial x(t)}{\partial t} = f'(u)$: characteristic

$\Rightarrow$ $\dfrac{\mathrm{d}u(x(t),t)}{\mathrm{d}t} \equiv 0$: Riemann Invariant (RI)

- flow with discontinuities:

$\Rightarrow$ $s = \dfrac{\Delta f}{\Delta u} = \dfrac{f(u_r) - f(u_l)}{u_r - u_l}$: Rankine Hugoniot (RH) relation

$\Rightarrow$ Riemann problem: shock or rarefaction (or compound shock)

1.3 Systems of Conservation Laws

1.4 Systems of Conservation Laws

recapitulation: scalar conservation laws

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \qquad \overline{u}(t_1) - \overline{u}(t_0) + \overline{\overline{f}}(x_1) - \overline{\overline{f}}(x_0) = 0$$

- continous flow

$\Rightarrow$ $x(t) : \dfrac{\partial x(t)}{\partial t} = f'(u)$: characteristic

$\Rightarrow$ $\dfrac{\mathrm{d}u(x(t),t)}{\mathrm{d}t} \equiv 0$: Riemann Invariant (RI)

- flow with discontinuities:

$\Rightarrow$ $s = \dfrac{\Delta f}{\Delta u} = \dfrac{f(u_r) - f(u_l)}{u_r - u_l}$: Rankine Hugoniot (RH) relation

$\Rightarrow$ Riemann problem: shock or rarefaction

1.4.1 Linear systems

Linear hyperbolic systems

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0 \qquad \text{with } U(x,t) = \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} \in R^n$$

$$\Downarrow F(U) = \mathsf{A} \cdot U$$

$$\frac{\partial U}{\partial t} + \mathsf{A} \cdot \frac{\partial U}{\partial x} = 0 \quad (1) \qquad \text{and } F(U) = \begin{bmatrix} f_1(U) \\ \vdots \\ f_n(U) \end{bmatrix}$$

(1) is a hyperbolic system of equations

$\Updownarrow$

A has n real eigenvalues and a complete set of eigenvectors

$\Updownarrow$

the system has n real characteristic curves

$\Rightarrow \mathsf{A} = \mathsf{R} \cdot \Lambda \cdot \mathsf{L}$ with

- $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n) = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \lambda_n \end{bmatrix}$

  diagonal eigenvalue (e-val) matrix

- $\mathsf{R} = \left[R_1 \middle| \cdots \middle| R_n \right]$: right eigenvectors (e-vect), $\mathsf{A} \cdot R_i = \lambda_i \, R_i$

- $\mathsf{L} = \begin{bmatrix} L_1 \\ \hline \vdots \\ \hline L_n \end{bmatrix}$: left eigenvectors (e-vect), $L_i \cdot \mathsf{A} = \lambda_i \, L_i$

  normalization: $\mathsf{R} = \mathsf{L}^{-1}$

  (if, additionally, $\mathsf{R} \cdot \mathsf{R}^T = \mathsf{I} \Rightarrow \mathsf{R}^T = \mathsf{L}$)

Characteristic variables

$$\frac{\partial U}{\partial t} + \mathsf{A} \cdot \frac{\partial U}{\partial x} = 0 \quad \text{with } \mathsf{A} = \mathsf{R} \cdot \Lambda \cdot \mathsf{L}$$

$$\frac{\partial U}{\partial t} + \mathsf{R} \cdot \Lambda \cdot \mathsf{L} \cdot \frac{\partial U}{\partial x} = 0$$

$$\frac{\mathsf{L} \cdot \partial U}{\partial t} + \Lambda \cdot \frac{\mathsf{L} \cdot \partial U}{\partial x} = 0 \quad \text{with } \mathsf{L} \cdot \partial U = \partial \mathsf{L} \cdot U \text{ (linear, } \mathsf{L} \text{ constant!)}$$

define $\boxed{W = \mathsf{L} \cdot U : \quad \text{characteristic variables } W}$ $\Rightarrow$ $\boxed{\frac{\partial W}{\partial t} + \Lambda \cdot \frac{\partial W}{\partial x} = 0}$

$$\forall i : \boxed{\frac{\partial w_i}{\partial t} + \lambda_i \cdot \frac{\partial w_i}{\partial x} = 0} \qquad (i = 1..n)$$

$\Rightarrow n$ scalar linear advection equations for $w_i(y_i = x - \lambda_i \, t)$ with wave speed λ_i

$\Rightarrow$ the equations fully decouple

Characteristics and Riemann Invariants

$$\forall i : \frac{\partial w_i}{\partial t} + \lambda_i \cdot \frac{\partial w_i}{\partial x} = 0 \qquad (i = 1..n)$$

$\forall i$: (n characteristic fields)

- $x_i(t) : \frac{\partial x_i(t)}{\partial t} = \lambda_i$: ith characteristic
- $\frac{\mathrm{d}w_i(x_i(t),t)}{\mathrm{d}t} \equiv 0$: w_i Riemann Invariant (RI) on characteristic x_i

$\Rightarrow n$ different (linear) waves

$\Rightarrow n$ characteristic curves

$\Rightarrow n$ Riemann Invariants

Wave decomposition

$U = \mathrm{R} \cdot W$

- excite one characteristic wave: simple wave, with one single wave speed λ_i

$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = \begin{bmatrix} \cdots & R_i & \cdots \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ 0 \\ w_i(x - \lambda_i\, t) \\ 0 \\ \vdots \end{bmatrix}$$

$\Rightarrow U(x - \lambda_i\, t) = R_i\, w_i(x - \lambda_i\, t)$: simple wave

- excite several characteristic waves

$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = \begin{bmatrix} R_1 & \cdots & R_n \end{bmatrix} \cdot \begin{bmatrix} w_1(x - \lambda_1\, t) \\ \vdots \\ w_n(x - \lambda_n\, t) \end{bmatrix}$$

$\Rightarrow U(x,t) = \sum_{j=1}^{n} R_j\, w_j(x - \lambda_j\, t)$: general wave

$W = \mathsf{L} \cdot U$

- excite one conserved variable u_i

$$\begin{bmatrix} w_1 \\ \\ \vdots \\ \\ w_n \end{bmatrix} = \begin{bmatrix} L_1 \\ \hline \vdots \\ \hline L_n \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ 0 \\ u_i \\ 0 \\ \vdots \end{bmatrix}$$

$\Rightarrow \forall j \; : \; w_j = L_{j,i}\, u_i \; : n$ characteristic waves are excited, each with speed λ_j

- excite several conserved variables

$$\begin{bmatrix} w_1 \\ \\ \vdots \\ \\ w_n \end{bmatrix} = \begin{bmatrix} L_1 \\ \hline \vdots \\ \hline L_n \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}$$

$\Rightarrow \forall j \; : \; w_j = L_j \cdot U$: general wave

A simple 2×2 example

$\mathsf{A} = \mathsf{R} \cdot \Lambda \cdot \mathsf{L}$ with

- $\Lambda = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
- $\mathsf{R} = \left[\begin{array}{c|c} R_1 & R_2 \end{array}\right] = \left[\begin{array}{c|c} 0.5 & 0.5 \\ 0.5 & -0.5 \end{array}\right]$
- $\mathsf{L} = \begin{bmatrix} L_1 \\ \hline L_2 \end{bmatrix} = \mathsf{R}^{-1} = \left[\begin{array}{cc} 1 & 1 \\ \hline 1 & -1 \end{array}\right]$

$\Rightarrow$ excite w_1 (profile in the first characteristic wave), $w_2 \equiv 0$: simple wave

$$W = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} w_1(y_1 = x - \lambda_1\, t) \\ 0 \end{bmatrix}$$

$$U(x - \lambda_1\, t) = \left[\begin{array}{c|c} R_1 & R_2 \end{array}\right] \cdot \begin{bmatrix} w_1 \\ 0 \end{bmatrix} = R_1\, w_1 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} w_1(x - \lambda_1\, t)$$

$\Rightarrow$ excite w_1 and w_2 : not a simple wave

$$U = R_1\, w_1 + R_2\, w_2 = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} w_1(x - \lambda_1\, t) + \begin{bmatrix} 0.5 \\ -0.5 \end{bmatrix} w_2(x - \lambda_2\, t)$$

$\Rightarrow$ excite conservative variable $u_2(x, 0)$, but take $u_1(x, 0) \equiv 0$

$$W = \left[\frac{L_1}{L_2}\right] \cdot \begin{bmatrix} u_1 \equiv 0 \\ u_2 \end{bmatrix} = \left[\frac{1 \quad 1}{1 \quad -1}\right] \cdot \begin{bmatrix} 0 \\ u_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \end{bmatrix} u_2$$

$\int u_1\, dx$ and $\int u_2\, dx$ are conserved !

Shocks

- integral conservation law:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

$$\Downarrow$$

$$\boxed{\overline{U}(t_1) - \overline{U}(t_0) + \overline{\overline{F}}(x_1) - \overline{\overline{F}}(x_0) = 0}$$

with $\overline{U}(t) = \int_{x_0}^{x_1} U(x,t)dx$ and $\overline{\overline{F}}(x) = \int_{t_0}^{t_1} F(U(x,t))dt$

- Rankine-Hugoniot relation:

$$\boxed{s(U_r - U_l) = F(U_r) - F(U_l) = \mathsf{A} \cdot (U_r - U_l)}$$

$s_i = \lambda_i$ and $U_r - U_l = R_i$

n wave families $\Rightarrow n$ shock waves

The Riemann problem

- Riemann problem:

$U(x,0) = U_l$ ($x < 0$)

$U(x,0) = U_r$ ($x > 0$)

- wave decomposition of initial state $W_l = \mathsf{L} \cdot U_l, W_r = \mathsf{L} \cdot U_r$
- characteristic waves propagate $w_i(y_i = x - \lambda_i\, t)$

$w_i(y_i) = w_{l,i}$ if $y_i = x - \lambda_i\, t < 0$

$w_i(y_i) = w_{r,i}$ if $y_i = x - \lambda_i\, t > 0$

- reconstruct conserved variables

$U = \mathsf{R} \cdot W = \sum_{i=1}^{n} R_i\, w_i(y_i = x - \lambda_i\, t)$

$= \sum_j^{y_j<0} R_j\, w_{l,j} + \sum_k^{y_k>0} R_k\, w_{r,k}$

$\Rightarrow n$ shocks propagating with speed λ_i

$\Rightarrow$ initial discontinuity $U_r - U_l$ splits up in n discontinuities

$$U_r - U_l = \mathsf{R} \cdot (W_r - W_l) = \sum_{i=1}^{n} R_i\,(w_{r,i} - w_{l,i})$$

that propagate with speed λ_i

$\Rightarrow$ jump over shock i equals $R_i\,(w_{r,i} - w_{l,i}) = R_i\,(\mathsf{L}\,(U_r - U_l))_i$

1.4.2 The linear wave equation

Classification of linear scalar 2nd order PDEs with two independent variables

$$\boxed{a\,u_{tt} + b\,u_{xt} + c\,u_{xx} + d\,u_t + e\,u_x = 0}$$

for $u(x,t)$, with $u_x = \frac{\partial u}{\partial x}$, $u_t = \frac{\partial u}{\partial t}$, $a \neq 0$

- write as first order system

define $v = u_t$ and $w = u_x$

$\Rightarrow u_{tt} = v_t$, $u_{xt} = v_x$, $u_{xx} = w_x$

then $v_t = u_{tt} = -(b\,u_{xt} + c\,u_{xx} + d\,u_t + e\,u_x)/a$

$= -(b\,v_x + c\,w_x + d\,v + e\,w)/a$

$w_t = u_{xt} = v_x$

$$\Rightarrow \frac{\partial U}{\partial t} + \mathsf{A} \cdot \frac{\partial U}{\partial x} + \mathsf{B} \cdot U = 0$$

with $U = \begin{bmatrix} v \\ w \end{bmatrix}$, $\mathsf{A} = \begin{bmatrix} b/a & c/a \\ -1 & 0 \end{bmatrix}$, $\mathsf{B} = \begin{bmatrix} d/a & e/a \\ 0 & 0 \end{bmatrix}$

$\Rightarrow$ eigenstructure A: $\quad \lambda = \dfrac{b \pm \sqrt{b^2 - 4ac}}{2a}$

$\Rightarrow$ the 2nd order equation is

- hyperbolic $\Leftrightarrow b^2 - 4ac > 0 \Leftrightarrow \lambda$ real, complete eigenvector set
- parabolic $\Leftrightarrow b^2 - 4ac = 0 \Leftrightarrow \lambda$ real, but incomplete eigenvector set
- elliptic $\Leftrightarrow b^2 - 4ac < 0 \Leftrightarrow \lambda$ complex

The wave equation

$$\boxed{u_{tt} - \alpha^2 u_{xx} = 0}$$

- $a = 1, c = -\alpha^2 \quad \Rightarrow \quad \mathsf{A} = \begin{bmatrix} 0 & -\alpha^2 \\ -1 & 0 \end{bmatrix}$
- $\lambda_1 = \alpha, \lambda_2 = -\alpha$ real

$\mathsf{R} = \left[\begin{array}{c|c} 1 & -1/\alpha \\ 1 & 1/\alpha \end{array}\right] \qquad \mathsf{L} = \mathsf{R}^{-1} = \left[\begin{array}{cc} 0.5 & -0.5\,\alpha \\ \hline 0.5 & 0.5\,\alpha \end{array}\right]$

$\Rightarrow$ hyperbolic

- remark: $(\frac{\partial}{\partial t} + \alpha \frac{\partial}{\partial x})\,(\frac{\partial}{\partial t} - \alpha \frac{\partial}{\partial x})u = 0$

  $\Rightarrow u(x,t) = f(x + \alpha\, t) + g(x - \alpha\, t)$

  (initial conditions: $u(x,0), u_t(x,0)$)

The heat equation

$$u_t - u_{xx} = 0$$

$$a' \, u_{xx} + b' \, u_{xt} + c' \, u_{tt} + d' \, u_x + e' \, u_t = 0$$

- $a' = -1$, $e' = 1 \quad \Rightarrow \quad \mathsf{A} = \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix}$
- $\lambda_{1,2} = 0$ real

$R_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, but no linearly independent R_2

$\Rightarrow$ parabolic ($b'^2 - 4a'c' = 0$)

The Poisson equation

$$u_{xx} + u_{yy} = 0$$

$$a' \, u_{xx} + b' \, u_{xy} + c' \, u_{yy} + d' \, u_x + e' \, u_y = 0$$

- $a' = 1$, $c' = 1 \quad \Rightarrow \quad \mathsf{A} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$
- $\lambda_{1,2} = \pm\sqrt{-4} = \pm 2\, i$ complex

$\Rightarrow$ elliptic ($b'^2 - 4a'c' < 0$)

1.4.3 Nonlinear systems

Nonlinear hyperbolic systems

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

$$\Downarrow$$

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial U}\frac{\partial U}{\partial x} = 0$$

$$\Downarrow \frac{\partial F(U)}{\partial U} = \mathsf{A}(U)$$

$$\boxed{\frac{\partial U}{\partial t} + \mathsf{A}(U) \cdot \frac{\partial U}{\partial x} = 0 \quad (1)}$$

with $U(x,t) = \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} \in R^n$

and $F(U) = \begin{bmatrix} f_1(U) \\ \vdots \\ f_n(U) \end{bmatrix}$

with Jacobian matrix $\mathsf{A}(U) = \dfrac{\partial F(U)}{\partial U} = \begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} & \cdots & \frac{\partial f_1}{\partial u_n} \\ \frac{\partial f_2}{\partial u_1} & \cdots & & \\ \vdots & & & \\ \frac{\partial f_n}{\partial u_1} & \cdots & \cdots & \frac{\partial f_n}{\partial u_n} \end{bmatrix}$

$$\boxed{\frac{\partial U}{\partial t} + \mathsf{A}(U) \cdot \frac{\partial U}{\partial x} = 0 \quad (1)}$$

(1) is a hyperbolic system of equations

$\Updownarrow$

$\mathsf{A}(U)$ has n real eigenvalues and a complete set of eigenvectors $\forall U$

$\Updownarrow$

the system has n real characteristic curves

$$\Rightarrow \mathsf{A}(U) = \mathsf{R}(U) \cdot \Lambda(U) \cdot \mathsf{L}(U)$$

Characteristic variables

$$\frac{\partial U}{\partial t} + \mathsf{R}(U) \cdot \Lambda(U) \cdot \mathsf{L}(U) \cdot \frac{\partial U}{\partial x} = 0$$

$$\frac{\mathsf{L}(U) \cdot \partial U}{\partial t} + \Lambda(U) \cdot \frac{\mathsf{L}(U) \cdot \partial U}{\partial x} = 0$$

define (formally) $\boxed{\partial W = \mathsf{L}(U) \cdot \partial U : \quad \text{characteristic variables } \partial W}$

$$\boxed{\frac{\partial W}{\partial t} + \Lambda(U) \cdot \frac{\partial W}{\partial x} = 0}$$

- n wave modes with wave speeds λ_i
- the definition of the characteristic variables ∂W only on the differential, local level

  $\Rightarrow$ the equations (and thus the wave modes) do generally not globally decouple due to the nonlinearity (see below)

Characteristics and Riemann Invariants

$$\frac{\mathsf{L}(U) \cdot \partial U}{\partial t} + \Lambda(U) \cdot \frac{\mathsf{L}(U) \cdot \partial U}{\partial x} = 0$$

$\forall i$: (n characteristic fields)

- $\boxed{x_i(t) : \frac{\partial x_i(t)}{\partial t} = \lambda_i(U)}$: ith characteristic

- if $\exists\, w_i(U)$: $\partial w_i(U) \approx L_i \cdot \partial U$

  $\Rightarrow \boxed{\frac{\mathrm{d}w_i(x_i(t), t)}{\mathrm{d}t} \equiv 0}$: w_i Riemann Invariant (RI) on characteristic x_i

$\Rightarrow$ n different (nonlinear) waves, n characteristic curves

$\Rightarrow$ less than n Riemann Invariants (wave information for wave i only locally determined)

$\Rightarrow$ characteristics are not straight lines !!

Shocks

- Rankine-Hugoniot relation:

$$s(U_r - U_l) = F(U_r) - F(U_l)$$

  - nonlinear
  - small-amplitude shocks: linearize

  $s(U_r - U_l) = \mathsf{A}(U_l)\,(U_r - U_l)$

  given U_l, there are n small-amplitude shocks, with speeds λ_i, and $U_r - U_l = R_i$

  - in general: n shock curves in phase plane (see Leveque)

The Riemann problem

- the initial jump $U_r - U_l$ splits up in n waves
- in general: some shocks (compressive), some rarefactions (like Burgers)
- (see Leveque)

1.4.4 The Euler equations

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

$$U = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho\, e \end{bmatrix} \qquad F(U) = \begin{bmatrix} \rho v_x \\ \rho v_x^2 + p \\ \rho v_x v_y \\ (\rho\, e + p) v_x \end{bmatrix}$$

- Euler = dissipationless hydrodynamics or gasdynamics, compressible

- 4 equations in 4 unknowns: ρ, v_x, v_y, p

  with $\rho\, e = \rho\, \epsilon(\rho, p) + \frac{1}{2}\rho v^2 = E$

  e: specific total energy (J/kg)

  $E = \rho\, e$: volumetric total energy (J/m^3), conserved quantity

  $\epsilon(\rho, p)$: specific internal energy (J/kg), equation of state (EOS)

- perfect (ideal) gas EOS: $\epsilon(\rho, p) = \dfrac{p}{\rho\,(\gamma - 1)}$

  $\Rightarrow \rho\, e = \dfrac{p}{\gamma - 1} + \dfrac{1}{2}\rho v^2$

- $\gamma = \dfrac{f+2}{f}$ adiabatic constant, with f =degrees of freedom

  $\gamma = 7/5 = 1.4$ for air: diatomic gas: $f = 3$ translational + 2 rotational

  $\gamma = 5/3 = 1.667$ for hydrogen: monatomic gas: $f = 3$ translational

Conservative and primitive variables

- vector of conservative variables:

$$U = \begin{bmatrix} \rho \\ m_x \\ m_y \\ E \end{bmatrix} = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho\, e = \frac{p}{(\gamma-1)} + \frac{1}{2}\rho v^2 \end{bmatrix} \text{ in } \frac{\partial U}{\partial t} + \mathsf{A}(U)_U \cdot \frac{\partial U}{\partial x} = 0$$

- vector of primitive variables: $V = \begin{bmatrix} \rho \\ v_x \\ v_y \\ p \end{bmatrix}$

- transformation: $\partial U = \dfrac{\partial U}{\partial V} \cdot \partial V$

$$\frac{\partial U}{\partial V} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ v_x & \rho & 0 & 0 \\ v_y & 0 & 1 & 0 \\ v^2/2 & \rho\, v_x & \rho\, v_y & 1/(\gamma-1) \end{bmatrix}$$

$$\frac{\partial V}{\partial U} = \frac{\partial U}{\partial V}^{-1}$$

$$\Rightarrow \frac{\partial U}{\partial V} \cdot \frac{\partial V}{\partial t} + \mathsf{A}(U)_U \cdot \frac{\partial U}{\partial V} \cdot \frac{\partial V}{\partial x} = 0$$

$$\frac{\partial V}{\partial t} + \frac{\partial V}{\partial U} \cdot \mathsf{A}(U)_U \cdot \frac{\partial U}{\partial V} \cdot \frac{\partial V}{\partial x} = 0$$

define $\mathsf{A}(V)_V = \frac{\partial V}{\partial U} \cdot \mathsf{A}(U)_U \cdot \frac{\partial U}{\partial V}$

with property $\lambda(\mathsf{A}(V)_V) = \lambda(\mathsf{A}(U)_U)$ (similarity transformation)

$$\Rightarrow \frac{\partial V}{\partial t} + \mathsf{A}(V)_V \cdot \frac{\partial V}{\partial x} = 0$$

Hyperbolic system

- $\frac{\partial V}{\partial t} + \mathsf{A}(V)_V \cdot \frac{\partial V}{\partial x} = 0$

with $V = \begin{bmatrix} \rho \\ v_x \\ v_y \\ p \end{bmatrix}$ and $\mathsf{A}_V = \begin{bmatrix} v_x & \rho & 0 & 0 \\ 0 & v_x & 0 & 1/\rho \\ 0 & 0 & v_x & 0 \\ 0 & c^2\rho & 0 & v_x \end{bmatrix}$

$c = \sqrt{\frac{\gamma p}{\rho}}$

$\Rightarrow$

$\lambda_1 = v_x$: entropy wave

$\lambda_2 = v_x$: shear wave

$\lambda_3 = v_x + c$: sound wave, right traveling

$\lambda_4 = v_x - c$: sound wave, left traveling

$$\Rightarrow \mathsf{R} = \left[\begin{array}{c|c|c|c} 1 & 0 & \rho & \rho \\ 0 & 0 & c & -c \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \rho\, c^2 & \rho\, c^2 \end{array}\right]$$

$$\Rightarrow \mathsf{L} = \left[\begin{array}{cccc} 1 & 0 & 0 & -1/c^2 \\ \hline 0 & 0 & 1 & 0 \\ \hline 0 & 1/(2c) & 0 & 1/(2\rho c^2) \\ \hline 0 & -1/(2c) & 0 & 1/(2\rho c^2) \end{array}\right]$$

$\Rightarrow$ hyperbolic system

Characteristics and Riemann Invariants

$$\frac{\partial V}{\partial t} + \mathsf{R}(V)\cdot\Lambda(V)\cdot\mathsf{L}(V)\cdot\frac{\partial V}{\partial x} = 0$$
$$\frac{\mathsf{L}(V)\cdot\partial V}{\partial t} + \Lambda(V)\cdot\frac{\mathsf{L}(V)\cdot\partial V}{\partial x} = 0$$

$\forall i$: (n characteristic fields)

- $\boxed{x_i(t) : \frac{\partial x_i(t)}{\partial t} = \lambda_i(V)}$: ith characteristic

- if $\exists\, w_i(V)$: $L_i(V)\cdot\partial V = \alpha(V)\,\partial w_i(V)$

$$\Rightarrow L_i(V)\cdot\frac{\partial V}{\partial t} + \lambda_i(V)L_i(V)\cdot\frac{\partial V}{\partial x} = 0$$
$$\alpha(V)\,\frac{\partial w_i(V)}{\partial t} + \lambda_i(V)\alpha(V)\,\frac{\partial w_i(V)}{\partial x} = 0$$

$$\Rightarrow \frac{\mathrm{d}w_i(x_i(t),t)}{\mathrm{d}t} = 0 \ : \quad w_i \text{ Riemann Invariant (RI) on characteristic } x_i$$

- $i = 1$: find $w_1(V)$ such that

$$L_1(V) \cdot \partial V = \partial\rho - \frac{1}{c^2}\partial p = \alpha(V)\,\partial w_1(V)$$

choose $w_1 = s = \dfrac{p}{\rho^\gamma}$

$$\Rightarrow \partial w_1 = -\frac{\gamma p}{\rho^{\gamma+1}}\partial\rho + \frac{\partial p}{\rho^\gamma} = \frac{-c^2}{\rho^\gamma}\left(\partial\rho - \frac{1}{c^2}\partial p\right)$$

$$\Rightarrow L_1(V) \cdot \partial V = \partial\rho - \frac{1}{c^2}\partial p = \alpha(V)\,\partial w_1(V)$$

with $\alpha(V) = \dfrac{-\rho^\gamma}{c^2}$ and $w_1 = s = \dfrac{p}{\rho^\gamma}$

$\Rightarrow s$ is a Riemann Invariant on $x_1(t)$ with $\dfrac{\partial x_1(t)}{\partial t} = v_x$

the entropy of a fluid element is conserved on its path

- $i = 2$: find $w_2(V)$ such that

$$L_2(V) \cdot \partial V = \partial v_y = \alpha(V)\,\partial w_2(V)$$

choose $w_2 = v_y$ and $\alpha(V) = 1$ (trivial)

$\Rightarrow v_y$ is a Riemann Invariant on $x_2(t)$ with $\dfrac{\partial x_1(t)}{\partial t} = v_x$

- $i = 3$: find $w_3(V)$ such that

$$L_3(V) \cdot \partial V = \frac{1}{2c}\partial v_x + \frac{1}{2\rho c^2}\partial p = \alpha(V)\,\partial w_3(V)$$

no solution, RI does not exist

- $i = 4$: no RI

Linear waves

$$\frac{\partial V}{\partial t} + A_V(V) \cdot \frac{\partial V}{\partial x} = 0$$

- assume $V(x,t) = V_0 + V_1(x,t)$

  with V_0 constant background, $V_1(x,t)$ small perturbation

- linearize: $A_V(V) \approx A_V(V_0) \;\Rightarrow\; \frac{\partial V_1}{\partial t} + A_V(V_0)\frac{\partial V_1}{\partial x} \approx 0$

  $\mathsf{A}_V(V_0) = \mathsf{R}(V_0) \cdot \Lambda(V_0) \cdot \mathsf{L}(V_0)$

- define $W_1 = \mathsf{L}(V_0) \cdot V_1$: characteristic variables W_1

$\Rightarrow \frac{\partial W_1}{\partial t} + \Lambda(V_0) \cdot \frac{\partial W_1}{\partial x} = 0$

$\Rightarrow n$ scalar linear advection equations

$$\mathsf{R} = \left[\begin{array}{c|c|c|c} 1 & 0 & \rho & \rho \\ 0 & 0 & c & -c \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \rho\, c^2 & \rho\, c^2 \end{array}\right] \text{ and } \mathsf{L} = \left[\begin{array}{cccc} 1 & 0 & 0 & -1/c^2 \\ \hline 0 & 0 & 1 & 0 \\ \hline 0 & 1/(2c) & 0 & 1/(2\rho c^2) \\ \hline 0 & -1/(2c) & 0 & 1/(2\rho c^2) \end{array}\right] \text{ with } V = \left[\begin{array}{c} \rho \\ v_x \\ v_y \\ p \end{array}\right]$$

$\lambda_1 = v_x$: entropy wave $\qquad \lambda_3 = v_x + c$: sound wave, right traveling

$\lambda_2 = v_x$: shear wave $\qquad \lambda_4 = v_x - c$: sound wave, left traveling

- $V_1 = \mathsf{R}(V_0) \cdot W_1$: properties of Euler waves
  - entropy: $\Delta\rho$
  - shear: Δv_y
  - sound: $\Delta\rho, \pm\Delta v_x, \Delta p$
- $W_1 = \mathsf{L}(V_0) \cdot V_1$: waves generated by perturbation of the primitive variables
- large-amplitude = nonlinear

  $\Rightarrow$ waves interact, steepen into shocks, rarefactions, wave coupling, . . .

1.4.5 The MHD equations

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

$$U = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho v_z \\ B_x \\ B_y \\ B_z \\ \rho\, e \end{bmatrix} \qquad F(U) = \begin{bmatrix} \rho\, v_x \\ \rho\, v_x^2 + p + B^2/2 - B_x^2 \\ \rho\, v_x v_y - B_x B_y \\ \rho\, v_x v_z - B_x B_z \\ 0 \\ B_y v_x - B_x v_y \\ B_z v_x - B_x v_z \\ (\rho\, e + p + B^2/2) v_x - B_x\, (\vec{v} \cdot \vec{B}) \end{bmatrix}$$

- MHD = dissipationless magnetohydrodynamics or magnetogasdynamics, compressible

- 8 equations in 8 unknowns: $\rho, v_x, v_y, v_z, B_x, B_y, B_z, p$

  with $\rho\, e = \rho\, \epsilon(\rho, p) + \frac{1}{2}\rho v^2 + \frac{1}{2}B^2 = E$

  e: specific total energy (J/kg)

  $E = \rho\, e$: volumetric total energy (J/m^3), conserved quantity

  $\epsilon(\rho, p)$: specific internal energy (J/kg), equation of state (EOS)

- perfect (ideal) gas EOS: $\epsilon(\rho, p) = \dfrac{p}{\rho\,(\gamma - 1)}$

  $$\Rightarrow \rho\, e = \frac{p}{\gamma - 1} + \frac{1}{2}\rho v^2 + \frac{1}{2}B^2$$

- $\gamma = 5/3 = 1.667$ for monatomic plasmas

• $\nabla \cdot \vec{B} = \dfrac{\partial B_x(x,t)}{\partial x} \equiv 0$ is a constraint

$\Rightarrow B_x$ constant in space (in 1D) = initial condition

then it follows from the equations that $\dfrac{\partial B_x(x,t)}{\partial t} \equiv 0$: the constraint is preserved by the evolution equations

we can leave B_x out as a variable in 1D

$\Rightarrow$ in general: the $\nabla \cdot \vec{B}$ constraint only needs to be specified as an initial condition (on the analytical level, numerically: more tricky, see later!)

'Physical' form of the MHD equations

• mass continuity equation: $\dfrac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$

• Newton's law of motion: $\rho \dfrac{d\vec{v}}{dt} = -\nabla p + (\nabla \times \vec{B}) \times \vec{B})$

Ampère's law $\vec{J} = \nabla \times \vec{B}$ (units such that $\mu = 1$)

• vector induction equation: $\dfrac{\partial \vec{B}}{\partial t} = \nabla \times (\vec{v} \times \vec{B}$

derives directly from one of Maxwell's equations, namely, Faraday's law of induction, and from Ohm's law for an ideal plasma: $\vec{E} = -\vec{v} \times \vec{B}$ with $\vec{E}$ the electric field

• evolution of the pressure (perfect (ideal) gas): $\dfrac{\partial p}{\partial t} + (\vec{v} \cdot \nabla)p + \gamma p \nabla \cdot \vec{v} = 0$

we can rewrite as $\dfrac{ds}{dt} = 0$ with the (specific) entropy $s = \dfrac{p}{\rho^\gamma}$

- magnetic monopoles do not exist in nature: $\nabla \cdot \vec{B} = 0$
- conservation of magnetic flux in time: $\Phi = \int_S \vec{A} \cdot \vec{n} dS$

$$\frac{d\Phi}{dt} = \int_S (\frac{\partial \vec{A}}{\partial t} + \vec{u}(\nabla \cdot \vec{A}) + \nabla \times (\vec{A} \times \vec{u})) \cdot \vec{n} dS$$

total time derivative of the flux Φ_B of the magnetic field $\vec{B}$ through a surface moving with the plasma speed $\vec{v}$

$$\frac{d\Phi_B}{dt} = \int_S (\frac{\partial \vec{B}}{\partial t} + \vec{v}(\nabla \cdot \vec{B}) + \nabla \times (\vec{B} \times \vec{v})) \cdot \vec{n} dS$$

using the induction equation: $\boxed{\frac{d\Phi_B}{dt} = 0}$

the magnetic field is frozen into the plasma for ideal MHD, or fluid elements which reside on a common field line at one time, remain on this magnetic field line at all times

Conservative and primitive variables

- vector of conservative variables:

$$U = \begin{bmatrix} \rho \\ m_x \\ m_y \\ m_z \\ B_x \\ B_y \\ B_z \\ E \end{bmatrix} = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho v_z \\ B_x \\ B_y \\ B_z \\ \rho\, e = \frac{p}{(\gamma-1)} + \frac{1}{2}\rho v^2 + \frac{1}{2}B^2 \end{bmatrix} \text{ in } \frac{\partial U}{\partial t} + \mathsf{A}(U)_U \cdot \frac{\partial U}{\partial x} = 0$$

- vector of primitive variables: $V = \begin{bmatrix} \rho \\ v_x \\ v_y \\ v_z \\ B_x \\ B_y \\ B_z \\ p \end{bmatrix}$
- transformation: $\partial U = \frac{\partial U}{\partial V} \cdot \partial V$

$$\Rightarrow \frac{\partial V}{\partial t} + \mathsf{A}(V)_V \cdot \frac{\partial V}{\partial x} = 0$$

- Hyperbolic system:

$$\text{with } \mathsf{A}_V = \begin{bmatrix} v_x & \rho & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & v_x & 0 & 0 & 0 & B_y/\rho & B_z/\rho & 1/\rho \\ 0 & 0 & v_x & 0 & 0 & -B_x/\rho & 0 & 0 \\ 0 & 0 & 0 & v_x & 0 & 0 & -B_x/\rho & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & B_y & -B_x & 0 & 0 & v_x & 0 & 0 \\ 0 & B_z & 0 & -B_x & 0 & 0 & v_x & 0 \\ 0 & c^2\rho & 0 & 0 & 0 & 0 & 0 & v_x \end{bmatrix} \qquad \left(c = \sqrt{\frac{\gamma p}{\rho}} \right)$$

$\lambda_1 = v_x + c_{fx}$: fast wave, right

$\lambda_2 = v_x - c_{fx}$: fast wave, left

$\lambda_3 = v_x + c_{Ax}$: Alfvén wave, right

$\lambda_4 = v_x - c_{Ax}$: Alfvén wave, left

$\lambda_5 = v_x + c_{sx}$: slow wave, right

$\lambda_6 = v_x - c_{sx}$: slow wave, left

$\lambda_7 = v_x$: entropy wave

$\lambda_8 = 0$: not Galilean invariant!!

with

$$c_{fx}^2 = \frac{1}{2}\left(\frac{\gamma p + B^2}{\rho} + \sqrt{\left(\frac{\gamma p + B^2}{\rho}\right)^2 - 4\frac{\gamma p B_x^2}{\rho^2}}\right)$$

$$c_{Ax}^2 = \frac{B_x^2}{\rho}$$

$$c_{sx}^2 = \frac{1}{2}\left(\frac{\gamma p + B^2}{\rho} - \sqrt{\left(\frac{\gamma p + B^2}{\rho}\right)^2 - 4\frac{\gamma p B_x^2}{\rho^2}}\right)$$

wave speeds anisotropic!! (depending on angle between propagation direction x and local magnetic field $\vec{B}$)

- a way to restore Galilean invariance: add a source term S

$$\boxed{\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = S}$$

$$U = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho v_z \\ B_x \\ B_y \\ B_z \\ \rho\, e \end{bmatrix} \quad F(U) = \begin{bmatrix} \rho\, v_x \\ \rho\, v_x^2 + p + B^2/2 - B_x^2 \\ \rho\, v_x v_y - B_x B_y \\ \rho\, v_x v_z - B_x B_z \\ 0 \\ B_y v_x - B_x v_y \\ B_z v_x - B_x v_z \\ (\rho\, e + p + B^2/2) v_x - B_x\, (\vec{v} \cdot \vec{B}) \end{bmatrix}$$

$$S = - \begin{bmatrix} 0 \\ B_x \\ B_y \\ B_z \\ v_x \\ v_y \\ v_z \\ \vec{v} \cdot \vec{B} \end{bmatrix} \nabla \cdot \vec{B}$$

$\Rightarrow$ source term S has no effect if $\nabla \cdot \vec{B} \equiv 0$ (which should be fulfilled on the analytical level), but regularizes the equations (Galilean invariant, complete set of eigenvectors)

useful when

- $\nabla \cdot \vec{B} = 0$ is not exactly satisfied, e.g. numerically

- entropy symmetrization of the MHD equations

- Hyperbolic system:

$$\mathsf{A}'_V = \begin{bmatrix} v_x & \rho & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & v_x & 0 & 0 & 0 & B_y/\rho & B_z/\rho & 1/\rho \\ 0 & 0 & v_x & 0 & 0 & -B_x/\rho & 0 & 0 \\ 0 & 0 & 0 & v_x & 0 & 0 & -B_x/\rho & 0 \\ 0 & 0 & 0 & 0 & v_x & 0 & 0 & 0 \\ 0 & B_y & -B_x & 0 & 0 & v_x & 0 & 0 \\ 0 & B_z & 0 & -B_x & 0 & 0 & v_x & 0 \\ 0 & c^2\rho & 0 & 0 & 0 & 0 & 0 & v_x \end{bmatrix}$$

$\lambda_i,\ i = 1..7$ remain unchanged

$\lambda_8 = v_x$: Galilean invariant!!

complete set of eigenvectors

$\Rightarrow$ use this form of the equations from now on

$\Rightarrow$ hyperbolic system, but: non-strictly hyperbolic, because wave speeds can coincide

- define $\mu_f = \dfrac{c_f}{c_f^2 - c_A^2}$ and $\mu_s = \dfrac{c_s}{c_s^2 - c_A^2}$

$$\Rightarrow \mathsf{R}_{1-4} = \left[\begin{array}{c|c|c|c} \rho & \rho & 0 & 0 \\ \mu_f\,(c_f^2 - c_A^2) & -\mu_f\,(c_f^2 - c_A^2) & 0 & 0 \\ -\mu_f\,(B_x B_y/\rho) & \mu_f\,(B_x B_y/\rho) & -B_z & B_z \\ -\mu_f\,(B_x B_z/\rho) & \mu_f\,(B_x B_z/\rho) & B_y & -B_y \\ 0 & 0 & 0 & 0 \\ \mu_f c_f\,(B_y/\sqrt{\rho}) & \mu_f c_f\,(B_y/\sqrt{\rho}) & -\sqrt{\rho}B_z & -\sqrt{\rho}B_z \\ \mu_f c_f\,(B_z/\sqrt{\rho}) & \mu_f c_f\,(B_z/\sqrt{\rho}) & -\sqrt{\rho}B_y & -\sqrt{\rho}B_y \\ \rho c^2 & \rho c^2 & 0 & 0 \end{array}\right]$$

$$\Rightarrow \mathsf{R}_{5-8} = \left[\begin{array}{c|c|c|c} \rho & \rho & 1 & 0 \\ \mu_s\,(c_s^2 - c_A^2) & \mu_s(c_s^2 - c_A^2) & 0 & 0 \\ -\mu_s\,(B_x B_y/\rho) & \mu_s(B_x B_y/\rho) & 0 & 0 \\ -\mu_s\,(B_x B_z/\rho) & \mu_s(B_x B_z/\rho) & 0 & 0 \\ 0 & 0 & 0 & 1 \\ \mu_s c_s\,(B_y/\sqrt{\rho}) & \mu_s c_s\,(B_y/\sqrt{\rho}) & 0 & 0 \\ \mu_s c_s\,(B_z/\sqrt{\rho}) & \mu_s c_s\,(B_z/\sqrt{\rho}) & 0 & 0 \\ \rho c^2 & \rho c^2 & 0 & 0 \end{array}\right]$$

Characteristics and Riemann Invariants

$\forall i$: (n characteristic fields)

- $\boxed{x_i(t) : \dfrac{\partial x_i(t)}{\partial t} = \lambda_i(V)}$: ith characteristic

- if $\exists\, w_i(V)$: $L_i(V) \cdot \partial V = \alpha(V)\, \partial w_i(V)$

$$\Rightarrow \frac{\mathrm{d}w_i(x_i(t), t)}{\mathrm{d}t} = 0 :$$ w_i Riemann Invariant (RI) on characteristic x_i

- $i = 7$: find $w_7(V)$ such that

$$L_7(V) \cdot \partial V = \partial \rho - \frac{1}{c^2}\partial p = \alpha(V)\, \partial w_7(V)$$

$\Rightarrow$ s is a Riemann Invariant on $x_7(t)$ with $\dfrac{\partial x_7(t)}{\partial t} = v_x$

the entropy of a fluid element is conserved on its path

- $i = 8$: find $w_8(V)$ such that

$$L_8(V) \cdot \partial V = \partial B_x = \alpha(V)\, \partial w_8(V)$$

$\Rightarrow B_x$ is a Riemann Invariant on $x_8(t)$ with $\dfrac{\partial x_8(t)}{\partial t} = v_x$

- $i = 1,2,3,4,5,6$: find $w_i(V)$ such that

$$L_i(V) \cdot \partial V = \alpha(V)\, \partial w_i(V)$$

no solution, RI does not exist

$$\mathsf{R}_{1-4} = \left[\begin{array}{c|c|c|c} \rho & \rho & 0 & 0 \\ \mu_f\,(c_f^2 - c_A^2) & -\mu_f\,(c_f^2 - c_A^2) & 0 & 0 \\ -\mu_f\,(B_x B_y/\rho) & \mu_f\,(B_x B_y/\rho) & 0 & 0 \\ 0 & 0 & B_y & -B_y \\ 0 & 0 & 0 & 0 \\ \mu_f c_f\,(B_y/\sqrt{\rho}) & \mu_f c_f\,(B_y/\sqrt{\rho}) & 0 & 0 \\ 0 & 0 & -\sqrt{\rho}B_y & -\sqrt{\rho}B_y \\ \rho c^2 & \rho c^2 & 0 & 0 \end{array}\right]$$

$$\mathsf{R}_{5-8} = \left[\begin{array}{c|c|c|c} \rho & \rho & 1 & 0 \\ \mu_s\,(c_s^2 - c_A^2) & \mu_s(c_s^2 - c_A^2) & 0 & 0 \\ -\mu_s\,(B_x B_y/\rho) & \mu_s(B_x B_y/\rho) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ \mu_s c_s\,(B_y/\sqrt{\rho}) & \mu_s c_s\,(B_y/\sqrt{\rho}) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \rho c^2 & \rho c^2 & 0 & 0 \end{array}\right]$$

- $V_1 = \mathsf{R}(V_0) \cdot W_1$: properties of MHD waves, take $B_{z0} = 0$

  - fast (1,2): $\Delta\rho, \pm\Delta v_x, \pm\Delta v_y, \Delta B_y, \Delta p$

    compressive, Δp in phase with $\Delta B (= \Delta B_y)$
  - slow (5,6): $\Delta\rho, \pm\Delta v_x, \pm\Delta v_y, \Delta B_y, \Delta p$

    compressive, Δp in anti-phase with $\Delta B (= \Delta B_y)$
  - Alfvén (3,4): $\pm\Delta v_z, \Delta B_z$

    non-compressive, non-planar
  - entropy (7): $\Delta\rho$
  - $\nabla \cdot \vec{B}$ wave (8): $\Delta B_x \sim \nabla \cdot \vec{B}$
- large-amplitude = nonlinear

  $\Rightarrow$ waves interact, steepen into shocks, rarefactions, wave coupling, . . .

Numerical simulation of flows with shocks

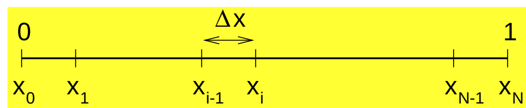
2.1 1D finite difference schemes

2.1.1 Scalar conservation laws

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

$$\frac{\partial u}{\partial t} + f'(u)\,\frac{\partial u}{\partial x} = 0 \qquad \text{with} \qquad f'(u) = \frac{\partial f(u)}{\partial u}$$

- continuous domain $\Rightarrow$ finite number of *grid points*



e.g. equidistant grid: $x_i = i\Delta x = \dfrac{i}{N}$

- point-values of functions $f(x)$ $\Rightarrow$ $\{f_i \equiv f(x_i), i = 0, 1, \ldots, N\}$
- in space and time: $f_i^n \equiv f(x_i, t_n)$

Finite difference approximations

- derivatives $\Rightarrow$ truncated Taylor series expansions, e.g.

$$u_{i\pm1} = u_i \pm \left.\frac{\partial u}{\partial x}\right|_i \Delta x + \left.\frac{\partial^2 u}{\partial x^2}\right|_i \frac{\Delta x^2}{2!} \pm \left.\frac{\partial^3 u}{\partial x^3}\right|_i \frac{\Delta x^3}{3!} + O(\Delta x^2)$$ [1a] and [1b]

[1a]: $\left.\frac{\partial u}{\partial x}\right|_i = \frac{u_{i+1}-u_i}{\Delta x} - \frac{\Delta x}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_i + O(\Delta x^2)$ '1st-order forward'

[1b]: $\left.\frac{\partial u}{\partial x}\right|_i = \frac{u_i-u_{i-1}}{\Delta x} + \frac{\Delta x}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_i + O(\Delta x^2)$ '1st-order backward'

[1a]–[1b]: $\left.\frac{\partial u}{\partial x}\right|_i = \frac{u_{i+1}-u_{i-1}}{2\Delta x} + 0\,\frac{\Delta x}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_i + O(\Delta x^2)$ '2nd-order central'

- 2nd-order derivatives:

[1a]+[1b]: $\left.\frac{\partial^2 u}{\partial x^2}\right|_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + O(\Delta x^2)$ (2nd-order)

Four schemes for the linear advection equation

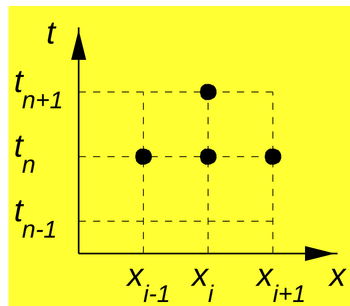
$$f(u) = a\,u \quad \Rightarrow \quad \frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

(linear equation; assume $a > 0$)

- 1. Forward Central (FC):

$$\underbrace{\frac{v_i^{n+1} - v_i^n}{\Delta t}}_{\text{1st-order forward FD}} + a \underbrace{\frac{v_{i+1}^n - v_{i-1}^n}{2\,\Delta x}}_{\text{2nd-order central FD}}$$

with stencil:



$$\Rightarrow \boxed{v_i^{n+1} = v_i^n - a\frac{\Delta t}{\Delta x}\frac{v_{i+1}^n - v_{i-1}^n}{2}}$$

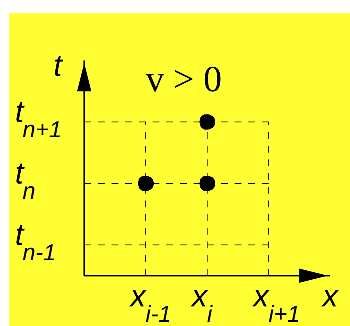
$O(\Delta x^2, \Delta t)$ ($\Rightarrow$ consistent!)

BUT: numerically unstable

- 2. First Order Upwind (FOU):

$$\underbrace{\frac{v_i^{n+1} - v_i^n}{\Delta t}}_{\text{1st-order forward FD}} + a \underbrace{\frac{v_i^n - v_{i-1}^n}{\Delta x}}_{\text{1st-order left FD}}$$

with stencil:



$$\Rightarrow \boxed{v_i^{n+1} = v_i^n - a\frac{\Delta t}{\Delta x}\left(v_i^n - v_{i-1}^n\right)}$$

$O(\Delta x, \Delta t)$ (consistent)

BUT: not accurate – high diffusion

$\Rightarrow$ if the sign of a is not specified in advance:

$$\frac{v_i^{n+1} - v_i^n}{\Delta t} + a^+\frac{v_i^n - v_{i-1}^n}{\Delta x} + a^-\frac{v_{i+1}^n - v_i^n}{\Delta x} = 0$$

with the definitions: $a^+ = max(0, a)$ and $a^- = min(0, a)$

- 3. Lax-Wendroff (LW):

$$\frac{\partial u}{\partial t} = -a\,\frac{\partial u}{\partial x} \quad \Rightarrow \quad \frac{\partial^2 u}{\partial t^2} = -a\,\frac{\partial^2 u}{\partial x \partial t} = a^2\,\frac{\partial^2 u}{\partial x^2}$$

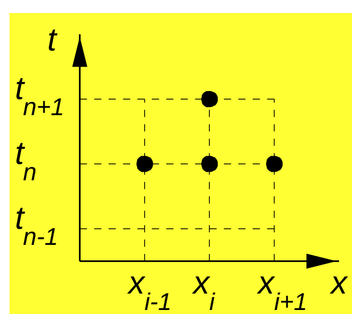
consider Taylor expansion in time:

$$u_i^{n+1} = u_i^n + \left.\frac{\partial u}{\partial t}\right|_i^n \Delta t + \left.\frac{\partial^2 u}{\partial t^2}\right|_i^n \frac{\Delta t^2}{2!} + O(\Delta t^3)$$

$$\Rightarrow u_i^{n+1} = u_i^n - a\left.\frac{\partial u}{\partial x}\right|_i^n \Delta t + a^2\left.\frac{\partial^2 u}{\partial x^2}\right|_i^n \frac{\Delta t^2}{2!} + O(\Delta t^3)$$

$$\boxed{\frac{v_i^{n+1} - v_i^n}{\Delta t} + a\,\frac{v_{i+1}^n - v_{i-1}^n}{2\,\Delta x} - \frac{a^2}{2}\,\Delta t\,\frac{v_{i+1}^n - 2v_i^n + v_{i-1}^n}{\Delta x^2} = 0} \quad O(\Delta x^2, \Delta t^2)$$

with stencil:



$O(\Delta x^2, \Delta t^2)$ (consistent)

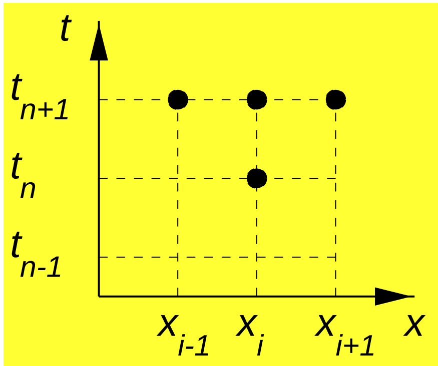
BUT: not positive – oscillations

- 4. Backward Central (BC):

$$\underbrace{\frac{v_i^{n+1}-v_i^n}{\Delta t}}_{\text{1st-order forward FD}} + a\underbrace{\frac{v_{i+1}^{n+1}-v_{i-1}^{n+1}}{2\,\Delta x}}_{\text{2nd-order central FD}} \Rightarrow \boxed{v_i^{n+1} = v_i^n - a\frac{\Delta t}{\Delta x}\frac{v_{i+1}^{n+1}-v_{i-1}^{n+1}}{2}}$$

$O(\Delta x^2, \Delta t)$ (consistent)

with stencil:



IMPLICIT scheme:

- all v_i at time level $n+1$ are coupled
- need matrix inversion in every time step
- schemes 1.–3. are EXPLICIT:

no matrix inversion needed

numerically stable, BUT: not positive – oscillations

$\Rightarrow$ REMARK: schemes 1.–4. are LINEAR in the v_i

Four requirements for a shock-capturing numerical scheme

1. Accurate – low diffusion
2. Numerically stable
3. Positive, no spurious oscillations – low dispersion
4. Conservative – the Lax-Wendroff theorem

1. Accurate – low diffusion

linear advection-diffusion equation: $$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \eta\frac{\partial^2 u}{\partial x^2}$$

consider discretization of spatial part:

- FC: $$\frac{v_i^{n+1} - v_i^n}{\Delta t} + a\,\frac{v_{i+1}^n - v_{i-1}^n}{2\,\Delta x} = 0$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\,\left.\frac{\partial u}{\partial x}\right|_i + 0\,\left.\frac{\partial^2 u}{\partial x^2}\right|_i + a\,\frac{\Delta x^2}{3!}\,\left.\frac{\partial^3 u}{\partial x^3}\right|_i + O(\Delta x^3) = 0$$

$\Rightarrow$ NO DIFFUSION (but: unstable)

linear advection-diffusion equation: $$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \eta\frac{\partial^2 u}{\partial x^2}$$

- FOU: $$\frac{v_i^{n+1} - v_i^n}{\Delta t} + a\,\frac{v_i^n - v_{i-1}^n}{\Delta x} = 0 \qquad (a > 0)$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\,\left.\frac{\partial u}{\partial x}\right|_i - a\,\frac{\Delta x}{2}\,\left.\frac{\partial^2 u}{\partial x^2}\right|_i + a\,\frac{\Delta x^2}{3!}\,\left.\frac{\partial^3 u}{\partial x^3}\right|_i + O(\Delta x^3) = 0$$

- also: rewrite FOU as

$$\frac{v_i^{n+1} - v_i^n}{\Delta t} + a\frac{v_{i+1}^n - v_{i-1}^n}{2\Delta x} - \frac{|a|\Delta x}{2}\frac{v_{i+1}^n - 2v_i^n + v_{i-1}^n}{\Delta x^2} = 0$$

- second order accurate discretization of the spatial part of the *linear advection-diffusion equation* with diffusion coefficient $\eta_{num} = |a|\Delta x/2$.
- this *numerical diffusion* vanishes in first order in Δx

$\Rightarrow$ NUMERICAL DIFFUSION: we want to minimize it, but necessary for stability (explicit schemes) and positivity (see below) linear advection-diffusion equation: $$\boxed{\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \eta\frac{\partial^2 u}{\partial x^2}}$$

REMARK: interaction of spatial and temporal discretization may lead to cancellation of errors:

- LW: diffusion term, but cancels with first order error in temporal discretization

$$\frac{v_i^{n+1} - v_i^n}{\Delta t} + a\,\frac{v_{i+1}^n - v_{i-1}^n}{2\,\Delta x} - \frac{a^2}{2}\Delta t\,\frac{v_{i+1}^n - 2v_i^n + v_{i-1}^n}{\Delta x^2} = 0 \quad O(\Delta x^2, \Delta t^2)$$

$\Rightarrow$ NO DIFFUSION (second order!), stable

LW is the unique explicit linear 2-level scheme which is second order in space and time (but: not positive)

linear advection-diffusion equation: $$\boxed{\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \eta\frac{\partial^2 u}{\partial x^2}}$$

REMARK: dispersion relation: $u(x,t) = \exp(i(kx - \omega t))$

$$-i\,\omega\,u + a\,i\,k\,u = \eta\,(i\,k)^2\,u$$

$$\boxed{\omega - a\,k + \eta\,i\,k^2 = 0}$$

$\Rightarrow$ complex dispersion relation = damped waves

($\eta = 0 \;\Rightarrow$ undamped waves with phase velocity $= \omega/k = a$, and group velocity $= \partial\omega/\partial k = a$)

2. Numerically stable

numerical solution=exact solution+error

$$v_j^n = u_j^n + e_j^n$$

- FOU:

$$\frac{v_j^{n+1} - v_j^n}{\Delta t} + a\,\frac{v_j^n - v_{j-1}^n}{\Delta x} = 0$$

$$\Rightarrow \underbrace{\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\,\frac{u_j^n - u_{j-1}^n}{\Delta x}}_{\text{new error: O}(\Delta x,\Delta t)} + \underbrace{\frac{e_j^{n+1} - e_j^n}{\Delta t} + a\,\frac{e_j^n - e_{j-1}^n}{\Delta x}}_{\text{amplification of error}} = 0 \qquad \text{(linear!)}$$

requirement for numerical stability: existing errors are not amplified

Fourier decomposition of error on grid (mode m): (von Neumann method)

$$e_j^n = \bar{e}_m^n \exp(i\, m\, \pi\, \Delta x\, j) = \bar{e}_m^n \exp(i \theta_m j)$$

in FOU:

$$\frac{\bar{e}_m^{n+1} \exp(i\theta_m j) - \bar{e}_m^n \exp(i\theta_m j)}{\Delta t} + a\,\bar{e}_m^n \exp(i\theta_m j)\frac{1 - \exp(-i\theta_m)}{\Delta x} = 0$$

$$\Rightarrow \frac{\bar{e}_m^{n+1}}{\bar{e}_m^n} = 1 - a\frac{\Delta t}{\Delta x}\underbrace{(1 - \exp(-i\theta_m))}_{0\ldots 2}$$

$$\left|\frac{\bar{e}_m^{n+1}}{\bar{e}_m^n}\right| \le 1 \quad \Leftrightarrow \quad |a|\frac{\Delta t}{\Delta x} \le 1$$

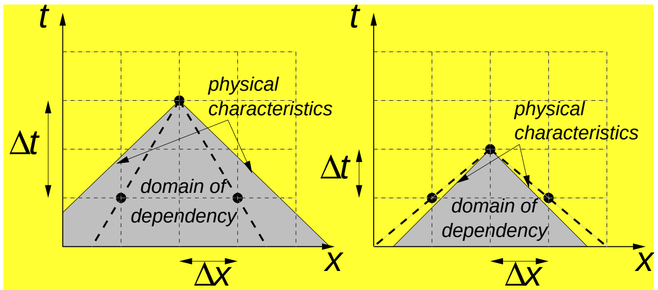
$$\Rightarrow \Delta t \le \frac{\Delta x}{|a|}$$

= CFL condition (Courant-Friedrichs-Levy)

$\Rightarrow$ FOU is conditionally stable

Physical interpretation of CFL condition

- hyperbolic system: information propagates along real characteristic curves $\Rightarrow$ domain of dependence



- for systems: several wave speeds, domain of dependence delineated by characteristics with smallest and largest wave speeds
- slopes of characteristics = wave speeds a_{min} and a_{max}

- $\Delta t \leq \dfrac{\Delta x}{|a|}$ $\Rightarrow$ numerical domain of dependence $\geq$ physical domain of dependence

- FC: (explicit, central in space)

$$\boxed{u_i^{n+1} = u_i^n - a\frac{\Delta t}{\Delta x}\frac{u_{i+1}^n - u_{i-1}^n}{2}}$$

$$\Rightarrow \frac{\bar{e}_m^{n+1}}{\bar{e}_m^n} = 1 - a\frac{\Delta t}{\Delta x}\underbrace{\frac{(\exp(i\theta_m) - \exp(-i\theta_m))}{2}}_{i\sin(\theta_m)}$$

$\Rightarrow$ unconditionally unstable!

- BC: (implicit, central in space)

$$\boxed{u_i^{n+1} = u_i^n - a\frac{\Delta t}{\Delta x}\frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2}}$$

$$\Rightarrow 1 = \frac{\bar{e}_m^n}{\bar{e}_m^{n+1}} - a\frac{\Delta t}{\Delta x}\underbrace{\frac{(\exp(i\theta_m) - \exp(-i\theta_m))}{2}}_{i\sin(\theta_m)}$$

$\Rightarrow$ unconditionally stable!

- LW: (explicit)

$\Rightarrow$ conditionally stable under CFL condition

- conclusion: numerical diffusion (FOU) or implicit time integration (BC) can make scheme stable

3. Positive, no spurious oscillations – low dispersion

linear advection equation with dispersive term: $$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \mu\frac{\partial^3 u}{\partial x^3}$$

dispersion relation: $u(x,t) = \exp(i(kx - \omega t))$

$$-i\,\omega\,u + a\,i\,k\,u = \mu(i\,k)^3\,u$$

$$\boxed{-\omega + a\,k = -\mu\,k^3} \quad \boxed{v_{ph} = \frac{\omega}{k} = a + \mu\,k^2} \quad \boxed{v_g = \frac{\partial\omega}{\partial k} = a + 3\,\mu\,k^2}$$

$\Rightarrow$ dispersion = Gibbs phenomenon = oscillations at discontinuities

$\Rightarrow$ central space discretization = no diffusion term ($\sim$ second derivative)

leading error term = dispersive term ! ($\sim$ third derivative) $\Rightarrow$ oscillations!

$\Rightarrow$ solution: we need diffusion, but will make schemes first order at discontinuities

Positivity properties of smooth exact solutions

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

$$\frac{\partial u}{\partial t} + f'(u)\,\frac{\partial u}{\partial x} = 0 \qquad \text{with} \qquad f'(u) = \frac{\partial f(u)}{\partial u} = a(u)$$

u is Riemann Invariant on characteristic $x(t)$

Properties:

- (1): local maximum cannot increase
  local minimum cannot decrease

- (2): no new local maxima or minima can arise
  (monotone profile remains monotone)

Positive schemes

- how can we know where to add diffusion, and how much?

$\Rightarrow$ one possible approach: consider positive schemes

(1): Local Extremum Diminishing (LED) spatial discretization

- $\dfrac{\partial v_j}{\partial t} = c_{j-1}\,v_{j-1} + c_j\,v_j + c_{j+1}\,v_{j+1}$

  consistency ($u(x,t)$ constant is a solution) $\Rightarrow c_{j-1} + c_j + c_{j+1} \equiv 0$

$\Rightarrow \dfrac{\partial v_j}{\partial t} = c_{j-1}\,(v_{j-1} - v_j) + c_{j+1}\,(v_{j+1} - v_j)$

- define LED scheme $\Leftrightarrow c_{j-1} \geq 0$ and $c_{j+1} \geq 0$

$\Rightarrow$ it follows that local extrema ($\sim$ oscillations) are suppressed:

if v_j is a local maximum $\Rightarrow \dfrac{\partial v_j}{\partial t} < 0$

if v_j is a local minimum $\Rightarrow \dfrac{\partial v_j}{\partial t} > 0$

- remark: requires compact stencil
- example: FOU:

$$\frac{\partial v_j}{\partial t} = \frac{a^+}{\Delta x}(v_{j-1} - v_j) - \frac{a^-}{\Delta x}(v_{j+1} - v_j)$$

$\Rightarrow c_{j-1} \geq 0$ and $c_{j+1} \geq 0$

$\Rightarrow$ FOU is LED! $\Rightarrow$ no increasing oscillations

- positivity is related to concept of Total Variation Diminishing (TVD) schemes, but more easily extendable to multiple spatial dimensions

(2): no new local extrema

- $v_j^{n+1} = v_j^n + \Delta t (c_{j-1}\, v_{j-1}^n + c_j\, v_j^n + c_{j+1}\, v_{j+1}^n)$

  consistency ($u(x,t)$ constant is a solution) $\Rightarrow 1 + \Delta t(c_{j-1} + c_j + c_{j+1}) \equiv 1$

  convex average, no new local extrema $\Leftrightarrow$ all coefficients positive

  - $c_i \geq 0 \ \forall i \neq j$ from LED condition
  - $1 + \Delta t\, c_j \geq 0$

$$\Delta t \leq \frac{1}{-c_j}$$

$$\Delta t \leq \frac{1}{\sum_{i \neq j} c_i}$$ new kind of CFL condition?

$$\Delta t \leq \frac{1}{\sum_{i \neq j} c_i}$$ new kind of CFL condition?

- example: FOU:

$$\frac{\partial v_j}{\partial t} = \frac{a^+}{\Delta x}(v_{j-1} - v_j) - \frac{a^-}{\Delta x}(v_{j+1} - v_j)$$

$$\Rightarrow \sum_{i \neq j} c_i = \frac{a^+}{\Delta x} - \frac{a^-}{\Delta x} = \frac{|a|}{\Delta x}$$

$$\Rightarrow \Delta t \leq \frac{\Delta x}{|a|}$$ (good old CFL condition)

4. Conservative – the Lax-Wendroff theorem

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

'natural' discretization: CONSERVATIVE

$$\frac{\partial v_j}{\partial t} + \frac{\tilde{f}_{j+1/2} - \tilde{f}_{j-1/2}}{\Delta x} = 0$$

with $\tilde{f}_{j+1/2}$ the numerical flux function at $j + 1/2$

$$\Rightarrow v_j^{n+1} = v_j^n - \frac{\Delta t}{\Delta x}(\tilde{f}_{j+1/2} - \tilde{f}_{j-1/2})$$

$$\Rightarrow \sum_j v_j^{n+1} = \sum_j v_j^n$$

$\Rightarrow$ exact conservation at the discrete level! (= natural discretization)

- remark: if (strictly) conservative as defined above, isolated discontinuity will propagate at exactly right speed, independent of grid size (need consistency here)

  $\Rightarrow$ Lax-Wendroff theorem (in 1D) : for a consistent and (strictly) conservative scheme:

  if the scheme converges for a given problem, then it will converge to a weak solution (with the right shock speed)

$\Rightarrow$ good if you can find numerical schemes that are strictly conservative

- BUT: strict conservation is not necessary; it is sufficient that $\tilde{f}_{j,r}$ and $\tilde{f}_{j+1,l}$ approach each other at least with order h, both for smooth and discontinuous flow; then numerical shock speed will converge to the right shock speed by refining (for isolated discontinuity)

- problem: for flows with shocks, some non-conservative schemes converge to solutions with wrong shock speed

BUT: how about 2D and 3D, systems, unstructured grids, some non-conservative schemes seem to give right shock speed, FE schemes, . . . ? open questions

- example: FOU is conservative:

$$\boxed{\frac{\partial v_j}{\partial t} + \frac{\tilde{f}_{j+1/2} - \tilde{f}_{j-1/2}}{\Delta x} = 0}$$

$$\frac{v_j^{n+1} - v_j^n}{\Delta t} + a^+ \frac{v_j^n - v_{j-1}^n}{\Delta x} + a^- \frac{v_{j+1}^n - v_j^n}{\Delta x} = 0$$

$$\frac{v_j^{n+1} - v_j^n}{\Delta t} + \frac{[a^+ v_j^n + a^- v_{j+1}^n] - [a^+ v_{j-1}^n + a^- v_j^n]}{\Delta x} = 0$$

$$\Rightarrow \tilde{f}_{j+1/2} = a^+ v_j^n + a^- v_{j+1}^n$$

$$\Rightarrow \tilde{f}_{j+1/2} = \underbrace{\frac{a\, v_j + a\, v_{j+1}}{2}}_{\text{central, second order}} - \underbrace{\frac{1}{2}|a|\,(v_{j+1} - v_j)}_{\text{numerical diffusion term}}$$

- example: simple extension of FOU for nonlinear equation is NOT conservative, and gives wrong shock speed! :

assume $v_j^n \geq 0$, Burgers equation

$$\frac{v_j^{n+1} - v_j^n}{\Delta t} + v_j^n \frac{v_j^n - v_{j-1}^n}{\Delta x} = 0$$

take Riemann problem with $u_l = 1, u_r = 0 \Rightarrow s = 1/2$

$v_j^n = 1$ (then also $v_{j-1}^n = 1$) $\Rightarrow v_j^{n+1} = 1$

$v_j^n = 0 \Rightarrow v_j^{n+1} = 0$

$\Rightarrow$ numerical $s = 0$, quite wrong

Nonlinear schemes – the Godunov theorem

- FOU: linear scheme

- 1. Accurate – low diffusion: NO (first order)
- 2. Numerically stable: yes, CFL
- 3. Positive, no spurious oscillations: yes
- 4. Conservative: yes

- BC: linear scheme

- 1. Accurate – low diffusion: yes (second order)
- 2. Numerically stable: yes, unconditionally
- 3. Positive, no spurious oscillations: NO (dispersion)
- 4. Conservative: yes

$\Rightarrow$ Godunov's theorem: a linear positive scheme cannot be second order

$\Rightarrow$ conversely: we need non-linear schemes to achieve both positivity and second order (away from shocks)

Linear reconstruction: the Minmod slope limiter

starting from FOU, construct a second order conservative scheme

FOU ($a > 0$): $\dfrac{u_j^{n+1} - u_j^n}{\Delta t} + a\,\dfrac{u_j^n - u_{j-1}^n}{\Delta x} = 0$

conservative: $v_j^{n+1} = v_j^n - \dfrac{\Delta t}{\Delta x}(\tilde{f}_{j+1/2} - \tilde{f}_{j-1/2})$

$\tilde{f}_{j+1/2} = a\,u_j^n$: first order

$\Rightarrow$ use the gradient to reconstruct u at the cell interface with c_1 and c_2 some constants ($c_1 + c_2 = 1/2$):

$$\tilde{f}_{j+1/2} = a\,(u_j^n + c_1\,(v_{j+1}^n - v_j^n) + c_2\,(v_j^n - v_{j-1}^n))$$

second order, but not positive: oscillations

$\Rightarrow$ use non-linear limiter function Ψ to determine the slope with which to reconstruct

$$\tilde{f}_{j+1/2} = a\,(u_j^n + \frac{1}{2}\,\Psi(\frac{v_{j+1}^n - v_j^n}{v_j^n - v_{j-1}^n})\,(v_j^n - v_{j-1}^n))$$

$\Rightarrow$ conditions on $\Psi(r)$ can be derived such that positivity is satisfied

$$r = \frac{v_{j+1}^n - v_j^n}{v_j^n - v_{j-1}^n}$$

- example: MINMOD limiter function

$$\Psi(r) = \max(0, \min(r, 1))$$

$\Rightarrow$ if slopes same sign ($r > 0$): take smallest slope

$\Rightarrow$ if slopes different sign (oscillation!): take slope 0 $\Rightarrow$ first order at shock

Nonlinear equations

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

$$\frac{\partial u}{\partial t} + f'(u)\,\frac{\partial u}{\partial x} = 0 \qquad \text{with} \qquad f'(u) = \frac{\partial f(u)}{\partial u} = a(u)$$

⇒ generalize the first order upwind scheme for linear equation:

$$\tilde{f}_{j+1/2} = \frac{a\,v_j + a\,v_{j+1}}{2} - \frac{1}{2}\,|a|\,(v_{j+1} - v_j)$$

becomes

$$\tilde{f}_{j+1/2} = \frac{f(v_j) + f(v_{j+1})}{2} - \frac{1}{2}\,|\tilde{a}(v_j, v_{j+1})|\,(v_{j+1} - v_j)$$

with, e.g., $\tilde{a}(v_j, v_{j+1}) = a(\frac{v_j + v_{j+1}}{2})$

⇒ this is the (local) Lax-Friedrichs scheme

other more sophisticated choices for $\tilde{a}$ are possible

positive second-order schemes can be obtained by taking non-linearly reconstructed values in stead of v_j and v_{j+1}

2.1.2 Systems of conservation laws

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

linear systems

Apply first order upwind to every equation separately:

$$\frac{\partial U}{\partial t} + \mathsf{A} \cdot \frac{\partial U}{\partial x} = 0$$

hyperbolic $\Rightarrow \mathsf{A} = \mathsf{R} \cdot \Lambda \cdot \mathsf{L}$

define $W = \mathsf{L} \cdot U$: characteristic variables W $\Rightarrow$ $\frac{\partial W}{\partial t} + \Lambda \cdot \frac{\partial W}{\partial x} = 0$

for every component of W (take, e.g., first component)

$$\frac{\hat{w}_{1i}^{n+1} - \hat{w}_{1i}^{n}}{\Delta t} + \lambda_1^+ \frac{\hat{w}_{1i}^{n} - \hat{w}_{1i-1}^{n}}{\Delta x} + \lambda_1^- \frac{\hat{w}_{1i+1}^{n} - \hat{w}_{1i}^{n}}{\Delta x} = 0$$

$\Rightarrow$ in matrix form: $\frac{\hat{W}_i^{n+1} - \hat{W}_i^{n}}{\Delta t} + \Lambda^+ \frac{\hat{W}_i^{n} - \hat{W}_{i-1}^{n}}{\Delta x} + \Lambda^- \frac{\hat{W}_{i+1}^{n} - \hat{W}_i^{n}}{\Delta x} = 0$

($\hat{W}_i$ is here numerical approximation of exact W) :

$\Rightarrow$ in conserved variables (V_i is here numerical approximation of exact U):

$$\frac{V_i^{n+1} - V_i^{n}}{\Delta t} + \mathsf{R} \cdot \Lambda^+ \cdot \mathsf{L} \frac{V_i^{n} - V_{i-1}^{n}}{\Delta x} + \mathsf{R} \cdot \Lambda^- \cdot \mathsf{L} \frac{V_{i+1}^{n} - V_i^{n}}{\Delta x} = 0$$

first order:

$\Rightarrow \tilde{F}_{j+1/2} = \mathsf{A}^+ V_j^n + \mathsf{A}^- V_{j+1}^n$

$$\Rightarrow \tilde{F}_{j+1/2} = \underbrace{\frac{\mathsf{A}\, V_j + \mathsf{A}\, V_{j+1}}{2}}_{\text{central, second order}} - \underbrace{\frac{1}{2} |\mathsf{A}| \left(V_{j+1} - V_j\right)}_{\text{numerical diffusion term}}$$

with $|\mathsf{A}| = \mathsf{R} \cdot |\Lambda| \cdot \mathsf{L}$

second order (away from shocks):

$$\Rightarrow \tilde{F}_{j+1/2} = \mathsf{A}^{+}(V_j^n + \frac{1}{2}\,\Psi(\frac{V_{j+1}^n - V_j^n}{V_j^n - V_{j-1}^n})\,(V_j^n - V_{j-1}^n)) + \mathsf{A}^{-}(\ldots)$$

$\Rightarrow$ this is the Roe scheme

- simplification: give every wave same (maximal) diffusion: Lax-Friedrichs (LF) scheme

$$\Rightarrow \tilde{F}_{j+1/2} = \underbrace{\frac{\mathsf{A}\,V_j + \mathsf{A}\,V_{j+1}}{2}}_{\text{central, second order}} \quad \underbrace{-\frac{1}{2}\,|\lambda|_{max}\,(V_{j+1} - V_j)}_{\text{numerical diffusion term}}$$

with $|\lambda|_{max}$ the largest eigenvalue (in absolute value)

$\Rightarrow$ more simple, more robust $\Rightarrow$ good scheme, but sometimes too diffusive

- the CFL time step limitation becomes (for Roe and LF)

$$\Delta t < \frac{\Delta x}{max_{k,j}(|\lambda_{j+1/2}^{(k)}|)}$$

with k running over the number n of waves in the system

nonlinear systems

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

generalize FOU for linear systems:

$$\Rightarrow \tilde{F}_{j+1/2} = \underbrace{\frac{F(V_j) + F(V_{j+1})}{2}}_{\text{central, second order}} - \underbrace{\frac{1}{2}\,|\tilde{\mathsf{A}}(V_j, V_{j+1})|\,(V_{j+1} - V_j)}_{\text{numerical diffusion term}}$$

with, e.g., $\tilde{\mathsf{A}}(V_j, V_{j+1}) = \mathsf{A}(\frac{V_j + V_{j+1}}{2})$

$\Rightarrow$ this is a simplified Roe scheme

other more sophisticated choices for $\tilde{\mathsf{A}}$ are possible (full Roe scheme uses Roe linearization, . . .)

positive second-order schemes can be obtained by taking non-linearly reconstructed values in stead of V_j and V_{j+1}

conclusions:

for 1D problems, using finite differences, the upwind idea, and nonlinear reconstruction, we obtain schemes that are

- 1: accurate: second order (except at shocks)
- 2: numerically stable (CFL for explicit, unconditionally for implicit)
- 3: positive: no oscillations at shocks
- 4: conservative: capture shocks with the right speed

$\Rightarrow$ the Lax-Friedrichs scheme is simple, robust, and thus very useful:

$$\tilde{F}_{j+1/2} = \underbrace{\frac{F(V_j) + F(V_{j+1})}{2}}_{\text{central, second order}} - \underbrace{\frac{1}{2}\,|\tilde{\lambda}|_{max}(V_j, V_{j+1})\,(V_{j+1} - V_j)}_{\text{numerical diffusion term}}$$

with $|\tilde{\lambda}|_{max}(V_j, V_{j+1}) = |\lambda|_{max}(\frac{V_j + V_{j+1}}{2})$

2.2 Finite volume schemes

- Finite Difference (FD) = v_j point values, upwind
- Finite Volumes (FV) = $\bar{v}_j$ cell averages,

  using fluxes at cell interfaces, Riemann problems

$\Rightarrow$ here we will make the link between the two

Recapitulation: FOU FD scheme

$$f(u) = a\,u \quad \Rightarrow \quad \frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$ (linear equation; assume $a > 0$)

$$\Rightarrow \boxed{v_j^{n+1} = v_j^n - a\,\frac{\Delta t}{\Delta x}\,(v_j^n - v_{j-1}^n)\text{=0}}$$

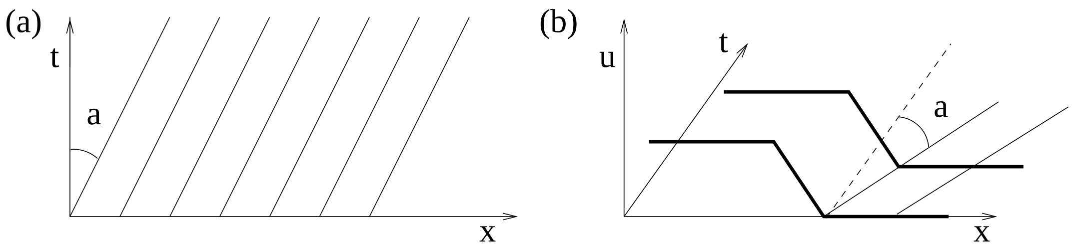
'natural' discretization: CONSERVATIVE, f^* numerical flux function

$$\frac{\partial v_j}{\partial t} + \frac{f^*_{j+1/2} - f^*_{j-1/2}}{\Delta x} = 0$$

$$\Rightarrow f^*_{j+1/2} = a\,v_j$$

$$\Rightarrow f^*_{j+1/2} = \underbrace{\frac{a\,v_j + a\,v_{j+1}}{2}}_{\text{central, second order}} - \underbrace{\frac{1}{2}\,|a|\,(v_{j+1} - v_j)}_{\text{numerical diffusion term}}$$

Recapitulation: Riemann problem



solution $u^*(x=0,t)$ at $x=0$ is constant in t

numerical Riemann problem at interface:

$v^*_{j+1/2} = v_j$!!

$\Rightarrow f_{j+1/2} = f(v^*_{j+1/2}) = a\, v_j$!!

$\Rightarrow$ Riemann flux = upwind flux !!

Finite Volume (FV) schemes

- repeat every time step

  - take averages in every cell $\Rightarrow$ Riemann problems at all interfaces!

  - propagate solution by solving Riemann problems (time step limitation!)

$\Rightarrow$ this is the *Godunov scheme*, uses a Riemann solver

we can approximate the exact Riemann flux (linearize, make continuous, cheaper, ...), and obtain the approximate Riemann flux f^*

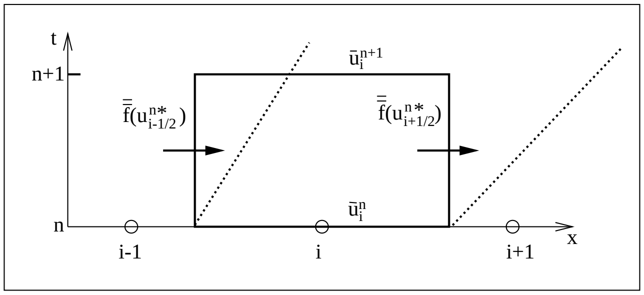
$f^*_{i+1/2} \approx f_{i+1/2}(u^*)$

$\Rightarrow$ this is called an approximate Riemann solver

$\Rightarrow$ this is completely analogous to the FD upwind idea

2.2.1 Spatial discretization

Cell averages define Riemann problems



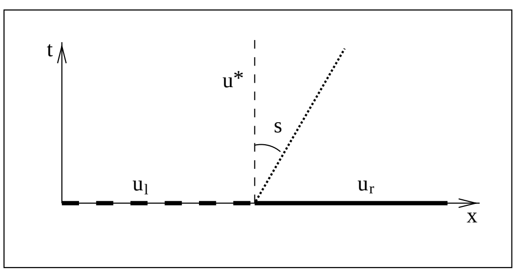
$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$

We integrate over a finite volume cell and obtain

$$(\overline{u}_i^{n+1} - \overline{u}_i^n)\,\Delta x + (\overline{\overline{f}}(u^{n*}_{i+1/2}) - \overline{\overline{f}}(u^{n*}_{i-1/2}))\,\Delta t = 0$$

with $\overline{u}(t) = \int_{x_0}^{x_1} u(x,t)dx/\Delta x$ and $\overline{\overline{f}}(x) = \int_{t_0}^{t_1} f(u(x,t))dt/\Delta t$

$\Rightarrow$ at every cell interface there is a Riemann problem: find state u^*



- approximate (linearized) Riemann solver: find an expression for numerical flux function f^* (in stead of u^*)

  e.g., $f^{n*}_{i+1/2} = \frac{f(u^n_{i+1})+f(u^n_i)}{2} - \frac{1}{2}|f'^{n*}_{i+1/2}|(u^n_{i+1} - u^n_i)$

  Lax-Friedrichs, with $f'^{n*}_{i+1/2} = f'(\dfrac{u^n_i + u^n_{i+1}}{2})$
- CFL = waves from neighbouring Riemann problems do not interfere
- FD upwind concept $\sim$ FV scheme with Riemann solver

1D finite volume schemes

$$\frac{\partial U}{\partial t} + \nabla \cdot \vec{F}(U) = 0$$

define cell average stored in cell center of cell i as $\overline{U}_i = \left(\int_{x_{i-1/2}}^{x_{i+1/2}} U(x,t)\, dx \right) / \Delta x$

time evolution equation for this average after integration in space over the *finite volume* cell with label i

$$\frac{\partial \overline{U}_i}{\partial t} + 1/\Delta x \, (F^*_{i+1/2} - F^*_{i-1/2}) = 0$$

Many numerical flux functions, including Roe and Lax-Friedrichs, can be cast in the following form

$$F^*(U_l, U_r) = \frac{F(U_l) + F(U_r)}{2} + D(U_l, U_r)$$

- second order in space: use linear reconstruction with slope limiter L

$$U_l = \overline{U}_i + 1/2\, L(\overline{U}_i - \overline{U}_{i-1}, \overline{U}_{i+1} - \overline{U}_i)$$

Conservation law in 2D

$$\frac{\partial u}{\partial t} + \frac{\partial f_x(u)}{\partial x} + \frac{\partial f_y(u)}{\partial y} = 0 \qquad \text{with } u(x,y,t)$$

or

$$\boxed{\frac{\partial u}{\partial t} + \nabla \cdot \vec{f}(u) = 0} \qquad \text{with } \vec{f}(u) = (f_x(u), f_y(u))$$

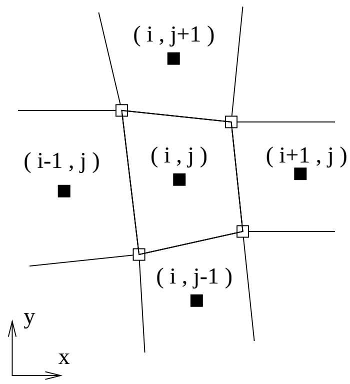
define $\overline{u}(t) = \int \int u(x,y,t) dx\, dy / \Omega_{i,j}$

and $\overline{\overline{\vec{f}}}(x,y) = \int_{t_0}^{t_1} \vec{f}(u(x,y,t)) dt / \Delta t$

$$\Rightarrow (\overline{u}(t_1) - \overline{u}(t_0))\, \Omega_{i,j} + \int \int \nabla \cdot \overline{\overline{\vec{f}}}(x,y) dx\, dy\, \Delta t = 0$$

$$\Rightarrow \boxed{(\overline{u}(t_1) - \overline{u}(t_0))\, \Omega_{i,j} + \oint \overline{\overline{\vec{f}}}(x,y) \cdot \vec{n} dl\, \Delta t = 0}$$

2D finite volume schemes



define cell averages $\overline{U}_{i,j} = \left(\int\int U(x,y,t)\, dx\, dy \right) / \Omega_{i,j}$

and obtain for the time evolution

$$\frac{\partial \overline{U}_{i,j}}{\partial t} + 1/\Omega_{i,j} \sum_{k=1}^{4} \vec{F}_k^* \cdot \vec{n}_k \, \Delta l_k = 0$$

- 3D: analogous

Numerical flux functions

- (approximate) Roe:

$$F^*(U_l, U_r) = \frac{F(U_l) + F(U_r)}{2} - |\mathsf{A}^*(U_j, U_{j+1})| \cdot \frac{U_r - U_l}{2}$$

with $\mathsf{A}^*(U_j, U_{j+1}) = \mathsf{A}(\frac{U_j + U_{j+1}}{2})$

- (local) Lax-Friedrichs:

$$F^*(U_l, U_r) = \frac{F(U_l) + F(U_r)}{2} - (|\lambda_i|_{max}) \frac{U_r - U_l}{2}$$

2.2.2 Boundary conditions

Ingoing and outgoing characteristics

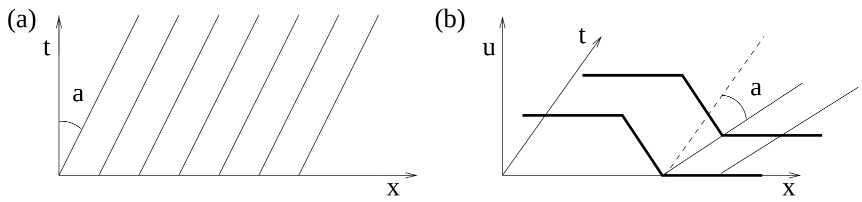
- hyperbolic system: wave perturbations propagate along characteristics

⇒ at domain boundary:

- impose wave perturbations along characteristics going into the domain as boundary conditions

- extrapolate from computational domain wave perturbations along characteristics coming out from the domain

- e.g., linear advection

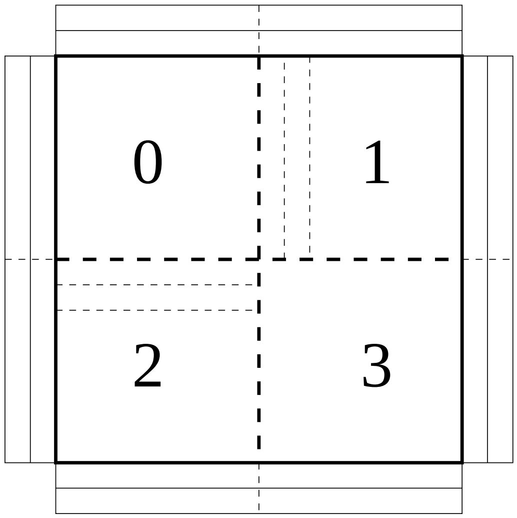


- nonlinear system: complication: nonlinear local relation between wave perturbations and conserved variables (Riemann Invariants do generally not exist)

⇒ at least take correct number of imposed and extrapolated quantities based on counting ingoing characteristics

⇒ how to decide which conservative variables to impose: trial and error, guided by physical intuition

Ghost cell approach



2.2.3 Temporal discretization

Two-stage Runge-Kutta scheme

$$\frac{\partial \overline{U}_{i,j}}{\partial t} = R^{(1),(2)}_{i,j}(\overline{U})$$

with $R^{(1),(2)}_{i,j}$ a first or second order accurate discretization of the *residual* in cell (i,j)

- first order in time:

$$\overline{U}^{t+\Delta t}_{i,j} = \overline{U}^{t}_{i,j} + R^{(1)}_{i,j}(\overline{U}^t)\,\Delta t$$

- second order in time: use two-stage Runge-Kutta:

$$\overline{U}^{*}_{i,j} = \overline{U}^{t}_{i,j} + R^{(2)}_{i,j}(\overline{U}^t)\,\Delta t/2$$

$$\overline{U}^{t+\Delta t}_{i,j} = \overline{U}^{t}_{i,j} + R^{(2)}_{i,j}(\overline{U}^*)\,\Delta t$$

- remark: LW: combine temporal and spatial discretization to achieve second order in one step (cancellation of error terms)

- time step Δt is derived from the following CFL-like time step limitation

$$\Delta t = c_{CFL} \min_{i,j} [\frac{\Omega_{i,j}}{\sum_{k=1}^{4} \max(0, (\vec{v}_{i,j} \cdot \vec{n}_k + c^f_{k,i,j}))\, \Delta l_k}]$$

conclusion

- FV Riemann ∼ FD upwind
- $\dfrac{\partial \overline{U}_{i,j}}{\partial t} + 1/\Omega_{i,j} \sum_{k=1}^{4} \vec{F}^*_k \cdot \vec{n}_k \, \Delta l_k = 0$
- good choice of numerical flux function:
  1. accurate – low diffusion (second order away from shocks)
  2. numerically stable (CFL or implicit)
  3. positive – no oscillations (at shocks)
  4. conservative – capture shocks with right speed

2.3 Example: 2D scalar problem on Cartesian grid

The problem – the solution

$$\frac{\partial u}{\partial t} + \nabla \cdot \vec{h}(u) = 0$$

$$\frac{\partial u}{\partial t} + \frac{\partial \frac{u^2}{2}}{\partial x} + \frac{\partial u}{\partial y} = 0$$

fluxes $f(u) = u^2/2$ and $g(u) = u$, $\vec{h}(u) = (f(u), g(u))$

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

$$\frac{\partial u}{\partial t} + (u, 1) \cdot (\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}) = 0$$

- domain: $(x, y) \in [0, 1] \times [0, 1]$
- initial condition: $u(x, y) \equiv 0$

- boundary conditions: impose value where $\vec{\lambda} \cdot \vec{n}$ goes into domain (locally 1D)

  choose bottom: u = 1.5 -> -0.5 linearly

$\Rightarrow$ left: impose u = 1.5 (ingoing characteristic)

$\Rightarrow$ right: impose u = -0.5 (ingoing characteristic)

$\Rightarrow$ top: u is free (outgoing characteristics)

- discretization:

$$\frac{\partial \overline{u}_{i,j}}{\partial t} + 1/\Omega_{i,j} \sum_{k=1}^{4} \vec{h}_k^* \cdot \vec{n}_k \, \Delta l_k = 0$$

choose regular Cartesian grid (Δx,Δy):

$$\frac{\partial \overline{u}_{i,j}}{\partial t} + 1/\Omega_{i,j} \left((f^*_{i+1/2,j} - f^*_{i-1/2,j}) \Delta y + (g^*_{i,j+1/2} - g^*_{i,j-1/2}) \Delta x \right) = 0$$

$$\frac{\partial \overline{u}_{i,j}}{\partial t} + \frac{f^*_{i+1/2,j} - f^*_{i-1/2,j}}{\Delta x} + \frac{g^*_{i,j+1/2} - g^*_{i,j-1/2}}{\Delta y} = 0$$

choose first order Lax Friedrichs flux function:

$$f^*{}_{i+1/2} = \frac{f(u_i) + f(u_{i+1})}{2} - \frac{1}{2} |a^*(u_i, u_{i+1})| \, (u_{i+1} - u_i)$$

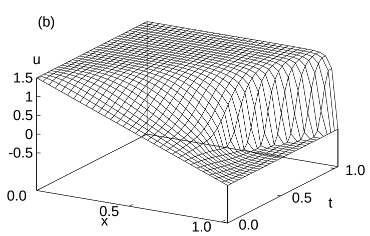
with $a^*(u_i, u_{i+1}) = a(\frac{u_i + u_{i+1}}{2})$

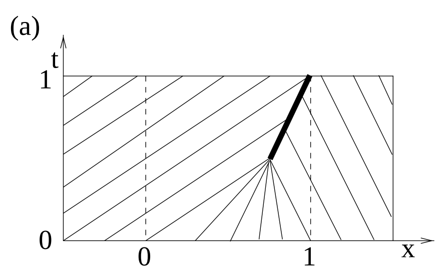
- after time evolution steady state is reached
- interpretation of steady state:

$$\frac{\partial \frac{u^2}{2}}{\partial x} + \frac{\partial u}{\partial y} = 0$$

$\Rightarrow$ this is the Burgers equation (y plays role of t), with $u_l = 1.5$ and $u_r = -0.5$

$\Rightarrow$ compressive wave steepens into shock!





A fortran90 implementation

- $u(-1 : ni + 2, -1 : nj + 2)$

  ni physical cells in i direction $(1 \ldots ni)$, nj cells in j direction

  two layers of ghost cells

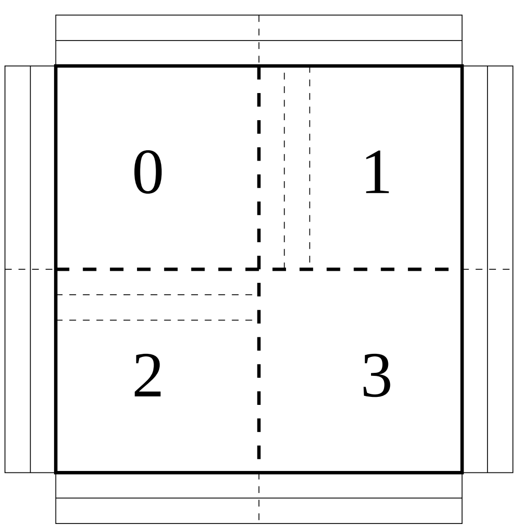
- loop

  - do boundary conditions

  - do update for new timestep

2.4 Implementation on parallel computers using MPI

Domain partitioning



MPI: Message Passing Interface

- single program, multiple processors
- MPI = library of routines (f90 or C)

⇒ commands:

- initialization and termination

call MPI_INIT(ierr)

call MPI_COMM_RANK(MPI_COMM_WORLD, myid, ierr)

call MPI_COMM_SIZE(MPI_COMM_WORLD, numprocs, ierr)

call MPI_ABORT(MPI_COMM_WORLD, 1, ierr)

call MPI_FINALIZE(ierr)

- timing

call MPI_BARRIER(MPI_COMM_WORLD,ierr)

t1=MPI_WTIME()

- broadcast information (tol0) from processor 0 to all the others: from one to all

call MPI_BCAST(tol0,1,MPI_DOUBLE_PRECISION,0,MPI_COMM_WORLD,ierr)

- reduce = from all to all with operation (sum, . . .)

call MPI_ALLREDUCE(resid,resid0,1,MPI_DOUBLE_PRECISION,MPI_SUM,
MPI_COMM_WORLD,ierr)

⇒ resid is collected from every processor, summed up, and sent to every processor in resid0

- non-blocking (do something else while waiting) send and receive

```
call MPI_ISEND(leftbufsend,2*nlj,MPI_DOUBLE_PRECISION,nbrleft,0,
  MPI_COMM_WORLD,req(1),ierr)
```

⇒ send leftbufsend of size 2*nlj to nbrleft

```
call MPI_IRECV(leftbufrec,2*nlj,MPI_DOUBLE_PRECISION,nbrleft,0,
  MPI_COMM_WORLD,req(5),ierr)
```

⇒ receive leftbufrec of size 2*nlj from nbrleft

```
call MPI_WAITALL(8,req,status_array,ierr)
```

⇒ wait until all sends and receives (info stored in status arrays) have completed

2.4.1 Parallel performance – scalability

Serial bottlenecks

- execution time
  - 1 processor:

$$T_1 = \underbrace{(1-\alpha)}_{parallel} + \underbrace{\alpha}_{serial} \qquad (=1)$$

  - n processors:

$$T_n = \frac{(1-\alpha)}{n} + \alpha$$

- parallel speedup:

$$S_n = \frac{T_1}{T_n} \qquad (\;= n \text{ ideally} \;)$$

$$\Rightarrow S_n = \frac{n}{(1-\alpha) + n\,\alpha} < \frac{1}{\alpha}$$

$$S_n = \frac{n}{(1-\alpha) + n\,\alpha} < \frac{1}{\alpha}$$

- $\alpha = 0 \;\Rightarrow S_n = n$: perfect scaling
- $S_{max} = S_\infty = \dfrac{1}{\alpha}$: speedup curve flattens

  e.g.: $\alpha = 0.1 \;\Rightarrow S_{max} = 10$

$\Rightarrow$ serial fraction α acts as bottleneck

- α is very small in our explicit algorithm (local!)
- α is large for standard implicit algorithms (global!)

  $\Rightarrow$ need to adapt algorithm to parallel execution

(Remark: S_n can become larger than n due to hardware effects (e.g. cache))

Communication overhead (for message passing)

- execution time

  - n processors:

  $$T_n = T_n^{calc} + T_n^{comm}$$

  - 1 processor:

  $$T_1 = T_n^{calc}\, n$$

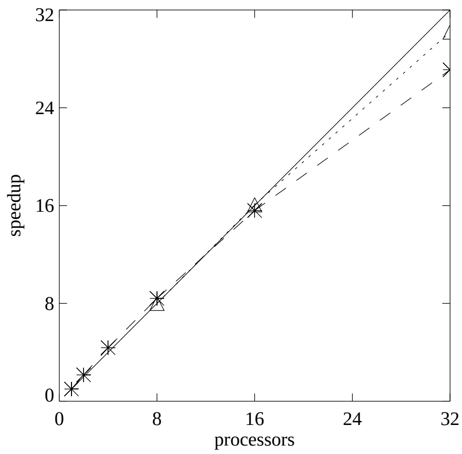
- parallel speedup:

$$S_n = \frac{T_1}{T_n} = \frac{n}{1 + \frac{T_n^{comm}}{T_n^{calc}}} = \frac{n}{1 + f_c}$$

$$f_c = \frac{T_n^{comm}}{T_n^{calc}} \sim \frac{n_x + n_y}{n_x\, n_y} \sim \frac{perimeter}{surface}$$

$\Rightarrow$ large domains (small f_c) are better, speedup curves flatten for large n

- example: 2D MHD code, Lax-Friedrichs, MPI



Speedup for the simulation of a 2D bow shock flow with a parallel MHD code on a relatively coarse grid (80×80, dashed with asterisks) and on a slightly finer grid (160×160, dotted with triangles). The theoretical speedup is given by the solid line.

2.4.2 Parallel computer architectures

- Distributed Memory (DM)
  - every processor has its own memory
  - communication over network (fast hardware or ... internet)
  - IBM SP2
  - scalable (clusters of $\sim$ 4000 Pentiums ...)
- Shared Memory (SM)
  - processors share memory
  - Alfven (sun)
  - limited number of processors, not (directly) scalable
- Hybrid (HY)
  - a cluster of SM machines

- communication over network (fast hardware or ... internet)

2.4.3 Parallellization methods

- MPI: explicit message passing
  - explicit calls to pass the messages
  - ‘hard’ for programmer
  - efficient (explicit control)
  - standard, portable, omnipresent
  - DM, but also SM, and best for HY
  - (machine-specific message passing libraries exist, slightly more efficient, but not portable (e.g. Cray SHMEM))

- HPF (High Performance Fortran): hidden message passing
  - compiler flags and directives
  - 'easier' for programmer
  - potentially much less efficient (less explicit control, 'hard' for compiler)
  - standard, portable, but not very widespread
  - DM, but also SM, HY

- application libraries: hidden message passing
  - (Petsc, Aztec, Cactus, ...)
  - higher level directives and calls, use MPI but hidden, for specific PDE applications
  - 'easier' for programmer
  - potentially less efficient, but efficient for specific problems
  - standard, portable, free
  - DM, but also SM, HY

- openMP: shared memory programming

  - compiler flags and directives

  - ‘easier’ for programmer

  - may not be very efficient (less explicit control, ‘hard’ for compiler)

  - new standard, portable, not very widespread yet

  - only SM (bad performance on DM, HY), limited number of processors

  - (machine-specific shared memory compilers exist, slightly more efficient, but not portable)

Derivation of MHD as a hyperbolic system

derivation of MHD from the Euler and Maxwell equations