Lecture Notes

Modelling with partial differential equations

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1 Traffic flow models – hyperbolic conservation laws

Aim of the lecture:
Introduction to several applied models involving differential equation: discussion of modelling, and of analytic and numerical aspects.

1.1 Modelling

Prototypical question: How long should traffic light phases be so that, during the green phase, the traffic jam in front of the traffic light dissolves?

simplifying model assumptions:

- single-track road without possibility to overtake
- no entry/exit points or junctions
- busy road: no description of individual vehicles, but instead vehicle density $\rho(x,t)$ (e.g. vehicles per km) at location $x \in \mathbb{R}$ and time $t > 0$

  Number of vehicles in interval (a,b) at time t:

  $$\int_a^b \rho(x,t)\mathrm{d}x$$

- let $v(x,t)$ be the speed of vehicles at (x,t)

  $\Rightarrow$ vehicles passing x at time t: $\rho(x,t)v(x,t) = J(x,t)$ ... flux density.

looking for: equation of motion for density ρ

Balance equation $\forall(a,b)$:

$$\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b \rho(x,t)\mathrm{d}x}_{\text{vehicles in }(a,b)} = \underbrace{\rho(a,t)v(a,t)}_{\text{inflow}} - \underbrace{\rho(b,t)v(b,t)}_{\text{outflow}} = -\int_a^b \frac{\partial(\rho v)}{\partial x}(x,t)\mathrm{d}x$$

⇒ Continuity equation

$$\rho_t + (\rho v)_x = 0, \quad x \in \mathbb{R}, t > 0 \tag{1.1}$$

with initial condition (IC): $\rho(x,0) = \rho_0(x)$, $x \in \mathbb{R}$.

looking for: (constitutive) equation for v; includes modelling information on traffic dynamics and driving behaviour

Suppose $v = v(\rho)$ with

- $v(\rho)$ monotonically decreasing (lower velocity for denser traffic)
- $v(\rho_{\max}) = 0$ (above some maximal vehicle density or below some minimum distance between vehicles, traffic stops)
- possibly: $v(0) = v_{\max}$ (maximum velocity on empty road)

1) Lighthill-Whitham-Richards (LWR) model (1955; simplest model, $v(\rho)$ linear):

$$v(\rho) = v_{\max}\left(1 - \frac{\rho}{\rho_{\max}}\right), 0 \le \rho \le \rho_{\max}$$

$$\Rightarrow \text{(1.1) becomes } \rho_t + \left[v_{\max}\rho\left(1 - \frac{\rho}{\rho_{\max}}\right)\right]_x = 0, x \in \mathbb{R}, t > 0 \tag{1.2}$$

2) Greenberg model:

$$v(\rho) = v_{\text{ref}} \ln \frac{\rho_{\max}}{\rho}, 0 < \rho \le \rho_{\max}$$

$$\Rightarrow \rho_t - v_{\text{ref}}\left(\rho \ln \frac{\rho}{\rho_{\max}}\right)_x = 0 \tag{1.3}$$

Drawback of Greenberg model: for density $\to 0$ velocity $v(\rho)$ is unbounded – this is unrealistic.

(1.2), (1.3) are *conservation laws*, as the total number of vehicles is conserved. Formal integration of (1.1) leads to:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathbb{R}} \rho(x,t)\mathrm{d}x = -\int\limits_{\mathbb{R}} \frac{\partial}{\partial x}[\rho(x,t)v(\rho(x,t))]\mathrm{d}x = 0.$$

(1.2), (1.3) are *hyperbolic equations:*

Definition 1.1. *The system of equations*

$$\begin{array}{rcl} u_t + \partial_x f(u) &=& 0, \quad x \in \mathbb{R}, t > 0 \\ u(x,0) &=& u_0(x), \quad x \in \mathbb{R} \end{array} \tag{1.4}$$

with $f : \mathbb{R}^m \to \mathbb{R}^m$ *is called* hyperbolic *if* $f'(u) \in \mathbb{R}^{m\times m}$ *is diagonalizable and has only real eigenvalues* ($\forall u \in \mathbb{R}^m$)*.*

A function $u : \mathbb{R}\times[0,\infty) \to \mathbb{R}^m$ *is called* classical solution *if* $u \in C^1(\mathbb{R}\times(0,\infty)) \cap C^0(\mathbb{R}\times[0,\infty))$ *and* (1.4) *holds pointwise.*

Simplification of the LWR model:

Transform (1.2) into non-dimensionalized form:

Let L and τ be typical length and time scales such that $L/\tau = v_{\max}$.

scaled variables:

$$x_s := \frac{x}{L} \quad , \quad t_s := \frac{t}{\tau} \quad , \quad u := 1 - \frac{2\rho}{\rho_{\max}}$$

$$\Rightarrow \partial_t \rho = \frac{1}{\tau}\partial_{t_s}\left[\frac{\rho_{\max}}{2}(1-u)\right] = -\frac{\rho_{\max}}{2\tau}\partial_{t_s} u,$$

$$\begin{aligned}\partial_x\left[v_{\max}\rho\left(1-\frac{\rho}{\rho_{\max}}\right)\right] &= \frac{1}{L}\partial_{x_s}\left[v_{\max}\underbrace{\frac{\rho_{\max}}{2}(1-u)}_{=\rho}\frac{1}{2}(1+u)\right]\\ &= -\frac{\rho_{\max}}{2\tau}\partial_{x_s}\left(\frac{u^2}{2}\right)\end{aligned}$$

$$\begin{aligned}\Rightarrow u_t + \left(\frac{u^2}{2}\right)_x &= 0, \qquad x\in\mathbb{R}, t>0\\ u(x,0) &= u_0(x), \quad x\in\mathbb{R},\end{aligned} \tag{1.5}$$

with $u_0 = 1 - 2\rho_0/\rho_{\max}$, omitting the index "$s$".

(1.5) is called *inviscid Burgers' equation.*

$$\begin{aligned}\rho = 0 \quad &\Leftrightarrow \quad u = 1; v = v_{\max} \text{ ... empty road}\\ \rho = \rho_{\max} \quad &\Leftrightarrow \quad u = -1; v = 0 \text{ ... traffic jam}\end{aligned}$$

Example 1.2.

$$u_0(x) = \begin{cases} 1, & x<0\\ 1-x, & 0\le x<1\\ 0, & x\ge 1\end{cases}$$

Method of characteristics for $u_t + uu_x = 0$:

$$\frac{\mathrm{d}t}{\mathrm{d}s} = 1, \quad \frac{\mathrm{d}x}{\mathrm{d}s} = u, \quad \frac{\mathrm{d}u}{\mathrm{d}s} = 0,$$

with $t(0) = 0, x(0) = x_0, u(0) = u_0(x_0) \Rightarrow s = t$.

$\Rightarrow u(t) = u_0(x_0)$ (const.) along the characteristic $x(t) = u_0(x_0)t + x_0$, $t \geq 0$

$\Rightarrow$ solution for $x \in \mathbb{R}$, $t < 1$:

$$u(x,t) = \begin{cases} 1, & x < t < 1 \\ \frac{1-x}{1-t}, & t \leq x < 1 \\ 0, & x \geq 1 > t \end{cases} \tag{1.6}$$

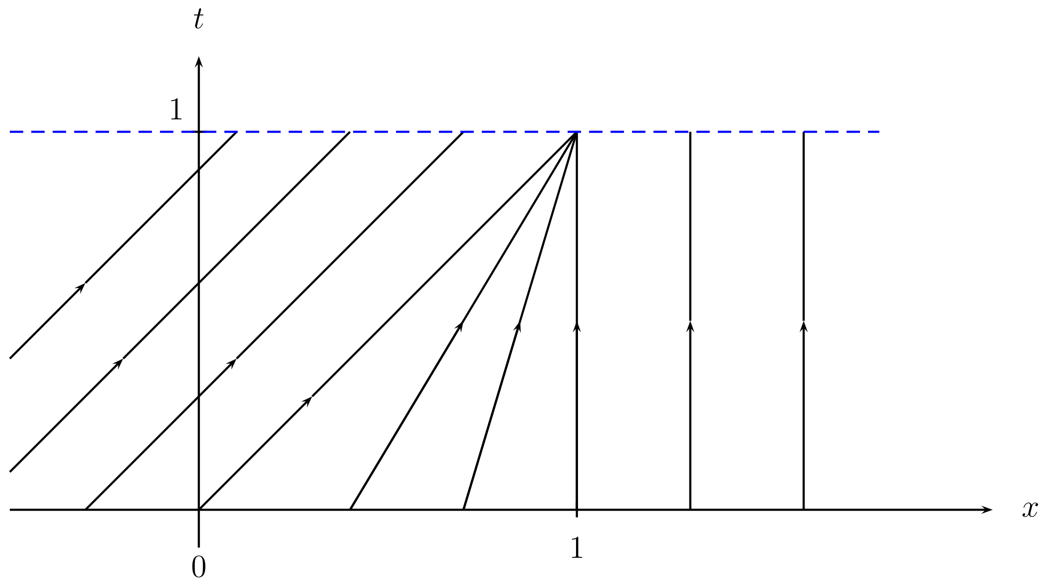


Figure 1.1: characteristics: *no* trajectories (= paths of movement) of vehicles, but propagation of density values $\rho(x,t)$

Solution for $t = 1$ is discontinuous in $x = 1$ (a *shock* is created). This is the case as well for a (slightly) smoothed IC with $u_0 \in C^1(\mathbb{R})$: a classical solution exists only for a finite time in this case. $\square$

Questions:

- $\exists$ solution for $t \geq 1$?
- Which solution concept?

References: [Jü] §1,3; [LV] §1-3.

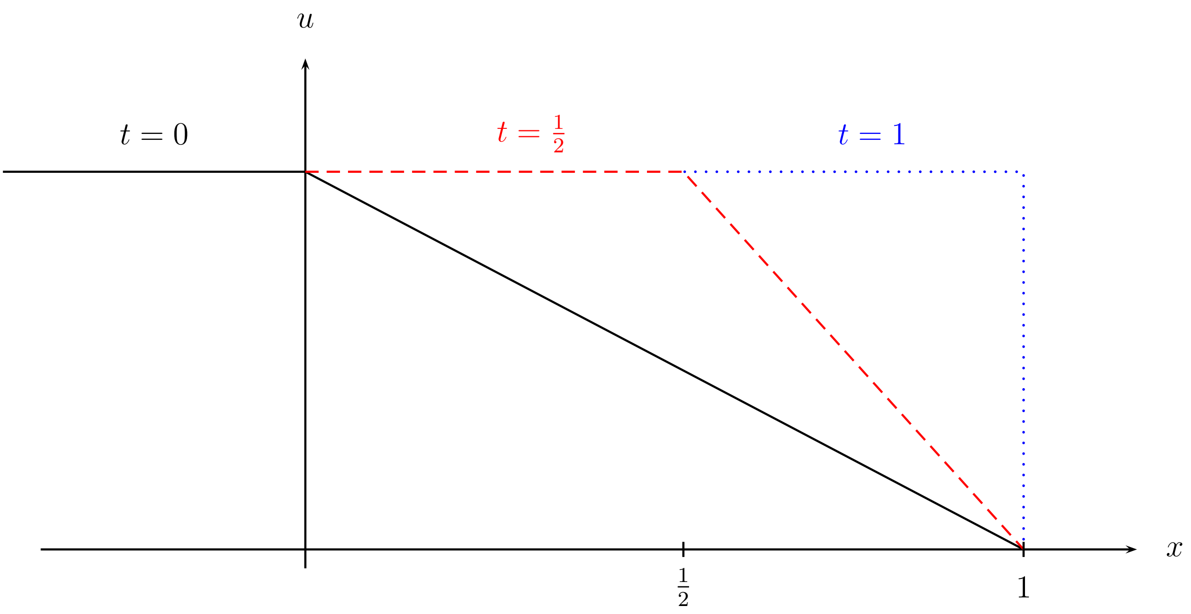


Figure 1.2: Solution (1.6)

1.2 Scalar hyperbolic conservation laws

Consider the hyperbolic conservation law

$$\begin{aligned} u_t + f(u)_x &= 0 \quad , \quad x \in \mathbb{R}, t > 0 \\ u(x,0) &= u_0(x) \quad , \quad x \in \mathbb{R} \end{aligned} \tag{1.7}$$

with $f : \mathbb{R} \to \mathbb{R}$.

We generally assume that $f''(u) > 0 \quad \forall u \in \mathbb{R}$ ("genuine nonlinearity")

<u>Motivation of a weak solution:</u> Multiply (1.7) with

$$\Phi \in C_0^1(\mathbb{R}^2) := \{\Phi \in C^1(\mathbb{R}^2) \mid \Phi \text{ has compact support }\},$$

integrate over $\mathbb{R}_x \times \mathbb{R}_t^+$:

$$\begin{aligned} 0 &= \int_0^\infty \int_{\mathbb{R}} (u_t + f(u)_x)\Phi \mathrm{d}x\mathrm{d}t \\ &= -\int_0^\infty \int_{\mathbb{R}} (u\Phi_t + f(u)\Phi_x)\mathrm{d}x\mathrm{d}t - \int_{\mathbb{R}} u(x,0)\Phi(x,0)\mathrm{d}x \end{aligned}$$

For the last two integrals only "u integrable" is needed.

Definition 1.3. *Let* $L^1_{\text{loc}} \ni u : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R}$ *with* $f(u) \in L^1_{\text{loc}}$. u *is called* weak solution *of* (1.7) *if*

$$\int_0^\infty \int_{\mathbb{R}} (u\Phi_t + f(u)\Phi_x)\mathrm{d}x\mathrm{d}t = -\int_{\mathbb{R}} u_0(x)\Phi(x,0)\mathrm{d}x \quad \forall \Phi \in C^1_0(\mathbb{R}^2). \tag{1.8}$$

Every classical solution is a weak solution; the converse is not true in general.

<u>another weak formulation:</u>

Integrate (1.7) over $(a,b) \times (s,t)$ for arbitrary $a, b \in \mathbb{R}; s, t > 0$:

$$\int_a^b u(x,t)\mathrm{d}x - \int_a^b u(x,s)\mathrm{d}x = -\int_s^t f(u(b,\tau))\mathrm{d}\tau + \int_s^t f(u(a,\tau))\mathrm{d}\tau. \tag{1.9}$$

One can show: each weak solution (as in Def. 1.3) satisfies (1.9).

Consider now conservation laws with discontinuous initial data; these appear e.g. in Ex. 1.2 at $t = 1$. Due to translation invariance of (1.7) in x and t we can assume that this discontinuity is situated in $(0,0)$.

Definition 1.4. *Equation* (1.7) *with IC*

$$u_0(x) = \begin{cases} u_l & , \quad x < 0 \\ u_r & , \quad x \geq 0 \end{cases} \tag{1.10}$$

with $u_l, u_r \in \mathbb{R}$ *is called* Riemann problem*.*

Let $u(x,t)$ be a solution of (1.7), (1.10).

$\Rightarrow u(\alpha x, \alpha t)$ also is a solution $\forall \alpha > 0$.

indicates: u depends only on $\xi = x/t$, i.e. $u = \tilde{u}(\xi)$.

Determination of $\tilde{u}(\xi)$:

$$\begin{aligned} \Rightarrow 0 = u_t + f(u)_x &= -\frac{x}{t^2}\tilde{u}'(\xi) + f'(\tilde{u}(\xi))\tilde{u}'(\xi)\frac{1}{t} \\ &= \frac{1}{t}\tilde{u}'(\xi)[f'(\tilde{u}(\xi)) - \xi] \qquad \forall \xi \end{aligned}$$

$\Rightarrow$ 3 possibilities:

- $\tilde{u}'(\xi) = 0 \quad \Rightarrow \tilde{u}(\xi) = \text{const.}$
- u is discontinuous along $\xi = x/t$, i.e., $\nexists \tilde{u}'(\xi)$.

- $f'(\tilde{u}(\xi)) = \xi \quad \Rightarrow \tilde{u}(\xi) = (f')^{-1}(\xi)$; $\exists$ inverse of f' (on $f'(\mathbb{R})$) because $f'' > 0$ on $\mathbb{R}$ (by assumption).

We consider 3 ICs corresponding to these possibilities:

Case 1, $u_l = u_r$: $u(x,t) = u_r = u_l \quad \forall x \in \mathbb{R}, t \geq 0$.

Case 2, $u_l > u_r$:

Consider Ex. 1.2 starting at $t = 1$: vehicle density for $x > 0$ greater than for $x < 0$.
$\Rightarrow$ greater (positive) speed for $x < 0$ than for $x > 0$.

$\Rightarrow$ We expect a shock curve, i.e., discontinuity of the solution at $x = \psi(t)$.

Lemma 1.5. *The function*

$$u(x,t) := \begin{cases} u_l & , \quad x < st \\ u_r & , \quad x \geq st \end{cases} \tag{1.11}$$

is a weak solution of (1.7), (1.10) *if and only if the shock speed s satisfies the* Rankine-Hugoniot (RH) condition*:*

$$s = \psi'(t) = \frac{f(u_l) - f(u_r)}{u_l - u_r}. \tag{1.12}$$

(In this case it is even the unique "entropy solution", see Theorem 1.13.)

Proof. Let $\Phi \in C_0^1(\mathbb{R}^2)$. u =const, except on $x = st$. $\Rightarrow$

$$\begin{aligned}
\int_0^\infty \int_{\mathbb{R}} u\Phi_t \mathrm{d}x\mathrm{d}t &= \int_0^\infty \left(\int_{-\infty}^{st} u\Phi_t \mathrm{d}x + \int_{st}^\infty u\Phi_t \mathrm{d}x \right) \mathrm{d}t \\
&\overset{\text{“}u_t=0\text{”}}{=} \int_0^\infty \Bigg(\partial_t \int_{-\infty}^{st} u\Phi \mathrm{d}x - su(st-0,t)\Phi(st,t) \\
&\qquad + \partial_t \int_{st}^\infty u\Phi \mathrm{d}x + su(st+0,t)\Phi(st,t) \Bigg) \mathrm{d}t \\
&= -\int_{\mathbb{R}} u(x,0)\Phi(x,0)\mathrm{d}x - s(u_l - u_r) \int_0^\infty \Phi(st,t)\mathrm{d}t.
\end{aligned}$$

$$\begin{aligned}\int_0^\infty \int_{\mathbb{R}} f(u)\Phi_x \mathrm{d}x\mathrm{d}t &\overset{\substack{\text{split,}\\ \text{int. by parts}}}{=} \int_0^\infty \Big(-\int_{-\infty}^{st} f(u)_x \Phi \mathrm{d}x + f(u(st-0,t))\Phi(st,t) \\ &\qquad - \int_{st}^{\infty} f(u)_x \Phi \mathrm{d}x - f(u(st+0,t))\Phi(st,t)\Big)\mathrm{d}t \\ &\overset{\text{“}f(u)_x=0\text{''}}{=} (f(u_l)-f(u_r)) \int_0^\infty \Phi(st,t)\mathrm{d}t.\end{aligned}$$

Hence

$$\int_0^\infty \int_{\mathbb{R}} (u\Phi_t + f(u)\Phi_x)\mathrm{d}x\mathrm{d}t = -\int_{\mathbb{R}} u_0(x)\Phi(x,0)\mathrm{d}x,$$

follows if and only if (1.12) holds. ■

Remark 1.6. Weak solutions of (1.7), (1.10) are *not* unique! Additionally to (1.11) there are more, e.g. consisting of 3 shocks (see exercises; cf. also Theorem 1.13).

Generalised Rankine-Hugoniot condition for u not piecewise continuous and s not constant:

$$s(t) = \psi'(t) = \frac{f(u_l(t)) - f(u_r(t))}{u_l(t) - u_r(t)} \tag{1.13}$$

with $u_l(t) = \lim_{x \nearrow \psi(t)} u(x,t)$, $u_r(t) = \lim_{x \searrow \psi(t)} u(x,t)$.

Example 1.7. Let $f(u) = u^2/2, u_l = 0, u_r = -1$.

$$\Rightarrow s = \frac{1}{2}\frac{u_l^2 - u_r^2}{u_l - u_r} = -\frac{1}{2}$$

Characteristics see Figure 1.3 □

Case 3, $u_l < u_r$: (1.11) is here still *one* weak solution:

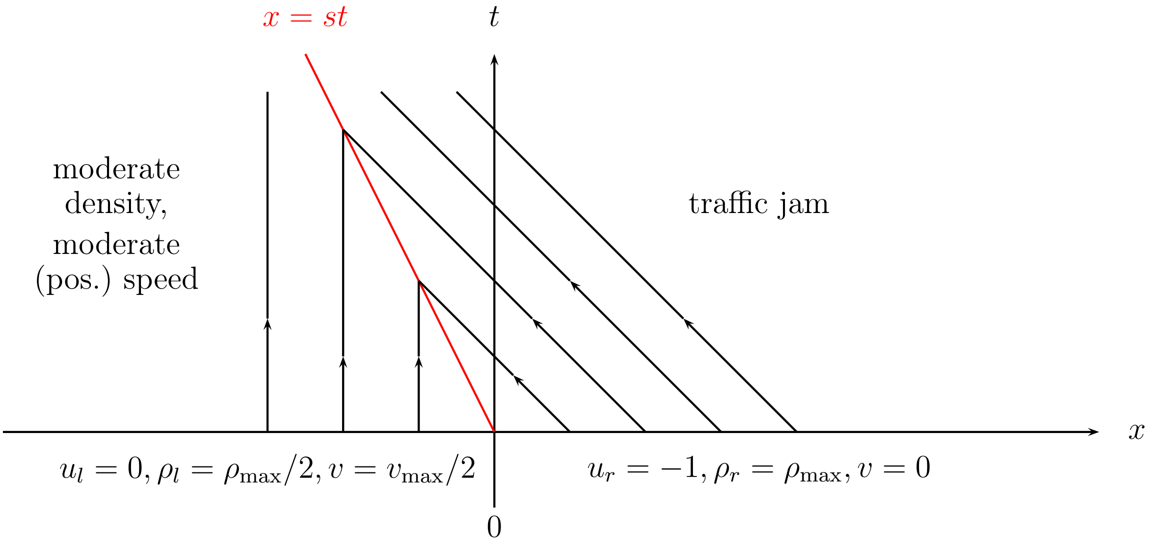
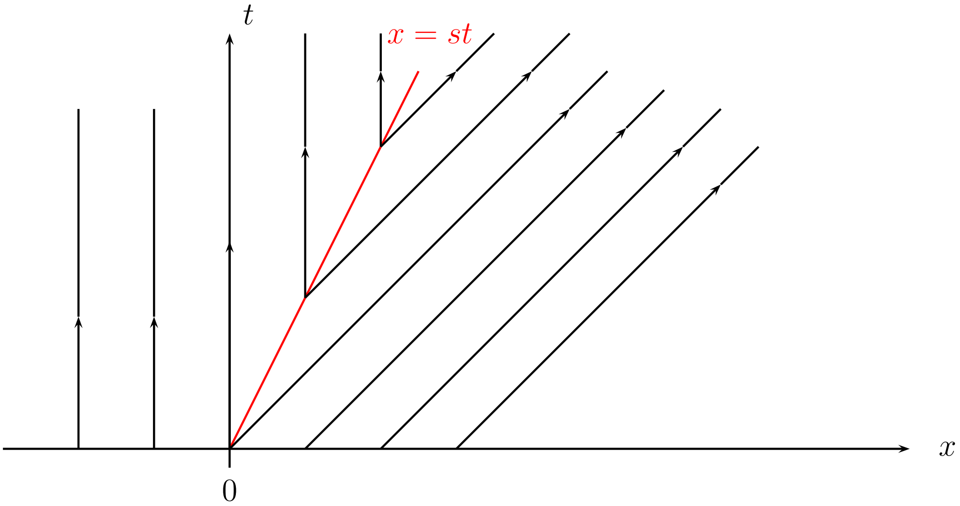


Figure 1.3: left end of traffic jam at $x = st$. Characteristics are not vehicle trajectories.

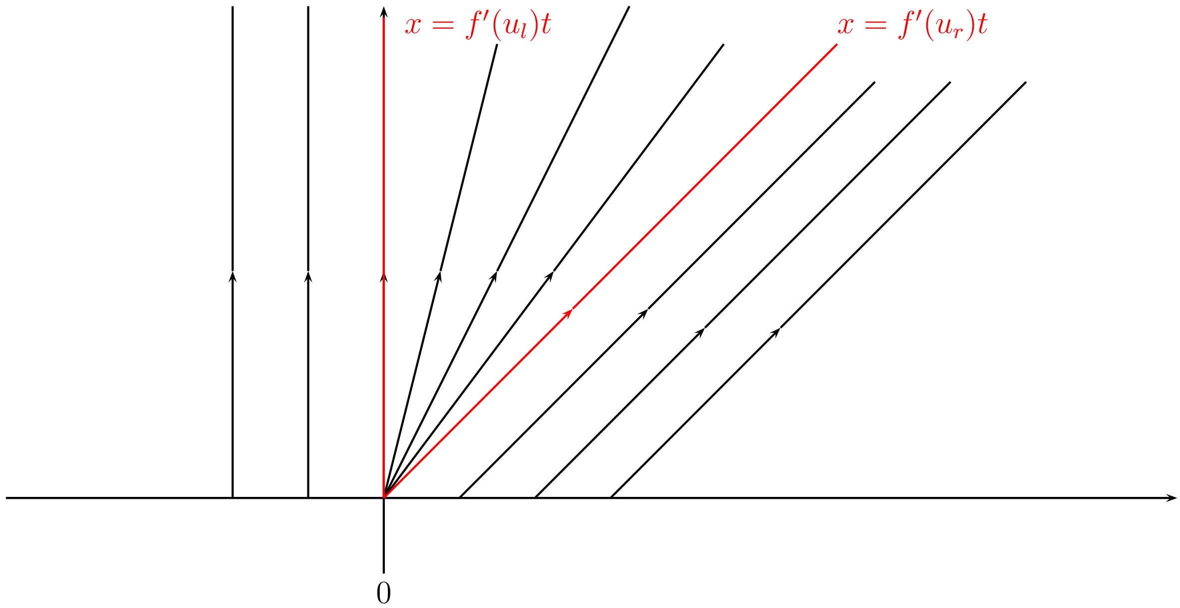


Characteristics of (1.7) for $f(u) = u^2/2, u_l = 0, u_r = 1, s = \dfrac{1}{2}$.

Solution is "instable" because characteristics begin in the shock curve. "Newly generated" information, which is not contained in u_0, is transported away from the shock.

Further weak solution of (1.7), (1.10):

$$u_2(x,t) := \begin{cases} u_l & , \quad x < f'(u_l)t \\ (f')^{-1}\left(\frac{x}{t}\right) & , \quad f'(u_l)t \le x \le f'(u_r)t \\ u_r & , \quad x > f'(u_r)t \end{cases} \tag{1.14}$$



Characteristics of *rarefaction wave* u_2 for $f(u) = u^2/2, u_l = 0, u_r = 1$, $(f')^{-1}(\xi) = \xi$: $u_2(x,t) = \frac{x}{t}$ for $0 \le x \le t$.

$\exists$ even infinitely many weak solutions!

Solution concept is so weak that uniqueness was lost.

Question: which is the "correct" or physically relevant solution?

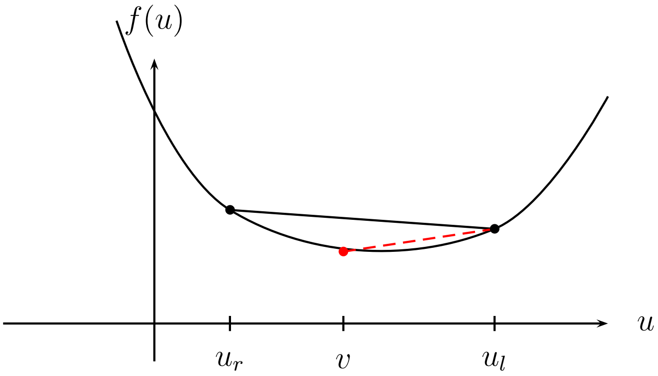
2 possibilities: first approach with entropy conditions:

Definition 1.8. *A weak solution* $u : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R}$ *of* (1.7), (1.10) *satisfies* Oleinik's entropy condition *if, along every curve of discontinuity* $x = \psi(t)$*, the following holds:*

$$\frac{f(u_l(t)) - f(v)}{u_l(t) - v} \ge \psi'(t) \ge \frac{f(u_r(t)) - f(v)}{u_r(t) - v} \tag{1.15}$$

$\forall t \in \mathbb{R}^+, \forall v$ *between* $u_l(t)$ *and* $u_r(t)$.

Rem: Solutions without discontinuities satisfy (1.15) trivially. (1.15) is also used for non-convex f.



RH-condition (1.13) implies

$$\sigma(v) := \underbrace{\frac{f(u_l) - f(v)}{u_l - v}}_{\nearrow \text{ in } v, \text{ since } f''>0} \overset{(1.15)}{\geq} \psi' = s \overset{\text{RH}}{=} \frac{f(u_l) - f(u_r)}{u_l - u_r} = \sigma(u_r) \qquad \forall v \text{ between } u_l \text{ and } u_r.$$

Due to the monotony of $\sigma(v)$, σ is maximal at $v = u_r$ if $u_l < u_r$ and minimal if $u_l > u_r$.

$$\Rightarrow u_l \geq u_r \text{ (for } f'' > 0)$$

In Case 3 ($u_l < u_r$), the shock-solution (1.11) does *not* satisfy the entropy condition. For u_2 from (1.14), the entropy condition is trivial because u_2 is continuous.

For $v \to u_{l,r}$ in (1.15): Propagation velocity of characteristics satisfies the *Lax entropy condition:*

$$f'(u_l) \geq \frac{f(u_l) - f(u_r)}{u_l - u_r} \geq f'(u_r), \quad \text{since } f'' > 0.$$

Interpretation: Characteristics have to run into the shock from the left and right sides and stop there, i.e., the "mathematical entropy", or "information", or range of $u(.,t)$ decreases with time (cf. second law of thermodynamics; physical entropy [= - mathematical entropy] increases there).

Second approach with entropy functions / viscosity solution:

Assumption: (1.7) is just an idealisation of the diffusion equation

$$u_t + f(u)_x = \varepsilon u_{xx}, \quad x \in \mathbb{R}, t > 0 \tag{1.16}$$

with (small) $\varepsilon > 0$. (1.16) has a unique smooth solution u^ε.
Convention: The limit function $u := \lim_{\varepsilon \to 0} u^\varepsilon$ shall be the physically relevant solution, *viscosity solution.*
Aim: Find a condition (only) on weak solution u such that it represents this limit.

Definition 1.9. *The pair of functions $\eta \in C^2(\mathbb{R})$ and $\psi \in C^1(\mathbb{R})$ are called* entropy *and (corresponding)* entropy flux*, if $\eta'' > 0$ and if it holds for all classical solutions u of* (1.7)*:*

$$\eta(u)_t + \psi(u)_x = 0, \quad x \in \mathbb{R}, t > 0 \tag{1.17}$$

Rem: *This implies $\psi' = f'\eta'$.*

Assumptions for the *vanishing viscosity limit* ($\forall\, T > 0$):

$$u^\varepsilon \stackrel{\varepsilon \to 0}{\longrightarrow} u \text{ pointwise a.e. in } \mathbb{R} \times (0,T),$$

$$u^\varepsilon \stackrel{\varepsilon \to 0}{\longrightarrow} u \text{ in } L^1_{loc}(\mathbb{R} \times (0,T)),$$
$$\|u^\varepsilon\|_{L^\infty(\mathbb{R}\times(0,T))} \leq \text{const.} \quad \forall 0 < \varepsilon < 1,$$
$$\|\eta'(u^\varepsilon)u^\varepsilon_x\|_{L^1(\mathbb{R}\times(0,T))} \leq \text{const.} \quad \forall 0 < \varepsilon < 1.$$

Then (without proof): u solves (1.7).

Modification of the entropy equation (1.17) for discontinuous u:
Multiply (1.16) by $\eta'(u^\varepsilon)$; choose ψ such that $\psi' = f'\eta'$:

$$\eta(u^\varepsilon)_t + \psi(u^\varepsilon)_x = \varepsilon\eta'(u^\varepsilon)u^\varepsilon_{xx} = \varepsilon(\eta'(u^\varepsilon)u^\varepsilon_x)_x - \varepsilon\eta''(u^\varepsilon)(u^\varepsilon_x)^2\,;$$

multiply by $\Phi \in C^1_0(\mathbb{R}^2), \Phi \geq 0$, integrate over $\mathbb{R} \times (0,\infty)$:

$$\int_0^\infty \int_{\mathbb{R}} [\eta(u^\varepsilon)_t + \psi(u^\varepsilon)_x]\, \Phi \mathrm{d}x\mathrm{d}t \tag{1.18}$$
$$= -\varepsilon \int_0^\infty \int_{\mathbb{R}} \eta'(u^\varepsilon)u^\varepsilon_x \Phi_x \mathrm{d}x\mathrm{d}t - \varepsilon \int_0^\infty \int_{\mathbb{R}} \underbrace{\eta''(u^\varepsilon)}_{>0}\, \underbrace{(u^\varepsilon_x)^2\Phi}_{\geq 0}\, \mathrm{d}x\mathrm{d}t$$
$$\leq \varepsilon\|\eta'(u^\varepsilon)u^\varepsilon_x\|_{L^1(\mathbb{R}\times(0,T))}\|\Phi_x\|_{L^\infty(\mathbb{R}\times(0,T))} \stackrel{\varepsilon \to 0}{\longrightarrow} 0 \qquad \text{with } T = T(\Phi)\,.$$

As $\Phi \geq 0$ is arbitrary, the limit $u := \lim u^\varepsilon$ satisfies:

$$\Rightarrow \quad \eta(u)_t + \psi(u)_x \leq 0 \qquad \text{(for smooth solutions).} \tag{1.19}$$

For weak solutions the following holds (from inequality (1.18) after integration by parts in x, t):

$$\int_0^\infty \int_{\mathbb{R}} [\eta(u)\Phi_t + \psi(u)\Phi_x]\, \mathrm{d}x\mathrm{d}t \geq -\int_{\mathbb{R}} \eta(u_0(x))\Phi(x,0)\mathrm{d}x \quad \forall \Phi \in C^1_0(\mathbb{R}^2),\ \Phi \geq 0. \tag{1.20}$$

Rem: For the (direct) limit $\varepsilon \to 0$ on the left hand side of (1.18) our assumptions are not strong enough to obtain (1.19). One should therefore take the limit in the ε–analogon of (1.20). After reversing the integration by parts one can conclude (1.19).

Definition 1.10. *Let* $u : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R}$ *be a weak solution of* (1.7). u *is called* entropy solution *if the inequality* (1.20) *holds* $\forall$ *strictly convex entropies* η *and their corresponding entropy fluxes* ψ *.*

Rem: 1) For shock waves, the entropy inequality (1.20) is equivalent to Oleinik's entropy condition (1.15) (see Th. II.1.1 in [LF]).
2) By [DeLellis-Otto-Westdieckenberg, 2003], for this equivalence *one* strictly convex η suffices in Definition 1.10.
3) The rarefaction wave u_2 is an entropy solution; it even satisfies the entropy equality (1.17) a.e. (as u_2 is continuous, $\exists$ weak derivative) resp. (1.20) with "=".
4) Entropy solutions are in general not reversible in time: a shock would become a rarefaction wave (and vice versa).

Example 1.11. Let $f(u) = \dfrac{u^2}{2}, \eta(u) = u^2 \Rightarrow \psi(u) = \dfrac{2}{3}u^3$ (as $\psi' = f'\eta'$). Let $\Phi \in C_0^1(\mathbb{R}^2), \Phi \geq 0$.

For $u_l < u_r$, the shock wave (1.11) is *no* entropy solution, as we have for (1.11) (with $s = \dfrac{u_l + u_r}{2}$):

$$
\begin{aligned}
&\int_0^\infty \int_{\mathbb{R}} \left[\underbrace{u^2}_{=\eta(u)} \Phi_t + \underbrace{\frac{2}{3}u^3}_{=\psi(u)} \Phi_x \right] \mathrm{d}x\mathrm{d}t \\
&\overset{\text{“}u_t \equiv 0\text{”}}{=} \int_0^\infty \left[\partial_t \int_{-\infty}^{st} u^2 \Phi \mathrm{d}x - s u_l^2 \Phi(st,t) + \partial_t \int_{st}^\infty u^2 \Phi \mathrm{d}x + s u_r^2 \Phi(st,t) \right. \\
&\left. + \frac{2}{3} u_l^3 \Phi(st,t) - \frac{2}{3} u_r^3 \Phi(st,t) \right] \mathrm{d}t \\
&= - \int_{\mathbb{R}} u_0(x)^2 \Phi(x,0) \mathrm{d}x - \underbrace{\frac{u_l + u_r}{2}}_{=s} (u_l^2 - u_r^2) \int_0^\infty \Phi(st,t) \mathrm{d}t \\
&+ \frac{2}{3}(u_l^3 - u_r^3) \int_0^\infty \Phi(st,t) \mathrm{d}t \\
&= - \int_{\mathbb{R}} \underbrace{u_0(x)^2}_{=\eta(u_0)} \Phi(x,0) \mathrm{d}x + \frac{1}{6}(u_l - u_r)^3 \int_0^\infty \underbrace{\Phi(st,t)}_{\geq 0} \mathrm{d}t \\
&\geq - \int_{\mathbb{R}} \eta(u_0(x)) \Phi(x,0) \mathrm{d}x \quad \Leftrightarrow \quad u_l \geq u_r. \qquad \square
\end{aligned}
$$

Conclusion: (1.11) satisfies the entropy inequality (1.20) exactly for $u_l \geq u_r$.

Similarly to the example for $u_l < u_r$ we have: Only the rarefaction wave u_2 is an entropy solution.

Summary:

Theorem 1.12. *Let $f \in C^2(\mathbb{R})$ with $f'' > 0$ on $\mathbb{R}$.*

(1) Let $u_l > u_r$:

$$\Rightarrow u(x,t) = \begin{cases} u_l & , \quad x < st \\ u_r & , \quad x > st \end{cases} \qquad \text{with} \quad s := \frac{f(u_l) - f(u_r)}{u_l - u_r}$$

is a weak entropy solution of (1.7).

(2) Let $u_l < u_r$: u_2 from (1.14) *is weak entropy solution of* (1.7).

Theorem 1.13 (Kruzkov, 1970)**.** *Let $f \in C^2(\mathbb{R}), u_0 \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$.*
$\Rightarrow \exists!$ weak entropy solution of (1.7).

Proof. difficult, [LF], [Wa]; for f uniformly convex see also §3.4.2 in [Ev]. ■

Summary for $f(u) = \dfrac{u^2}{2}$:

$$\begin{tikzcd}[column sep=huge, row sep=huge]
\boxed{u_t + uu_x = \varepsilon u_{xx}} \arrow[r, "\text{“}\varepsilon \to 0\text{”}"] \arrow[d, "\begin{array}{l}\exists!\ \text{class. solution}\\ \text{for all t>0}\end{array}"] & \boxed{u_t + uu_x = 0} \arrow[d, "\begin{array}{l}\exists!\ \text{class. solution for } t < t_0.\\ \exists\ \text{weak solutions}\\ \text{for } t \geq t_0 \text{ (satisfy RH-}\\ \text{jump conditions);}\\ \text{but they are \underline{not} unique}\\ \\ \text{+entropy condition}\\ \Rightarrow \text{unique}\\ \text{weak solution}\end{array}"] \\
\boxed{u^\varepsilon(x,t)} \arrow[r, "\varepsilon \to 0"] & \boxed{u(x,t)}
\end{tikzcd}$$

References: [Jü] §2, [LV] §3, [Ho] §5.

1.3 Traffic light problem

LWR-model for $u = 1 - \dfrac{2\rho}{\rho_{\max}}$:

$$u_t + \left(\frac{u^2}{2}\right)_x = 0 \quad , \quad x \in \mathbb{R} \tag{1.21}$$

IC:

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

$\overline{u} := 1 - 2\overline{\rho}/\rho_{\max} \in (-1, 1)$

Traffic light at $x = 0$ turns red at $t = 0$; traffic light phase has duration $\omega > 0$.

Question: Does the traffic jam dissolve during the green phase $[\omega, 2\omega)$?

Step 1: Red phase $(0 \le t \le \omega)$

Solve (1.21) on $(-\infty, 0)$ with boundary condition (BC) $u(x = 0, t) = -1 \ldots$ models red traffic light.

Solution from (1.11) for $0 < t \le \omega$:

$$u(x,t) = \begin{cases} \overline{u} & , \quad x < st \\ -1 & , \quad st < x < 0\,; \\ 1 & , \quad x > 0 \end{cases} \qquad s = \frac{u_l + u_r}{2} = \frac{\overline{u} - 1}{2} < 0$$

Step 2: Green phase $(t \ge \omega)$

Solve (1.21) on $\mathbb{R}$ with IC

$$u(x,\omega) = \begin{cases} \overline{u} & , \quad x < s\omega \\ -1 & , \quad s\omega < x < 0 \\ 1 & , \quad x > 0 \end{cases}$$

i.e. 2 Riemann problems:

a) As $\overline{u} > -1$: shock $\psi(t) = st, s = \dfrac{\overline{u} - 1}{2}$

b) As $-1 < 1$: rarefaction wave, originating in $(0, \omega)$

$\Rightarrow$ Solution for $t \ge \omega$:

$$u(x,t) = \begin{cases} \overline{u} & , \quad x < st \\ -1 & , \quad st < x < \omega - t \\ \frac{x}{t-\omega} & , \quad \omega - t \le x \le t - \omega \\ 1 & , \quad x > t - \omega \end{cases}$$

correct as long as $st < \omega - t$ or $t < t_1 := \dfrac{\omega}{s+1} = \dfrac{2\omega}{\overline{u}+1}$ ($t_1 \leq 2\omega$ as well as $t_1 > 2\omega$ possible).

Step 3: Green phase ($t > t_1$)

At $t = t_1$ shock and rarefaction wave interact.

Solve (1.21) on $\mathbb{R}$ with IC $u(x, t_1)$ and generalised RH-condition for shock starting from (st_1, t_1):

$$\begin{aligned} s(t) = \psi'(t) &= \frac{1}{2}[u(\psi(t)+0,t) + u(\psi(t)-0,t)] \\ &= \frac{1}{2}\left(\frac{\psi(t)}{t-\omega} + \overline{u}\right), \quad t > t_1; \end{aligned}$$

i.e. linear ODE for $\psi(t)$ with IC $\psi(t_1) = st_1 = \omega\dfrac{\overline{u}-1}{\overline{u}+1}$

Solution:

$$\psi(t) = \underbrace{\overline{u}(t-\omega)}_{\substack{\text{dominant} \\ \text{for } t\to\infty}} - \sqrt{t-\omega}\sqrt{\omega(1-\overline{u}^2)}, \quad t \geq t_1$$

2 cases:

a) $\underline{\overline{u} \leq 0}$ (high traffic density): $\Rightarrow\ t_1 \geq 2\omega$, only relevant for longer green phases.

   $\psi(t) \overset{t\to\infty}{\longrightarrow} -\infty \Rightarrow \exists$ shock $\forall t$.

   It moves to $-\infty$ with speed $\psi'(t) \overset{t\to\infty}{\longrightarrow} \overline{u}$;

   hence reduction of shock speed from $s = \dfrac{\overline{u}-1}{2} < 0$ to $\overline{u}$ with $|\overline{u}| \leq |s|$.

   Because $\psi'(t) = \dfrac{u_l + u_r(t)}{2} = \dfrac{\overline{u} + u_r(t)}{2} \overset{t\to\infty}{\longrightarrow} \overline{u}$: Jump distance $u_l - u_r(t) \overset{t\to\infty}{\longrightarrow} 0$

b) $\underline{\overline{u} > 0}$ (low traffic density): $\Rightarrow\ t_1 < 2\omega$

   $\psi(t) \overset{t\to\infty}{\longrightarrow} \infty$, i.e., shock curve $\psi(t)$ moves in positive x-direction.

   $\psi(t_2) = 0$ has unique solution $t_2 = \omega/\overline{u}^2$:

   Traffic jam or disturbance *behind* traffic light completely dissolved.

Traffic disturbance (behind the traffic light) dissolves during green phase $[\omega, 2\omega) \Leftrightarrow t_2 \leq 2\omega$, i.e. $\overline{u} \geq 1/\sqrt{2}$ or

$$\overline{\rho} \leq \rho_0 := \frac{\rho_{\max}}{2}\left(1 - \frac{1}{\sqrt{2}}\right) \approx 0.146\rho_{\max},$$

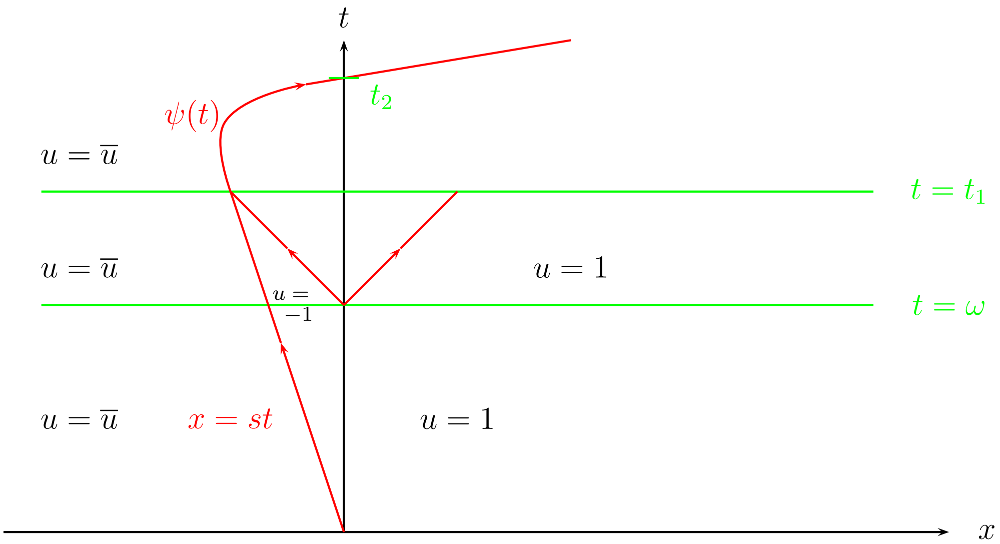


Figure 1.4: Shock curve for $\overline{u} > 0$

independently of duration of green phase!

For $\overline{\rho} > \rho_0$: traffic jam or disturbance grows with t.

Summary:

- $\overline{\rho} \geq \rho_{\max}/2$: already one red phase disturbs traffic permanently, even if afterwards traffic light stays green forever.
- $(1 - 1/\sqrt{2})\rho_{\max} - \overline{\rho} < \rho_{\max}/2$: traffic jam accumulates with time, but vanishes after traffic light stays green.
- $\overline{\rho} \leq (1 - 1/\sqrt{2})\rho_{\max}/2$: influence of red phase (behind traffic light) vanishes before end of green phase.

• current research of traffic modelling includes: stochastic models, interaction with (partially) automatic vehicles

References: [Jü] §3

1.4 Numerical methods

1.4.1 Linear advection equation

- only *finite difference methods*, almost always explicit

- for linear advection equation (with $a > 0$):

$$\begin{aligned} u_t + au_x &= 0, \quad x \in \mathbb{R}, t > 0 \\ u(x,0) &= u_0(x), \quad x \in \mathbb{R}. \end{aligned} \tag{1.22}$$

For $u_0 \in L^1_{\text{loc}}(\mathbb{R})$ the explicit weak solution is

$$u(x,t) = u_0(x - at)\,. \tag{1.23}$$

- here: uniform mesh (x_j, t_n) with

$$x_j = jh \quad (j \in \mathbb{Z}) \quad , \quad t_n = nk \quad (n \in \mathbb{N}_0), \quad h,\, k > 0.$$

Approximation $u_j^n \sim u(x_j, t_n)$

Definition 1.14 (Difference quotients)**.**

$$\begin{aligned} \mathrm{D}_x^+ v_j &= \frac{v_{j+1} - v_j}{h} && \ldots \quad \text{forward difference} \\ \mathrm{D}_x^- v_j &= \frac{v_j - v_{j-1}}{h} && \ldots \quad \text{backward difference} \\ \mathrm{D}_x^0 v_j &= \frac{v_{j+1} - v_{j-1}}{2h} && \ldots \quad \text{central difference} \\ \mathrm{D}_x^2 v_j &= \frac{v_{j+1} - 2v_j + v_{j-1}}{h^2} && \ldots \quad \text{second difference} \end{aligned}$$

We have $\mathrm{D}_x^0 v_j = \frac{1}{2}(\mathrm{D}_x^+ + \mathrm{D}_x^-)v_j$ and by Taylor's formula:

$$\mathrm{D}_x^+ v_j = v'(x_j) + O(h) \quad (\text{for } v \in C^2(\mathbb{R}))$$

$$\mathrm{D}_x^0 v_j = v'(x_j) + O(h^2) \quad (\text{for } v \in C^3(\mathbb{R})).$$

Replacing derivatives in (1.22) by corresponding difference quotients gives finite difference scheme.

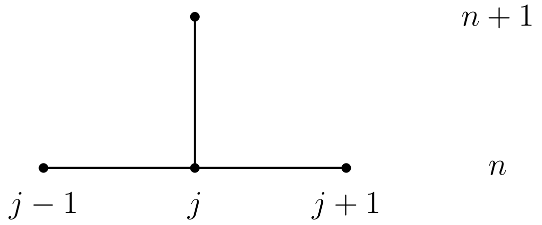
1st idea: <u>central scheme:</u>

$$\frac{u_j^{n+1} - u_j^n}{k} = -a\frac{u_{j+1}^n - u_{j-1}^n}{2h}, \quad n \geq 0, j \in \mathbb{Z};$$

or

$$u_j^{n+1} = u_j^n - \frac{ak}{2h}(u_{j+1}^n - u_{j-1}^n).$$

$\rightarrow$ *explicit* scheme with *numerical stencil*:



Disadvantage: method is unstable, i.e., develops (artificial) oscillations (→ Exercises).

2nd idea: *implicit* scheme:

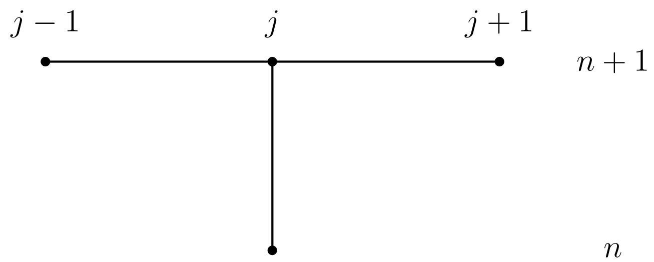
$$\frac{u_j^{n+1}-u_j^n}{k} = -a\frac{u_{j+1}^{n+1}-u_{j-1}^{n+1}}{2h}, \quad ,n \geq 0, j \in \mathbb{Z},$$

or

$$\frac{ak}{2h}u_{j+1}^{n+1} + u_j^{n+1} - \frac{ak}{2h}u_{j-1}^{n+1} = u_j^n.$$

Disadvantage: in each time step a (tridiagonal) system of linear equations needs to be solved.

Numerical stencil:



3rd idea: Lax-Friedrichs scheme:

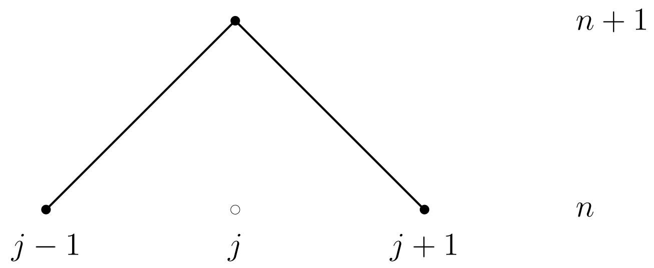
Approximation of t-derivative (first for $u(x,t)$):

$$\frac{1}{k}\left(u(x,t+k) - \frac{1}{2}[u(x+h,t)+u(x-h,t)]\right) ,$$

hence

$$u_j^{n+1} = \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right) - \frac{ak}{2h}\left(u_{j+1}^n - u_{j-1}^n\right), \quad n \geq 0, j \in \mathbb{Z} \tag{1.24}$$

Numerical stencil:



Advantage: (conditionally) stable (for $\frac{k}{h}$ small enough → Exercises)

Disadvantage: Solution is (strongly) smoothed out.

$\forall$ schemes: exact solution (1.23) does *not* satisfy difference scheme. Hence:

Definition 1.15. *Inserting the exact solution into difference scheme* $U^{n+1} = \mathcal{H}_k U^n$ *gives* local truncation error *– as residuum.*
Notation: $U^n = \{u_j^n,\ j \in \mathbb{Z}\}$*; the operator* $\mathcal{H}_k$ *is the propagator of the scheme for time step size* k*.*

Example: local truncation error for Lax-Friedrichs scheme (1.24):

$$
\begin{aligned}
L_k(x,t) &:= \frac{1}{k}\big(u(x,t+k) - \mathcal{H}_k(u(.,t);x)\big) \\
&= \frac{1}{k}\left(u(x,t+k) - \frac{1}{2}[u(x+h,t) + u(x-h,t)]\right) \\
&\quad + \frac{a}{2h}[u(x+h,t) - u(x-h,t)]\,.
\end{aligned}
$$

Leading factor $\frac{1}{k}$ is important for the right order of the scheme; the global order is one order less than the local order.

$u(x,t+k)$ is the exact solution at time $t+k$; $\mathcal{H}_k(u(.,t);x)$ is the result of one numerical step, starting with the *exact* solution at time t.

Taylor expansion in t, x around the continuously varying argument (x,t) for u smooth enough:

$$
\begin{aligned}
\Rightarrow \quad L_k(x,t) &= \frac{1}{k}\left[\left(u + u_t k + \frac{1}{2}u_{tt}k^2 + O(k^3)\right) - \frac{1}{2}\left(2u + u_{xx}h^2 + O(h^4)\right)\right] \\
&\quad + \frac{a}{2h}\left(2u_x h + O(h^3)\right) \\
&= \underbrace{u_t + a u_x}_{=0} + \frac{1}{2}\left(u_{tt}k - u_{xx}\frac{h^2}{k}\right) + O(k^2) + O\left(\frac{h^4}{k}\right) + O(h^2) \qquad (1.25)
\end{aligned}
$$

From (1.22): $\quad u_{tt} = -au_{xt} = a^2 u_{xx}$.
Let $\dfrac{k}{h}$ = const (henceforth our standard assumption).

$$\Rightarrow \quad L_k(x,t) = \frac{k}{2}\left(a^2 - \left(\frac{h}{k}\right)^2\right) u_{xx}(x,t) + O(h^2) = O(k)\,, \tag{1.26}$$

hence

$$|L_k(x,t)| \le Ck \quad \forall k < k_0$$

$\forall (x,t)$, because C is determined by $\|(u_0)_{xx}\|_{L^\infty(\mathbb{R})}$.

$\to$ "First order method (in k)"; numerical solution gets better for smaller $k > 0$.

Definition 1.16. *A method is* consistent *if* $\|L_k(.,t)\|_{L^1(\mathbb{R})} \to 0$ *for* $k \to 0$ *($\forall$ fixed $t > 0$).*

2 approaches for better match between PDE and numerical scheme:

1. (different) scheme of higher order for the given PDE (see 6. idea);
2. same scheme (1.24) but modified PDE (depending on h and k!).

From (1.26): Lax-Friedrichs is even method of second order for the *modified equation*:

$$u_t + au_x = \underbrace{-\frac{k}{2}\left(a^2 - \left(\frac{h}{k}\right)^2\right)}_{=:D} u_{xx} \quad , x \in \mathbb{R}, t > 0. \tag{1.27}$$

Here we are looking for those modified equations which, for the considered scheme, are solved better than Equation (1.22). Modified equations are not uniquely determined.

(1.27) is an advection-diffusion equation if $D \ge 0$ (for $D < 0$ it would be backwards parabolic and unstable!). Hence the following has to hold:

$$a^2 - \left(\frac{h}{k}\right)^2 \le 0 \quad \left(\Leftrightarrow \frac{|a|k}{h} \le 1 \ldots \text{ stability condition}\right).$$

Hence: (max.) numerical speed of propagation $\frac{h}{k}$ has to be $\ge$ real speed of propagation $|a|$.

For $k \to 0$ and $\frac{h}{k}$ =const, (1.27) formally converges to $u_t + au_x = 0$ (cf. *vanishing viscosity limit* in (1.16)).

The Lax-Friedrichs scheme for (1.22) hence implies *artificial diffusion* (with constant $D > 0$) and thus prevents discontinuities and oscillations.

Stability means that error propagation remains bounded (for $k \to 0$).

Definition 1.17. *For a given norm the numerical method* $\mathcal{H}_k$ *is called* stable *if* $\forall T$: $\exists C > 0$ *and* $k_0 > 0$ *such that:*

$$\|(\mathcal{H}_k)^n\| \leq C \quad \forall\, nk \leq T\,,\; 0 < k < k_0$$

e.g. for $\|\mathcal{H}_k\| \leq 1 + \alpha k \quad \Rightarrow \quad \|(\mathcal{H}_k)^n\| \leq (1+\alpha k)^n \leq e^{\alpha k n} \leq e^{\alpha T}$.

Definition 1.18. *A method is* convergent, *if* $u_j^n \overset{h,k\to 0}{\longrightarrow} u(x_j, t_n)\ \forall\, j,\, n$.

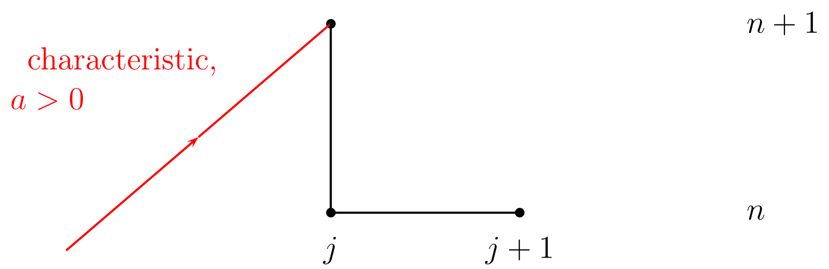
Theorem 1.19 (Lax equivalence theorem; fundamental theorem of numerical analysis)**.** *For linear consistent difference methods: stabil* $\Leftrightarrow$ *convergent.*

4th idea: Downwind scheme:

Aim: reduction of numerical diffusion (in comparison to Lax-Friedrichs schema)

$$u_j^{n+1} = u_j^n - \frac{ak}{h}\left(u_{j+1}^n - u_j^n\right) \quad \text{[for } a > 0\text{, otherwise exchange (1.28), (1.29)]} \tag{1.28}$$

Numerical stencil:



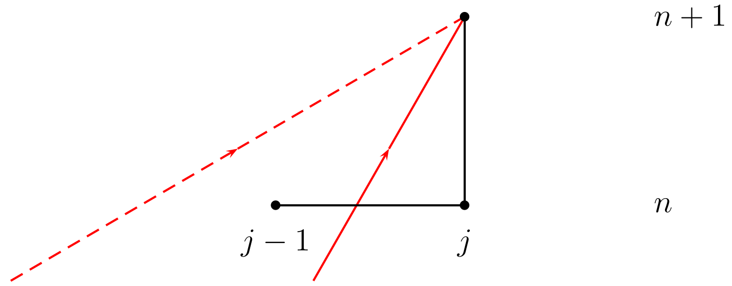
exact solution (1.23): wave travelling to the right

Disadvantage: scheme not useful (unstable), because information is transported into the wrong direction.

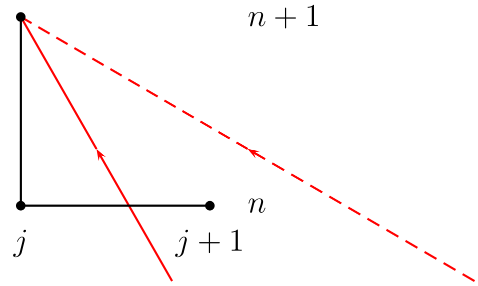
5th idea: Upwind scheme:

$$u_j^{n+1} = u_j^n - \frac{ak}{h}(u_j^n - u_{j-1}^n), \quad n \geq 0, j \in \mathbb{Z} \qquad \text{[for } a > 0\text{]} \tag{1.29}$$

Numerical stencil:



possible characteristics for 2 values of $a > 0$



possible characteristics for 2 values of $a < 0$

Advantage: no oscillations; less artificial diffusion (smaller D) than Lax-Friedrichs.

local truncation error:

$$\begin{aligned} L_k(x,t) &:= \frac{1}{k}\left(u(x,t+k) - u(x,t) + \frac{ak}{h}\left(u(x,t) - u(x-h,t)\right)\right) \\ &\overset{\text{Taylor}}{=} \frac{ak}{2}\left(a - \frac{h}{k}\right) u_{xx} + O(h^2) + O(k^2) \quad \ldots \text{1st order method (in } k) \end{aligned}$$

Modified equation of second order (with $k/h = \text{const}$):

$$u_t + a u_x = \underbrace{-\frac{ak}{2}\left(a - \frac{h}{k}\right)}_{=:D} u_{xx} \tag{1.30}$$

$$\text{(1.30) well posed} \quad \Leftrightarrow \quad D \geq 0 \quad \Leftrightarrow \quad 0 \leq \frac{ak}{h} \leq 1. \tag{1.31}$$

This is an indicator for the stability of a numerical scheme, but no proof.

(1.31) is called *Courant-Friedrichs-Levy (CFL) condition*; here it is a stability condition (cp. to the slope of characteristics in numerical stencil).
typical value in practice: $\frac{ak}{h} \approx 0.8$

6th idea: Lax-Wendroff scheme (for $a \in \mathbb{R}$):

Derivation via Taylor series:

$$u(x, t+k) = u(x,t) + k u_t(x,t) + \frac{k^2}{2} u_{tt}(x,t) + O(k^3);$$

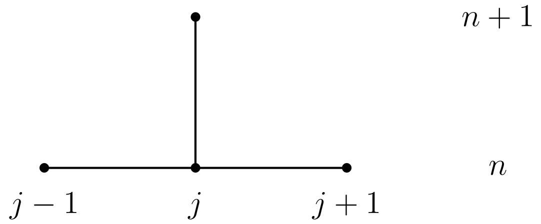
use

$$u_t = -a u_x, u_{tt} = a^2 u_{xx}$$

and central and second difference approximations for u_x, u_{xx}:

$$\Rightarrow u_j^{n+1} = u_j^n - \frac{k}{2h} a (u_{j+1}^n - u_{j-1}^n) + \frac{k^2}{2h^2} a^2 (u_{j+1}^n - 2u_j^n + u_{j-1}^n)$$

Numerical stencil:



CFL condition: $\dfrac{|a|k}{h} \leq 1$.

Lax-Wendroff is second order scheme. The modified equation of third order is

$$u_t + a u_x = \frac{h^2}{6} a \left(\frac{k^2}{h^2} a^2 - 1 \right) u_{xxx} \, . \tag{1.32}$$

which is a *dispersive equation*; no numerical diffusion.

numerical solution for discontinuous data:

$$\text{e.g. } u_0(x) = \begin{cases} 1 & , \quad x < 0 \\ 0 & , \quad x > 0 \end{cases}$$

Phenomena:

- 1st order schemes smooth the discontinuity.

- 2nd order schemes develop oscillations (cp. Gibbs phenomenon).
- All (discussed) schemes calculate the correct "shock" speed.
- Order of convergences is reduced from 1 to $\frac{1}{2}$ resp. from 2 to $\frac{2}{3}$ (consider L^1-error, *not* L^∞-error)

Referenzen: [Jü] §4, [LV] §10.

1.4.2 Nonlinear conservation laws

Consider the example: Burgers' equation or LWR-model:

$$\begin{cases} u_t + uu_x &= 0, \quad x \in \mathbb{R}, t > 0 \\ u(x,0) &= u_0(x) \end{cases} \tag{1.33}$$

1st idea: modified upwind scheme

e.g. for $u_0 \geq 0$:

$$u_j^{n+1} = u_j^n - \frac{k}{h} u_j^n (u_j^n - u_{j-1}^n), n \in \mathbb{N}_0, j \in \mathbb{Z} \tag{1.34}$$

For $u_j^0 = \begin{cases} 1 & , \quad j < 0 \\ 0 & , \quad j \geq 0 \end{cases}$ we have: $u_j^0 = u_j^1 = u_j^2 = \dots \ \forall j \in \mathbb{Z}$.

$\Rightarrow$ numerical solution converges to $u(x,t) = u_0(x)$!

But this is *not* a weak solution of (1.33) or of $u_t + \frac{1}{2}(u^2)_x = 0$!

For other Riemann problems: numerical method gives moving shock wave, but with wrong velocity!

$\Rightarrow$ method useless.

Problem: scheme (1.34) discretizes (1.33), but *not* Burgers' equation in *conservation form*: $u_t + \dfrac{1}{2}(u^2)_x = 0$. See exercise: $u_t + \frac{1}{2}(u^2)_x = 0$, $(u^2)_t + \frac{2}{3}(u^3)_x = 0$ have different weak solutions.

Definition 1.20. *(a) A difference scheme of the form*

$$u_j^{n+1} = u_j^n - \frac{k}{h}[F(u_{j-p}^n, \dots, u_{j+q}^n) - F(u_{j-1-p}^n, \dots, u_{j-1+q}^n)] \tag{1.35}$$

with a numerical flux function $F : \mathbb{R}^{p+q+1} \to \mathbb{R}$ *is called* conservative.

(b) A conservative scheme is called consistent *(with $u_t + f(u)_x = 0$), if F is locally Lipschitz continuous and $F(u, \dots, u) = f(u)\ \forall u \in \mathbb{R}$.*

simple case: $p = 0, q = 1$

$$\to u_j^{n+1} = u_j^n - \frac{k}{h}[F(u_j^n, u_{j+1}^n) - F(u_{j-1}^n, u_j^n)] \tag{1.36}$$

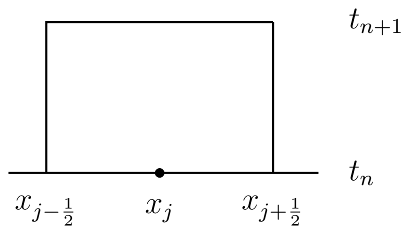
conservative scheme $\Rightarrow$ discrete conservation of mass (due to telescopic sum in j) $\Rightarrow$ correct speed of (smoothed) shocks.

Interpretation of (1.36):

weak solution of $u_t + f(u)_x = 0$ satisfies (see (1.9))

$$\begin{aligned}\frac{1}{h}\int_{x_{j-1/2}}^{x_{j+1/2}} u(x,t_{n+1})\mathrm{d}x &= \frac{1}{h}\int_{x_{j-1/2}}^{x_{j+1/2}} u(x,t_n)\mathrm{d}x \\ &\quad - \frac{k}{h}\left[\frac{1}{k}\int_{t_n}^{t_{n+1}} f(u(x_{j+1/2},t))\mathrm{d}t - \frac{1}{k}\int_{t_n}^{t_{n+1}} f(u(x_{j-1/2},t))\mathrm{d}t\right]\end{aligned} \tag{1.37}$$

with cell centers $x_{j\pm\frac{1}{2}} := (j \pm \frac{1}{2})h$.



Interpret u_j^n as approximation for cell average of $u(x,t)$:

$$u_j^n \sim \overline{u}_j^n := \frac{1}{h}\int_{x_{j-1/2}}^{x_{j+1/2}} u(x,t_n)\mathrm{d}x$$

and $F(u_j^n, u_{j+1}^n)$ as approximation of mean flow through $x_{j+1/2}$ during (t_n, t_{n+1}):

$$F(u_j^n, u_{j+1}^n) \sim \frac{1}{k}\int_{t_n}^{t_{n+1}} f(u(x_{j+\frac{1}{2}},t))\mathrm{d}t$$

$\Rightarrow$ scheme (1.36) follows from (1.37) .

Example 1.21. Upwind-scheme for Burgers' equation:

$$u_j^{n+1} = u_j^n - \frac{k}{h}\left[\frac{1}{2}(u_j^n)^2 - \frac{1}{2}(u_{j-1}^n)^2\right], \quad n \geq 0, j \in \mathbb{Z}$$

for $u_j^n \geq 0 \quad \forall n, j$.

$F(u_j, u_{j-1}) = \frac{1}{2}u_j^2$; first order scheme. $\square$

Example 1.22. Lax-Friedrichs scheme:

$$u_j^{n+1} = \frac{1}{2}(u_{j-1}^n + u_{j+1}^n) - \frac{k}{2h}(f(u_{j+1}^n) - f(u_{j-1}^n)),$$

$$F(u_j, u_{j+1}) = \frac{h}{2k}(u_j - u_{j+1}) + \frac{1}{2}(f(u_j) + f(u_{j+1})),$$

First order scheme, conservative, consistent □

Example 1.23. Lax-Wendroff scheme:

$$\begin{aligned} u_j^{n+1} = u_j^n &- \frac{k}{2h}\left(f(u_{j+1}^n) - f(u_{j-1}^n)\right) \\ &+ \frac{k^2}{2h^2}\left[f'(u_{j+1/2}^n)(f(u_{j+1}^n) - f(u_j^n)) - f'(u_{j-1/2}^n)(f(u_j^n) - f(u_{j-1}^n))\right] \end{aligned}$$

with $u_{j\pm\frac{1}{2}}^n := (u_j^n + u_{j\pm1}^n)/2$.

Scheme conservative, consistent, second order. □

Convergence:

vague idea: numerical solution from Examples 1.21-1.23 converges to a weak solution of $u_t + f(u)_x = 0$ (for $h, k \to 0$).

Problem: weak solution is not unique in general!

Definition 1.24. Total variation *of a function* $v : \mathbb{R} \to \mathbb{R}$*:*

$$\mathrm{TV}(v) := \sup \sum_{j=1}^{N} |v(\xi_j) - v(\xi_{j-1})|,$$

Supremum over all subdivisions $-\infty = \xi_0 < \xi_1 < \ldots < \xi_N = \infty$ *of* $\mathbb{R}$.

For $v \in C^1(\mathbb{R}) : \mathrm{TV}(v) = \int\limits_{\mathbb{R}} |v'(x)|\mathrm{d}x$

Necessary for $\mathrm{TV}(v) < \infty : \exists \lim_{x\to\pm\infty} v(x)$.

Theorem 1.25 (Lax-Wendroff)**.** *Let* $\{u_l(x,t),\ l \in \mathbb{N}\}$ *be a sequence of numerical solutions, calulated via a consistent and conservative method on a mesh sequence with* $h_l, k_l \xrightarrow{l\to\infty} 0$ *. (u_l is e.g. a constant extension of u_j^n on the cells.)*

Suppose there is a function $u(x,t)$ such that:

(1) $u_l \xrightarrow{l\to\infty} u$ *in* $L^1(\Omega) \quad \forall \Omega = (a,b) \times (0,T)$,

(2) $\forall T > 0 : \exists R > 0$ *with*

$$\mathrm{TV}(u_l(.,t)) < R \quad \forall 0 \le t \le T, \quad \forall l \in \mathbb{N}.$$

$\Rightarrow u(x,t)$ *is weak solution of* $u_t + f(u)_x = 0$

Proof. [LV] §12. ■

Remark 1.26. Theorem 1.25 does *not* imply the convergence of the numerical approximation sequence u_l; is also does *not* imply that u is the entropy solution.

Theorem 1.27. *Additionally to the assumptions of Theorem 1.25 suppose:* $(\eta,\psi) \in C^2(\mathbb{R}) \times C^1(\mathbb{R})$ *with* $\eta'' > 0$ *is* one *entropy / entropy flux pair (see Def. 1.9). Let* $\Psi : \mathbb{R}^{p+q+1} \to \mathbb{R}$ *be a numerical entropy flux function, consistent with* ψ *(i.e.,* $\Psi(u,\dots,u) = \psi(u)\ \forall u \in \mathbb{R}$*) and*

$$\eta(u_j^{n+1}) \le \eta(u_j^n) - \frac{k}{h}\left[\Psi(u_{j-p}^n,\dots,u_{j+q}^n) - \Psi(u_{j-1-p}^n,\dots,u_{j-1+q}^n)\right] \quad \forall j,n \tag{1.38}$$

$\Rightarrow u(x,t)$ *(from Theorem 1.25) satisfies the (weak) entropy inequality* (1.20)*:*

$$\int_0^\infty \int_{\mathbb{R}} \left[\eta(u)\Phi_t + \psi(u)\Phi_x\right] \mathrm{d}x\mathrm{d}t \ge -\int_{\mathbb{R}} \eta(u_0(x))\Phi(x,0)\mathrm{d}x \quad \forall \Phi \in C_0^1(\mathbb{R}^2),\ \Phi \ge 0. \tag{1.39}$$

Hence, u *is also entropy solution.*

Proof. [LV] §12. ■

Remark 1.28.

1. Compare (1.38) with entropy inequality (1.19):

   $$\eta(u)_t + \psi(u)_x \le 0.$$

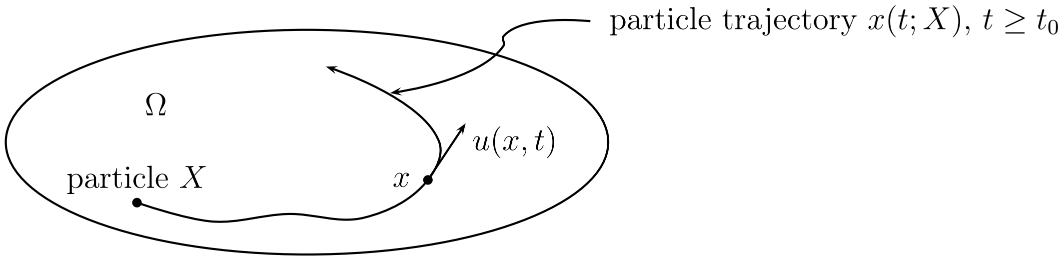
2. By [DeLellis-Otto-Westdieckenberg, 2003], already one strictly convex η is enough for entropy solutions in Def. 1.10.
3. Condition (1.38) holds e.g. for the *Godunov scheme*, a special version of the upwind method (details in [LV] §13, [Jü] §5).

<u>References</u>: [Jü] §4, [LV] §12.

2 Fluid mechanics

2.1 Euler equations

Consider the flow of a fluid (=liquid or gas) in the domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$.



$\rho(x,t) \geq 0 \ldots$ mass density

$u(x,t) \ldots$ velocity (vector) field

$p(x,t) \ldots$ pressure

- here: description by *Euler coordinates*, i.e., x is a fixed point of space, through which different material points of the fluid flow.
- alternative description by *Lagrange coordinates* (mostly in §3): $X \in \Omega$ is a fluid material point (or particle), $t \mapsto x(t;X)$ with $x(t_0;X) = X$ its movement or trajectory.

Aim: derivation of the 3 Euler equations:

(a) conservation of mass:

consider (arbitrary) temporally fixed region $R \subset \Omega$ with smooth boundary ∂R and outer normal vector ν:

Balance equation:

$$\underbrace{\frac{\mathrm{d}}{\mathrm{d}t} \int\limits_R \rho(x,t)\mathrm{d}x}_{\text{total mass in } R} = \underbrace{-\int\limits_{\partial R} \rho u \cdot \nu \mathrm{d}S}_{\substack{\text{mass flow through} \\ \text{surface } \partial R}}$$

$$\text{divergence theorem} \quad \Rightarrow \quad \int_R \rho_t + \operatorname{div}(\rho u) \mathrm{d}x = 0 \quad \forall R \subset \Omega$$

$$\Rightarrow \quad \boxed{\rho_t + \operatorname{div}(\rho u) = 0, x \in \Omega} \quad \ldots \textit{ continuity equation} \tag{2.1}$$

<u>(b) conservation of momentum:</u>

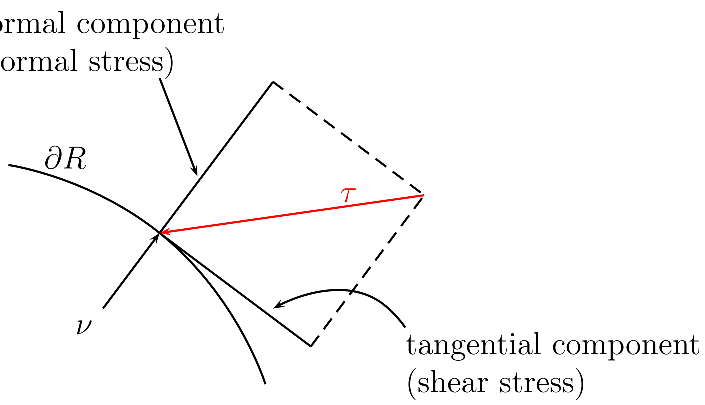
from Newton's second law: <u>mass × acceleration = force</u>,

hence change of momentum is due to external/volume forces and surface forces

$R \subset \Omega \ldots$ arbitrary (fixed) domain

momentum of mass in R: $\int_R \rho u \mathrm{d}x$

- external/volume forces: $\int_R \underbrace{\rho f}_{\substack{\text{force density,}\\ \text{given vector field } f}} \mathrm{d}x$ (e.g. gravitation, electromagnetic)
- surface forces on ∂R with outer normal ν: *stress vector* $\tau = \tau(x, t, \nu)$



One can show:

1. $\tau(x, -\nu) = -\tau(x, \nu) \ \ldots$ local equilibrium of stress (from Newton's 3rd law)
2. τ depends linearly on ν, so $\tau(x, \nu) = T(x) \cdot \nu$;

   matrix $T \ \ldots$ stress tensor (from conservation of momentum)
3. $T = T^\top$, rotation invariance (from conservation of angular momentum)

total surface force:

$$\int_{\partial R} \tau(x,t,\nu)\mathrm{d}S = \int_{\partial R} T(x,t)\cdot\nu\mathrm{d}S \overset{\text{div. theorem}}{=} \int_R \operatorname{div} T\mathrm{d}x = \int_R \nabla\cdot T\mathrm{d}x$$

$\Rightarrow$ force density on fluid: $\rho f + \nabla\cdot T$

Let $X \in \Omega$ be a particle; $x(t;X) = (x_1(t), x_2(t), x_3(t))$ its trajectory.

Speed of particle X: $\dot{x}(t) = u(x(t),t)$ [The label X shall be skipped in the sequel.]

Acceleration of particle X:

$$\begin{aligned} a(t) = \ddot{x}(t) &= \frac{\mathrm{d}}{\mathrm{d}t}u(x(t),t) \\ &= u_{x_1}\underbrace{\dot{x_1}}_{=u_1} + u_{x_2}\underbrace{\dot{x_2}}_{=u_2} + u_{x_3}\underbrace{\dot{x_3}}_{=u_3} + u_t = u_t + \underbrace{(u\cdot\nabla)}_{\substack{\text{scalar}\\ \text{diff. operator}}} u = \frac{\mathrm{D}u}{\mathrm{D}t}, \end{aligned}$$

with material derivative $\dfrac{\mathrm{D}}{\mathrm{D}t} := \partial_t + u\cdot\nabla$

It describes the temporal rate of change of an x- and t-dependent physical quantity (e.g. temperature) in a volume element which is transported in a flow field with speed u. It hence describes the rate of change in the reference frame which moves with the flow.

<u>Ex.:</u> Let the temperature distribution (in 1D) change only because it is transported by the flow, i.e., $\tilde{T}(x,t) = \tilde{T}_0(x-ut) \Rightarrow \frac{\mathrm{D}\tilde{T}}{\mathrm{D}t} = 0$.

Newton's second law $\Rightarrow$ balance equation for densities:

$$\rho\frac{\mathrm{D}}{\mathrm{D}t}u = \rho f + \nabla\cdot T$$

add $u\rho_t + u\operatorname{div}(\rho u) = 0$

$$\Rightarrow \partial_t(\underbrace{\rho u}_{\substack{\text{momentum}\\ \text{density}}}) + \underbrace{u\operatorname{div}(\rho u) + \rho(u\cdot\nabla)u}_{=\nabla\cdot(\rho u\otimes u)\ldots\nabla \text{ from momentum flux density}} = \rho f + \nabla\cdot T$$

$$\Rightarrow \boxed{\partial_t(\rho u) + \nabla\cdot(\rho u\otimes u - T) = \rho f} \quad \ldots \text{ momentum balance equation} \tag{2.2}$$

Special case: inviscid fluid $\to$ no shear stress

$\tau(x,\nu) = -p(x)\nu$, $p \ldots$ pressures $\Rightarrow T = -p(x)I, \nabla\cdot T = -\nabla p$

$$\Rightarrow \partial_t(\rho u) + \nabla\cdot(\rho u\otimes u) + \nabla p = \rho f \tag{2.3}$$

Rem.: no tangential forces $\Rightarrow$ rotation cannot be started/stopped.

(c) conservation of energy

Balance: change of energy = $\underbrace{\text{power}}_{\text{force}\,\cdot\,\text{velocity.}}$ − heat loss

Energy density: $\rho\Big(\underbrace{\frac{|u|^2}{2}}_{\text{kin. energy}} + \underbrace{e}_{\text{internal energy}}\Big)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_R \rho\left(\frac{|u|^2}{2}+e\right)\mathrm{d}x = \underbrace{-\int\limits_{\partial R}\rho\left(\frac{|u|^2}{2}+e\right)u\cdot\nu\,\mathrm{d}S}_{\text{energy flux through }\partial R}$$
$$+\int\limits_R \rho \underbrace{f\cdot u}_{\substack{\text{power}\\ \text{due to}\\ \text{volume forces}}} dx + \int\limits_{\partial R}\Big(\underbrace{\tau\cdot u}_{\substack{\text{power}\\ \text{due to}\\ \text{surface forces}}} - \underbrace{h}_{\substack{\text{heat flux}\\ \text{through }\partial R}}\Big)\mathrm{d}S \quad \forall R\subset\Omega$$

$$\int\limits_{\partial R}(\tau\cdot u-h)\,\mathrm{d}S = \int\limits_{\partial R}\nu\cdot(T\cdot u-q)\,\mathrm{d}S;$$

with $h(x,t)=\nu\cdot q(x,t)$; q ... heat flux density (=vector)

Divergence theorem $\Rightarrow$ energy balance equation:

$$\boxed{\frac{\partial}{\partial t}\left[\rho\left(\frac{|u|^2}{2}+e\right)\right]+\operatorname{div}\left[\rho u\left(\frac{|u|^2}{2}+e\right)+q-T\cdot u\right]=\rho f\cdot u} \tag{2.4}$$

(2.1), (2.2), (2.4) ... general balance equations; so far these do not incorporate physics resp. material properties, but they are the starting point for *Euler* (with $T=-pI$) and *Navier-Stokes equations* (in §2.2). In total we will examine 2×2 models: inviscid / viscous $\times$ (in)compressible.

Special cases:

a) Fourier's law of thermal conduction: $q=-\kappa\nabla\tilde{T}$, κ ... thermal conductivity, $\tilde{T}$ ... temperature

b) inviscid fluid: $T=-pI \Rightarrow \operatorname{div}(T\cdot u)=-\operatorname{div}(pu)$

c) inviscid ideal gas:

$$T=-pI, p=\rho R\tilde{T}, \quad R \ldots \text{gas constant}$$

frequently: $e=c_V\tilde{T}+\text{const}$ (for polytropic gases), c_V ... specific heat with constant volume

d) inviscid ideal fluid with $f = 0, q = 0$:

compressible Euler equations (for inviscid ideal fluid):

$$\begin{cases} \rho_t + \operatorname{div}(\rho u) = 0 \\ \partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla p = 0 \\ \partial_t \left[\rho\left(\frac{|u|^2}{2} + e\right)\right] + \operatorname{div}\left[\rho u \left(\frac{|u|^2}{2} + e\right) + pu\right] = 0 \end{cases}$$

This is a hyperbolic conservation law: 5 equations for 6 variables (ρ, u, p, e). One needs one additional (physical) constitutive equation, e.g. $e = c_V \tilde{T} + \text{const}, p = \rho R \tilde{T}$.

e) inviscid incompressible fluid with $f = 0, q = 0$:

Flow $u(x,t)$ is *incompressible* if $\forall$ domains $R(t) \subset \Omega$, which move with the flow, the following holds:

$$\text{vol }(R(t)) = \int_{R(t)} \mathrm{d}x = \text{const in } t.$$

This holds if and only if $\operatorname{div} u = 0$, because:

$$0 = \frac{d}{dt}\text{vol }(R(t)) = \frac{d}{dt}\int_{R(t)} \mathrm{d}x \overset{(*)}{=} \int_{\partial R(t)} u(x,t)\cdot \nu \mathrm{d}S = \int_{R(t)} \operatorname{div} u \mathrm{d}x$$

1D-illustration of (*): $\frac{d}{dt}\int_{a(t)}^{b(t)} \mathrm{d}x = \dot{b}(t) - \dot{a}(t) = u(b(t)) - u(a(t))$
(detailed proof of (*): [CM] §1.1).

Incompressibility of good approximation for "small speeds" (e.g. mach number $Ma := |u|/c < 0.3$, with c ... speed of sound).

Additionally suppose $\frac{\mathrm{D}e}{\mathrm{D}t} = 0$ (e.g. $e = \text{const}$):

incompressible Euler equations:

$$\begin{cases} \rho_t + \operatorname{div}(\rho u) = 0 \\ \partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla p = 0 \\ \operatorname{div} u = 0 \end{cases}$$

5 equations for 5 variables

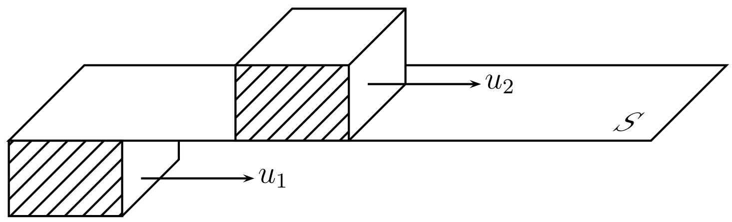
energy equation is satiesfied "automatically" ($\to$ Exercises).

References: [CM] §1.1

2.2 Navier-Stokes equations

Aim: Derivation of NS equations

Shear stress in fluid (=gas or liquid) depends only on local changes of velocity $u(x)$, i.e., on $\frac{\partial u}{\partial x} = \left(\frac{\partial u_i}{\partial x_j}\right)_{i,j=1,2,3}$



Fluid at rest (i.e. $u = 0$) or in homogeneous movement (i.e. $u = \text{const}$): no shear stress, τ has only normal component:

$$\tau(x, \nu) = -p(x)\nu, \quad p \ldots \textit{ pressure}, \quad \Rightarrow \quad T = -p(x)I$$

in general: $T = \underbrace{-pI}_{\text{normal stress}} + \sigma$

Matrix $\sigma = (\sigma_{ij})_{i,j=1,2,3} \ldots$ viscous stress tensor (shear forces due to friction, viscosity)

Assumptions on σ — as function of $\frac{\partial u}{\partial x}$:

1. $\sigma\left(\frac{\partial u}{\partial x}\right)$ is linear, i.e. *Newtonian fluid* (Ex.: water, oil):

   $$\sigma_{ij}(x) = \sum_{k,l=1}^{3} C_{ijkl} \frac{\partial u_k}{\partial x_l}(x) \quad (3^4 = 81 \text{ coefficients})$$

   non-Newtonian examples: ketchup, shampoo, blood, starch suspension (non-constant viscosity).

2. fluid is isotropic, i.e., $\nexists$ distinguished direction

   $\Rightarrow \sigma$ is invariant under (rigid body) rotations, i.e.

   $$\sigma\left(U \cdot \frac{\partial u}{\partial x} \cdot U^{-1}\right) = U \cdot \sigma\left(\frac{\partial u}{\partial x}\right) \cdot U^{-1} \quad \forall \text{ orthogonal matrices } U \tag{2.5}$$

   Fluid crystals are an example of anisotropic fluids.

3. σ is symmetric (follows from conservation of angular momentum)

From (2.) we deduce:

$$\sigma = \sigma(D) \quad \text{with} \quad D := \frac{1}{2}\left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial x}^{\top}\right) \quad \ldots \textit{ deformation tensor (or strain tensor)}$$

Proof. $\sigma = 0$ for rotations with constant angular velocity; e.g. rotation around x_3-axis: $\tilde{u} = \omega(-x_2, x_1, 0)^{\top}$, $\frac{\partial \tilde{u}}{\partial x} = \omega \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

$$\sigma(\frac{\partial \tilde{u}}{\partial x}) = 0 \Rightarrow C_{ij21} = C_{ij12} \quad ; \quad i, j = 1, 2, 3$$

analogously for x_1-, x_2-axis: $C_{ij23} = C_{ij32}, C_{ij13} = C_{ij31}$.

$$\begin{aligned}\Rightarrow \sigma_{ij} = {} & C_{ij11}(u_1)_{x_1} + C_{ij22}(u_2)_{x_2} + C_{ij33}(u_3)_{x_3} \\ & + C_{ij12}((u_1)_{x_2} + (u_2)_{x_1}) + C_{ij13}((u_1)_{x_3} + (u_3)_{x_1}) \\ & + C_{ij23}((u_2)_{x_3} + (u_3)_{x_2}),\end{aligned}$$

hence $\sigma = \sigma(D)$. ∎

• $\sigma = \sigma^T$ is a linear, isotropic (i.e. satisfying (2.5)) function of D. One can show that σ, D commute[1] (cf. theorem of Rivlin-Ericksen, [EGK] §5.9).

$\Leftrightarrow \sigma, D$ simultaneously diagonalisable

$\Rightarrow \sigma_i$ (=eigenvalues of σ) are linear functions of d_i (=eigenvalues of D)

Due to rotation invariance (2.): σ_i is symmetric function with respect to index permutations

$$\Rightarrow \sigma_i = \lambda(\underbrace{d_1 + d_2 + d_3}_{=\operatorname{Sp} D = \operatorname{div} u}) + 2\mu d_i \quad ; \quad i = 1, 2, 3.$$

Transforming back to basis of σ, D:

$$\Rightarrow \boxed{\sigma = \lambda(\operatorname{div} u)I + 2\mu D} \tag{2.6}$$

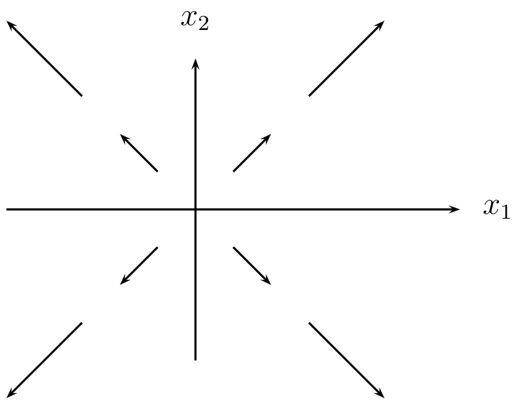
Only 2 coefficients left; interpretation of λ, μ:

Example 2.1. isotropic expansion: $u = cx, c > 0$

$$\operatorname{div} u = 3c, D = cI$$

stress tensor:

$$T = -pI + \sigma = -pI + \lambda(\operatorname{div} u)I + 2\mu D = -(\underbrace{p - (3\lambda + 2\mu)c}_{\text{effective pressure}})I$$



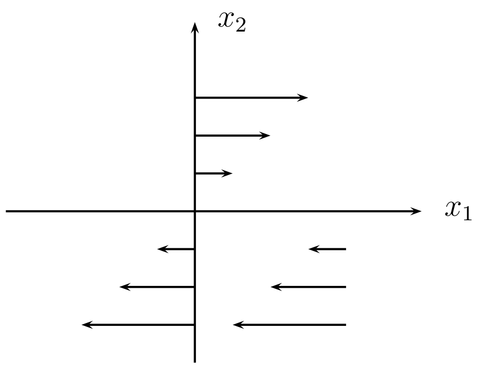
$\mu_d := \lambda + \frac{2}{3}\mu \geq 0$ ... *pressure viscosity* resp. *2nd viscosity coefficient*

$\rightarrow$ effective pressure is lower than thermodynamic pressure. $\square$

Example 2.2. Shear flow $u = (\kappa x_2, 0, 0)^\top, \kappa = \text{const}, \ p = 0$

$$\Rightarrow \operatorname{div} u = 0, D = \frac{1}{2}\begin{pmatrix} 0 & \kappa & 0 \\ \kappa & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\Rightarrow T = \lambda(\operatorname{div} u)I + 2\mu D = \mu\kappa\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



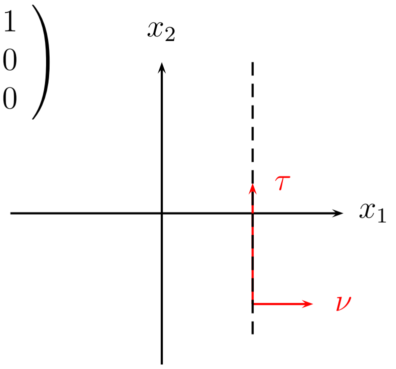
Stress vector $\tau = T \cdot \nu = \mu\kappa(\nu_2, \nu_1, 0)^\top$

τ is pure shear force.

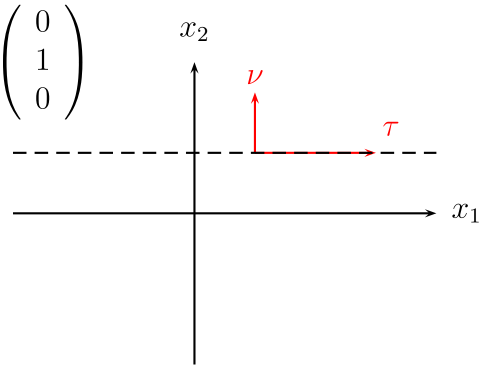
$\mu \geq 0$ ... *shear viscosity, 1st viscosity coefficient* $\square$

[1]M.E. Gurtin, A short proof of the representation theorem for isotropic, linear stress-strain relations; J. of Elasticity 4, 1974

$\nu = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$



$\nu = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$



$$\Rightarrow \sigma = \underbrace{\mu_d(\operatorname{div} u)I}_{\text{normal component of stress}} + \underbrace{2\mu\left(D - \frac{1}{3}(\operatorname{div} u)I\right)}_{\text{tangential component of stress}}$$

$\operatorname{Sp}(D - \frac{1}{3}(\operatorname{div} u)I) = \operatorname{div} u - \frac{1}{3}\operatorname{div} u \cdot 3 = 0$

Inserting $T = -pI + \sigma$ in balance equation of momentum (2.2):

$$\nabla \cdot T = -\nabla p + \nabla(\lambda \operatorname{div} u) + 2\nabla \cdot (\mu D)$$

$\Rightarrow$ compressible Navier-Stokes equations:

$$\begin{cases} \rho_t + \operatorname{div}(\rho u) = 0 \\ \partial_t(\rho u) + \nabla \cdot (\rho u \otimes u - 2\mu D) + \nabla(p - \lambda \operatorname{div} u) = \rho f \\ \partial_t \left[\rho\left(\frac{|u|^2}{2} + e\right)\right] + \operatorname{div}\left[\rho u\left(\frac{|u|^2}{2} + e\right) + q - T \cdot u\right] = \rho f \cdot u \end{cases}$$

5 equations for 9 variables (ρ, p, u, e, q)

special cases:

a) $\lambda = \mu = 0 \quad \Rightarrow \quad$ compressible Euler equations

b) $\lambda = \text{const}, \mu = \text{const}$ (henceforth assumed):

$$(2\nabla \cdot D)_i = \left(\nabla \cdot \left(\frac{\partial u}{\partial x} + \left(\frac{\partial u}{\partial x}\right)^\top\right)\right)_i = \sum_{j=1}^{3} \frac{\partial}{\partial x_j}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)$$
$$= \partial_{x_i}(\operatorname{div} u) + \Delta u_i$$

$$\Rightarrow \partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla(p - (\lambda + \mu)\operatorname{div} u) = \mu \Delta u + \rho f$$

c) incompressible homogeneous fluid: (e.g. water, oil)

$\operatorname{div} u = 0, \rho(x,t) = \rho_0 = \text{const} \Rightarrow$ continuity equation trivially satisfied

$\Rightarrow$incompressible Navier-Stokes equations for homogeneous fluid:

$$\begin{cases} \rho_0\left[u_t + \nabla \cdot (u \otimes u)\right] + \nabla p = \mu \Delta u + \rho_0 f \quad \text{(parabolic for } u\text{)} \\ \operatorname{div} u = 0 \end{cases} \tag{2.7}$$

4 equations for 4 variables $(u, p) \to$ closed system

possible boundary conditions: $u(x,t) = 0, x \in \partial\Omega$ (no slip condition)

If $\mu = 0$ (i.e. shear forces, viscosity negligible) $\Rightarrow$

incompressible homogeneous Euler equations:

$$\begin{cases} \rho_0[u_t + \nabla \cdot (u \otimes u)] + \nabla p = \rho_0 f \quad \text{(hyperbolic for } u\text{)} \\ \operatorname{div} u = 0 \end{cases} \tag{2.8}$$

possible boundary conditions: $u(x,t) \cdot \nu = 0, x \in \partial\Omega$

Solution theory:
in $\mathbb{R}^2$: $\exists\,!$ solution $\forall\, t \geq 0$ for (2.7) resp. (2.8)
in $\mathbb{R}^3$: $\exists\,!$ solution for "small times" for (2.7) resp. (2.8). It is not clear whether a solution exists $\forall\, t \geq 0$.
Problem in $\mathbb{R}^3$: there can be turbulences or "chaotic behaviour"; but not in $\mathbb{R}^2$.

d) ideal compressible gas: (e.g. air, rarefied gases)

constant shear viscosity $\mu \geq 0$

vanishing pressure viscosity: $\mu_d = \lambda + \frac{2}{3}\mu = 0$

$\Rightarrow \sigma = 2\mu[D - \frac{1}{3}(\operatorname{div} u)I]$

The rest is analogous to the Euler equations.

e) homogeneous incompressible "slow" flow:

Let $f = 0$. If the nonlinear term $(u \cdot \nabla)u$ in (2.7) is negligible:

$$\nabla \cdot (u \otimes u) = (\underbrace{\operatorname{div} u}_{=0})u + (u \cdot \nabla)u \approx 0$$

$\Rightarrow$ Stokes equations (linear for u, p):

$$\begin{cases} u_t = -\frac{1}{\rho_0}\nabla p + \nu_0 \Delta u, \quad \nu_0 := \mu/\rho_0 \ \ldots \ \textit{kinematic viscosity} \\ \operatorname{div} u = 0 \end{cases} \tag{2.9}$$

Motivation: let $\tilde{x} := x/L$, $\tilde{u} := u/U$ with typical reference length L and reference velocity U.
$\Rightarrow \ (u \cdot \nabla_x)u = \frac{U^2}{L}(\tilde{u} \cdot \nabla_{\tilde{x}})\tilde{u}, \quad \nu_0 \Delta_x u = \nu_0 \frac{U}{L^2} \Delta_{\tilde{x}} \tilde{u}$
Disregarding this nonlinear term is OK for $\frac{U^2}{L} \ll \nu_0 \frac{U}{L^2}$ resp. for $Re := \frac{LU}{\nu_0} \ll 1$ ... *Reynolds number* (dimensionless)

Rem:

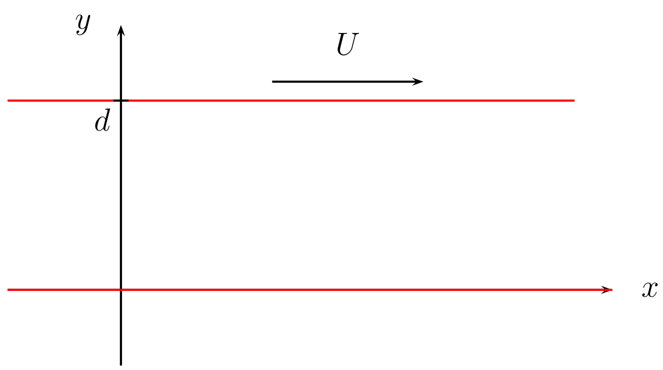
- Typical scales of ∇u, Δu are actually still missing;
- Only $(u \cdot \nabla)u$ and Δu are compared because these "drive" the flow; ∇p is only the response to the constraint $\operatorname{div} u = 0$, see (2.14).

Flows with equal Reynolds numbers allow for scaled (down) wind tunnel experiments.

some viscosity numbers:
air $\mu = 1.8 \times 10^{-5}\,\mathrm{Pa\,s}$
water $\mu = 0.89 \times 10^{-3}\,\mathrm{Pa\,s}$
olive oil $\mu = 0.8 \times 10^{-1}\,\mathrm{Pa\,s}$

Example 2.3. incompressible, homogeneous, stationary flow between 2 parallel moving plates (based on Navier-Stokes (2.7)):

Assumptions: $f = 0$, $2D$-flow, infinite plates, no pressure drop in x, hence $p = p(y)$.



$$\Rightarrow \operatorname{div} u = 0, \rho = \rho_0, \frac{\partial u}{\partial t} = 0$$

$$\begin{cases} \rho_0 \nabla \cdot (u \otimes u) + \nabla p = \mu \Delta u \\ \operatorname{div} u = 0 \end{cases} \tag{2.10}$$

Look for special x–independent solution because problem is x–independent:
$u(y) = (u_1(y), u_2(y))^\top, p = p(y)$

$\operatorname{div} u = \underbrace{\partial_x u_1}_{=0} + \partial_y u_2 = 0 \ \Rightarrow \ u_2 = 0$ (due to boundary condition $u(x,0) = 0$)

$\Rightarrow \nabla \cdot (u \otimes u) = (\underbrace{\operatorname{div} u}_{=0})u + (\underbrace{u \cdot \nabla}_{u_1 \partial_x + u_2 \partial_y = 0})u = 0$

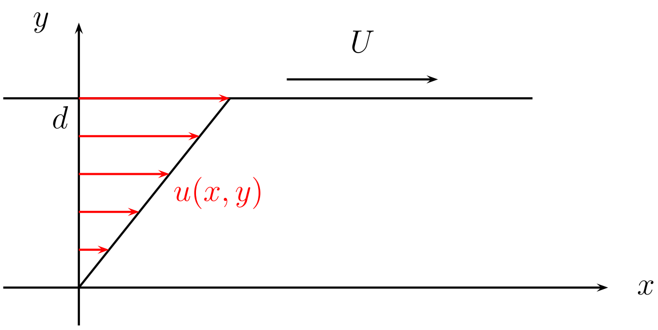
$$\Rightarrow \begin{cases} 0 = \mu \Delta u_1 = \mu \partial_y^2 u_1 \\ p_y = 0 \end{cases}$$

$\Rightarrow p = \text{const} = p_0, \partial_y^2 u_1 = 0$

No-slip condition: $u_1(0) = 0, u_1(d) = U$

$$\Rightarrow u = u(y) = \left(\frac{Uy}{d}, 0\right)^\top$$

This is pure shear flow, "planar Couette flow".



Force on (lower) plate at rest:

$$\tau(\nu) = T \cdot \nu = -p_0 \nu + \mu \frac{U}{d}(\nu_2, \nu_1)^\top \quad \text{(cp. Ex. 2.2 with } \frac{U}{d})$$

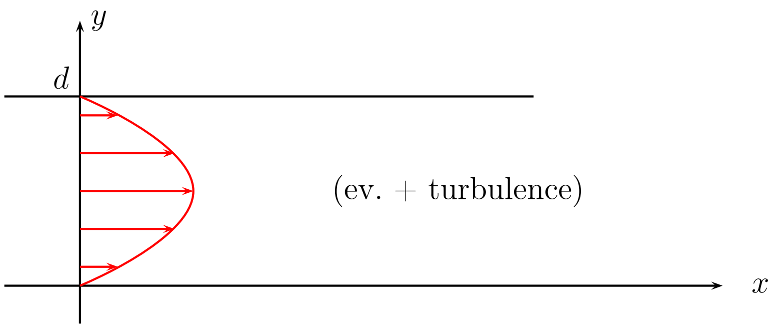
For $\nu = (0,1)^\top$: $\tau = (\mu \frac{U}{d}, -p_0)^\top$ $\square$

Example 2.4. like Ex. 2.3; both plates at rest (i.e. $U = 0$) with pressure drop $p_x = -c < 0$. (2.10) is still x-independent. $\Rightarrow$ look for x-independent solution. $\Rightarrow$ 1st line of (2.10):

$$\begin{cases} p_x = \mu (u_1)_{yy} \quad \Rightarrow \quad (u_1)_{yy} = -\frac{c}{\mu} \\ u_1(0) = u_1(d) = 0 \end{cases}$$

$$\Rightarrow u(y) = \left(\frac{c}{2\mu} y(d-y), 0\right)^\top, p(x) = -cx + \underbrace{p_0}_{=\text{const}}$$

This is a "planar Poiseuille flow" (balance between pressure drop and friction)



Application: measurement of viscosity (in practice: viscometer with 2 concentric cylinders):

$$\text{transported mass per time per length} = \int_0^d \rho_0 u_1(y)\mathrm{d}y = \frac{\rho_0 c d^3}{12\mu}$$

Poiseuille flow is unstable for large Reynolds numbers (i.e. small viscosity); transition to turbulent flow.

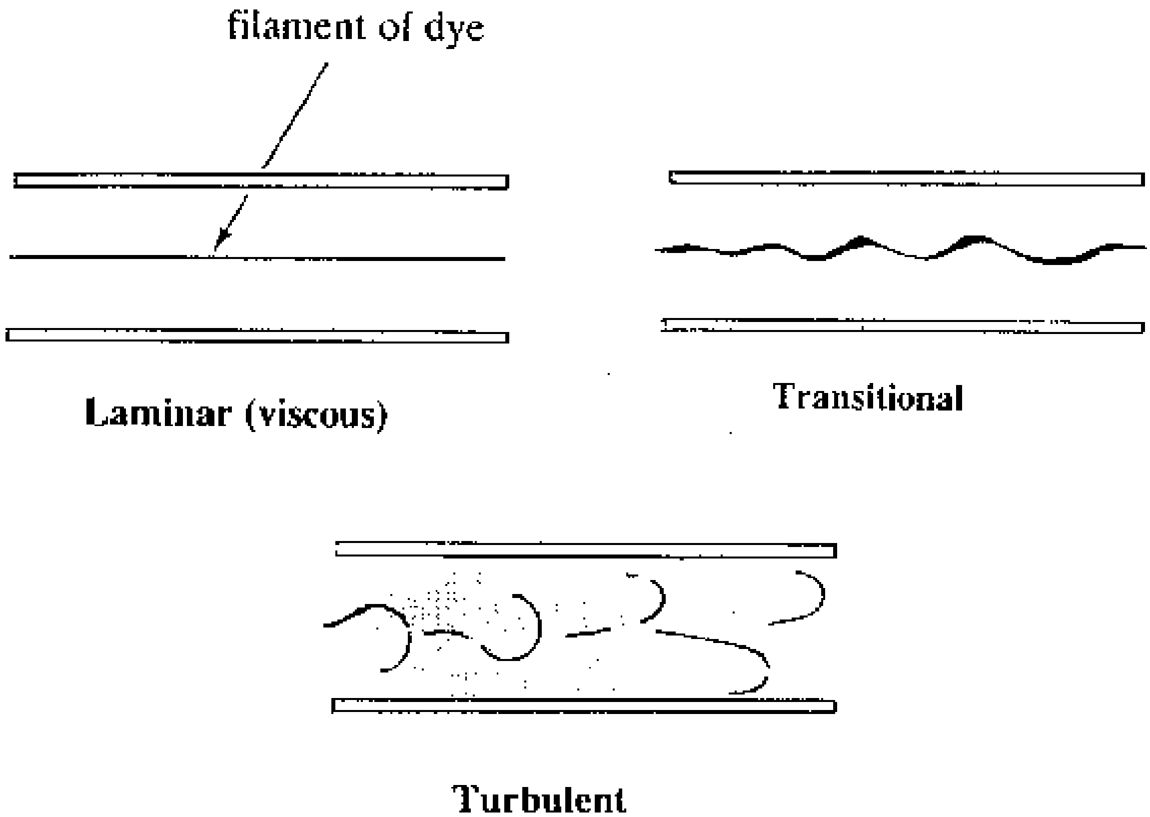


Figure 2.1: tube flow for increasing Re: transition from laminar to turbulent flow

References: [CM] §1.3, [EGK] §5.9

2.2.1 Helmholtz-Hodge decomposition

Aim: interpretation of incompressible (Navier-)Stokes equations as evolution equations for u with p as Lagrange multiplier for the constraint $\operatorname{div} u = 0$.

$$\begin{cases} u_t + (u \cdot \nabla)u = -\frac{1}{\rho_0}\nabla p + \nu_0 \Delta u & , \quad \Omega \\ \operatorname{div} u = 0 & , \quad \Omega \\ u \cdot \nu = 0 & , \quad \partial\Omega \end{cases} \tag{2.11}$$

Physically, the stricter boundary condition $u\big|_{\partial\Omega} = 0$ would be better, but for the following (purely analytical) lemma $u \cdot \nu = 0$ suffices.

Lemma 2.5 (Helmholtz-Hodge decomposition)**.** *Let* $\Omega \subset \mathbb{R}^d, d \geq 2$ *be bounded with* $\partial\Omega \in C^{2,\alpha}(0 < \alpha < 1), w \in C^{1,\alpha}(\overline{\Omega}; \mathbb{R}^d)$. [2]

$\Rightarrow \exists! u \in C^{1,\alpha}(\overline{\Omega}; \mathbb{R}^d), p \in C^{2,\alpha}(\overline{\Omega})$: *(p scalar; unique up to additive constant)*

$$w = u + \nabla p \tag{2.12}$$

with $\operatorname{div} u = 0$ *in* Ω, $u \cdot \nu = 0$ *on* $\partial\Omega$. *($u, w \dots$ vector fields)*

Proof. 1. Show the orthogonality relation:

$\forall u$ with $\operatorname{div} u = 0, u \cdot \nu = 0$ on $\partial\Omega$ holds $\int\limits_\Omega u \cdot \nabla p \mathrm{d}x = 0$ (i.e. $u \perp \nabla p$ in $L^2(\Omega)$), because:

$$\operatorname{div}(pu) = (\operatorname{div} u)p + u \cdot \nabla p = u \cdot \nabla p$$

$$\Rightarrow 0 \overset{\text{BC}}{=} \int\limits_{\partial\Omega} pu \cdot \nu \mathrm{d}s = \int\limits_\Omega \operatorname{div}(pu) \mathrm{d}x = \int\limits_\Omega u \cdot \nabla p \mathrm{d}x \quad \checkmark$$

hence: (2.12) is orthogonal decomposition in $L^2(\Omega)$.

[2] Hölder seminorm: $|f|_{C^{0,\alpha}(\overline{\Omega})} := \sup\limits_{x \neq y \in \Omega} \frac{|f(x) - f(y)|}{|x - y|^\alpha}, 0 \leq \alpha \leq 1$;

Hölder norm: $\|f\|_{C^{n,\alpha}} := \|f\|_{C^n} + \max\limits_{|\beta|=n} |D^\beta f|_{C^{0,\alpha}}, n \in \mathbb{N}_0$.

2. Uniqueness: let $w = u_1 + \nabla p_1 = u_2 + \nabla p_2$

$$\Rightarrow 0 = (u_1 - u_2) + \nabla(p_1 - p_2),\ (u_1 - u_2) \cdot \nu\big|_{\partial\Omega} = 0,\ \operatorname{div}(u_1 - u_2) = 0 \quad (2.13)$$

$\Rightarrow$ (due to 1.) $\quad (u_1 - u_2) \perp \nabla(p_1 - p_2)$ in $L^2(\Omega)$ and

$$0 \overset{(2.13)}{=} \int_\Omega [(u_1 - u_2) + \underbrace{\nabla(p_1 - p_2)] \cdot (u_1 - u_2)\mathrm{d}x}_{=0} = \int_\Omega |u_1 - u_2|^2 \mathrm{d}x$$

$\Rightarrow u_1 = u_2 \quad \Rightarrow \quad \nabla p_1 = \nabla p_2 \quad \checkmark$

3. Existence: We want: $w = u + \nabla p \Rightarrow \operatorname{div} w = \operatorname{div} u + \operatorname{div} \nabla p = \Delta p$ and on $\partial\Omega$: $w \cdot \nu = \nabla p \cdot \nu$. Thus solve for p:

$$\Delta p = \operatorname{div} w \quad \text{in } \Omega,\ \nabla p \cdot \nu = w \cdot \nu \quad \text{on } \partial\Omega \qquad (= \text{Neumann problem for Poisson equation})$$

Due to $\operatorname{div} w \in C^{0,\alpha}(\overline{\Omega})$ and $w \cdot \nu \in C^{1,\alpha}(\partial\Omega)$ there exists $p \in C^{2,\alpha}(\overline{\Omega})$ (see PDE course). Let $u := w - \nabla p \in C^{1,\alpha}(\overline{\Omega})$

$$\begin{aligned} \Rightarrow \quad & \operatorname{div} u = \operatorname{div} w - \Delta p = 0 \quad \checkmark \\ & u \cdot \nu\big|_{\partial\Omega} = w \cdot \nu\big|_{\partial\Omega} - \nabla p \cdot \nu\big|_{\partial\Omega} = 0. \quad \checkmark \end{aligned}$$

■

Definition 2.6. *Projection operator:* $\mathbb{P}w := u$, *where* $w = u + \nabla p, \operatorname{div} u = 0$ *and* $u \cdot \nu = 0, \partial\Omega$.

$\mathbb{P} : C^{1,\alpha}(\overline{\Omega}) \to C^{1,\alpha}(\overline{\Omega})$ *is well defined due to above Lemma.*

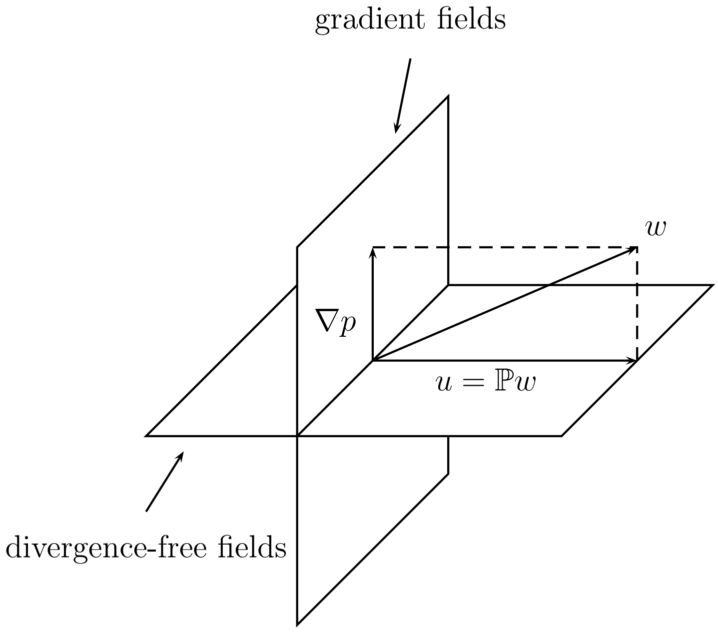
Properties:

(a) $\mathbb{P}$ is linear

(b) $w = u + \nabla p = \mathbb{P}w + \nabla p$

(c) $\mathbb{P}u = u \quad \forall u$ with $\operatorname{div} u = 0, u \cdot \nu\big|_{\partial\Omega} = 0$

(d) $\mathbb{P}(\nabla p) = 0$.



Apply $\mathbb{P}$ to (2.11):

$$\mathbb{P}\left(\partial_t u + \frac{1}{\rho_0}\nabla p\right) = \mathbb{P}(-(u \cdot \nabla)u + \nu_0 \Delta u)$$

Due to $\operatorname{div} \partial_t u = \partial_t \operatorname{div} u = 0$ and $(\partial_t u) \cdot \nu = \partial_t (u \cdot \nu) = 0$:

$$\mathbb{P}(\partial_t u) = \partial_t u \quad \text{(lt. (c))}.$$

From (d): $\mathbb{P}(\nabla p) = 0$

$$\Rightarrow \partial_t u = \mathbb{P}(-(u \cdot \nabla)u + \nu_0 \Delta u) \tag{2.14}$$

This is an evolution equation only for u; p eliminated!

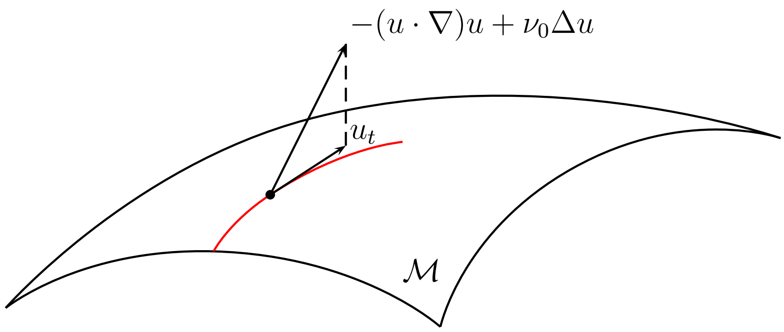


Figure 2.2: manifold $\mathcal{M}$ determined by $\operatorname{div} u = 0$.

Caution: $\operatorname{div}(\Delta u) = \Delta(\operatorname{div} u) = 0$, but in general $(\Delta u) \cdot \nu\big|_{\partial\Omega} \neq 0$.

$\Rightarrow$ in general $\mathbb{P}(\Delta u) \neq \Delta u$

(2.14) also useful for numerical algorithms.

Determination of pressure p from u:

$$
\begin{aligned}
(2.11): \quad \nabla p &= -\rho_0[u_t + (u \cdot \nabla)u - \nu_0 \Delta u] \\
&\overset{(2.14)}{=} \rho_0(\mathbb{I} - \mathbb{P})[-(u \cdot \nabla)u + \nu_0 \Delta u]
\end{aligned}
$$

References: [CM] §1.3

2.2.2 Rotation

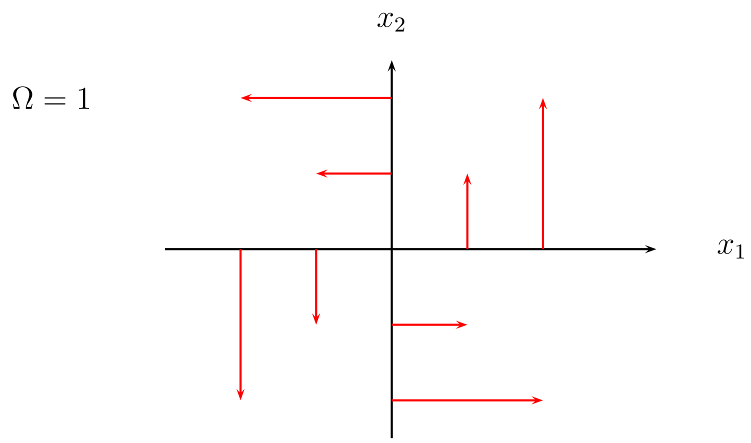
Definition 2.7. *$\omega := \operatorname{rot} u := \nabla \times u$ is called* rotation *or* "vorticity field" *of the 3D velocity field u.*
In 2D ω is scalar: $\omega := \operatorname{rot} u := \partial_{x_1} u_2 - \partial_{x_2} u_1$ (embedded in $\mathbb{R}^3$).

Example 2.1 (continuation)**.** $u(x) = cx, c \in \mathbb{R}$

$$
\omega = c \begin{pmatrix} \partial_{x_1} \\ \partial_{x_2} \\ \partial_{x_3} \end{pmatrix} \times \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}
$$

□

Example 2.8. $u(x) = \Omega(-x_2, x_1, 0)^\top \Rightarrow \omega = \operatorname{rot} u = (0, 0, 2\Omega)^\top$



ω_3 = double angular velocity around x_3-axis (= axis of rotation).
In general: direction of ω defines (as normal vector) local plane of rotation, its length the local intensity of vorticity. □

local decomposition of flow:

Movement $\approx$ (rigid) translation + deformation + (rigid) rotation

Lemma 2.9. *Let $u(x)$ be a smooth 3D vector field.*

$$u(y) = u(x) + D(x)\cdot(y-x) + \frac{1}{2}\omega(x)\times(y-x) + O(\|y-x\|^2) \quad \forall x,y\in\mathbb{R}^3$$

Proof. From Taylor's theorem:

$$u(y) = u(x) + \frac{\partial u}{\partial x}(x)\cdot(y-x) + O(\|y-x\|^2)$$

Moreover:

$$\begin{aligned}
\left(D\cdot(y-x)+\frac{1}{2}\omega\times(y-x)\right)_1 &= \partial_1 u_1(y_1-x_1)\\
&\quad+\frac{1}{2}(\partial_1 u_2+\partial_2 u_1)(y_2-x_2)+\frac{1}{2}(\partial_1 u_3+\partial_3 u_1)(y_3-x_3)\\
&\quad+\frac{1}{2}[(\underbrace{\partial_3 u_1-\partial_1 u_3}_{=\omega_2})(y_3-x_3)-(\underbrace{\partial_1 u_2-\partial_2 u_1}_{=\omega_3})(y_2-x_2)]\\
&= \partial_1 u_1(y_1-x_1)+\partial_2 u_1(y_2-x_2)+\partial_3 u_1(y_3-x_3)\\
&= \sum_{j=1}^{3}\partial_j u_1(y_j-x_j) = \left[\frac{\partial u}{\partial x}\cdot(y-x)\right]_1
\end{aligned}$$

other components analogously. ∎

References: [CM] §1.3, [MP] §1.2

2.3 Vorticity models

Aim: Vorticity formulation for homogeneous incompressible Euler equation

2.3.1 Vector fields from sources and vortices

Let $G\subset\mathbb{R}^d; d=2,3$; simply connected domain;[3] let $u\in C^1(G,\mathbb{R}^d)$ (in this chapter).

Definition 2.10. *u is called* irrotational *[or* curl-free*] if* $\operatorname{rot} u = 0$ *in G.*

u is called conservative *if* $\int_C u\,ds$ *is path-independent.*

[3] Every closed path can be contracted continuously to a point.

Theorem 2.11. *u curl-free* $\Leftrightarrow$ *u conservative* $\Leftrightarrow$ $\exists$ potential $\varphi : u = \nabla\varphi$

Proof. Analysis course. ∎

Lemma 2.12. *Let $u \in C^1(G)$ be a vector field. Then*

(i) $\operatorname{rot} u = 0 \quad \Leftrightarrow \quad \exists\varphi : u = \nabla\varphi$

(ii) $\operatorname{div} u = 0 \quad \Leftrightarrow \quad \exists$ vector potential $A : u = \operatorname{rot} A$ *(only in 3D)*

(2D-interpretation only via embedding in 3D:
$\exists A = (0,0,A_3)^\top : u = \operatorname{rot} A = (\partial_2 A_3, -\partial_1 A_3, 0)^\top$*, bzw.* $u = (\partial_2 A_3, -\partial_1 A_3)^\top =: \nabla^\perp A_3$ *)*

Aim: solution $u \in C^1(G)$ of system

$$\begin{cases} \operatorname{rot} u = \omega & \text{in } G \quad (\text{vortex of } u\text{: } \omega \in C^1(G)) & (2.15) \\ \operatorname{div} u = f & \text{in } G \quad (\text{source of } u\text{: } f \in C^0(G)) & (2.16) \end{cases}$$

Solution of (2.15):

Because $\operatorname{div}\operatorname{rot} u = 0$: (2.15) is solvable $\Leftrightarrow$ $\operatorname{div}\omega = 0$:

First look for special solution $u_0 = (u_1, u_2, u_3)^\top$ with $u_3 = 0$.

$\operatorname{rot} u_0 = \omega \quad \Leftrightarrow$

$$\begin{cases} -\partial_3 u_2 = \omega_1 \\ \partial_3 u_1 = \omega_2 \\ \partial_1 u_2 - \partial_2 u_1 = \omega_3 \end{cases}$$

Choose special solution

$$u_1 := \int \omega_2(x_1,x_2,x_3)\mathrm{d}x_3$$
$$u_2 := -\int \omega_1(x_1,x_2,x_3)\mathrm{d}x_3 + g(x_1,x_2)$$

with $\partial_1 g = \partial_1 \int \omega_1 \mathrm{d}x_3 + \partial_2 \int \omega_2 \mathrm{d}x_3 + \omega_3$.

General solution according to Lemma 2.12(i):

$$u = u_0 + \nabla\varphi \quad , \quad \forall\varphi \in C^2(G)$$

in 2D: via embedding into $\mathbb{R}^3$:

$$\operatorname{rot} u = \begin{pmatrix} \partial_1 \\ \partial_2 \\ 0 \end{pmatrix} \times \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \partial_1 u_2 - \partial_2 u_1 \end{pmatrix} \tag{2.17}$$

$\Rightarrow \omega_1 = \omega_2 = 0$ (necessary condition on data) $\Rightarrow u_0 = (0, \int \omega_3 \mathrm{d}x_1)^\top$

Rest is analogous.

<u>Solution of (2.16):</u>

General solution according to Lemma 2.12 (ii):

$$u = \underbrace{\left(\int f \mathrm{d}x_1, 0, 0\right)^\top}_{\text{special solution}} + \operatorname{rot} A, \quad \forall A \in C^2(G)$$

<u>in 2D:</u>

With $\psi = A_3$.

$$u = \begin{pmatrix} \int f \mathrm{d}x_1 \\ 0 \\ 0 \end{pmatrix} + \operatorname{rot} \begin{pmatrix} 0 \\ 0 \\ \psi \end{pmatrix} = \begin{pmatrix} \int f \mathrm{d}x_1 + \partial_2 \psi \\ -\partial_1 \psi \\ 0 \end{pmatrix} \quad \forall \psi \in C^2(G).$$

<u>System (2.15), (2.16)</u>: Let f, ω be given with $\operatorname{div} \omega = 0$ (because $\operatorname{div} \operatorname{rot} u = 0$).

<u>Strategy:</u> Decomposition $u = u_q + u_w$ where u_q is divergence-free and u_w curl-free.

Lemma 2.13. *Let* $\operatorname{div} \omega = 0$. *Solution* u *of* (2.15), (2.16) *has the general form* $u = u_q + u_w$, *where* $u_q := \operatorname{rot} A$, $u_w := \nabla \varphi$, *and* A, φ *solve:*

$$-\Delta A = \omega \quad \textit{and} \quad \operatorname{div} A = 0$$

resp. $\Delta \varphi = f$.

Proof. First solve

$$\begin{cases} \operatorname{div} u_q = 0 \\ \operatorname{rot} u_q = \omega \qquad \text{(solvable because } \operatorname{div} \omega = 0\text{)} \end{cases}$$

According to Lemma 2.12 (ii): $u_q = \operatorname{rot} A$

$\Rightarrow \omega = \operatorname{rot} u_q = \operatorname{rot} \operatorname{rot} A = \nabla(\operatorname{div} A) - \Delta A$

Let for example $\operatorname{div} A = 0$.

$\Rightarrow -\Delta A = \omega$; is compatible with $\operatorname{div} A = 0$ because:

$$-\operatorname{div}(\Delta A) = -\Delta(\operatorname{div} A) = 0 = \operatorname{div} \omega.$$

Now solve

$$\begin{cases} \operatorname{div} u_w = f \\ \operatorname{rot} u_w = 0 \end{cases}$$

According to Lemma 2.12 (i): $u_w = \nabla\varphi$

$\Rightarrow \operatorname{div} u_w = \operatorname{div} \nabla\varphi = f$, hence $\Delta\varphi = f$

$\Rightarrow u_0 := u_q + u_w$ is special solution of (2.15), (2.16).

General solution: $u = u_0 + \nabla\tilde{\varphi}$, $\forall\tilde{\varphi}$ with $\Delta\tilde{\varphi} = 0$. ■

Remark 2.14. A function $u = \nabla\varphi$ with $\Delta\varphi = 0$ is called *Laplace field*. It is divergence-free and curl-free because

$$\operatorname{rot} u = \operatorname{rot} \nabla\varphi = 0 \quad , \quad \operatorname{div} u = \Delta\varphi = 0.$$

In fluid dynamics u describes an incompressible *potential flow*.

2.3.2 The vorticity equation

Homogeneous, incompressible Euler equation in $\mathbb{R}^2$, $\mathbb{R}^3$:

$$\begin{cases} \frac{\partial u}{\partial t} + (u \cdot \nabla)u = -\frac{1}{\rho_0}\nabla p \\ \operatorname{div} u = 0 \end{cases} \tag{2.18}$$

We have: $(u \cdot \nabla)u = \frac{1}{2}\nabla|u|^2 - u \times \omega$ with $\omega := \operatorname{rot} u$

rot of (2.18) $\Rightarrow$

$$\partial_t \underbrace{\operatorname{rot} u}_{=\omega} + \frac{1}{2} \underbrace{\operatorname{rot}(\nabla|u|^2)}_{=0} - \operatorname{rot}(u \times \omega) = -\frac{1}{\rho_0} \underbrace{\operatorname{rot} \nabla p}_{=0}$$

$$\begin{aligned} \operatorname{rot}(u \times \omega) &= (\omega \cdot \nabla)u - \omega \underbrace{\operatorname{div} u}_{=0} - (u \cdot \nabla)\omega + u \underbrace{\operatorname{div} \omega}_{=\operatorname{div} \operatorname{rot} u = 0} \\ &= (\omega \cdot \nabla)u - (u \cdot \nabla)\omega \end{aligned}$$

$\Rightarrow \partial_t\omega - (\omega \cdot \nabla)u + (u \cdot \nabla)\omega = 0$ Here we have eliminated p.

$$\Rightarrow \boxed{\frac{\mathrm{D}\omega}{\mathrm{D}t} = (\omega \cdot \nabla)u} \quad \text{with } \operatorname{rot} u = \omega, \operatorname{div} u = 0 \ \dots \ \textit{vorticity equation} \text{ in } \mathbb{R}^3$$

$(\omega \cdot \nabla)u$ describes the vortex stretching in 3D (with simultaneous thinning out of the vortex and increase of vortex intensity).

Simplification in 2D:

$$\omega = (0, 0, \partial_1 u_2 - \partial_2 u_1)^\top, \nabla = (\partial_1, \partial_2, 0) \Rightarrow (\omega \cdot \nabla) u = 0$$

$$\Rightarrow \boxed{\frac{\mathrm{D}\omega}{\mathrm{D}t} = 0} \quad \text{resp. } \frac{\partial \omega}{\partial t} + u \cdot \nabla \omega = 0 \ldots \textit{vorticity equation} \text{ in } \mathbb{R}^2$$

ω here is a scalar function! The vorticity equation is nonlinear because $u = u[\omega]$.

A-priori estimates of ω:

Lemma 2.15. *For the vorticity equation in $D \subset \mathbb{R}^2$ with $u \cdot \nu = 0$ on ∂D the following holds:*

$$\Rightarrow \|\omega(\cdot, t)\|_{L^p(D)} = \|\omega_0\|_{L^p(D)} \quad , 1 \leq p \leq \infty, \forall t \geq 0 \ . \tag{2.19}$$

Proof. For $1 \leq p < \infty$ multiply the vorticity equation by $|\omega|^{p-1} \operatorname{sign}(\omega)$:

$$(\partial_t \omega)|\omega|^{p-1} \operatorname{sign}(\omega) + (u \cdot \nabla \omega)|\omega|^{p-1} \operatorname{sign}(\omega) = 0,$$

$$\Rightarrow \partial_t |\omega|^p + u \cdot \nabla |\omega|^p = 0$$

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \int_D |\omega|^p \mathrm{d}x = - \int_D u \cdot \nabla |\omega|^p \mathrm{d}x \quad &= \quad - \int_D \operatorname{div}(u|\omega|^p) \mathrm{d}x + \int_D (\underbrace{\operatorname{div} u}_{=0}) |\omega|^p \mathrm{d}x \\ &= \quad - \int_{\partial D} (\underbrace{u \cdot \nu}_{=0}) |\omega|^p \mathrm{d}s = 0 \end{aligned}$$

This gives (2.19) for $1 \leq p < \infty$. The case $p = \infty$ follows from $\|\omega(\cdot, t)\|_{L^\infty(D)} = \lim\limits_{p \to \infty} \|\omega(\cdot, t)\|_{L^p(D)}$. ∎

This is an important estimate for the proof of existence in $\mathbb{R}^2$ (much more difficult in $\mathbb{R}^3$).

Reconstruction of u from ω:

1st case: Let $D \subset \mathbb{R}^2$ be simply connected and bounded

$$\begin{cases} \partial_1 u_2 - \partial_2 u_1 = \omega & , \quad D \\ \partial_1 u_1 + \partial_2 u_2 = 0 & , \quad D \\ u \cdot \nu = 0 & , \quad \partial D \end{cases} \tag{2.20}$$

$\operatorname{div} u = 0 \Rightarrow \exists A = (0, 0, \psi)^\top : u = \operatorname{rot} A$, i.e. $u_1 = \partial_2 \psi, u_2 = -\partial_1 \psi$, resp. $u = \nabla^\perp \psi$ with $\nabla^\perp := \begin{pmatrix} \partial_2 \\ -\partial_1 \end{pmatrix}$

Definition 2.16. *For given u, ψ with $u = \nabla^\top \psi$ is called* stream function*; it is unique up to an additive constant.*

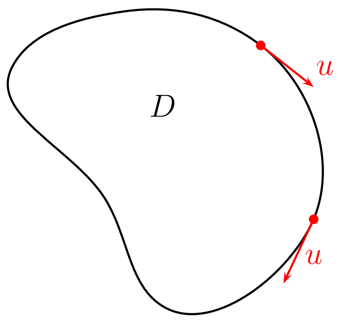
Definition 2.17. *The integral curves $x(s) = \begin{pmatrix} x_1(s) \\ x_2(s) \end{pmatrix}$, $s \in \mathbb{R}$ of $u(x,t)$ for $\underline{t \text{ fixed}}$ are called* stream lines / flow lines*. They solve $\frac{\mathrm{d}x}{\mathrm{d}s} = u(x;t)$.*

Caution: stream lines $\neq$ particle trajectories (except in stationary flow).

Interpretation:

Stream lines are level curves of $\psi(x,t)$ for t fixed because:

$$\frac{\mathrm{d}}{\mathrm{d}s}\psi(x(s);t) = \partial_1\psi\,\dot{x}_1 + \partial_2\psi\,\dot{x}_2 = -u_2u_1 + u_1u_2 = 0$$



Integration of the tangential vector field u along ∂D gives $x(s)$.

Due to $u \cdot \nu = 0$ on ∂D (i.e. tangential field): One integral curve of u lies on ∂D, so ∂D (with suitable parameterisation) is a stream line $\Rightarrow \psi = \text{const}$ on ∂D.

Convention: Choose the additive constant for ψ such that $\psi = 0$ on ∂D.

This way, ψ is uniquely determined:

Lemma 2.18. *$u = u[\omega] = \nabla^\perp\psi$ is the unique solution of* (2.20)*, where ψ solves the* potential problem

$$\begin{cases} -\Delta\psi = \omega & , \quad D \\ \psi = 0 & , \quad \partial D. \end{cases} \tag{2.21}$$

Proof. Existence follows from (2.21) and $\omega = -\Delta\psi = \mathrm{rot}(\underbrace{\nabla^\perp\psi}_{=u})\checkmark$

$\mathrm{div}\, u = \mathrm{div}(\nabla^\perp\psi) = 0\checkmark$

$\psi\big|_{\partial D} = 0 \Rightarrow \nabla\psi \perp \partial D \Rightarrow u = \nabla^\perp\psi \,||\, \partial D\checkmark$

Uniqueness: Let $v := u - \tilde{u}$ be the difference between two solutions, hence

$$\operatorname{rot} v = \operatorname{div} v = 0 \text{ in } D; v \cdot \nu = 0, \partial D$$

According to Lemma 2.12 (i): $v = \nabla\varphi$

$\Rightarrow 0 = \operatorname{div} v = \operatorname{div} \nabla\varphi = \Delta\varphi$ in D, $\nabla\varphi \cdot \nu = 0$ on ∂D

$\Rightarrow \varphi = \text{const} \quad \Rightarrow \quad v = \nabla\varphi \equiv 0$ ■

With Lemma 2.18 the "coefficient function" $u[\omega]$ in the 2D vorticity equation

$$\frac{\partial\omega}{\partial t} + u[\omega] \cdot \nabla\omega = 0$$

is defined. For proof of well-posedness of this evolution problem the a-priori estimate (2.19) is essentiell (see §2.3 in [MP]; §3.2.3, 3.3, 4.2 in [MB]).

Representation of ω from (2.21):

Theorem 2.19.

$$\psi(x) = \int_D G_D(x, x')\omega(x')\mathrm{d}x';$$

the Green's function G_D *solves*

$$\begin{aligned} \Delta_x G_D(x, x') &= -\delta(x - x') \text{ in } D, \\ G_D(x, x') &= 0 \quad \forall x \in \partial D \text{ or } x' \in \partial D. \end{aligned}$$

We have:

$$G_D(x, x') = G(x, x') + \gamma(x, x') \text{ with } G(x, x') = -\frac{1}{2\pi}\log|x - x'|, \ \Delta_x\gamma = \Delta_{x'}\gamma = 0, \ + \ BC \text{ for } \gamma.$$

$$\Rightarrow u(x) = \nabla^\perp\psi(x) = \int_D \underbrace{\nabla_x^\perp G_D(x, x')}_{=:K_D(x,x')}\omega(x')\mathrm{d}x'.$$

Proof. PDE course. ■

Remark 2.20. Under which condition does one obtain a stationary flow?

We have

$$\begin{aligned} u \cdot \nabla\omega &= u_1\partial_1\omega + u_2\partial_2\omega = \partial_2\psi \cdot \partial_1\omega - \partial_1\psi \cdot \partial_2\omega \\ &= \det \begin{pmatrix} \partial_1\omega & \partial_2\omega \\ \partial_1\psi & \partial_2\psi \end{pmatrix} =: \det J(\omega, \psi) \end{aligned}$$

Hence:

$$\frac{\partial\omega}{\partial t} = 0 \quad \Leftrightarrow \quad \det J(\omega,\psi) = 0 \quad \forall x \in D.$$

Then $\omega(x), \psi(x)$ are (functionally) dependent, i.e., $\omega = f(\psi)$ or $\psi = g(\omega)$.

<u>2nd case:</u> $D = \mathbb{R}^2$

Therefore solve:

$$\begin{cases} \operatorname{div} u = 0 \\ \operatorname{rot} u = \begin{pmatrix} 0 \\ 0 \\ \omega \end{pmatrix} \end{cases} \tag{2.22}$$

Analogously to Lemma 2.18 u can be determined from $u = \nabla^\perp\psi$ and $-\Delta\psi = \omega$ in $\mathbb{R}^2$.

A *special solution* can be given by means of *Green's function* for the Poisson equation in $\mathbb{R}^2$,

$$G(x, x') = -\frac{1}{2\pi} \log|x - x'|; x, x' \in \mathbb{R}^2$$

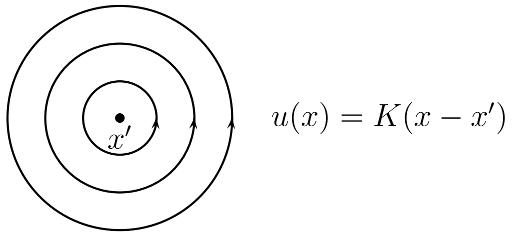
$$\begin{aligned} \psi(x) &= \int_{\mathbb{R}^2} G(x,x')\omega(x')\mathrm{d}x', \\ u_0(x) &= \nabla^\perp\psi(x) = \int_{\mathbb{R}^2} K(x - x')\omega(x')\mathrm{d}x' \end{aligned} \tag{2.23}$$

with

$$K(x - x') = -\frac{1}{2\pi}\frac{(x-x')^\perp}{|x-x'|^2} \quad ; \quad x^\perp = \begin{pmatrix} x_2 \\ -x_1 \end{pmatrix} \text{ for } x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}.$$

Remark for analyis regarding existence of u: The *generalised Young inequality*

$$\|u\|_{L^r(\mathbb{R}^2)} \leq C\|\omega\|_{L^p(\mathbb{R}^2)} \quad ; 1 < p < 2, 2 < r < \infty \text{ with } \frac{1}{r} = \frac{1}{p} - \frac{1}{2}; \ \frac{1}{|x|} \in L^2_w(\mathbb{R}^2).$$



holds.

Interpretation of $K(x - x')$:

Let $\omega(x) = \delta(x - x'), x' \in \mathbb{R}^2$ be given.

$\Rightarrow K(x - x')$ = velocity vector field $u(x)$, "produced" by *unit vortex* $\omega(x) = \delta(x - x')$ at x':

General solution of (2.22) (cf. Rem. 2.14):

$$u = \nabla^\perp \psi + \underbrace{\nabla \varphi}_{\text{Laplace field}} \qquad \text{with } \Delta\varphi = 0 \text{ in } \mathbb{R}^2$$

Without "boundary condition at infinity" the solution is *not* unique.

Possible boundary conditions:

$$u(x) \overset{|x|\to\infty}{\longrightarrow} u_\infty (= \text{const}) \quad \text{(i.e., uniform flow at infinity)} \tag{2.24}$$

$\Rightarrow$ *unique* solution of (2.22), (2.24) (e.g. for ω with compact support):

$$u = \nabla^\perp \psi + u_\infty$$

References: [MP] §1.2

2.3.3 Motion of point vortices in $\mathbb{R}^2$

We first consider the vorticity equation in $D \subset \mathbb{R}^2$ simply connected and bounded:

$$\omega_t = -u \cdot \nabla \omega \quad , \tag{2.25}$$

and u satisfies: div $u = 0$ in D, $u \cdot \nu = 0$ on ∂D.

Aim: Reduce the PDE "vorticity equation" to a system of ODEs.

Consider the initial condition (linear combination of *point vortices*):

$$\omega_0(x) := \sum_{i=1}^{N} a_i \delta(x - x_i), \quad x \in D \subset \mathbb{R}^2 \tag{2.26}$$

with given *positions* $x_i \in D \subset \mathbb{R}^2$ and *intensities* $a_i \in \mathbb{R}$.
In Euler equations, the conservation of N point vortices for $t > 0$ is plausible because the model contains no diffusion/viscosity.

Problems: a distributional formulation of PDE (2.25) is "delicate" because already the coefficient function $u[\omega_0]$ is singular at x_i, hence is not usable in weak formulation. $\Rightarrow$ regularisation needed:

The following step function approximates ω_0:

$$\omega_0^\varepsilon(x) := \frac{1}{\varepsilon^2\pi}\sum_{i=1}^{N} a_i \chi_{\underbrace{K(x_i,\varepsilon)}_{\text{ball}}}(x)$$

We have $\chi_{K(x_i,\varepsilon)}\frac{1}{\varepsilon^2\pi} \to \delta(x - x_i)$ in $\mathcal{D}'(D)$.

For the reformulation we consider $\forall f \in C^1(\bar{D})$ (and sufficiently smooth u, ω):

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_D \omega f \mathrm{d}x = -\int_D (u\cdot\nabla\omega) f \mathrm{d}x &\overset{\operatorname{div} u=0}{=} -\int_D \operatorname{div}(fu\omega)\mathrm{d}x + \int_D \omega u\cdot\nabla f \mathrm{d}x \\ &\overset{\text{div.thm}}{=} -\int_{\partial D} f\omega \underbrace{u\cdot\nu}_{=0}\mathrm{d}s + \int_D \omega u\cdot\nabla f \mathrm{d}x.\end{aligned}$$

$\Rightarrow$ this motivates the *weak formulation* of the vorticity equation:
Find $\omega \in C^1([0,T], L^2(D))$ with

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\omega(t), f\rangle = \langle\omega(t), u(t)\cdot\nabla f\rangle \quad \forall f \in C^1(\bar{D}), \omega(t=0) = \omega_0, \tag{2.27}$$

and $\langle f, g\rangle := \int_D f(y)g(y)\mathrm{d}y$. Same form for $D = \mathbb{R}^2$.

Properties of solution $\omega^\varepsilon(t)$ of (2.27) in $D = \mathbb{R}^2$ with IC ω_0^ε:

Theorem 2.21. *For $D = \mathbb{R}^2$ we have:*

$$\lim_{\varepsilon\to 0}\langle\omega^\varepsilon(t), f\rangle = \sum_{i=1}^{N} a_i f(x_i(t)) = \langle\omega(t), f\rangle, \quad \forall\, f \in C^1(\mathbb{R}^2),$$

with $\omega(x,t) = \sum_{i=1}^{N} a_i\delta(x - x_i(t))$.

$x_i(t)$ *solves the ODE ("discrete vorticity model"):*

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}x_i(t) = u(x_i(t),t) = \underbrace{\sum_{j\neq i} K(x_i(t) - x_j(t))a_j}_{(*)} \\ x_i(0) = x_i \quad ; \quad i = 1,\dots,N. \end{cases} \tag{2.28}$$

(*) ... velocity field of the "other" vortices $\Rightarrow$ one (single) vortex is stationary.

Proof. [MP] Th. 4.2.3. ∎

Remark 2.22. Is $\omega(x,t)$ (measure valued) solution of (2.27) with IC ω_0 from (2.26)? Almost, because ω solves

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\omega(t),f\rangle = \langle\omega(t),u_r\cdot\nabla f\rangle \quad \forall f\in C^1(\mathbb{R}^2) \tag{2.29}$$

with the "regularised velocity"

$$u_r(x,t) := \int_{\mathbb{R}^2} \underbrace{\nabla^\perp G(x,x')}_{=K(x-x')}\underbrace{\chi_{\{x\neq x'\}}\omega(x',t)}_{=0\text{ for }x=x'}\,\mathrm{d}x' \tag{2.30}$$

(in mathematically sloppy notation).

$\chi_{\{x\neq x'\}}$ prevents the "self interaction" of the point vortices; this is used now as additional physical assumption. (2.30) with singularities of the integral kernel at positions of the deltas would not even be defined. That one single point vortex has to be stationary is also seen from the fact that in this case there is no distinguished direction.

Source of problem: weak formulation (2.27) with velocity field u from (2.23) is not defined for distributional solution.

Solution $\omega(t)$ with $x_i(t)$ solves the PDE (2.29)-(2.30) by reduction to a system of ODEs (2.28). □

<u>Vorticity model as Hamiltonian system:</u>

(2.28) is equivalent to

$$\begin{cases} a_i\frac{\mathrm{d}}{\mathrm{d}t}x_i^1 = \frac{\partial}{\partial x_i^2}H, & i=1,...,N,\\ a_i\frac{\mathrm{d}}{\mathrm{d}t}x_i^2 = -\frac{\partial}{\partial x_i^1}H, \end{cases} \tag{2.31}$$

with *Hamiltonian* ("energy")

$$H := -\frac{1}{4\pi}\sum\sum_{j\neq i} a_i a_j \ln|x_i-x_j|;$$

Notation $x_i = (x_i^1, x_i^2)^\top$.

Compare to *Hamilton's equations* of point mechanics:

a particle with mass m, kinetic energy $\frac{p^2}{2m}$, momentum $p = m\,u$ and potential energy $V(x)$.

With Hamiltonian $H(x,p) := \frac{p^2}{2m} + V(x)$ we have:

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}x = \frac{\partial}{\partial p}H = \frac{p}{m} = u,\\ \frac{\mathrm{d}}{\mathrm{d}t}p = -\frac{\partial}{\partial x}H = -\frac{\mathrm{d}V}{\mathrm{d}x} = F \quad \dots \quad \text{Newton's second law.} \end{cases}$$

Hamiltonian sytems always have the following property:

"Energy" is constant in time, hence: $H(t) = \text{const} \quad \forall t$.

Moreover:

Vortex center $B(t) := \dfrac{\sum_{i=1}^N a_i x_i(t)}{\sum_{i=1}^N a_i}$ is constant in time (for $\sum_{i=1}^N a_i \neq 0$) $\Rightarrow M(t) := \sum_{i=1}^N a_i x_i(t) = \text{const}$.

Inertia is constant in time, i.e.: $I(t) := \sum_{i=1}^N a_i |x_i(t)|^2 = \text{const}$

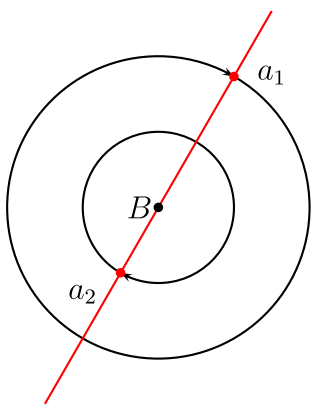
Hence: 4 (scalar) *first integrals* of the motion $\Rightarrow$ ODE system (2.31) for max. 3 point vortices ($N \leq 3$) is explicitly solvable (because a Hamiltonian system in $\mathbb{R}^{2N}$ with $N+1$ Poisson-commuting conserved quantities is completely integrable [V.I. Arnold, Dynamical Systems III]).

Example 2.23. N=2:

$$H = -\frac{1}{2\pi} a_1 a_2 \ln |x_1 - x_2| = \text{const} \quad \Rightarrow \quad |x_1(t) - x_2(t)| = \text{const}$$

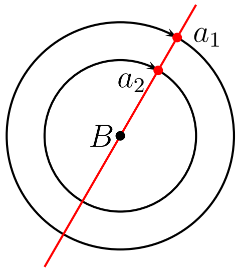
Vortex center ... $B := \dfrac{M}{a_1 + a_2} = \text{const}$ and it is on line connecting $x_1(t)$ and $x_2(t)$.

<u>1st case:</u> $\operatorname{sign} a_1 = \operatorname{sign} a_2$



here $a_{1,2} < 0$

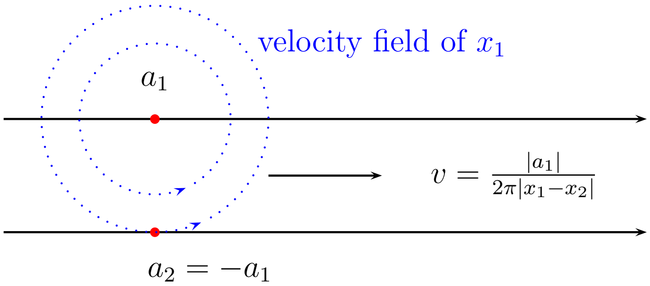
<u>2nd case:</u> $\operatorname{sign} a_1 \neq \operatorname{sign} a_2$ and $|a_1| \neq |a_2|$



here $a_1 > 0$, $|a_2| > |a_1|$

We have: radius of rotation $\to \infty$ for $|a_1| \to |a_2|$

3rd case: $a_1 = -a_2$



hier $a_1 > 0$

$\square$

Question: Does system (2.28) have a global (in time) solution? 2 possible problems:

a) $|x_i| \to \infty$ for $t \to T^*$.

b) $|x_i(t) - x_j(t)| \to 0$ for $t \to T^*$, which means 2 "particles" at one place and the right hand side of (2.28) is not well-defined anymore.

Solution: Global solvability depends on $\{\operatorname{sign} a_i\}$.

Theorem 2.24. *Let* $\operatorname{sign} a_i = \operatorname{sign} a_1 \neq 0$, $\forall i = 2, \dots, N \Rightarrow$ *The solution of* (2.28) $\exists$ *for* $0 \leq t < \infty$.

Proof. 1st claim: System stays in finite region, i.e., $|x_i(t)| \leq \text{const}\,\forall t$, because:

$$|x_i(t)|^2 \leq \frac{1}{|a_i|} \sum_j |a_j||x_j|^2 = \frac{|I(t)|}{|a_i|} = \text{const} \quad \checkmark \tag{2.32}$$

2nd claim: All pairs $k \neq l$ have fixed minimal distance $|x_k(t) - x_l(t)|$, i.e., velocity is always finite $\forall t < \infty$, because:

$$
\begin{aligned}
&- \underbrace{a_k a_l}_{>0} \ln |x_k(t) - x_l(t)| = 4\pi H(t) + \sum_{\substack{i \neq j \\ (i,j) \neq (k,l)}} \sum a_i a_j \ln \underbrace{|x_i(t) - x_j(t)|}_{\leq |x_i| + |x_j|} \\
&\overset{(2.32)}{\leq} 4\pi H(t) + \sum_{\substack{i \neq j \\ (i,j) \neq (k,l)}} \sum a_i a_j \ln \left(\sqrt{\frac{|I|}{|a_i|}} + \sqrt{\frac{|I|}{|a_j|}} \right) =: C = \text{const} \quad \forall t.
\end{aligned}
$$

$$
\Rightarrow |x_k(t) - x_l(t)| \geq \exp\left(-\frac{C}{a_k a_l} \right) > 0 \quad \forall t \checkmark
$$

■

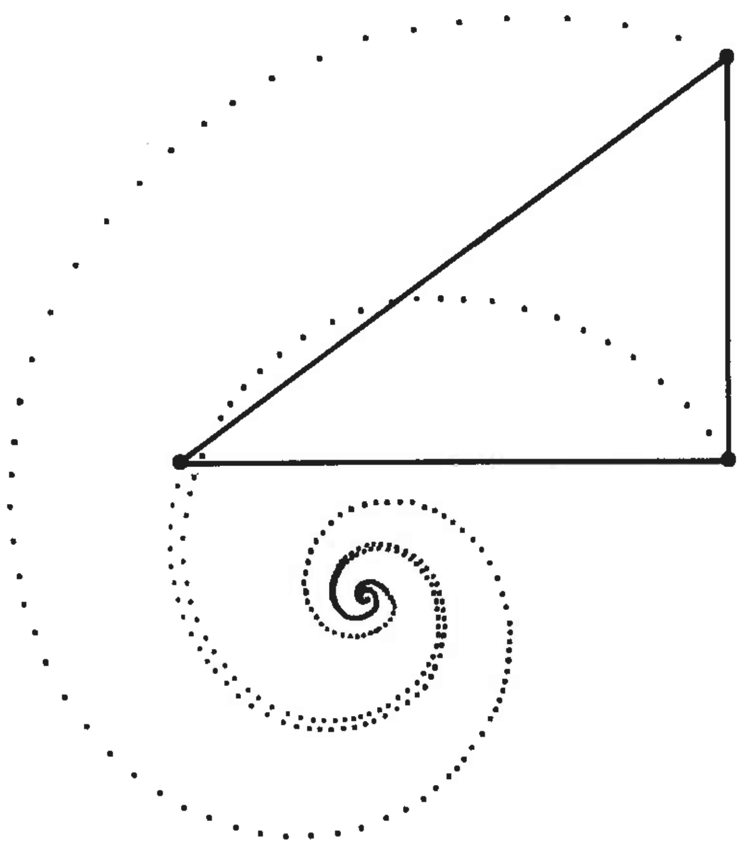
For different signs of a_i and $N \geq 3$ a "collapse" (i.e. $x_i(T^*) = x_j(T^*)$) is possible in finite time.

Example 2.25. $N = 3, a_1 = a_2 = 2, a_3 = -1;$

$x_1 = (-1, 0)^\top, x_2 = (1, 0)^\top, x_3 = (1, \sqrt{2})^\top$

$B = \left(-\frac{1}{3}, -\frac{\sqrt{2}}{3}\right)^\top$ . . . vortex center,

self-similar evolution, collapse at $T^* = 3\sqrt{2}\pi$.



After collapse: continues as (stationary) 1-vortex-flow; is not time-reversible!

□

Due to 2.24 the system stays in finite region for $\operatorname{sign} a_i = \operatorname{sign} a_1$; velocities also stay finite. Generalisation:

Theorem 2.26. *Suppose:*

$$\forall J \subset \{1, \dots, N\} : \sum_{i \in J} a_i \neq 0\,. \tag{2.33}$$

Then $\forall R > 0,\, T > 0$*:* $\exists \tilde{R} = \tilde{R}(a_i, R, N, T)$ *(independently of* $x_1, \dots, x_N$ *!) with*

$$x_1, \dots, x_N \in K_R(0) \quad \Rightarrow \quad x_i(t) \in K_{\tilde{R}}(0) \quad \forall i = 1, \dots, N; \forall 0 \leq t \leq T$$

(if trajectory exists up to that time).

Proof. Corollary 4.2.1 [MP] ■

Rem: Condition (2.33) is necessary – see Ex. 2.23, 3rd case with $x_1 \to x_2$.

Using this one can show:

Theorem 2.27. *Suppose that* $\forall J \subset \{1, \dots, N\} : \sum_{i \in J} a_i \neq 0, N \geq 3.$

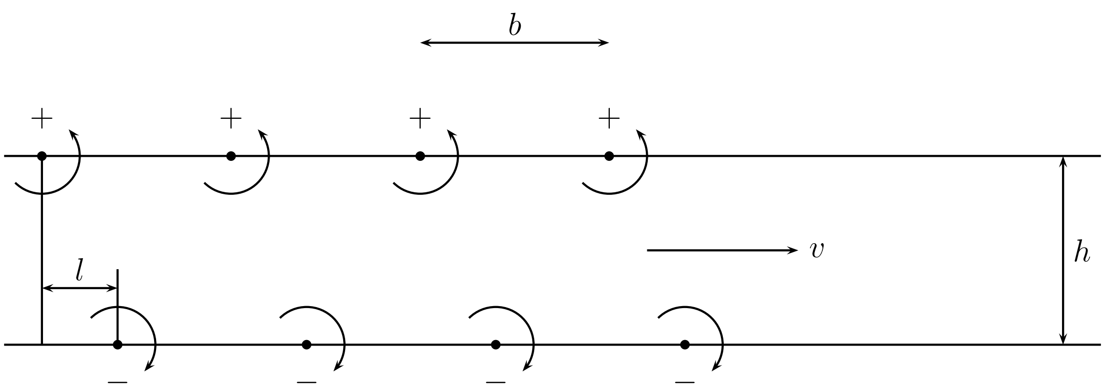
$\Rightarrow$ *for* almost all *initial conditions* $(x_1, \dots, x_N) \in \mathbb{R}^{2N}$:

$\exists$ *global solution* $(x_1(t), \dots, x_N(t))$ *of* (2.28)*;i.e.: let* $A \subset \mathbb{R}^{2N}$ *be bounded and* $B \subset A$ *the set of initial conditions which lead to a collapse in finite time. Then:*

$\mu(B) = 0.$

Proof. Th. 4.2.2 [MP] ■

Example 2.28 (von Kármán vortex street)**.**
• ∞ many vortices of intensity $\pm a$



System is subject to rigid translation with constant $v, \forall t > 0$.

- Application: Flow around rigid body $\Rightarrow$ viscosity (only important near surface) produces counter-rotating vortices, then: transport of vortices by Euler flow for (quite) long time
- vortex street for suitable a, b, h, l linearly stable. □

References: [MP] §4.1-3

2.4 Boundary layers for Navier-Stokes equations

Consider incompressible, homogeneous (scaled) Navier-Stokes equations with no-slip boundary conditions:

$$\begin{cases} u_t + (u\cdot\nabla)u + \nabla p &= \frac{1}{Re}\Delta u \quad ,\Omega \\ \operatorname{div} u &= 0 \quad ,\Omega \\ u &= 0 \quad ,\partial\Omega \\ u(x,0) &= u_0(x) \quad ,\Omega \end{cases} \tag{2.34}$$

In "interior" of Ω: friction term $\nu_0\Delta u$ often negligible in contrast to convective term $(u\cdot\nabla)u$ $\to$ Euler equations (easier to solve).

In Boundary layer at $\partial\Omega$: friction term essential, because u "small" and influence of boundary conditions.

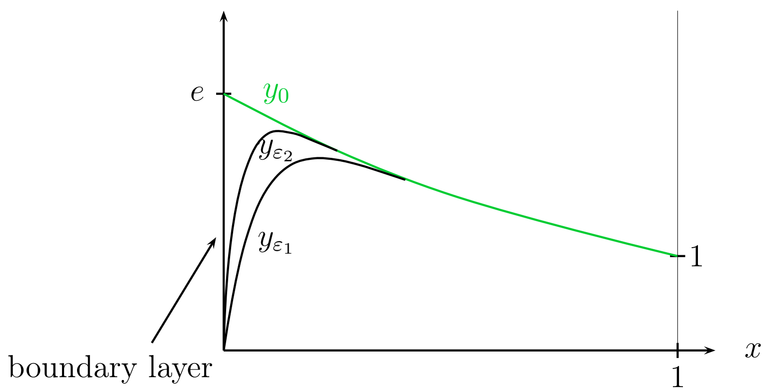
Aim: coupling of Euler equations in interior of Ω with boundary layer equations.

Model problem for *Method of asymptotic expansion*:

$$\begin{cases} \varepsilon y'' + 2y' + 2y = 0\,, \quad 0 < x < 1\,, \quad \varepsilon \ll 1\,, \\ y(0) = 0,\ y(1) = 1 \end{cases} \tag{2.35}$$

Exact solution: $y_\varepsilon(x) = \frac{1}{e^{\lambda_1} - e^{\lambda_2}}\left(e^{\lambda_1 x} - e^{\lambda_2 x}\right) \approx e\left(e^{-x} - e^{-\frac{2x}{\varepsilon}}\right) \xrightarrow{\varepsilon\to 0, x>0} e^{1-x}$,

$$\lambda_1 = \frac{-1+\sqrt{1-2\varepsilon}}{\varepsilon} \overset{\text{Taylor}}{\approx} -1\,,\ \lambda_2 = \frac{-1-\sqrt{1-2\varepsilon}}{\varepsilon} \overset{\text{Taylor}}{\approx} -\frac{2}{\varepsilon} + 1$$



$y_0 = e^{1-x}$ solves *reduced equation*

$$\begin{cases} 2y' + 2y &= 0, \\ y(1) &= 1; \end{cases} \tag{2.36}$$

is for $x \gg \varepsilon$ good approximation for y_ε, but not for $x \approx 0$.

Idea of asymptotic expansion: approximation of solution of (2.35), seperatly on $(0, \delta(\varepsilon))$ and $(\delta(\varepsilon), 1)$; here $\delta(\varepsilon) = O(\varepsilon)$.

Step 1 (outer expansion):

Formal ansatz for solution on $(\delta(\varepsilon), 1)$:

$$y(x) = y_0(x) + \varepsilon\, y_1(x) + \varepsilon^2\, y_2(x) + \dots$$

Rem.: Convergence of this "series" does not matter as it is always truncated after a few terms.

Plug into (2.35) $\Rightarrow$

$$\begin{aligned} \varepsilon^0(2y_0' + 2y_0) + \varepsilon^1(y_0'' + 2y_1' + 2y_1) + \varepsilon^2(y_1'' + 2y_2' + 2y_2) + \dots &= 0 \\ \varepsilon^0\, y_0(1) + \varepsilon^1\, y_1(1) + \varepsilon^2\, y_2(1) + \dots &= 1 \end{aligned}$$

Equating the coefficients suggests:

$$\begin{aligned} 2y_0' + 2y_0 = 0 \quad &, \quad y_0(1) = 1 \\ y_0'' + 2y_1' + 2y_1 = 0 \quad &, \quad y_1(1) = 0 \\ y_1'' + 2y_2' + 2y_2 = 0 \quad &, \quad y_2(1) = 0 \\ &\vdots \end{aligned} \tag{2.37}$$

$\Rightarrow y_0(x) = e^{1-x}, \dots$

Step 2 (inner expansion):

The inner expansion should approximate the solution on $(0, \delta(\varepsilon))$.

Let $\xi := \frac{x}{\varepsilon}$ (fast variable), $Y(\xi) := y(\varepsilon\,\xi)$.

$Y(\xi)$ satisfies

$$\frac{1}{\varepsilon} Y'' + \frac{2}{\varepsilon} Y' + 2Y = 0\,, \quad Y(0) = 0\,. \tag{2.38}$$

Expansion ansatz:

$$Y(\xi) = Y_0(\xi) + \varepsilon\, Y_1(\xi) + \varepsilon^2\, Y_2(\xi) + \dots$$

Plug into (2.38) $\Rightarrow$

$$\varepsilon^{-1}[Y_0'' + 2Y_0'] + \varepsilon^0[Y_1'' + 2Y_1' + 2Y_0] + \varepsilon[Y_2'' + 2Y_2' + 2Y_1] + \dots = 0$$

Equating coefficients suggests:

$$\begin{aligned} Y_0'' + 2Y_0' = 0 \quad &, \quad Y_0(0) = 0 \\ Y_1'' + 2Y_1' + 2Y_0 = 0 \quad &, \quad Y_1(0) = 0 \\ Y_2'' + 2Y_2' + 2Y_1 = 0 \quad &, \quad Y_2(0) = 0 \end{aligned} \tag{2.39}$$

$\Rightarrow Y_0(\xi) = a(1 - e^{-2\xi})$ for some $a \in \mathbb{R}$.

Step 3 (matching):

Compatibility condition for y_0 and Y_0 for $\varepsilon \to 0$ (Y_0 gives boundary layer transition between boundary condition at $x = 0$ and $y_0(\delta(\varepsilon))$; for $\varepsilon > 0$ it is still discontinuous):

$$\lim_{\xi\to\infty} Y_0(\xi) \stackrel{!}{=} \lim_{x\to 0} y_0(x) \quad \Rightarrow \quad a = e.$$

Step 4 (composite solution):

$$\tilde{y}(x) := \begin{cases} Y_0(\frac{x}{\varepsilon}), & x \in (0, \delta(\varepsilon)) \\ y_0(x), & x \in (\delta(\varepsilon), 1) \end{cases}$$

is discontinuous and *not* an approximation of order $O(\varepsilon)$ to the exact solution y (compare for $\delta(\varepsilon) = \varepsilon :\ y_0(\varepsilon) = e^{1-\varepsilon},\ y_\varepsilon(\varepsilon)$).

Step 5 (uniform approximation):

$$\hat{y}(x) := Y_0\left(\frac{x}{\varepsilon}\right) + y_0(x) - \lim_{x\to 0} y_0(x) = \cdots = e\left(e^{-x} - e^{-\frac{2x}{\varepsilon}}\right) \qquad \text{(cf. Taylor expansion of } y_\varepsilon)$$

is *uniform approximation (w.r.t.* $x \in [0,1]$*)* of order $O(\varepsilon)$ (follows from Taylor expansion of y_ε).

Rem.: In $\hat{y}$ the sum of the last two terms vanishes for $x \to 0$, as well as the first and third term for $x \to \infty$. For small and large x one thus obtains $\tilde{y}(x) \approx \hat{y}(x)$.

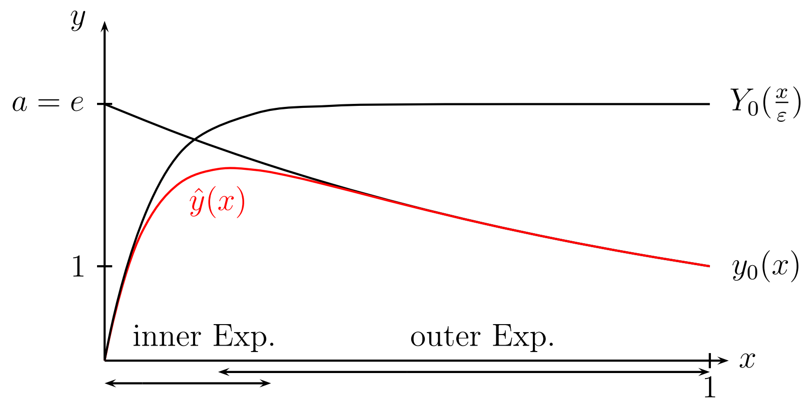
Remark 2.29. 1) In the outer expansion $\varepsilon y''$ plays no role, but in the inner expansion - because of rescaling to $\xi = \frac{x}{\varepsilon}$.

2) The further expansion terms $y_1(x), Y_1(\xi)$ can be calculated from the *inhomogeneous* ODEs in (2.37) resp. (2.39).

3) General inner expansion with $\xi := \frac{x}{\varepsilon^\alpha}$ and

$$Y(\xi) = Y_0(\xi) + \varepsilon^\beta Y_1(\xi) + \varepsilon^{2\beta} Y_2(\xi) + \ldots$$

Plausible values for $\alpha > 0$, $\beta > 0$ can be found by inserting into ODE and balancing dominant ε-terms (i.e. smallest ε-exponents). Aim: as many such terms as possible.



Prandtl's boundary layer equations (1904)

Consider 2D Navier-Stokes equations above a flat plate, $u = (v, w)^\top \in \mathbb{R}^2$; $(x, y)^\top \in \Omega := \mathbb{R} \times \mathbb{R}^+$; let $\varepsilon = \frac{1}{Re} \ll 1$ (but fixed):

$$\begin{cases} \partial_t v + v\,\partial_x v + w\,\partial_y v + \partial_x p &= \varepsilon \Delta v \\ \partial_t w + v \partial_x w + w\,\partial_y w + \partial_y p &= \varepsilon \Delta w \\ \partial_x v + \partial_y w &= 0 \\ v|_{y=0} = w|_{y=0} &= 0 \\ v(0, x, y) = v_I(x, y); & w(0, x, y) = w_I(x, y) \end{cases} \tag{2.40}$$

Step 1 (outer expansion): Ansatz ("away from $\{y = 0\}$"):

$$\begin{aligned} v &= v_0 + \varepsilon\, v_1 + \varepsilon^2\, v_2 + \dots \\ w &= w_0 + \varepsilon\, w_1 + \varepsilon^2\, w_2 + \dots \\ p &= p_0 + \varepsilon\, p_1 + \varepsilon^2\, p_2 + \dots \end{aligned}$$

Plugging into (2.40) gives in lowest order (ε^0) the Euler equations:

$$\begin{cases} \partial_t v_0 + v_0\,\partial_x v_0 + w_0\,\partial_y v_0 + \partial_x p_0 &= 0 \\ \partial_t w_0 + v_0 \partial_x w_0 + w_0\,\partial_y w_0 + \partial_y p_0 &= 0 \\ \partial_x v_0 + \partial_y w_0 &= 0 \\ v_0(0, x, y) = v_I(x, y); & w_0(0, x, y) = w_I(x, y) \end{cases} \tag{2.41}$$

(but no BC at $y = 0$)

Step 2 (inner expansion):

We expect large changes of the solution in y-direction, but not in x-direction $\Rightarrow$ Scaling ansatz near $\{y = 0\}$:

$$T := t,\ X := x,\ Y := \frac{y}{\varepsilon^\alpha},\ \text{with } \alpha > 0 \text{ to be determined;}$$

$$\begin{aligned} V(T, X, Y) &:= v(t, x, \varepsilon^\alpha Y), \\ W(T, X, Y) &:= w(t, x, \varepsilon^\alpha Y), \\ P(T, X, Y) &:= p(t, x, \varepsilon^\alpha Y). \end{aligned}$$

Plug into (2.40):

$$\begin{cases} \partial_T V + V\,\partial_X V + \varepsilon^{-\alpha}\, W\,\partial_Y V + \partial_X P = \varepsilon\,\partial_X^2 V + \varepsilon^{1-2\alpha}\,\partial_Y^2 V \\ \partial_T W + V\,\partial_X W + \varepsilon^{-\alpha}\, W\,\partial_Y W + \varepsilon^{-\alpha}\,\partial_Y P = \varepsilon\,\partial_X^2 W + \varepsilon^{1-2\alpha}\,\partial_Y^2 W \\ \partial_X V + \varepsilon^{-\alpha}\,\partial_Y W = 0 \\ V|_{Y=0} = W|_{Y=0} = 0 \end{cases} \tag{2.42}$$

Expansion ansatz for V, W, P:

$$\begin{aligned} V &= V_0 + \varepsilon^{\beta} V_1 + \varepsilon^{2\beta} V_2 + \dots \\ W &= W_0 + \varepsilon^{\beta} W_1 + \varepsilon^{2\beta} W_2 + \dots \\ P &= P_0 + \varepsilon^{\beta} P_1 + \varepsilon^{2\beta} P_2 + \dots \end{aligned} \tag{2.43}$$

with $\beta > 0$ to be determined.

Plugging into 3rd equation of (2.42) $\Rightarrow$

$$\left[\partial_X V_0 + \varepsilon^{\beta}\partial_X V_1 + \varepsilon^{2\beta}\partial_X V_2 + \dots\right] + \varepsilon^{-\alpha}\left[\partial_Y W_0 + \varepsilon^{\beta}\partial_Y W_1 + \varepsilon^{2\beta}\partial_Y W_2 + \dots\right] = 0$$

Leading ε-power is $\partial_Y W_0$; this suggests:

$$\partial_Y W_0 = 0,\ W_0(T, X, 0) = 0, \quad \forall T, X \Rightarrow \boxed{W_0 \equiv 0\ .}$$

Hence the vertical velocity in the boundary is of order at most $O(\varepsilon^{\beta})$.

Balance of next hieher ε-power suggests $\alpha = \beta$, hence

$$\boxed{\partial_X V_0 + \partial_Y W_1 = 0.}$$

Inserting (2.43) into 1st equation of (2.42) $\Rightarrow$

$$\begin{aligned} &[\partial_T V_0 + \varepsilon^{\alpha}\,\partial_T V_1 + \dots] + [V_0 + \varepsilon^{\alpha}\,V_1 + \dots]\cdot[\partial_X V_0 + \varepsilon^{\alpha}\,\partial_X V_1 + \dots] \\ &+\varepsilon^{-\alpha}\,[0 + \varepsilon^{\alpha}\,W_1 + \dots]\cdot[\partial_Y V_0 + \varepsilon^{\alpha}\,\partial_Y V_1 + \dots] + [\partial_X P_0 + \varepsilon^{\alpha}\,\partial_X P_1 + \dots] \\ &= \varepsilon\left[\partial_X^2 V_0 + \varepsilon^{\alpha}\,\partial_X^2 V_1 + \dots\right] + \varepsilon^{1-2\alpha}\left[\partial_Y^2 V_0 + \varepsilon^{\alpha}\,\partial_Y^2 V_1 + \dots\right]. \end{aligned}$$

If $1 - 2\alpha < 0$, there was only one leading term: $\partial_Y^2 V_0 = 0$.

The choice $1 - 2\alpha = 0$ gives the maximal number of leading terms:

$$\boxed{\partial_T V_0 + V_0\,\partial_X V_0 + W_1\,\partial_Y V_0 + \partial_X P_0 = \partial_Y^2 V_0,}$$

and $\alpha = \beta = \frac{1}{2}$ gives the bondary layer thickness $\delta(\varepsilon) = O(\varepsilon^{\frac{1}{2}})$.

Inserting (2.43) into 2nd equation of (2.42) $\Rightarrow$

$$\begin{aligned} &\left[\partial_T W_0 + \varepsilon^{\frac{1}{2}}\,\partial_T W_1 + \dots\right] + \left[V_0 + \varepsilon^{\frac{1}{2}}\,V_1 + \dots\right]\cdot\left[0 + \varepsilon^{\frac{1}{2}}\,\partial_X W_1 + \dots\right] \\ &+\varepsilon^{-\frac{1}{2}}\left[0 + \varepsilon^{\frac{1}{2}}\,W_1 + \dots\right]\cdot\left[0 + \varepsilon^{\frac{1}{2}}\,\partial_Y W_1 + \dots\right] + \varepsilon^{-\frac{1}{2}}\left[\partial_Y P_0 + \varepsilon^{\frac{1}{2}}\,\partial_Y P_1 + \dots\right] \\ &= \varepsilon\left[0 + \varepsilon^{\frac{1}{2}}\,\partial_X^2 W_1 + \dots\right] + \left[0 + \varepsilon^{\frac{1}{2}}\,\partial_Y^2 W_1 + \dots\right]. \end{aligned}$$

For the leading order we have $\boxed{\partial_Y P_0 = 0.}$ (Pressure is const in Y in boundary layer.)

Step 3 (matching):

Matching conditions:

$$\begin{array}{rrcl} & \lim_{Y\to\infty} V_0(T,X,Y) & \overset{!}{=} & \lim_{y\to 0} v_0(t,x,y) \\ [0 = W_0 =] & \lim_{Y\to\infty} W_0(T,X,Y) & \overset{!}{=} & \lim_{y\to 0} w_0(t,x,y) \\ [P_0(T,X) =] & \lim_{Y\to\infty} P_0(T,X,Y) & \overset{!}{=} & \lim_{y\to 0} p_0(t,x,y) \end{array}$$

2nd row and $W_0 \equiv 0$ lead to: $w_0(t,x,0) = 0$ (i.e., typical Euler BC $u_0 \cdot \nu = 0$.)

Solution step 1: Solve the Euler equations (2.41) for v_0, w_0, p_0 with $w_0(t,x,0) = 0$ in exterior domain (for $y > 0$).
The 3rd line of the coupling conditions and $\partial_Y P_0 = 0$ give $P_0(T,X) = p_0(t,x,0)$, $\forall T = t,\ X = x$.

Hence: pressure in boundary layer = pressure of outer flow at boundary ($y = 0$).

Solution step 2: Using the functions $p_0|_{y=0}$, $v_0|_{y=0}$ which are known from the outer flow, solve the *Prandtl boundary layer equations* in the boundary layer. (for V_0, W_1; $X \in \mathbb{R}$, $0 < Y < \infty$):

$$\left\{ \begin{array}{rcl} \partial_T V_0 + V_0\, \partial_X V_0 + W_1\, \partial_Y V_0 + \partial_X(p_0|_{y=0}) & = & \partial_Y^2 V_0, \\ V_0|_{Y=0} = W_1|_{Y=0} & = & 0, \quad \text{(from (2.42), last line)} \\ \lim_{Y\to\infty} V_0(T,X,Y) & = & v_0(t,x,0), \\ \partial_X V_0 + \partial_Y W_1 & = & 0, \quad \text{(from (2.42), 3rd line)} \\ V_0(0,X,Y) & = & v_I(x,0),\ Y > 0,\ \text{if } u_I \text{ contains no boundary layer.} \end{array} \right.$$

This is a degenerate parabolic equation for V_0 (the term $\partial_X^2 V_0$ is missing), wherein V_0 and W_1 are coupled by a linear equation of first order.

Combined approximation:

$$\begin{array}{rcll} \hat{v}(t,x,y) & = & V_0\left(t, x, \frac{y}{\varepsilon^{\frac{1}{2}}}\right) + v_0(t,x,y) - \underbrace{v_0(t,x,0)}_{\lim_{y\to 0} v_0}, & \\ \hat{w}(t,x,y) & = & w_0(t,x,y), & \text{(no correction of order } O(\varepsilon^0) \text{ because } W_0 \equiv 0), \\ \hat{p}(t,x,y) & = & p_0(t,x,y), & \text{(because pressure=const in } Y \text{ in boundary layer).} \end{array}$$

Result: In a boundary layer of vertical thickness $O(\sqrt{\varepsilon})$ the horizontal velocity component v_0 is corrected such that at $y = 0$ the no-slip condition $u = 0$ is satisfied. The vertical velocity component already satisfies $w_0(t,x,0) = 0$ because it solves the Euler equations and hence does not need to be corrected.

References: [EGK] §6.6

3 Theory of elasticity

Aim: Model how a body deforms subject to external forces.

3.1 Notation

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$: *Reference configuration* = region occupied by the body when no forces are applied
- $x \in \Omega$: particle
- $\Phi : \Omega \to \mathbb{R}^d$: *deformation field*. The particle x is moved by the deformation to $\Phi(x)$ (description in Lagrance coordinates; Φ does not have to be volume preserving)
- $\frac{\partial \Phi}{\partial x} \in \mathbb{R}^{d\times d}$: *deformation gradient*. We only consider orientation preserving deformations, i.e., such that $\det \frac{\partial \Phi}{\partial x} > 0$ (i.e. no reflections)
- $u(x) := \Phi(x) - x$: *displacement field*

We now consider the relative change of length effected by Φ.

Let $\Delta x \in \mathbb{R}^d$ be a small distance between 2 material points $\to$

$$\frac{\|\Phi(x+\Delta x) - \Phi(x)\|^2}{\|(x+\Delta x) - x\|^2} = \frac{\|\frac{\partial \Phi}{\partial x}(x) \cdot \Delta x + \mathcal{O}(\|\Delta x\|^2)\|^2}{\|\Delta x\|^2}$$
$$= \frac{(\Delta x)^\top \cdot \left(\frac{\partial \Phi}{\partial x}(x)\right)^\top \cdot \frac{\partial \Phi}{\partial x}(x) \cdot \Delta x}{\|\Delta x\|^2} + \mathcal{O}(\|\Delta x\|)$$

Definition 3.1. *The symmetric matrix*

$$C := \frac{\partial \Phi}{\partial x}^\top \cdot \frac{\partial \Phi}{\partial x} = \left(\frac{\partial u}{\partial x} + I\right)^\top \cdot \left(\frac{\partial u}{\partial x} + I\right) \tag{3.1}$$

is called Cauchy-Green strain tensor *and describes the local relative change of length in the body.*

We have

$$C = I \;\Leftrightarrow\; \exists Q \in \underbrace{O(d)}_{\text{orthog. matrices in } \mathbb{R}^d};\; b \in \mathbb{R}^d \;:\; \Phi(x) = Q \cdot x + b$$

(hence for rigid body movements there is no change of length).

Definition 3.2. *The symmetric matrix*

$$E := \frac{1}{2}(C - I) \;=\; \frac{1}{2}\left(\frac{\partial u}{\partial x}^\top + \frac{\partial u}{\partial x} + \frac{\partial u}{\partial x}^\top \cdot \frac{\partial u}{\partial x}\right)$$

is called Green strain tensor *and vanishes for such rigid body movements (and is quadratic in u).*
The matrix

$$\epsilon := \frac{1}{2}\left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial x}^\top\right) \approx E \qquad \textit{(for small variations of the displacement)}$$

is called linear strain tensor.

3.2 Hyperelastic materials

A body is deformed by some force. The work done is saved as *deformation energy*. An *elastic* body completely returns this energy if the applied force is removed. A material is called *hyperelastic* if the deformation energy depends pointwise on the Cauchy-Green strain tensor C:

$$E_{def} = \int_\Omega W(C(x))\mathrm{d}x,$$

with *energy density* $W : \{A \in \mathbb{R}^{d\times d} \,|\, A = A^\top\} \to \mathbb{R}$

(resp. general $W(x, C)$ for inhomogeneous materials).

Ex.: Rubber (isotropic; linear elasticity would be too inaccurate)

We only consider *isotropic* materials, i.e., material properties are the same in all directions $\Rightarrow W$ is invariant under (rigid body) rotations $\Rightarrow \tilde{W}(E) := W(\underbrace{I + 2E}_{=C})$ depends only on $\operatorname{Sp} E$, $\operatorname{Sp}(E^2)$ (for $d = 2$) and for $d = 3$ additionally on $\det E$. Derivation analogous to the proof of the form of the viscous stress tensor $\sigma\left(\frac{\partial u}{\partial x}\right)$ in §2.2: E is symmetric, hence diagonalisable $\to W$ only depends on its eigenvalues.

Lemma 3.3 (Hooke's law)**.** *Let $E = 0$ be a local minimum of $\tilde{W}$ with (w.l.o.g.) $\tilde{W}(0) = 0$. Then it holds in quadratic approximation:*

$$\tilde{W}(E) \approx \frac{1}{2}\lambda(\mathrm{Sp}\, E)^2 + \mu\, \mathrm{Sp}(E^2),$$

with Lamé-constants $\lambda, \mu \in \mathbb{R}$ (cf. (2.6)*: $\sigma = \lambda(\operatorname{div} u)I + 2\mu D$).*

Proof (for $d = 3$).

$$\text{Let} \quad \tilde{W}(E) = \hat{W}(\mathrm{Sp}\, E, \mathrm{Sp}(E^2), \underbrace{\det E}_{\text{cubic in } E}) \quad \text{with} \quad \hat{W} : \mathbb{R}^3 \to \mathbb{R}.$$

If $E = 0$ is a local minimum of $\tilde{W}$, Taylor's formula gives

$$\tilde{W}(E) = \underbrace{\hat{W}(0,0,0)}_{=0} + \underbrace{\partial_1 \hat{W}(0,0,0)}_{=0} \mathrm{Sp}\, E + \frac{1}{2} \underbrace{\partial_1^2 \hat{W}(0,0,0)}_{=:\lambda} (\mathrm{Sp}\, E)^2 + \underbrace{\partial_2 \hat{W}(0,0,0)}_{=:\mu} \mathrm{Sp}(E^2) + \mathcal{O}(\|E\|^3).$$

■

Rem: Hooke's law corresponds linear material law (cf. force-deformation relation in spring)

3.3 Variational formulation

Let $\partial\Omega = \Gamma_D \cup \Gamma_N$ (Dirichlet- resp. Neumann-boundary). Assume the body is fixed at Γ_D and on Γ_N an external surface force b is acting. Moreover, assume that on Ω a volume force is acting, e.g. gravitation. The displacement u caused by the forces implicates a total energy

$$E_{tot}(u) = \underbrace{\int_\Omega W(C(u(x)))\mathrm{d}x}_{\text{deformation energy}} - \underbrace{\int_\Omega f \cdot u \mathrm{d}x}_{\substack{\text{work} \\ \text{of volume force}}} - \underbrace{\int_{\Gamma_N} b \cdot u \mathrm{d}S}_{\substack{\text{work} \\ \text{of surface force}}} \tag{3.2}$$

Rem: domain of integration Ω ... undeformed reference configuration

Aim: find equation for displacement u — by minimizing $E_{tot}(u)$.

Admissible displacements satisfy $u|_{\Gamma_D} = 0$.

Let u be the minimizing displacement and v another admissible displacement, i.e., $v|_{\Gamma_D} = 0$.

$\Rightarrow \Psi : \mathbb{R} \to \mathbb{R},\ \Psi(t) := E_{tot}(u + t\, v)$ has a minimum at $t = 0$ so

$$0 \;=\; \Psi'(0) = \int_\Omega \underbrace{\left[\frac{\mathrm{d}W}{\mathrm{d}C}(C(u))\right]}_{\frac{\partial W}{\partial C_{ij}} \in \mathbb{R}^{d\times d}} : \underbrace{\left[\frac{\mathrm{d}C}{\mathrm{d}u}(v)\right]}_{\in \mathbb{R}^{d\times d}} \mathrm{d}x - \int_\Omega f \cdot v \,\mathrm{d}x - \int_{\Gamma_N} b \cdot v \,\mathrm{d}S \tag{3.3}$$

$\forall$ admissible $v \Rightarrow$ gives minimality condition for u.

$\Psi'(0) = \delta E_{tot}(u, v)$ ... *first variation* of E_{tot} at u in direction v

Notation:

- $A : B := \sum_{i\,j} A_{ij}\, B_{ij} = \mathrm{Sp}(A^\top \cdot B)$ ... Frobenius scalar product for (real) matrices.
- $\left(\frac{\partial v}{\partial x}\right)_{ij} = \left(\frac{\partial v_i}{\partial x_j}\right)$
- $(\mathrm{div}\, A)_i = \sum_j \partial_{x_j} A_{ij}$ ... divergence of a matrix function $A(x)$ is a vector field.

First variation of $E_2(u) := \int_\Omega f \cdot u \,\mathrm{d}x$:

$$\frac{\mathrm{d}\Psi_2}{\mathrm{dt}} = \frac{\mathrm{d}}{\mathrm{dt}} \int\limits_\Omega f \cdot (u + t\, v)\, \mathrm{d}x = \int\limits_\Omega f \cdot v \,\mathrm{d}x \quad \checkmark$$

next aim: representation of $\frac{\mathrm{d}W}{\mathrm{d}C}(C) : \frac{\mathrm{d}C}{\mathrm{d}u}(v)$.
- $\forall$ (small) symmetric matrices $\Delta \in \mathbb{R}^{d\times d}$:

$$W(C + \Delta) \overset{\text{Taylor}}{=} W(C) + \left[\frac{\mathrm{d}W}{\mathrm{d}C}(C)\right] : \Delta + \mathcal{O}(\|\Delta\|^2)$$

The matrix $\Sigma := 2\frac{\mathrm{d}W}{\mathrm{d}C}(C)$ is called *2nd Piola-Kirchhoff stress tensor* $\Sigma_{ij} = 2\frac{\partial W}{\partial C_{ij}}$. Because C is symmetric, Σ is symmetric; in general it depends on $\frac{\partial u}{\partial x}$.

- $\forall$ (small) $t > 0$: $C(u + t\,v) = C(u) + \frac{\mathrm{d}C}{\mathrm{d}u}(v)t + \mathcal{O}(t^2)$

$$\text{Laut (3.1):} \quad C(u + t\,v) = \left(\frac{\partial u}{\partial x} + t\,\frac{\partial v}{\partial x} + I\right)^\top \cdot \left(\frac{\partial u}{\partial x} + t\,\frac{\partial v}{\partial x} + I\right)$$
$$= C(u) + t\left[\left(\frac{\partial u}{\partial x} + I\right)^\top \cdot \frac{\partial v}{\partial x} + \frac{\partial v}{\partial x}^\top \cdot \left(\frac{\partial u}{\partial x} + I\right)\right] + \mathcal{O}(t^2)$$

$\Rightarrow \frac{\mathrm{d}C}{\mathrm{d}u}(v) = \left(\frac{\partial u}{\partial x} + I\right)^\top \cdot \frac{\partial v}{\partial x} + \frac{\partial v}{\partial x}^\top \cdot \left(\frac{\partial u}{\partial x} + I\right)$ ... directional derivative of C at u in direction v

- From (3.3): $\displaystyle\int_\Omega f\cdot v\,\mathrm{d}x + \int_{\Gamma_N} b\cdot v\,\mathrm{d}S = \int_\Omega \left[\frac{\mathrm{d}W}{\mathrm{d}C}(C)\right] : \left[\frac{\mathrm{d}C}{\mathrm{d}u}(v)\right]\mathrm{d}x$

$$= \frac{1}{2}\int_\Omega \Sigma : \left[\left(\frac{\partial u}{\partial x}+I\right)^\top\cdot\frac{\partial v}{\partial x} + \frac{\partial v}{\partial x}^\top\cdot\left(\frac{\partial u}{\partial x}+I\right)\right]\mathrm{d}x$$

$$\overset{\Sigma\text{ symm.}}{=} \int_\Omega \Sigma : \left[\left(\frac{\partial u}{\partial x}+I\right)^\top\cdot\frac{\partial v}{\partial x}\right]\mathrm{d}x \overset{(*)}{=} \int_\Omega \left[\left(\frac{\partial u}{\partial x}+I\right)\cdot\Sigma\right] : \frac{\partial v}{\partial x}\,\mathrm{d}x$$

$$\overset{\text{Gauß}}{=} -\int_\Omega \operatorname{div}\left(\left(\frac{\partial u}{\partial x}+I\right)\cdot\Sigma\right)\cdot v\,\mathrm{d}x + \int_{\Gamma_N}\left[\left(\frac{\partial u}{\partial x}+I\right)\cdot\Sigma\cdot n\right]\cdot v\,\mathrm{d}S$$

$\forall$ admissible v and outer normal vector n.

$(*)$ with $\quad A:(B\cdot C) = (B^\top\cdot A):C$

$\Rightarrow$ equation as well for integrand $\Rightarrow$

- *Equations of elasticity theory* (for $\frac{\partial u}{\partial x}$ and $\Sigma = \Sigma\left(\frac{\partial u}{\partial x}\right)$):

$$\begin{cases} -\operatorname{div}\left(\left(\frac{\partial u}{\partial x}+I\right)\cdot\Sigma\right) &= f \text{ in } \Omega \\ \left(\frac{\partial u}{\partial x}+I\right)\cdot\Sigma\cdot n &= b \text{ on } \Gamma_N \end{cases} \tag{3.4}$$

These are the *Euler-Lagrange equations* of E_{tot} in (3.2).

From $\frac{\partial u}{\partial x}$ and $u|_{\Gamma_D} = 0$ we obtain $u(x),\ \forall x\in\Omega$.

3.4 Linear elasticity

Assumptions:

- small displacements u
- small distortion, $E \approx \epsilon$
- Hooke's law holds: $W(C) = \frac{\lambda}{2}(\mathrm{Sp}\,\epsilon)^2 + \mu \underbrace{\epsilon:\epsilon}_{=\mathrm{Sp}(\epsilon^2)}$

$\Rightarrow$ Minimization problem: find admissible displacement u (i.e., satisfying $u|_{\Gamma_D} = 0$), such that

$$E_{tot}(u) = \int_\Omega \left(\frac{\lambda}{2}(\mathrm{Sp}\,\epsilon)^2 + \mu\epsilon:\epsilon - f\cdot u\right)\mathrm{d}x - \int_{\Gamma_N} b\cdot u\,\mathrm{d}S \ \to \min, \tag{3.5}$$

with $\epsilon(u) := \frac{1}{2}\left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial x}^\top\right)$. Further assumption: $\lambda,\mu > 0$

Notation:

$$a(u,v) := \int_\Omega \frac{\lambda}{2} \underbrace{(\operatorname{Sp}\epsilon(u))}_{=\operatorname{div} u} (\operatorname{Sp}\epsilon(v)) + \mu\epsilon(u) : \epsilon(v)\,\mathrm{d}x,$$

$$l(u) := \int_\Omega f \cdot u\,\mathrm{d}x + \int_{\Gamma_N} b \cdot u\,\mathrm{d}S,$$

hence: $J(u) := a(u,u) - l(u) \to \min$

next aim: bilinear form a is coercive on "space of admissible displacements" $H^1_D := \{u \in (H^1(\Omega))^d : u|_{\Gamma_D} = 0\}$.

Lemma 3.4 (Korn's inequality)**.** *Let Ω be a bounded domain with piecewise smooth boundary and $\mu_{d-1}(\Gamma_D) > 0$. $\Rightarrow \exists\, c > 0$ with*

$$\int_\Omega \epsilon(u) : \epsilon(u)\,\mathrm{d}x \geq c \sum_{i=1}^d \|u_i\|^2_{H^1(\Omega)} \qquad \forall u \in H^1_D\,. \tag{3.6}$$

Proof. (here only for smooth u satisfying $u|_{\partial\Omega} = 0$)

We have the formula

$$2\epsilon(u) : \epsilon(u) - \frac{\partial u}{\partial x} : \frac{\partial u}{\partial x} - (\operatorname{div} u)^2 = \operatorname{div}\left(\frac{\partial u}{\partial x} \cdot u - (\operatorname{div} u)\, u\right).$$

$$\Rightarrow \int_\Omega 2\epsilon(u) : \epsilon(u) - \frac{\partial u}{\partial x} : \frac{\partial u}{\partial x} - (\operatorname{div} u)^2\,\mathrm{d}x = \int_\Omega \operatorname{div}\left(\frac{\partial u}{\partial x} \cdot u - (\operatorname{div} u)\, u\right)\mathrm{d}x$$

$$\overset{\text{Gauß}}{=} \int_{\partial\Omega} \left(\frac{\partial u}{\partial x} \cdot u - (\operatorname{div} u)\, u\right) \cdot n\,\mathrm{d}S = 0, \quad \text{da } u|_{\partial\Omega} = 0. \tag{3.7}$$

From (3.7), Poincaré inequality for u_i:

$$2\int_\Omega \epsilon(u) : \epsilon(u)\,\mathrm{d}x \geq \int_\Omega \frac{\partial u}{\partial x} : \frac{\partial u}{\partial x}\,\mathrm{d}x = \sum_{i=1}^d \|\,|\nabla u_i|\,\|^2_{L^2(\Omega)} \geq c_p \sum_{i=1}^d \|u_i\|^2_{H^1(\Omega)},$$

with a constant $c_p > 0$.

for extension of proof: Poincaré inequality also holds for (smooth) u vanishing only on Γ_D. ∎

Rem.: For $d = 1$, (3.6) corresponds to the Poincaré inequality. For $d > 1$, (3.6) is non-trivial because the left hand side includes only the symmetric part of $\frac{\partial u}{\partial x}$, that is $\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$, but not all derivatives separately.

Theorem 3.5. *Let $f \in L^2(\Omega)$, $b \in L^2(\Gamma_N)$. Under the conditions of Lemma 3.4, E_{tot} in (3.5) has a unique minimizer $u \in H^1_D$.*

Proof. The (symmetric) bilinear form a is on H^1_D continuous and coercive (due to Korn's inequality). For a minimum the following (weak formulation) has to hold:

$$0 \stackrel{!}{=} \delta E_{tot}(u, v) \;=\; 2a(u, v) - l(v), \quad \forall v \in H^1_D.$$

Claim follows with Lemma of Lax-Milgram. ∎

[compare: the minimizer of $\frac{1}{2}\|\nabla u\|^2_{L^2} - \int_\Omega f u \mathrm{d}x$ satisfies $-\Delta u = f$.]

Analogously to the derivation of (3.4) one obtains the *linear equations of static elasticity* as *Euler-Lagrange equations* of (3.5):

$$\begin{cases} -\lambda \nabla (\operatorname{div} u) - 2\mu \operatorname{div}(\epsilon(u)) & = f, \;\; \Omega \\ \left(\lambda \operatorname{div} u + 2\mu \frac{\partial u}{\partial x}\right) \cdot n & = b, \;\; \Gamma_N \end{cases} \tag{3.8}$$

This is a linear 2nd order PDE system.

<u>References</u>: [EGK] §5.10, §6.1.9, [Schö] §1,§2

4 Diffusion filtering in image processing

Diffusion filters are

- optical lens attachment for photographic special effects $\to$ blur, softener;
- software-driven, digital image (post)processing, e.g. "Gaussian blur" in *Photoshop*.

Application/Aim: Smoothing of noisy images, blurring of too sharp/hard images, image sharpening, edge detection (e.g. for image segmentation)

We only consider greyscale images with scale $f(x) \in [0,1], x \in \Omega \subset \mathbb{R}^2$. Real-world application: f discrete (pixel) on a bounded region.

Here only $\Omega = \mathbb{R}^2$ to avoid problems with boundary conditions. Moreover, let $f \in L^1(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2)$.

4.1 Linear diffusion filter

Simplest image smoothing by convolution with 2D Gauss function

$$K_\sigma(x) := \frac{1}{2\pi\sigma^2} \exp\left(-\frac{|x|^2}{2\sigma^2}\right)$$

with standard deviation ("width") $\sigma > 0$:

$$(K_\sigma * f)(x) = \int\limits_{\mathbb{R}^2} K_\sigma(x-y) f(y) \mathrm{d}y \tag{4.1}$$

Effects:

- Because $K_\sigma \in C^\infty(\mathbb{R}^2) \Rightarrow K_\sigma * f \in C^\infty(\mathbb{R}^2)$, also for $f \in L^1(\mathbb{R}^2)$.
- In frequency domain:

$$\widehat{K_\sigma * f}(\omega) = \widehat{K_\sigma}(\omega) \cdot \widehat{f}(\omega) \tag{4.2}$$

with $\widehat{f}(\omega) = (\mathcal{F}f)(\omega) := \int\limits_{\mathbb{R}^2} f(x) e^{-i\omega \cdot x} \mathrm{d}x$

Because $\widehat{K_\sigma}(\omega) = 2\pi \exp\left(-\frac{|\omega|^2}{2/\sigma^2}\right)$:

(4.1) is *low pass filter*, which (monotonously) dampens high (spatial) frequencies $\Rightarrow$ edge smoothing, denoising.

Equivalence to linear diffusion filter:

$$\begin{cases} u_t &= \Delta u \quad , \quad x \in \mathbb{R}^2, t > 0 \\ u(x,0) &= f(x) \quad , \quad f \in L^1(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2) \end{cases} \tag{4.3}$$

has the unique solution (e.g. assuming Gaussian decay of u for $|x| \to \infty$):

$$u(x,t) = T_t f = \begin{cases} f(x) & , \quad t = 0 \\ (K_{\sqrt{2t}} * f)(x) & , \quad t > 0. \end{cases}$$

$\{T_t | t \geq 0\}$ ... evolution semigroup of the diffusion equation

Hence: time t corresponds to (spatial) width $\sqrt{2t}$ of the Gauss function; smoothing of image structures up to order σ corresponds to *stopping time* $T = \sigma^2/2$ of diffusion process.

Maximum-minimum-principle:

$$\inf_{\mathbb{R}^2} f \leq u(x,t) \leq \sup_{\mathbb{R}^2} f \quad \text{auf } \mathbb{R}^2 \times [0, \infty)$$

- Images typically contain structures on a large bandwidth of scales (e.g. portrait with resolution of every single pore)
- Often it is a-priori unclear which scale represents the "desired information". $\Rightarrow$ It is desirable to have a representation of the image in different scales.
- Original image f is embedded in evolution process resp.*scale of smoothed/simplified images* $\{u(x,t) | t \geq 0\}$.
- $u(x,t) \overset{t \to \infty}{\longrightarrow} 0$ (uniformly on bounded domains)

  $\Rightarrow$ More and more image structure gets lost. $\Rightarrow$ Only "small" t is practically relevant.
- An image can only be seen as representative of an equivalence class which contains all images of the same object. The difference between two images of a class can be e.g. grey value adjustment, translation, rotation, ...

Numerical aspects:

- Discrete version of convolution (4.1), multiplication (4.2) in frequency domain (via FFT), and discretization of diffusion equation are *not* equivalent.
- For this application mostly explicit finite difference schemes for (4.3).

Disadvantages of linear Gauss filtering:

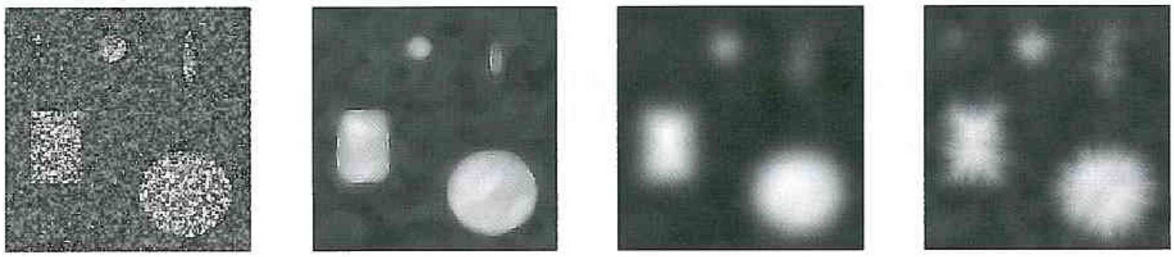


Figure 4.1: noisy original f, diffusion smoothing with *mean curvature equation*, Gaussian diffusion smoothing, diffusion smoothing with anisotropic diffusion orthogonal to the edges [Ma]

a) Isotropic diffusion smoothens noise but also image structures (e.g. edges).

   Local diffusion orthogonal to the edges is not desired.

b) Linear diffusion filters may move edges in the transition from fine to coarse image scale (i.e. for large t).

c) Topology of contour lines can change (in 2D), e.g. splitting in two contour lines when moving to a coarser scale.

d) Smoothing does not commute with (nonlinear, monotonic) mappings F which change contrast or grey value: $T_t(F(f)) \neq F(T_t f)$

(a), (b) can be ameliorated with *nonlinear diffusion filters*; (c), (d) using *morphological equations*.

References: [We] §1.1, [Ma] §10

4.2 Nonlinear diffusion filters

Aim:

- Nonlinear PDEs as improved model of (4.3);

  Image scale $\{T_t f \mid t \geq 0\}$ is still represented by an evolution semigroup $\{T_t \mid t \geq 0\}$.
- Use of *scalar* diffusivity which depends on local properties of the image.
- Extension to adaptive diffusion matrices for anisotropic diffusion filters.

4.2.1 The Perona-Malik model

Model:

scalar diffusivity $g(|\nabla u|^2) > 0$ with

$$g(s) \searrow \;;\quad g(0) = 1, \quad g(s) \overset{s\to\infty}{\longrightarrow} 0$$

e.g.

$$g(s^2) = \frac{1}{1 + s^2/\lambda^2} \quad \text{(with parameter } \lambda > 0\text{)} \tag{4.4}$$

hence:

$$\begin{cases} u_t - \operatorname{div}(g(|\nabla u|^2)\nabla u) & = \; 0 \quad ; x \in \mathbb{R}^2, t > 0 \\ u(x, 0) & = \; f(x) \end{cases} \tag{4.5}$$

Motivation: little diffusion at edges, because there $|\nabla u(x)|$ is large.

Edge sharpening:

1D-variant of (4.5) with flux function $\Phi(s) := sg(s^2)$:

$$u_t = \partial_x(\Phi(u_x)) = \Phi'(u_x)u_{xx} \tag{4.6}$$

For g of (4.4) we have:

$\Phi'(u_x) \geq 0$ for $|u_x| \leq \lambda \Rightarrow$ (4.6) is *forward parabolic*,

$\Phi'(u_x) < 0$ for $|u_x| > \lambda \Rightarrow$ (4.6) ist *backwards parabolic*

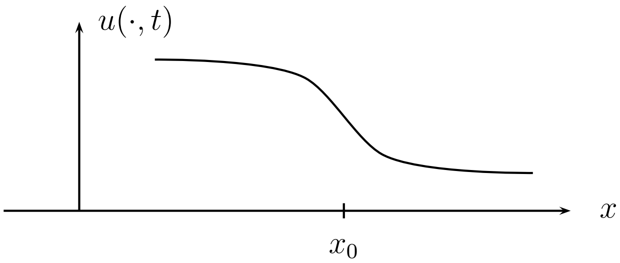
(i.e. indication for *ill-posedness* of (4.6)).

λ is a contrast parameter:

For $|u_x| \leq \lambda$ (low local contrast): smoothing;

for $|u_x| > \lambda$ (high local contrast): edge sharpening (for "small time", then growing oscillations).

We now consider the local behaviour (in x and t) of edge sharpening:



Edge position for a "smoothened edge"

For a "smoothened edge" we define the edge position x_0 (at time t) as the inflection point of u, i.e. as maximum of u_x^2. Hence: $(u_x u_{xx})(x_0) = 0$ (with $u_x(x_0) \neq 0$) and $(u_x u_{xxx})(x_0) < 0$. Calculate $\partial_t(u_x^2)(x_0, t)$:

$$\partial_t(u_x^2) = 2u_x u_{xt} \overset{(4.6)}{=} 2u_x \Phi''(u_x) \underbrace{u_{xx}^2}_{=0 \text{ at } (x_0,t)} + 2\Phi'(u_x) \underbrace{u_x u_{xxx}}_{<0 \text{ an } (x_0,t)} > 0 \text{ at } (x_0, t) \text{ exactly for } \Phi'(u_x) < 0,$$

hence exactly for $|u_x| > \lambda$. Then we have temporal growth of $|u_x(x_0)|$, i.e., edge sharpening.

<u>2D-equation</u> (4.5): Introduction of (local) coordinates ξ, η tangential resp. orthogonal to level curves of $u \Rightarrow$

$$u_t = g(|\nabla u|^2) \underbrace{\Delta u}_{=u_{\xi\xi}+u_{\eta\eta}} + g'(|\nabla u|^2) 2 \underbrace{\nabla^\top u \cdot \frac{\partial^2 u}{\partial x^2} \cdot \nabla u}_{=|\nabla u|^2 u_{\eta\eta}} = \underbrace{g(|\nabla u|^2)}_{>0} u_{\xi\xi} + \underbrace{\Phi'(|\nabla u|)}_{\in\mathbb{R}} u_{\eta\eta}, \quad (4.7)$$

$$\Phi'(s) = g(s^2) + 2s^2 g'(s^2),$$

hence forward diffusion along level curves (e.g. parallel to the edges) and forwards/backwards diffusion (corresponding to sign of Φ') in normal direction.

<u>Results:</u>

- Smoothing of small fluctuations (for $|\nabla u|$ small),
- Edge sharpening (normal to the edges) (for $|\nabla u|$ large);
- PM-filter works very well practically (i.e., numerically) (although tending to be *ill posed*, which is not proven yet though).

  Reason: numerical schemes give "implicit" regularization/stabilization (disappearing for finer and finer meshes).
- Disadvantage: noise (with $|\nabla u|$ large) is misinterpreted as "edge" $\Rightarrow$ is retained or even amplified.

systematic way out with following regularization ...

<u>References</u>: [We] §1.2, [Ma] §10, [TE]

4.2.2 Regularized Perona-Malik model

Replace diffusivity $g(|\nabla u|^2)$ in (4.5) by $g(|\nabla u_\sigma|^2) =: \alpha(x)$ with $u_\sigma := K_\sigma * u \Rightarrow$

$$\begin{cases} u_t = \operatorname{div}(g(|\nabla u_\sigma|^2)\nabla u), t > 0, \\ u(x, 0) = f(x). \end{cases} \quad (4.8)$$

$\sigma > 0$ is another scale parameter: noise on length scale smaller than σ is smoothened.

Consider (4.8) on $\Omega := (0, a_1) \times (0, a_2)$ with "extension by reflection" of $f\big|_\Omega$ on $\mathbb{R}^2$ (necessary for definition of u_σ).

Theorem 4.1. *Let $f \in L^\infty(\Omega)$. $\Rightarrow$ (4.8) has a unique distributional solution $u(x,t)$ with:*

$$u \in C([0,\infty); L^2(\Omega)) \cap L^2_{\text{loc}}(0,\infty; H^1(\Omega)) \cap C^\infty(\overline{\Omega} \times (0,\infty)),$$

$\partial_t u \in L^2_{\text{loc}}(0,\infty; H^2(\Omega))$.

For $a \le f \le b$ u satisfies the minimum/maximum principle:

$$a \le u(x,t) \le b \quad \forall x \in \Omega, t \ge 0.$$

Idea of proof. a) Existence by Schauder fixed point theorem for the mapping $v \mapsto w =: \mathcal{U}(v)$ in $W(0,T) := \left\{ w, \frac{\mathrm{d}w}{\mathrm{d}t} \in L^2(0,T; H^1(\Omega)) \right\}$ for fixed $T > 0$. w solves the linear equation

$$\begin{cases} w_t = \operatorname{div}(g(|\nabla v_\sigma|^2)\nabla w), t > 0 \\ w(x,0) = f(x) \end{cases} \tag{4.9}$$

b) Regularity via "bootstrapping" argument; i.e. from $u(t) \in H^1(\Omega)$ $\forall t > 0$ follows $u(t) \in H^2(\Omega)$ $\forall t > 0$, and so on.

c) Uniqueness & continuous dependence on initial conditions via Gronwall Lemma for difference of two solutions.

d) Minimum/Maximum principle with truncation method.

Details: [CLMC], Th. 2.1 in [We] ∎

Remark 4.2. 1) Iteration of (4.9) converges in $C([0,T]; L^2(\Omega))$ $\forall T > 0$ (see [CLMC]).

2) possible discretization of (4.8): finite differences; $g(|\nabla u_\sigma|^2)$ explicitly, rest implicitly in time [CLMC].

regular grid $(ih, jh, n\Delta t)$,

$$h = \frac{1}{N+1}, 0 \le i,j \le N+1, u^n_{i,j} \approx u(ih, jh, n\Delta t)$$

Let $\alpha^n_{i,j} \approx g(|\nabla K_\sigma * u|^2)(ih, jh, n\Delta t)$.

Discretization of $\partial_{x_1}(\alpha(x) u_{x_1})$ an $(ih, jh, n\Delta t)$:

$$\frac{1}{2h^2}\left[(\alpha^n_{i+1,j} + \alpha^n_{i,j})(u^{n+1}_{i+1,j} - u^{n+1}_{i,j}) - (\alpha^n_{i,j} + \alpha^n_{i-1,j})(u^{n+1}_{i,j} - u^{n+1}_{i-1,j})\right],$$

analogously for $\partial_{x_2}(\alpha(x) u_{x_2})$.

$\rightarrow$ semi-implicit scheme:

$$\frac{u_{i,j}^{n+1}-u_{i,j}^{n}}{\Delta t} - \frac{1}{2h^2}\Big[(\alpha_{i-1,j}^n+\alpha_{i,j}^n)u_{i-1,j}^{n+1}+(\alpha_{i,j-1}^n+\alpha_{i,j}^n)u_{i,j-1}^{n+1}$$
$$+(\alpha_{i,j}^n+\alpha_{i+1,j}^n)u_{i+1,j}^{n+1}+(\alpha_{i,j}^n+\alpha_{i,j+1}^n)u_{i,j+1}^{n+1}$$
$$-(4\alpha_{i,j}^n+\alpha_{i-1,j}^n+\alpha_{i,j-1}^n+\alpha_{i+1,j}^n+\alpha_{i,j+1}^n)u_{i,j}^{n+1}\Big]=0,$$

IC: $u_{i,j}^0 = f(ih,jh), \quad 1 \le i,j \le N$

$$\text{Neumann-BC:}\quad \begin{array}{ll} u_{i,0}^{n+1}=u_{i,1}^{n+1}, u_{i,N}^{n+1}=u_{i,N+1}^{n+1}, & 0\le i\le N+1,\\ u_{0,j}^{n+1}=u_{1,j}^{n+1}, u_{N,j}^{n+1}=u_{N+1,j}^{n+1}, & 0\le j\le N+1 \end{array}$$

total structure: $\dfrac{u^{n+1}-u^n}{\Delta t}+A_h(u^n)u^{n+1}=0$. Hence one has to solve the following linear system:

$$(I+\Delta t A_h(u^n))u^{n+1}=u^n, \quad n\ge 0,$$

with A_h block-tridiagonal, positive definit $\Rightarrow I+\Delta t A_h(u^n)$ invertible.

Invariances:

Let $\{T_t, t\ge 0\}$ be the solution semigroup of (4.8).

a) Grey value shift:

Diffusivity $g(|\nabla u_\sigma|^2)$ only depends on ∇u but *not* on u. $\Rightarrow$

$$\begin{aligned} T_t(0)&=0 \quad , \quad t\ge 0\\ T_t(f+C)&=T_t(f)+C \quad , \quad \forall t\ge 0;\forall C\in\mathbb{R} \end{aligned}$$

On bounded domains one additionally needs homogeneous Neumann-BCs.

b) Contrast inversion:

$g(|-\nabla u_\sigma|^2)=g(|\nabla u_\sigma|^2)$

$\Rightarrow T_t(-f)=-T_t(f) \quad \forall t\ge 0$

c) mean grey value:

$$\mu := \frac{1}{|\Omega|}\int_\Omega f(x)\mathrm{d}x = \frac{1}{|\Omega|}\int_\Omega T_t(f)\mathrm{d}x \quad t>0 \tag{4.10}$$

follows from divergence form of (4.8) and homogeneous Neumann-BC (compare extension by reflection).

d) Translation and rotation invariance for $\Omega=\mathbb{R}^2$.

Reduction of information for $t>0$:

Local Extrema of u are not amplified in (4.8):

Theorem 4.3. *Let $x_0 \in \Omega$ be a local extremum of $u(\cdot, t_0)$ for some $t_0 > 0$.* $\Rightarrow$
$u_t(x_0, t_0) \leq 0$ *if x_0 local maximum,*
$u_t(x_0, t_0) \geq 0$ *if x_0 local minimum.*

Proof. Let x_0 be a local maximum, hence $\nabla_x u(x_0, t_0) = 0, \Delta_x u(x_0, t_0) \leq 0$.
At (x_0, t_0) we have by (4.8):

$$u_t = \underbrace{g(|\nabla u_\sigma|^2)}_{\geq 0} \underbrace{\Delta u}_{\leq 0} + \nabla(g(|\nabla u_\sigma|^2)) \cdot \underbrace{\nabla u}_{=0} \leq 0.$$

■

Convergence of solution u from (4.8) towards mean grey value μ:

Theorem 4.4. *Let $f \in L^\infty(\Omega)$, $\Omega = (0, a_1) \times (0, a_2)$.*

$$\Rightarrow \|u(t) - \mu\|_{L^p(\Omega)} \leq C e^{-\lambda t} \quad , 1 \leq p < \infty, t \geq 0,$$

with C, λ depending on $\Omega, p, \|f\|_\infty$.

Proof. $e(x,t) := u(x,t) - \mu$ satisfies (4.8).
According to maximum principle in Theorem 4.1:

$$\|e(t)\|_{L^\infty(\Omega)} \leq \|f\|_{L^\infty(\Omega)} + |\mu| \quad \forall t \geq 0. \tag{4.11}$$

$\Rightarrow \nabla e_\sigma(t) = (\nabla K_\sigma) * e(t)$ satisfies (with Young inequality for convolution):

$$\|\nabla e_\sigma(t)\|_{L^\infty(\Omega)} \leq \|\nabla K_\sigma\|_{L^1(\mathbb{R}^2)} \|e(t)\|_{L^\infty(\Omega)} \overset{(4.11)}{\leq} C_1 \quad \forall t \geq 0$$

$\Rightarrow \exists \nu > 0$ with $g(|\nabla e_\sigma(x,t)|^2) \geq \nu \quad \forall t > 0, \forall x \in \Omega$.
First proof for $p = 2$: From (4.8) for $e(t)$ we infer, using $\nabla e \cdot n\big|_{\partial\Omega} = 0$:

$$\int\limits_\Omega e e_t \mathrm{d}x = \int\limits_\Omega e \operatorname{div}(g(|\nabla e_\sigma|^2)\nabla e)\mathrm{d}x = -\int\limits_\Omega |\nabla e|^2 \underbrace{g(|\nabla e_\sigma|^2)}_{\geq \nu} \mathrm{d}x,$$

hence

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|e(t)\|^2_{L^2(\Omega)} \leq -\nu \|\nabla e(t)\|^2_{L^2(\Omega)} \quad , \quad t > 0.$$

For $t > 0$ fixed: $e(t) \in C^\infty(\overline{\Omega})$, $\int\limits_\Omega e(x,t)\mathrm{d}x = 0$ (due to (4.10)) $\Rightarrow \exists x_0 \in \Omega$ with $e(x_0, t) = 0$. According to Poincaré inequality with $C_2 = C_2(\Omega) > 0$:

$$\|e(t)\|^2_{L^2(\Omega)} \leq C_2 \|\nabla e(t)\|^2_{L^2(\Omega)} \quad \forall t > 0,$$

hence

$$\frac{\mathrm{d}}{\mathrm{d}t}\|e(t)\|^2_{L^2(\Omega)} \leq -2\nu C_2^{-1}\|e(t)\|^2_{L^2(\Omega)} \quad , t \geq 0.$$

$$\Rightarrow \text{(by Gronwall's lemma)} \quad \|e(t)\|_{L^2(\Omega)} \leq e^{-\nu C_2^{-1}t}\|f-\mu\|_{L^2(\Omega)} \quad , t \geq 0. \tag{4.12}$$

Same decay for $\|e(t)\|_{L^p(\Omega)}$ with $1 \leq p < 2$ because $L^2(\Omega) \subset L^p(\Omega)$. Result for $2 < p < \infty$ follows from (4.11) and (4.12) by interpolation (Hölder inequality). ■

References: [We] §1.2, 2.3-4

4.2.3 Anisotropic diffusion filter

- so far only scalar, i.e., isotropic diffusivity in $u_t = \operatorname{div}(\Phi(\nabla u))$; flux

  $$j = -\Phi(\nabla u) = -g(|\nabla u|^2)\nabla u \quad \text{always } \| \text{ zu } \nabla u$$

- compare to PM-model written in local coordinates (ξ tangential, η normal to level curves of u):

  $$u_t = g(|\nabla u|^2)u_{\xi\xi} + \Phi'(\nabla u)u_{\eta\eta}$$

- an efficient anisotropic diffusion model: diffusion *only* tangential to level curves/contour lines (i.e. $\|$ to edges)

Ex.: mean curvature filter:

linear diffusion filter in local coordinates:

$$u_t = u_{\xi\xi} + u_{\eta\eta}$$

anisotropic analogon (with diffusion only tangential to level curves):

$$\begin{cases} u_t = u_{\xi\xi} & , \quad t > 0 \\ u(x,0) = f(x) \end{cases} \tag{4.13}$$

This is a nonlinear *degenerate* parabolic equation; in local coordinates the diffusion matrix reads $A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$.

Transformation to $x = (x_1, x_2)$-coordinates gives mean curvature equation:

$$\begin{aligned} u_t &= \frac{(\nabla^\perp u)^\top \cdot \frac{\partial^2 u}{\partial x^2} \cdot \nabla^\perp u}{|\nabla u|^2} = \frac{u_{x_2}^2 u_{x_1x_1} - 2u_{x_1}u_{x_2}u_{x_1x_2} + u_{x_1}^2 u_{x_2x_2}}{u_{x_1}^2 + u_{x_2}^2} \qquad \text{(cp. to (4.7))} \\ &= |\nabla u| \operatorname{div}\left(\frac{\nabla u}{|\nabla u|}\right). \end{aligned} \tag{4.14}$$

$\kappa(x,t) := \operatorname{div}\left(\frac{\nabla u}{|\nabla u|}\right)$ ... (mean) curvature of level curve of $u(\cdot,t)$ through x.

Theorem 4.5. *Assume that f is bounded and uniformly continuous on $\mathbb{R}^2$. ⇒*

(4.14) hat a unique viscosity solution *$u(x,t)$ on $\mathbb{R}^2 \times [0,\infty)$. It satisfies a max/min-principle:*

$$\inf_{\mathbb{R}^2} f \le u(x,t) \le \sup_{\mathbb{R}^2} f.$$

Solution is L^∞-stable, i.e., for 2 solutions $u_{1,2}(t)$ with ICs $f_{1,2}$ we have:

$$\|u_1(t) - u_2(t)\|_{L^\infty(\mathbb{R}^2)} \le \|f_1 - f_2\|_{L^\infty(\mathbb{R}^2)} \qquad \forall\, t \ge 0$$

Rem.: vague motivation of viscosity solution: because (4.13) is degenerate parabolic, consider $u_t = u_{\xi\xi} + \varepsilon\Delta u$, $\varepsilon \to 0$ (precise notions is very technical).

Reformulation of (4.14) as transport equation:

$$u_t + \kappa(x,t)n(x,t) \cdot \nabla u = 0; \tag{4.15}$$

with

$$n(x,t) := -\frac{\nabla u(x,t)}{|\nabla u(x,t)|} \ \ldots \text{ unit normal vector on level curve of } u(\cdot,t)$$

(nonlinear, because κ, n depend on u!)

Solution of (4.15) using method of characteristics:

$u = $ const along characteristics, given by $\dot{x} = \kappa(x,t)n(x,t)$.

Result:

- Velocity of level curves is proportional to local curvature;
  in direction of decreasing u
- Smoothing by alignment of curvature of each level curve:

  Each level curve asymptotically tends to a circle and collapses to a point in finite time.
- (4.15) *cannot* amplify contrast:

References: [We] §1.2.3, 1.4-5, [Ma]§10

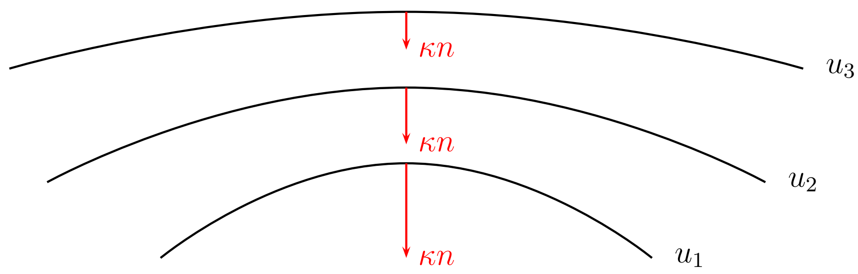


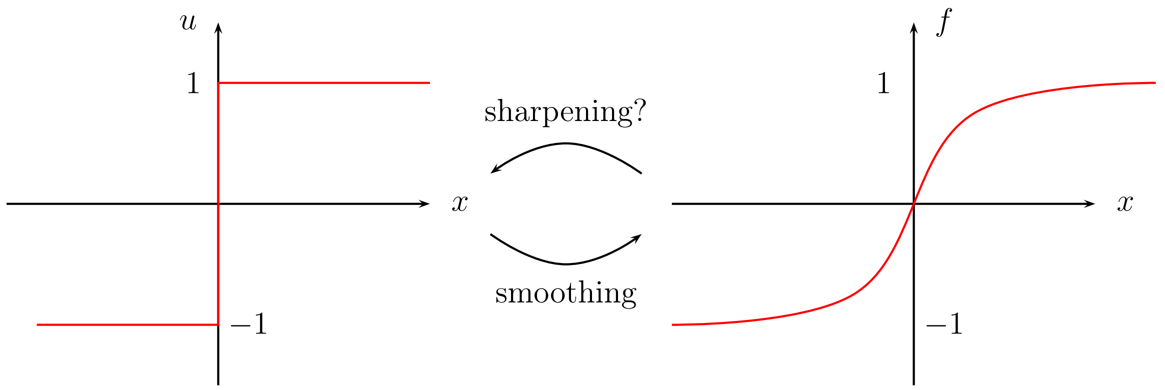
Figure 4.2: Level curves of u (at fixed time t with $u_1 < u_2 < u_3$); the move *apart*.

4.3 Edge sharpening, shock filter

opposing processes:

- smoothing, blur
- sharpening, deblur

1D-situation:



Aim: find a PDE for image sharpening as "time" evolution process

Example 4.6. Let $f(x) = \cos(x)$.

□

Conclusion:

- Direction of movement of 1D-"level points" $u(x,t)$ depends on $\operatorname{sign}[u_x(x,t)u_{xx}(x,t)]$.
- for $u_x(x,t) = 0$ or $u_{xx}(x,t) = 0$: no movement desired

Proposed model (in 1D): "shock filter" by Osher & Rudin:

$$\begin{cases} u_t = -\operatorname{sign}(u_x u_{xx}) u_x = -|u_x| \operatorname{sign}(u_{xx}), x \in \mathbb{R}, t > 0 \\ u(x,0) = f(x) \end{cases} \tag{4.16}$$

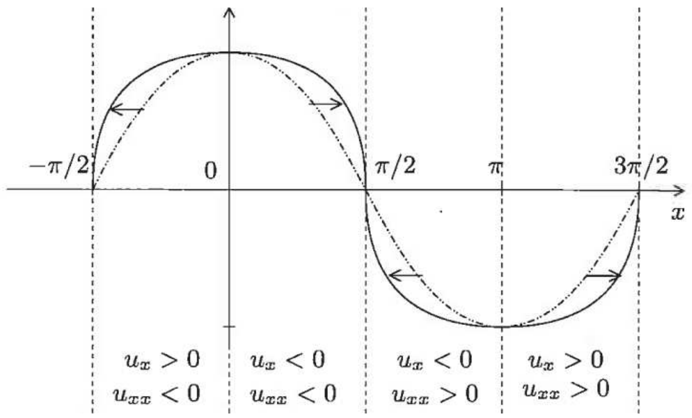


Figure 4.3: desired edge sharpening in 1D, [AK]

This is a transport equation with velocity ± 1, e.g. in the region where $u_x(x,t) > 0, u_{xx}(x,t) > 0$: $u_t + u_x = 0$. But in total the equation is fully nonlinear.

Preliminary study of a simplified model:
In the above example the local convexity/concavity do not change.

$$\begin{cases} u_t = -|u_x| \operatorname{sign}(f_{xx}), x \in \mathbb{R}, t > 0 \\ u(x,0) = f(x) := \cos(x) \end{cases} \tag{4.17}$$

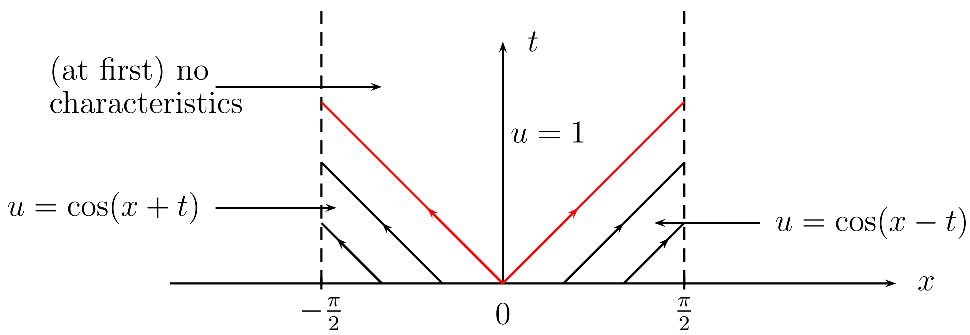
1st case: consider (4.17) on $\left(-\frac{\pi}{2}, \frac{\pi}{2}\right) \times \mathbb{R}^+$

$$\to \operatorname{sign}(f_{xx}) = -1 \quad \Rightarrow \quad u_t = |u_x| \qquad \text{(a Hamilton-Jacobi equation.)}$$

Solution by method of characteristics:

$$u(x,t) = \begin{cases} \cos(x+t) & , \quad -\frac{\pi}{2} < x < -t \\ 1 & , \quad t \geq |x| \\ \cos(x-t) & , \quad t < x < \frac{\pi}{2} \end{cases}$$

This is a *rarefaction wave*, analogously to §1.2; weak solution is only unique if we demand continuity.



2nd case: consider (4.17) on $\left(\frac{\pi}{2}, \frac{3\pi}{2}\right) \times \mathbb{R}^+$

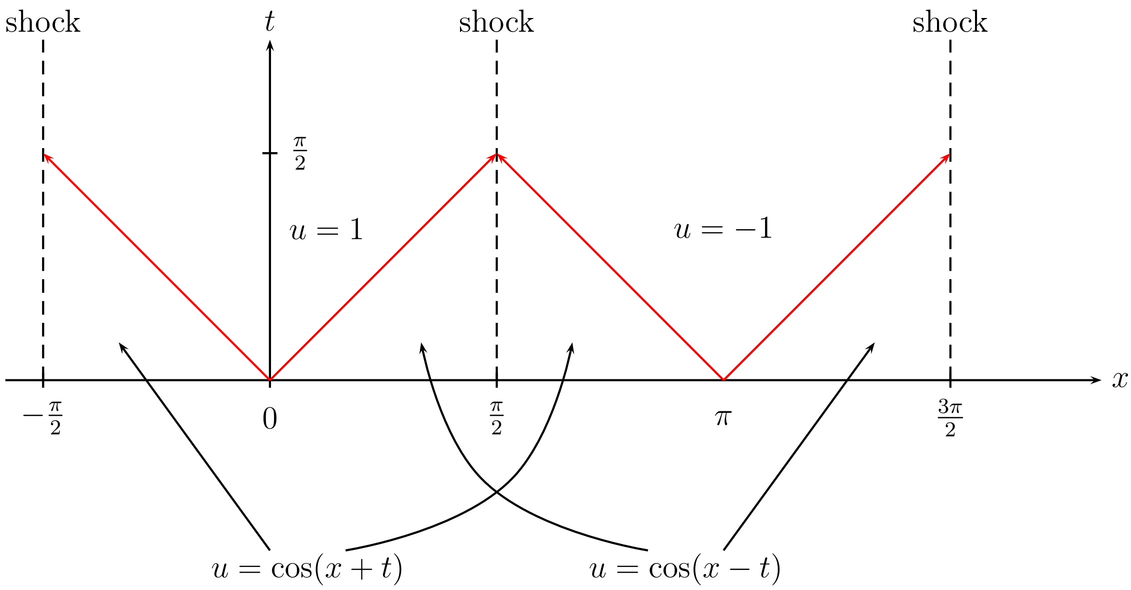
$$\to \operatorname{sign}(f_{xx}) = 1 \quad \Rightarrow \quad u_t = -|u_x|$$

analogous rarefaction wave:

$$u(x,t) = \begin{cases} \cos(x+t) & , \quad \frac{\pi}{2} < x < \pi - t \\ -1 & , \quad t \geq |x - \pi| \\ \cos(x-t) & , \quad t + \pi < x < \frac{3\pi}{2} \end{cases}$$

Solution of (4.17) by periodic extension:

has shocks at $x = (2k+1)\frac{\pi}{2}, k \in \mathbb{Z}$:



For $t \geq \frac{\pi}{2} : u(x,t) = (-1)^k$ for $(2k-1)\frac{\pi}{2} < x < (2k+1)\frac{\pi}{2}$. $\Rightarrow$ (4.17) sharpens the curves up to perfect step functions (in finite time!) with jumps where $f_{xx} = 0$.
Information gain (because of sharpening) seemingly possible because of restriction to $u \in \{-1, 1\}$.

Generalization of "shock filters" (4.16):

$$\begin{cases} u_t = -|u_x| F(u_{xx}), x \in \mathbb{R}, t > 0 \\ u(x,0) = f(x) \end{cases} \tag{4.18}$$

with $F \in \operatorname{Lip}(\mathbb{R})$ and $F(0) = 0; \operatorname{sign}(s)F(s) > 0,\ \forall s \neq 0.$

e.g. with $F(s) = s$:

$$u_t = -|u_x| u_{xx} = -(u_{xx} \operatorname{sign}(u_x)) u_x\,, \quad x \in \mathbb{R}, t > 0. \tag{4.19}$$

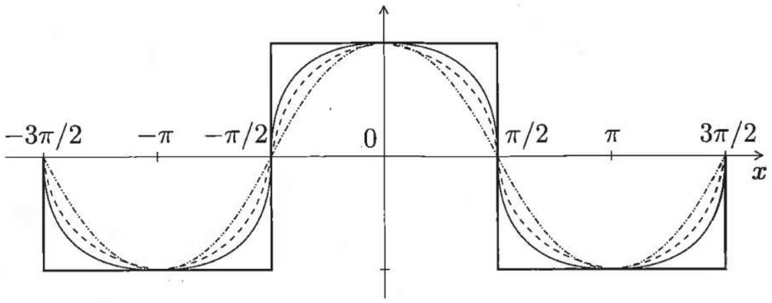


Figure 4.4: $u(\cdot, t)$ for $t = 0, \ldots, \frac{\pi}{2}$

This is a transport equation with local propagation speed $c(x,t) = \text{sign}(u_x)u_{xx}$.

Edge positions x_0 are defined as maxima of $u_x^2 \Rightarrow u_{xx}(x_0) = 0$, u_{xx} changes sign at x_0.

$\Rightarrow$ sign change of $c(x)$ is "detector" for edges (and extrema of u).

(4.19) is ill posed (backwards parabolic!), but works very well numerically (reason still unclear).

Conjecture 4.7 (Osher-Rudin, 1990)**.** Let $f \in C(\mathbb{R})$. $\Rightarrow$ (4.18) has a unique solution with jumps (for $t > 0$) only at inflection points of $f(x)$. The total variation of $u(.,t)$ is constant in t, the same holds for positions and values of local extrema.

<u>2D-generalization:</u>

$$u_t = -|\nabla u| F(\Delta u), \quad x \in \mathbb{R}^2,\ t > 0;$$

e.g. with $F(s) := \text{sign}(s)$.

<u>References</u>: [AK] §3.3.3, [Ma]§10

5 Pattern formation / reaction-diffusion equations

Examples for pattern formation processes:

- chemical reactions, e.g. spiral waves
- two-phase mixtures of liquids, e.g. "fingering" in oil-water flow in porous medium
- in biology: leaf structures, animal skin ("animal coat"), ...

in biology: only the "recipe" for pattern formation processes is "stored" genetically, but *not* the pattern itself.

Aim: (nonlinear) mathematical models (e.g. parabolic PDEs) producing "such" patterns $\to$ as possible mechanism for pattern formation.

5.1 Reaction-diffusion equations

Derivation:

$c(x,t)$ ... (scalar) density function of a substance; $x \in \mathbb{R}^3$
$J(c,x,t)$ ... flux function
$f(c,x,t)$ ... production rate of substance

Balance equation in domain $\Omega \subset \mathbb{R}^3$:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_\Omega c(x,t)\mathrm{d}x &= -\int\limits_{\partial\Omega} J\cdot\nu\mathrm{d}s + \int\limits_\Omega f(c,x,t)\mathrm{d}x \\ &\overset{\substack{\text{div.}\\ \text{theorem}}}{=} \int\limits_\Omega (-\operatorname{div} J + f)\mathrm{d}x\end{aligned}$$

Ω arbitrary $\Rightarrow$

$$c_t + \operatorname{div} J = f(c,x,t) \tag{5.1}$$

classical diffusion: $J = -D\nabla c$; here only $D = \text{const.}$

Generalization on multiple interacting species or chemicals $c_i(x,t)$; $i = 1,\ldots,m$.

Rate of production/reaction here only $f = f(c) \in \mathbb{R}^m$ (nonlinear!):

$$c_t = f(c) + D\Delta c. \tag{5.2}$$

here: $0 \leq D =$ constant diagonal matrix; hence no *cross-diffusion*.

References: [Mu] §9.2

5.2 Turing mechanism

let $m = 2$; $c = (u, v)^\top$, after suitable scaling (spatial scale parameter $\gamma > 0, d > 0$):

$$\begin{cases} u_t = \gamma f(u,v) + \Delta u \\ v_t = \gamma g(u,v) + d\Delta v \end{cases} \tag{5.3}$$

Turing mechanism:

1. Let $(u_0, v_0)^\top \in \mathbb{R}^2$ be a spatially homogeneous, asymptotically stable stationary point of

$$u_t = \gamma f(u,v), v_t = \gamma g(u,v). \tag{5.4}$$

2. For suitable f, g and $1 \neq d$ we have: (5.3) is *linearly instable* at $(u_0, v_0)^\top$, although diffusion "usually" stabilizes.

$\Rightarrow$ small disturbances of the homogeneous stationary state can produce spatially inhomogeneous patterns in the time evolution: "regular" (but usually not perfectly periodic) patterns as stationary states $u_\infty(x) = \lim_{t\to\infty} u(x,t)$ resp. $v_\infty(x) = \lim_{t\to\infty} v(x,t)$. They are *not* unique!

Consider (5.3) on $\Omega \subset \mathbb{R}^2$ with BC:

$$\frac{\partial u}{\partial \nu} = \frac{\partial v}{\partial \nu} = 0\,, \quad x \in \partial\Omega\,,$$

i.e. 0-flux-BC to permit *self-organizing patterns* (without BC-effect!).

IC: $u(x,0), v(x,0)$ given.

Definition 5.1 (linear asymptotic stability)**.** *For an autonomous dynamical system $y' = F(y)$ a point $y_0 \in \mathbb{R}^m$ is called a* linearly asymptotically stable stationary point *if $F(y_0) = 0$ and for all eigenvalues of $\frac{\partial F}{\partial y}(y_0)$ we have:* $\mathrm{Re}(\lambda_i) < 0$. *If there is an eigenvalue satisfying* $\mathrm{Re}(\lambda_i) > 0$ *then y_0 is called a* linearly unstable stationary point.

The case $\mathrm{Re}(\lambda_i) = 0$ is not covered here because it does not allow for a stability statement about the nonlinear system.

Conditions for diffusion-driven instability:

Lemma 5.2. $(u_0, v_0)^\top \in \mathbb{R}^2$ *is a linearly* asymptotically stable *stationary point of* (5.4) $\Leftrightarrow$

$$\begin{aligned} f(u_0, v_0) = g(u_0, v_0) &= 0, \\ f_u + g_v\big|_{u_0,v_0} &< 0, \\ f_u g_v - f_v g_u\big|_{u_0,v_0} &> 0. \end{aligned} \tag{5.5}$$

Proof. Linearization of ODE (5.4):

$$w := \begin{pmatrix} u - u_0 \\ v - v_0 \end{pmatrix};$$

for $|w|$ small we have:

$$w_t \approx \gamma A w, \quad A = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}_{u_0,v_0} \in \mathbb{R}^{2\times 2}.$$

$w = 0$ is linearly asymptotically stable $\Leftrightarrow \mathrm{Re}\,\lambda_{1,2}(A) < 0 \Leftrightarrow$

Conditions:

$$\begin{aligned} \operatorname{tr} A = \lambda_1 + \lambda_2 = f_u + g_v\big|_{u_0,v_0} &< 0, \\ \det A = \lambda_1 \lambda_2 = f_u g_v - f_v g_u\big|_{u_0,v_0} &> 0. \end{aligned}$$ ∎

Theorem 5.3 (necessary condition for instability)**.** *Suppose* (5.5) *holds. Let* $(u_0, v_0)^\top \in \mathbb{R}^2$ *be a linearly* unstable *stationary point of* (5.3) $\Rightarrow$

$$\begin{aligned} d f_u + g_v\big|_{u_0,v_0} &> 0, \\ (d f_u + g_v)^2 - 4d(f_u g_v - f_v g_u)\big|_{u_0,v_0} &> 0. \end{aligned} \tag{5.6}$$

(1st condition and middle condition of (5.5) *imply that $d \neq 1$, $f_u g_v < 0$)*

Proof. Step 1: Solution formula for linearized RD-equations, via eigenfunction expansion: Linearization of (5.3) around stationary state (with $w(x,t) \in \mathbb{R}^2$):

$$\begin{cases} w_t = \gamma A w + D \Delta w \quad , \quad D = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix}. \\ \text{BC: } \frac{\partial w_{1,2}}{\partial \nu} = 0, \quad x \in \partial\Omega, \\ \text{IC: } w(x,0) \text{ is "small" disturbance of } (u_0, v_0)^\top. \end{cases} \tag{5.7}$$

Consider first the scalar eigenvalue problem (=*Helmholtz equation*), $z(x) \in \mathbb{R}$:

$$\begin{cases} -\Delta z = \mu^2 z & , \quad \Omega \ldots \text{bounded domain} \\ \frac{\partial z}{\partial \nu} = 0 & , \quad \partial\Omega \end{cases} \tag{5.8}$$

$\mu_n^2 \in \mathbb{R}_0^+$, $n \in \mathbb{N}_0$ ...discrete eigenvalues of $-\Delta$ (increasing), μ ... "wavenumbers"; $\frac{1}{\mu}$ proportional to wave length
$z_n(x)$, $n \in \mathbb{N}_0$ ... (scalar) eigenfunctions; form ONB of $L^2(\Omega)$ (due to "expansion theorem" for self-adjoint compact operators).
In particular: $\mu_0 = 0$, $z_0 \equiv |\Omega|^{-1/2}$. This x-homogene mode is asymptotically stable by assumption (5.5).

Ansatz for system of two parabolic equations (5.7): based on eigenfunction expansion for (5.8):

$$w(x,t) = \sum_{n=0}^{\infty} c_n e^{\lambda_n t} z_n(x), \tag{5.9}$$

Main question: When can there be a λ_n with $\operatorname{Re}\lambda_n > 0$?

Calculation of $\lambda_n \in \mathbb{C}$, $c_n \in \mathbb{C}^2$; $n \in \mathbb{N}_0$ by inserting in (5.7) and matching the coefficients of z_n:

$$\lambda_n z_n c_n = \gamma z_n A c_n + \Delta z_n D c_n \overset{(5.8)}{=} z_n(\gamma A - \mu_n^2 D)c_n \qquad \forall\, n \in \mathbb{N}_0$$

This is a homogeneous linear system of equations for c_n. Its solvability condition (because $z_n \not\equiv 0$):

$$0 = \det(\lambda_n I - \gamma A + \mu_n^2 D) = \lambda_n^2 + l(\mu_n^2)\lambda_n + h(\mu_n^2) = 0, \qquad \text{(quadratic eq. for } \lambda_n) \tag{5.10}$$

$$l(\mu^2) := \mu^2(1+d) - \gamma(f_u + g_v) \in \mathbb{R},$$
$$h(\mu^2) := d\mu^4 - \gamma(d\, f_u + g_v)\mu^2 + \gamma^2 \det A \in \mathbb{R}.$$

Let $\lambda_n^j \in \mathbb{C}, j = 1,2$ be solutions of (5.10), i.e., eigenvalues of $\gamma A - \mu_n^2 D$, and $c_n^j \in \mathbb{C}^2$ the corresponding eigenvectors. (Here we assume that $\gamma A - \mu_n^2 D$ is diagonalizable $\forall n \in \mathbb{N}_0$.[1])
$\Rightarrow \quad c_n^j e^{\lambda_n^j t} z_n(x)$ solves (5.7).

$\lambda_n^{1,2}$ resp. $c_n^{1,2}$ are conjugate complex or both real because $\gamma A - \mu_n^2 D$ is real.

$$\Rightarrow \quad w(x,t) = \sum_{n=0}^{\infty} \left[\alpha_n c_n^1 e^{\lambda_n^1 t} + \beta_n c_n^2 e^{\lambda_n^2 t}\right] z_n(x), \tag{5.11}$$

and the coefficients α_n, $\beta_n \in \mathbb{C}$ are uniquely determined by the Fourier expansion of the IC$w(\cdot, 0) \in L^2(\Omega; \mathbb{R}^2)$.

Step 2: proof of the two inequalities (5.6):

[1] This also implies that the eigenfunctions $c_n^j z_n$ are complete for (5.7); it would not follow from the "expansion theorem" as (5.7) is not symmetric.

Homogeneous stationary state (u_0, v_0) of (5.3) is linearly asymptotically stable $\Leftrightarrow$ both solutions of (5.10) satisfy: $\operatorname{Re}\lambda_n^{1,2} < 0\ \forall\, n \in \mathbb{N}_0$.

In any case we have

$$l(\mu^2) = \underbrace{\mu^2(1+d)}_{\geq 0} \underbrace{-\gamma}_{<0} (\underbrace{f_u + g_v}_{<0 \text{ lt. (5.5)}}) > 0 \quad \forall \mu.$$

If λ_n is a double eigenvalue $\overset{(5.10)}{\Rightarrow}$ $\lambda_n = -l(\mu_n^2)/2 < 0$, i.e., asymptotically stable mode.

Stationary state (u_0, v_0) is linearly *instable* $\Leftrightarrow \exists n \in \mathbb{N}$, $\exists j \in \{1, 2\}$ with $\operatorname{Re}\lambda_n^j > 0$. (Rem.: $n = 0$ is asymptotically stable mode.)

This happens exactly for $h(\mu_n^2) < 0$ in (5.10) for one $n \in \mathbb{N}$; because (5.10) implies:

$$2\lambda_n^{1,2} = \underbrace{-l(\mu_n^2)}_{<0} \pm \sqrt{l^2(\mu_n^2) - 4h(\mu_n^2)}\,, \tag{5.12}$$

and $\lambda_n^1 > 0 \iff h(\mu_n^2) < 0$.

$$h(\mu^2) = \underbrace{d\mu^4}_{\geq 0} - \gamma(d\, f_u + g_v)\mu^2 + \underbrace{\gamma^2 \det A}_{>0 \text{ from (5.5)}} \tag{5.13}$$

$\Rightarrow h(\mu^2) < 0$ only for $d\, f_u + g_v > 0$ possible (= Condition 1).

As $f_u + g_v < 0$ (from (5.5)) $\Rightarrow d \neq 1, f_u g_v < 0$.

Minimum of $h(\mu^2)$ as function of μ^2:

$$h_{\min} = \gamma^2 \left(\underbrace{\det A}_{>0} - \underbrace{\frac{(d\, f_u + g_v)^2}{4d}}_{>0} \right), \quad \mu_{\min}^2 = \gamma \frac{d\, f_u + g_v}{2d} \overset{\text{Cond.1}}{>} 0$$

$\Rightarrow$ condition for $h(\mu^2) < 0$ for one $\mu \neq 0$:

$$\frac{(d\, f_u + g_v)^2}{4d} > \det A > 0, \quad (= \text{condition 2}).$$

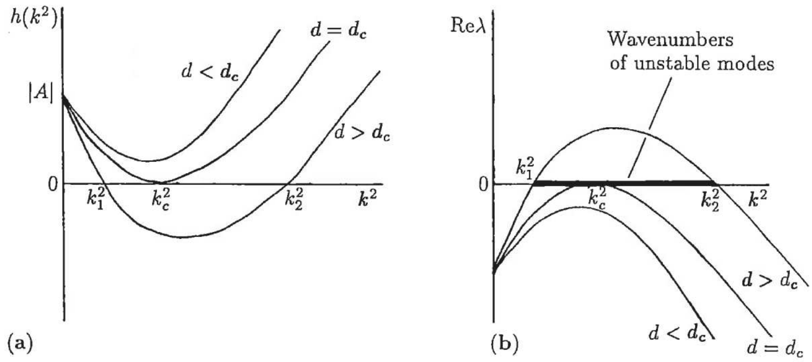
i.e. for $0 < d \ll 1$ or $d \gg 1$. ■

Remark 5.4. $h(\mu^2) < 0 \quad \Leftrightarrow \quad \underline{\mu}^2 < \mu^2 < \overline{\mu}^2$ (possibly empty set, <u>depending on d</u>, γ) with

$$\underline{\mu}^2, \overline{\mu}^2 = \gamma \frac{d\, f_u + g_v \mp \sqrt{(d\, f_u + g_v)^2 - 4d \det A}}{2d} \tag{5.14}$$

(=zeros of (5.13)).

Above conditions are necessary but not sufficient because $\mu_{\min}^2$ isn't an eigenvalue in general.



Remark 5.5 (sufficient condition for instability)**.** Exactly for the discrete eigenvalues $\mu_n^2 \in (\underline{\mu}^2, \overline{\mu}^2)$ (if they exist!) we have $\operatorname{Re}\lambda_n^1 > 0$ (unstable modes! Follows from (5.12)).

Following (5.11), the asymptotic behaviour of w (for large t) then is:

$$w(x,t) \sim \sum_{\underline{\mu} \le \mu_n \le \overline{\mu}} \alpha_n c_n^1 e^{\lambda_n^1 t} z_n(x)$$

Sum only over discrete eigenvalues of (5.8) (possibly empty set) $\Rightarrow$ only finitely many wavenumbers μ_n (of the "pattern") are unstable. Mode with maximal λ_n is domainant.

Idea: Linearly instable eigenfunctions are bounded by nonlinear effects $\Rightarrow$ spatially inhomogeneous stationary states develop (proof exists only for special cases)

Java-Demo for Brusselator: http://crossgroup.caltech.edu/Patterns/Demo4_5.html
(runs in Internet Explorer 11; not in Firefox)

Scale parameter γ ($\sqrt{\gamma}$ proportional to typical length scale) appears only in the interval boundaries (5.14) for instable μ-interval: the larger γ is, the more instable (pattern) modes there are.

Remark 5.6. Let $\Omega = \mathbb{R}^2 \Rightarrow$ Helmholtz equation (5.8) has continuous spectrum $\mu^2 \ge 0$.

For all modes with $\mu^2 \in (\underline{\mu}^2, \overline{\mu}^2)$ (5.9) is linearly instable.

$\Rightarrow$ spatial pattern develops; with wavenumber μ for maximal λ_μ^1.

References: [Mu] §14.2-3; [EGK] §16.2.12

5.3 Pattern formation in a sample system

Example for (5.3), first in 1D:

$$\begin{cases} u_t = \gamma f(u,v) + u_{xx} := \gamma(a - u + u^2 v) + u_{xx} \\ v_t = \gamma g(u,v) + d v_{xx} := \gamma(b - u^2 v) + d v_{xx} \end{cases} \tag{5.15}$$

$t > 0, x \in (0,p); a,b,d > 0$

Schnakenberg-System: Model for biochemical reaction between 2 substances with densities $u(x,t), v(x,t)$ and 3-molecule reaction (e.g. additional encyme reaction in system dynamics).

Pattern formation is independent from exact form of f, g.

Homogeneous, positive stationary state:

$$u_0 = a+b, v_0 = \frac{b}{(a+b)^2} \quad , \quad b > 0, a+b > 0;$$

at (u_0, v_0):

$$f_u = \frac{b-a}{a+b}, \quad f_v = (a+b)^2 > 0, \quad g_u = \frac{-2b}{a+b}, \quad g_v = -(a+b)^2 < 0\,.$$

Consequence of (5.6): $f_u g_v < 0 \Rightarrow b > a$.

Conditions (5.5), (5.6) for linear ODE-stability resp. linear PDE-instability:

$$\begin{cases} f_u + g_v < 0 \quad \Rightarrow \quad 0 < b-a < (a+b)^3, \\ \det A = f_u g_v - f_v g_u = (a+b)^2 > 0 \quad \checkmark \\ d\,f_u + g_v > 0 \quad \Rightarrow \quad d(b-a) > (a+b)^3 \\ (d\,f_u + g_v)^2 - 4d(f_u g_v - f_v g_u) > 0 \quad \Rightarrow \quad [d(b-a) - (a+b)^3]^2 > 4d(a+b)^4 \end{cases} \tag{5.16}$$

These inequality for (a,b,d) define area of instability ("Turing space").

Eigenvalue problem (5.8) on $\Omega = (0,p)$:

$$z_{xx} + \mu^2 z = 0, \quad z_x(0) = z_x(p) = 0$$

$$\Rightarrow \mu_n = \frac{n\pi}{p}, z_n(x) = \cos\frac{n\pi x}{p}, n \in \mathbb{N}_0$$

Let (a,b,d) be in the Turing space defined by (5.16).

$\Rightarrow$ from (5.14): band of instable wavenumbers $= (\underline{\mu}, \overline{\mu}) = (\sqrt{\gamma}\underline{\sigma}, \sqrt{\gamma}\overline{\sigma})$ with

$$\underline{\sigma}^2, \overline{\sigma}^2 := \frac{d(b-a) - (a+b)^3 \mp \sqrt{[d(b-a)-(a+b)^3]^2 - 4d(a+b)^4}}{2d(a+b)} \tag{5.17}$$

$\Rightarrow$ all discrete modes with $\mu_n = \dfrac{n\pi}{p} \in (\underline{\mu}, \overline{\mu})$ are linearly instable.

asymptotic behaviour (for large t) of $w(x,t) \approx (u(x,t) - u_0, v(x,t) - v_0)$ from (5.15):

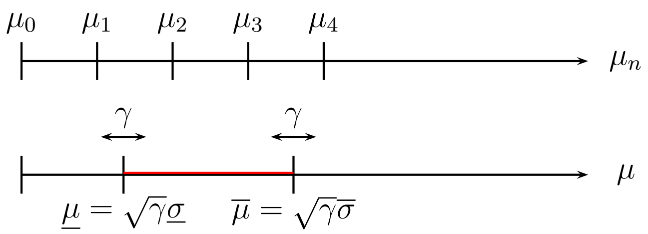
$$w(x,t) \sim \sum_{n=\underline{n}}^{\overline{n}} \alpha_n \underbrace{c_n}_{\in\mathbb{C}^2} e^{\lambda_n^1 t} \cos\frac{n\pi x}{p}, \tag{5.18}$$

$\lambda_n^1 \ldots$ positive solution of quadratic equation (5.10).

$\underline{n}, \overline{n}$ choosen such that the corresponding wavenumbers are in the band $(\underline{\mu}, \overline{\mu})$.

Influence of scale parameter $\gamma > 0$:

typical length scale / system size $\propto \sqrt{\gamma}$:



Instable interval $(\underline{\mu}, \overline{\mu})$ shiftable by γ. Depending on γ there are 0, 1, ... linearly instable modes:

- For $\gamma < \gamma_c = \left(\frac{\mu_1}{\bar{\sigma}}\right)^2$: all modes are linearly asymptotically stable $\Rightarrow (u_0, v_0)$ is stable $\Rightarrow$ no "pattern" possible.
- *Bifurcation* at $\gamma = \gamma_c$ (critical value)
- For $\gamma > \gamma_c$ with $\underline{\mu} < \mu_1 < \overline{\mu} < \mu_2 \Rightarrow$ only mode 1 is linearly instable:

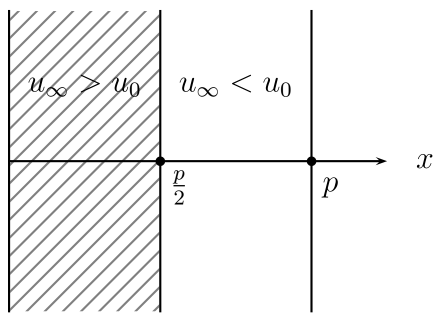
  $$u(x,t) \sim u_0 + ce^{\lambda_1^1 t} \cos \frac{\pi x}{p}, \mathrm{Re}\, \lambda_1^1 > 0.$$

  (valid in "linear regime")

  exponential growth of u is restricted by nonlinear effects.

  Hypothesis: $u_\infty(x) \approx u_0 + \tilde{c} \cos \frac{\pi x}{p}$

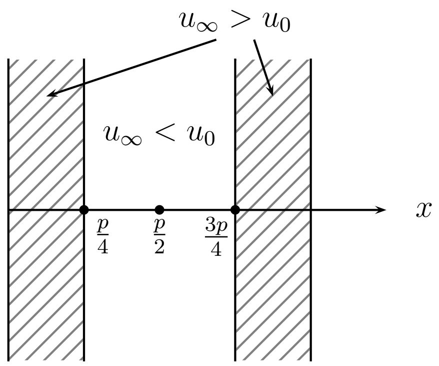
  expected 1D-pattern (for $\tilde{c} > 0$):

- If $\mu_1 < \underline{\mu} < \mu_2 < \overline{\mu} < \mu_3 \Rightarrow$ only mode 2 is linearly instable:

  $$u(x,t) \sim u_0 + ce^{\lambda_2^1 t} \cos \frac{2\pi x}{p}, \mathrm{Re}\, \lambda_2^1 > 0.$$

  expected 1D pattern:



Analogously for even lager systems. Also: system size and geometry (in 2D) are decisive for possible patterns.

2D-case:

Eigenvalue problem (5.8) on $\Omega = (0,p) \times (0,q)$:

$$\Delta z + \mu^2 z = 0 \quad , \quad \frac{\partial z}{\partial \nu} = 0 \text{ on } \partial\Omega$$

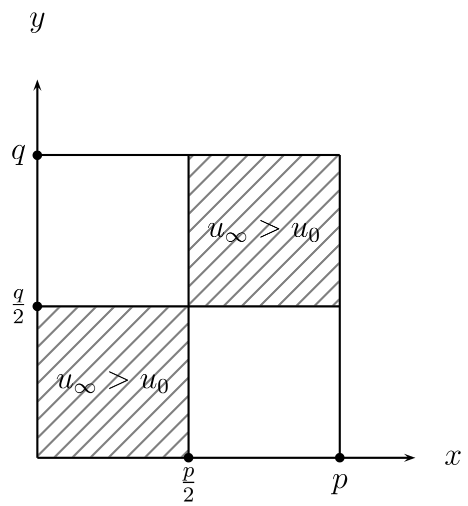
$$\Rightarrow \mu^2_{n,m} = \pi^2 \left(\frac{n^2}{p^2} + \frac{m^2}{q^2} \right), z_{n,m}(x,y) = \cos \frac{n\pi x}{p} \cos \frac{m \pi y}{q}; n, m \in \mathbb{N}_0$$

All discrete modes $z_{n,m}(x,y)$ with $\mu_{n,m} \in (\underline{\mu}, \overline{\mu})$ (from (5.17)) are instable.

asymptotic behaviour:

$$w(x,y,t) \sim \sum_{n,m} \alpha_{n,m} \underbrace{c_{n,m}}_{\in \mathbb{C}^2} e^{\lambda^1_{n,m} t} \cos \frac{n \pi x}{p} \cos \frac{m \pi y}{q} \quad \text{(sum over instable modes)}$$

Expected 2D-pattern, mode $(1,1)$:



References: [Mu] §14.4

5.4 Animal coat color patterns

Explanation ansatz: coat color patterns correspond to a bio-chemical "prototypical pattern" which is formed during pregnancy.

"experimental" reaction-diffusion model:

$$\begin{cases} u_t = \gamma f(u,v) + \Delta u \\ v_t = \gamma g(u,v) + d\Delta v \end{cases} \tag{5.19}$$

$f(u,v) := a - u - h(u,v), g(u,v) := \alpha(b-v) - h(u,v),$

$h(u,v) := \dfrac{\rho uv}{1+u+Ku^2}$ (rather "invented" function)

Parameter $a, b, \alpha, \rho, K > 0; d > 1$

Scale parameter $\sqrt{\gamma}$ proportional to typical length scale.

Region Ω for animal leg or tail: surface of cylinder (resp. trunacted pyramid)

Eigenvalue problem (5.8) on Ω with $0 < x < s, 0 < \theta < 2\pi$ leads to (with periodic BCs in θ; r =radius):

$$\mu_{n,m}^2 = \frac{n^2}{r^2} + \frac{m^2\pi^2}{s^2}, z_{n,m}(\theta,x) = \cos n\theta \cos\frac{m\pi x}{s}; n,m \in \mathbb{N}_0$$

and

$$z_{-n,m}(\theta,x) = \sin n\theta \cos\frac{m\pi x}{s}; n \in \mathbb{N}, m \in \mathbb{N}_0$$

All discrete modes $z_{n,m}$ with $\mu_{n,m} \in (\underline{\mu}, \overline{\mu})$ are instable.

Effects:

from numerical simulations with FEM; solution of (5.19) for "$t \to \infty$" (up to stationary state).

- long, thin cylinder ($0 < r \ll 1$): all circumferential modes $n \geq 1$ are outside the band of instability $(\underline{\mu}, \overline{\mu}) \Rightarrow$ only vertical stripes (with $n = 0$)
- the thicker the cylinder, the higher circumferential modes are possible

Conclusion:

- Effects are described qualitatively correctly.
- Whether model (5.19) describes their evolution correctly, is (still) unclear. The qualitative influence of the length scale on the possible patterns is "quite independent" of the equation.

References: [Mu] §15.1

5.5 Pattern formation in 2-component mixtures / Cahn-Hilliard equation

Application: Phase separation (under dominant diffusion) in binary fluid mixtures (e.g. (liquid) metallic alloys, emulsions: vinegar-oil, Ouzo-water microemulsion).

$$0 \le c_{1,2}(x,t) \le 1 \quad \dots \quad \text{local concentration of 2 components}$$

Derivation of Cahn-Hilliard equation:

$$\partial_t c_i + \operatorname{div} J_i = 0\ ; \quad i = 1,2$$

Assumptions: system isotherm, isobar, incompressible

$$\Rightarrow\ c_1 + c_2 = 1, \quad \partial_t(c_1 + c_2) = 0, \quad J_1 + J_2 = 0$$

choose $c := c_1 - c_2 \in [-1,1], \quad J := J_1 - J_2$

$$\Rightarrow\ c_t + \operatorname{div} J = 0, \quad \Omega \subset \mathbb{R}^d. \tag{5.20}$$

phenomenological Derivation of flux $J = -L\nabla\mu$:

$L \ge 0$	...	(const.) mobility
μ	...	chemical "potential" (e.g.. $\mu = c$ with diffusion); defined as derivative of a potential (resp. variational derivative of free energy); $\nabla\mu$ is *driving force* for evolution

- free energy for mixture (= necessary energy for "generation" of a system with def. temperature T which is in balance with the environment.)

$$E(c) := \int_\Omega \left[f(c) + \frac{\gamma}{2}\,|\nabla c|^2 \right] \mathrm{d}x \in \mathbb{R}, \quad \gamma > 0 \ \text{ const.}$$

$\frac{\gamma}{2}\,|\nabla c|^2 \quad \dots \quad$ energy of phase boundary between $c = \pm 1$; "penalizes" phase transitions

$f : \mathbb{R} \to \mathbb{R}$, given function, bistable (i.e. with 2 minima), e.g.

$f(c) = \alpha(c^2 - a^2)^2; \quad \alpha,\, a > 0.$

- system desires minimization of $E(c)$

- μ ist variational derivative of (non-convex) functional E (cf. Gâteaux derivative):

$$\delta E \underbrace{(c,v)}_{(*)} := \lim_{\varepsilon\to 0} \frac{E(c+\varepsilon v) - E(c)}{\varepsilon}$$

$$= \lim_{\varepsilon\to 0} \int_\Omega \frac{f(c+\varepsilon v) - f(c)}{\varepsilon} + \frac{\gamma}{2} \frac{|\nabla(c+\varepsilon v)|^2 - |\nabla c|^2}{\varepsilon} \, \mathrm{d}x$$

$$\overset{\text{int. by parts}}{=} \int_\Omega f'(c)v - \gamma\Delta c\, v \, \mathrm{d}x$$

$(*)$: at position c; in direction $v \in C_0^1(\Omega)$

$$\Rightarrow \mu(c) = \underbrace{\delta E(c)}_{\text{as lin. functional}} = -\gamma\Delta c + f'(c) \quad \dots \quad \text{Riesz-representant on} L^2(\Omega) \tag{5.21}$$

insert into (5.20) $\Rightarrow$ *Cahn-Hilliard equation*:

$$c_t = L\,\Delta(-\gamma\Delta c + f'(c)), \quad \Omega \quad \text{(semilinear, 4th order)} \tag{5.22}$$

- possible BCs:
  a) periodic BC
  b) $\frac{\partial c}{\partial \nu} = 0$, $J\cdot\nu = -L\frac{\partial}{\partial\nu}\left(-\gamma\Delta c + f'(c)\right) = 0$, i.e. vanishing flux through boundary

- Idea of evolution:

  const. solutions c with $f''(c) < 0$ can be unstable (because diffusion term $L\,\mathrm{div}(f''(c)\nabla c)$ appears; is dominant for small variations) $\longrightarrow$ pattern formation (coarsening for $t \nearrow 0$; "grains" develop out of almost one substance)

Theorem 5.7. *Let c be classical solution of the Cahn-Hilliard eq. in $\Omega := (0,l)^d$ with periodic or 0-flux BCs.* $\Rightarrow$

1. $\frac{d}{dt}\int_\Omega c\,\mathrm{d}x = 0$

   ($\Rightarrow$ $\int_\Omega c_i\,\mathrm{d}x =$ const, because $\int c_1 + c_2\,\mathrm{d}x = \int 1\,\mathrm{d}x =$ const)

2. $\frac{d}{dt}E(c(t)) \le 0$ *(free energy is Lyapunov-functional)*

Proof.

1.
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega c\,\mathrm{d}x = L\int_\Omega \Delta(-\gamma\Delta c + f'(c))\,\mathrm{d}x$$

$$\overset{\text{div Thm}}{=} L\int_{\partial\Omega} \nu\cdot\nabla(-\gamma\Delta c + f'(c))\,\mathrm{d}s \overset{\text{BC}}{=} 0$$

2.

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{dt}} \int_\Omega \left(\frac{\gamma}{2} |\nabla c|^2 + f(c)\right) \mathrm{d}x &= \int_\Omega \gamma \nabla c \cdot \nabla c_t + f'(c) c_t \,\mathrm{d}x \\
&\overset{\text{int. by parts}}{=} \int_\Omega \left[-\gamma \Delta c + f'(c)\right] c_t \,\mathrm{d}x \\
&= L \int_\Omega \left[-\gamma \Delta c + f'(c)\right] \Delta \left[-\gamma \Delta c + f'(c)\right] \,\mathrm{d}x \\
&\overset{\text{int. by parts}}{=} -L \int_\Omega \left|\nabla \left[-\gamma \Delta c + f'(c)\right]\right|^2 \,\mathrm{d}x \le 0
\end{aligned}$$

□

Remark: also holds for weak solution

Theorem 5.8 ([EF], Th. 2.1)**.** *Let $\Omega = (0,l)$, f be double sink potential with $f(c) = \gamma_2 c^4 + \gamma_1 c^3 + \gamma_0 c^2$, $c_0 \in H_E^2(\Omega) := \{y \in H^2(\Omega) \mid y_x(0) = y_x(l) = 0\}$.*
For the Cahn-Hilliard equation (5.22) with boundary condition (b) we have:

(i) $\forall T > 0 \, \exists!$ solution $c \in L^2\left((0,T); H^4(\Omega)\right)$ with $c_t \in L^2\left((0,T); L^2(\Omega)\right)$.

(ii) If $c_0 \in H^6(\Omega) \cap H_E^2(\Omega)$ and $\frac{\partial^2}{\partial x^2} c_0 \in H_E^2(\Omega)$ then the solution c is classical.

linear instability:

All constants $c = c_m \in \mathbb{R}$ solve the Cahn-Hilliard equation (5.22) (homogeneous stationary solution).
Disturbance $c = c_m + u$, u small with $\int_\Omega u \,\mathrm{d}x = 0$ (conservation of mass); let e.g. $L = 1$.
Linearization at c_m:

$$\begin{aligned}
u_t = c_t &= \Delta\left[-\gamma \Delta u + f'(c) - f'(c_m)\right] \\
&\approx \Delta\left[-\gamma \Delta u + f''(c_m)(c - c_m)\right] \\
&= -\Delta\left[\gamma \Delta u - f''(c_m)\, u\right] \qquad (5.23)
\end{aligned}$$

Eigenfunctions of operator $u \mapsto -\Delta(\gamma \Delta u - f''(c_m)\, u)$ on $\Omega = (0,l)^d$ with periodic BCs:

$$\begin{aligned}
\varphi_k(x) &= \mathrm{e}^{\mathrm{i}\, k \cdot x}, \quad k \in K := \frac{2\pi}{l} \mathbb{Z}^d \setminus \{0\} \quad \left(\text{because } \textstyle\int u \,\mathrm{d}x = 0\right), \\
\lambda_k &= |k|^2 \left(-\gamma |k|^2 - f''(c_m)\right) \\
&= -\gamma \left(|k|^2 + \frac{f''(c_m)}{2\gamma}\right)^2 + \frac{f''(c_m)^2}{4\gamma} \in \mathbb{R} \qquad (5.24)
\end{aligned}$$

Remark: $\{\varphi_k\}_{k\in K}$ ... Basis of $\{L^2(\Omega) \mid \text{periodic BC}, \int f \mathrm{d}x = 0\}$

$\Rightarrow$ solution of (5.23) as linear combination:

$$u(x,t) = \sum_{k\in K} \alpha_k \mathrm{e}^{\lambda_k t}\, \mathrm{e}^{\mathrm{i}\, k\cdot x}$$

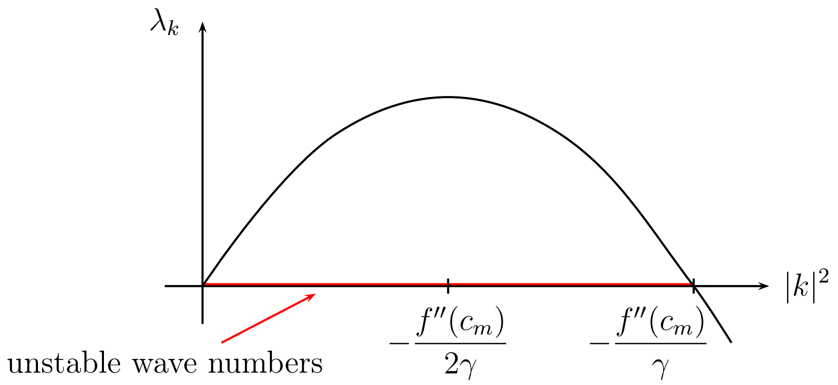
- $u \equiv 0$ is unstable if an eigenvalue $\lambda_k > 0$; only possible for $f''(c_m) < 0$. Let $f''(c_m) < 0$.
- from (5.24): most unstable mode for largest eigenvalue, hence

  $$\Big[|k|^2 + \underbrace{\frac{f''(c_m)}{2\gamma}}_{<0}\Big]^2 \longrightarrow \mathit{min}$$

  Let the solution be k_0.

  $\longrightarrow$ most unstable wave length:

  $$l_0 := \frac{2\pi}{|k_0|} \approx 2\,\pi \sqrt{-\frac{2\gamma}{f''(c_m)}} \quad \text{(because } k \text{ discrete).}$$



- wave numbers $|k|^2 > -\frac{f''(c_m)}{\gamma}$ are (linearly) stable

  $\longrightarrow$ Region with $l = \frac{2\pi}{|k|} < 2\pi\sqrt{-\frac{\gamma}{f''(c_m)}}$ does not allow for instability, i.e., no pattern formation.

Long term behaviour:

Theorem 5.9 ([EF], Th. 2.1)**.** *Assumption of Thm 5.8: let $\frac{1}{l}\int c_0 \,\mathrm{d}x =: M$, and c be the unique solution of the Cahn-Hilliard Eq. with BC (b) $\Rightarrow$*

(1) $c(t) \overset{t\to\infty}{\longrightarrow} c_\infty$ in $L^2(\Omega)$ with c_∞ is one solution of the stationary problem:

$$\begin{cases} \gamma c_\infty'' &= f'(c_\infty) - \alpha, \quad 0 < x < l, \\ c_\infty'(0) = c_\infty'(l) &= 0, \\ \int c_\infty \,\mathrm{d}x &= \int c_0 \,\mathrm{d}x, \end{cases} \tag{5.25}$$

and integration constant $\alpha \in \mathbb{R}$ *to be determined.*

(2) *Solution of* (5.25) *is equivalent to finding* critical points *of* $E(c)$ *in* $H^1(\Omega) \cap L^1(\Omega)$ *under constraint* $\mathcal{G}(c) := \int_\Omega c \,\mathrm{d}x \overset{!}{=} Ml$. *(by calculus of variations then* c_∞ *satisfies:* $\delta E(c) + \lambda\, \delta\mathcal{G}(c) \overset{(5.21)}{=} \underbrace{-\gamma\Delta c + f'(c)}_{=\mu(c)} + \lambda = 0$, *with* $\delta\mathcal{G}(c) = 1$ *and Lagrange multiplicator* $\lambda \in \mathbb{R}$.*)*

(3) $c(t) \overset{t\to\infty}{\longrightarrow} M$ *(= const) in* $L^2(\Omega)$ *(hence no phase separation), if one of the 3 following conditions holds:*

a) $\gamma > \frac{l^2}{\pi^2}$ *and* $\|c_0\|_2$ *small enough;*

b) $|M|$ *large (because then solution of* (5.25) *is unique);*

c) $\int (f(c_0(x)) - f_m)\,\mathrm{d}x + \frac{\gamma}{2}\,\|c_0'\|^2_{L^2}$ *small enough and* $f(c_0(x)) > f_m \quad \forall x \in (0,l)$, *where* $f_m := f(c_m)$ *is a local minimum of* f *and* $|c_m - M|$ *is small enough.*

Remark 5.10.

(1) Solution of (5.25) in general not unique; $c_\infty \equiv M$ is always a solution.

(2) Stationary problem of Cahn-Hilliard Eq. (5.22):

$$\begin{aligned} (-\gamma c_{xx} + f'(c))_{xx} &= 0\,, \quad 0 < x < l \quad \text{with} \quad c_x(0) = c_x(l) = 0 \\ (-\gamma c_{xx} + f'(c))_x\Big|_{x=0,l} &= 0 \end{aligned}$$

integrating twice gives (5.25).

(3) ad stationary problem (5.25):
For $M = 0$ and $f(c) := \frac{c^4}{4} - \frac{c^2}{2}$ (5.25) has exactly $2N_0 + 1$ solutions, where $N_0 = \left\lfloor \frac{4}{\pi l \sqrt{\gamma}} \right\rfloor$ ... Gauss bracket. One solution is $c_\infty \equiv 0$. If $c(x)$ is solution $\Rightarrow$ $-c(x)$ is solution.

Proof. of Theorem 5.9 (3c):

from $E(c(t)) \searrow$:

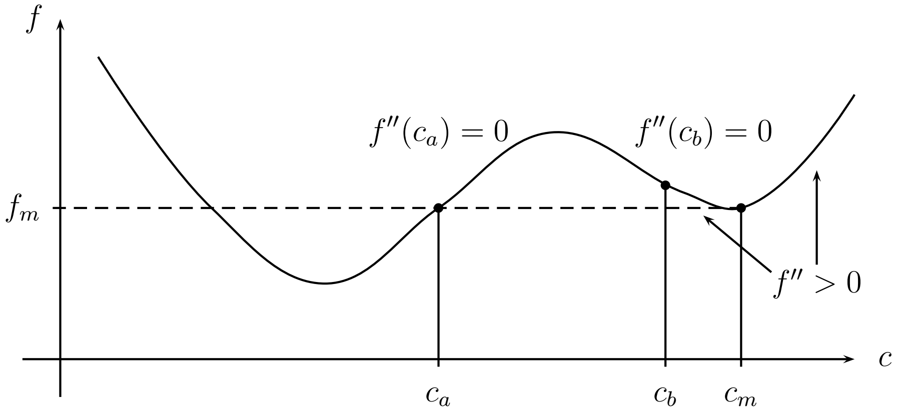
$$E(c) = \int_0^l f(c(x))\,\mathrm{d}x + \frac{\gamma}{2}\,\|c'\|^2_{L^2} \le E(c_0)$$

Sobolev embedding + Poincaré inequality (for $c - M \in H^1(\Omega)$, $\int_0^l (c-M)\mathrm{d}x = 0$) $\Rightarrow$

$$\int_0^l f(c)\,\mathrm{d}x + \frac{C\gamma}{2}\,\|c - M\|^2_{L^\infty} \le E(c) \le \int_0^l f(c_0)\,\mathrm{d}x + \frac{\gamma}{2}\,\|c_0'\|^2_{L^2} \quad \Big| - f_m l$$

$\Rightarrow$ with $\frac{1}{2}\|c-c_m\|^2_{L^\infty} \le \|c-M\|^2_{L^\infty} + |c_m - M|^2$:

$$\int_0^l (f(c)-f_m)\,\mathrm{d}x + \frac{C\gamma}{4}\,\|c-c_m\|^2_{L^\infty} \le \int_0^l \underbrace{(f(c_0)-f_m)}_{>0 \text{ lt. VS}}\,\mathrm{d}x + \frac{C\gamma}{2}\,|c_m - M|^2 + \frac{\gamma}{2}\,\|c_0'\|^2_{L^2} =: \varepsilon \tag{5.26}$$



by assumption ε "small enough".

Now let c_0 such that $\varepsilon < \frac{C\gamma}{8}\,(c_m - c_b)^2$ and $\int_0^l f(c_0) - f_m\,\mathrm{d}x \ge 0$

Claim:

$$\|c(t) - c_m\|_{L^\infty} < c_m - c_b \quad \forall t \ge 0. \tag{5.27}$$

Proof: From (5.26) for $t = 0$, hence $c = c_0$:

$$\|c_0 - c_m\|^2_{L^\infty} \le \frac{4}{C\gamma}\,\varepsilon < \frac{1}{2}\,(c_m - c_b)^2 < (c_m - c_b)^2;$$

c continuous in t $\Rightarrow$ (5.27) holds on maximal interval $[0, t^*)$. Let $t^* < \infty$ and

$$\|c(t^*) - c_m\|_{L^\infty} \ge c_m - c_b. \tag{5.28}$$

From (5.27): for $t \in [0, t^*)$: $\quad c(x,t) \in (c_b\,, 2c_m - c_b)$; $\quad f$ is convex

$$\Rightarrow \quad f(c(x,t)) \ge f_m \quad \forall x \in (0,l), \quad t \in [0, t^*)$$

$$\Rightarrow \quad \int_0^l f(c(t)) - f_m\,\mathrm{d}x \ge 0 \quad \text{on} \quad [0, t^*)$$

$$\Rightarrow \text{ (from (5.26)) } \quad \frac{C\gamma}{4}\,\|c(t) - c_m\|^2_{L^\infty} \le \varepsilon < \frac{C\gamma}{8}\,(c_m - c_b)^2$$

$$\Rightarrow \quad \|c(t) - c_m\|_{L^\infty} < \frac{1}{\sqrt{2}}\,(c_m - c_b) \quad \text{on} \quad [0, t^*) \;\ldots\; \text{contradiction to (5.28).}$$

Hence (5.27) $\forall\, t \geq 0$. □

From (5.27): $f''(c(x,t)) \geq 0 \quad \forall x \in (0,l), \quad t \geq 0$

$$c_t = (-\gamma c_{xx} + f'(c))_{xx} \qquad \Big|\; \cdot (c - M)\,, \quad \int_0^l \,\mathrm{d}x$$

$$\Rightarrow \quad \frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\,\|c - M\|_{L^2}^2 + \gamma\,\|c_{xx}\|_{L^2}^2 \overset{\text{int. by parts}}{=} -\int_0^l \underbrace{f''(c)}_{\geq 0}\,(c_x)^2\,\mathrm{d}x \leq 0\;.$$

With 2x Poincaré inequality (due to $\int_0^l (c - M)\,\mathrm{d}x = 0$) and with $c_x(0) = 0$ we obtain:

$$\begin{aligned} \|c - M\|_{L^2} &\leq C_p\,\|c_x\|_{L^2} \leq \frac{C_p\,l}{\sqrt{2}}\,\|c_{xx}\|_{L^2}\,. \\ \Rightarrow \quad \frac{\mathrm{d}}{\mathrm{dt}}\,\|c - M\|_{L^2}^2 &\leq -\frac{4\gamma}{C_p^2 l^2}\,\|c - M\|_{L^2}^2 \\ \Rightarrow \quad \|c(t) - M\|_{L^2} &\leq \mathrm{e}^{-\frac{2\gamma}{C_p^2 l^2}\,t}\,\|c_0 - M\|_{L^2}\,, \quad t \geq 0 \end{aligned}$$

■

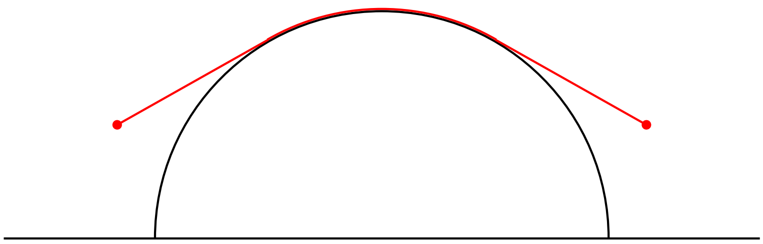
<u>Remark:</u> In Theorem 5.9 (3) $f'' \geq 0$ is essential, while for linear instability $f''(c_m) < 0$ was necessary.

<u>References</u>: [EGK] §6.2.13, [EF], [TE]

6 Problems with free boundary / thin-film equation

Examples:

- Flow in porous medium ($u_t = \Delta u^\alpha$, $\alpha > 1$); $\partial(\text{supp } u(t))$ is *free boundary*: dependent on time and solution
- Phenomena of melting and solidifying ("Stefan-Problem"): interface between liquid and solid phase is *free boundary*
- Obstacle problem for elastic membrane $\to$ course "calculus of variations"



- Evolution (resp. flow) of thin (wetting) liquid films on flat surface; free boundary $= \partial(\text{supp } h(t))$

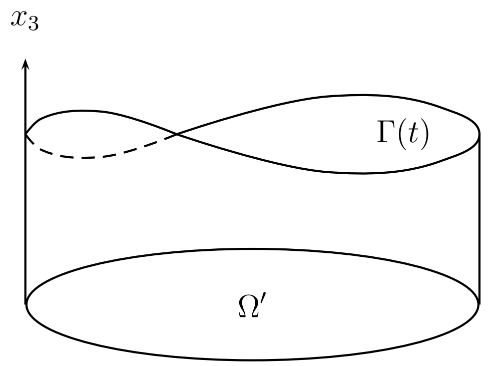
6.1 Derivation from Navier-Stokes equation

NS-equation for homogeneous incompressible flow:

$$\left.\begin{aligned} \varrho_0\,[u_t + (u\cdot\nabla)u] + \nabla p &= \mu\,\Delta\,u \\ \operatorname{div} u &= 0 \end{aligned}\right\} \tag{6.1}$$

in domain

$$\Omega(t) = \left\{(x', x_3) = (x_1, x_2, x_3) \in \mathbb{R}^3 \;\middle|\; x' \in \Omega',\ 0 < x_3 < \underbrace{h(x', t)}_{\text{smooth, pos.}} \right\};\ \Omega' \subset \mathbb{R}^2 \ldots \text{bounded domain}$$



- on fixed boundary ((x', x_3) with $x' \in \partial\Omega'$ or $x_3 = 0$): no-slip boundary condition $u = 0$.
- wanted: BC on free surface $\Gamma(t) = \{(x', h(x', t)) \mid x' \in \Omega'\}$.
  particle trajectory: $(x'(t),\, x_3(t))$ with tangential vector $u(x'(t), x_3(t))$.

  Idea: free boundary moves along with fluid:

  $$\begin{aligned} \frac{\mathrm{d}}{\mathrm{dt}}\, x'(t) &= (u_1, u_2)(x'(t), h(x'(t), t), t) \quad \ldots \text{ projected trajectory,} \\ \frac{\mathrm{d}}{\mathrm{dt}}\, h(x'(t), t) &= u_3(x'(t), h(x'(t), t), t) \end{aligned}$$

  $\Rightarrow$ *kinematic BC* on $\Gamma(t)$:

  $$u_3 = \partial_t\, h + u_1\, \partial_{x_1} h + u_2\, \partial_{x_2} h \tag{6.2}$$

- Balance of forces on surface between stress and capillary forces:

  $$T\nu \stackrel{!}{=} \gamma\, \kappa\, \nu \quad \ldots \text{ surface tension (acts in normal direction)} \tag{6.3}$$

  Hence: tangential components of $T\nu$ vanish:

  $$(T\nu)_{tang} = 0; \quad (T\nu)_{norm} = \gamma\kappa \tag{6.4}$$

  Stress tensor $\qquad T = 2\,\mu\, D - p\, I \qquad$ (as $\operatorname{div} u = 0$)
  Deformation tensor $\quad 2\, D = \nabla \otimes u + (\nabla \otimes u)^T$

  $$\begin{aligned} &\gamma \quad \ldots \quad \text{const} \quad (\sim \text{capillary number}) \\ &\kappa \quad = \quad \operatorname{div}_{x'} \left(\frac{\nabla_{x'}\, h}{\sqrt{1 + |\nabla_{x'}\, h|^2}} \right) \qquad \ldots \quad \text{mean curvature} \end{aligned}$$

Scaling:

L	...	typical length scale (horizontal)
H	...	typical height of film
V	...	typical velocity scale (horizontal)

$$
\begin{aligned}
x_i &= L\,\hat{x}_i\,; \quad i=1,2\,; \quad x_3 = H\,\hat{x}_3\,; \quad h = H\,\hat{h} \quad \text{with} \quad \varepsilon := \frac{H}{L} \ll 1 \\
u_i &= V\,\hat{u}_i\,; \quad i=1,2\,; \quad u_3 = \varepsilon\,V\,\hat{u}_3\,; \quad t = \frac{L}{V}\,\hat{t}; \quad p = \frac{\varepsilon\gamma}{L}\,\hat{p}; \quad V := \frac{\varepsilon^3\gamma}{\mu} \\
Re &:= \frac{\varrho_0\,L\,V}{\mu} \quad \ldots \quad \text{Reynolds number}
\end{aligned}
$$

The scalings of u_i, t, p arise naturally; the choice of V (later on) gives the "correct" balance between pressure term and viscosity.

Scaled NS-equation (notation '$\hat{\ }$' for scaled variable is omitted from now on):

$$
\begin{aligned}
\varepsilon^2\,Re\,[\partial_t\,u_i + (u\cdot\nabla)u_i] + \partial_{x_i}\,p &= \left(\varepsilon^2\,\partial_{x_1}^2 + \varepsilon^2\,\partial_{x_2}^2 + \partial_{x_3}^2\right)u_i\,; \quad i=1,2 && (6.5)\\
\varepsilon^2\,Re\,[\partial_t\,u_3 + (u\cdot\nabla)u_3] + \varepsilon^{-2}\,\partial_{x_3}\,p &= \left(\varepsilon^2\,\partial_{x_1}^2 + \varepsilon^2\,\partial_{x_2}^2 + \partial_{x_3}^2\right)u_3 && (6.6)\\
\operatorname{div} u &= 0
\end{aligned}
$$

Assumptions: $\varepsilon^2\,Re \ll 1$, $\varepsilon \ll 1$

$\Rightarrow$ dominant ε-order in (6.5), (6.6) ($\to$ "lubrication-approximation"):

$$
\begin{aligned}
\partial_{x_3}^2\,u_i &= \partial_{x_i}\,p\,; \quad i=1,2 && (6.7)\\
\partial_{x_3}\,p &= 0 \qquad (\text{hence } p = p(x',t))
\end{aligned}
$$

Solutions of (6.7) with BCs $u_i(x_3\!=\!0)\!=\!0$, $\partial_{x_3}u_i(x_3\!=\!h)\!=\!0$ (see (6.9) below); $i=1,2$:

$$
u_i(x,t) = \partial_{x_i}\,p(x',t)\left[\frac{x_3^2}{2} - h(x',t)\,x_3\right]; \quad i=1,2 \qquad (6.8)
$$

(cf. Poiseuille-flow)

On free boundary $x_3 = h(x',t)$ (with $\partial_{x_i}h = O(\varepsilon)$):

$$
\nu = \begin{pmatrix} 0\\0\\1 \end{pmatrix} + O(\varepsilon)\,, \quad \kappa = \varepsilon\Delta h + O(\varepsilon^2)\,.
$$

Consider (6.3) (unscaled !) for this particular ν:

$$T\begin{pmatrix}0\\0\\1\end{pmatrix} = \mu\begin{pmatrix}\frac{\partial u_1}{\partial x_3}+\frac{\partial u_3}{\partial x_1}\\ \frac{\partial u_2}{\partial x_3}+\frac{\partial u_3}{\partial x_2}\\ 2\frac{\partial u_3}{\partial x_3}\end{pmatrix} - \begin{pmatrix}0\\0\\p\end{pmatrix}$$

Magnitude of above terms after scaling: $O(\varepsilon^2)$, $O(\varepsilon^4)$; $O(\varepsilon^3)$, $O(\varepsilon)$

Dominant ε-order of tangential component (x_1, x_2) in balance (6.4) at $x_3 = h(x')$ is $O(\varepsilon^2)$:

$$\partial_{x_3} u_i(h(x')) = 0\,; \quad i = 1, 2\,. \tag{6.9}$$

Dominant ε-order of normal component (x_3) in (6.4) is $O(\varepsilon)$:

$$-p = \Delta h \qquad \text{(in scaled variables)} \tag{6.10}$$

• Integrate $\operatorname{div} u = 0$ in x_3:

$$0 = \int_0^{h(x_1,x_2,t)} (\partial_{x_1}u_1 + \partial_{x_2}u_2)\ dx_3 + u_3(x', h(x',t), t) - \underbrace{u_3(x', 0, t)}_{=0};$$

from kinematic BCs (6.2) at $x_3 = h(x')$:

$$\begin{aligned}
\partial_t h &= u_3 - u_1\partial_{x_1}h - u_2\partial_{x_2}h \\
&= -\int_0^{h(x_1,x_2,t)} (\partial_{x_1}u_1 + \partial_{x_2}u_2)\ dx_3 - u_1\,\partial_{x_1}h - u_2\,\partial_{x_2}h \\
&= -\operatorname{div}_{x'}\underbrace{\left(\int_0^{h(x_1,x_2,t)} \begin{pmatrix}u_1\\u_2\end{pmatrix} dx_3\right)}_{\text{flux function}} \overset{(6.8)}{=} -\operatorname{div}_{x'}\left(-\nabla_{x'}\,p(x',t)\,\frac{h^3}{3}\right)
\end{aligned}$$

With (6.10):

$$h_t = -\operatorname{div}\left(\frac{h^3}{3}\,\nabla\,\Delta h\right) \quad \ldots \quad \textit{thin film equation for } h(x_1,x_2,t), \tag{6.11}$$

(quasilin., 4th order)

- Evolution driven by surface tension, slowed down by viscosity
- While Navier-Stokes describes the full flow inside the film/droplet, (6.11) describes the evolution of its shape (due to the underlying liquid flow).
- Applications: movement of drop of water, (oil) lubrication, (paint) coating processes

References: [EGK] §7.10-11, [My]

6.2 Boundary conditions

more general thin film equations:

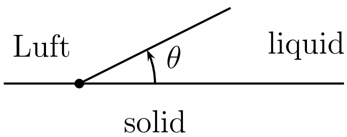
$$\begin{cases} h_t = -\operatorname{div}(h^n \nabla \Delta h)\,, \quad x \in \mathbb{R}^d\,; \quad 0 < n \leq 3 \\ h(\,\cdot\,,0) = h_0 \geq 0 \end{cases} \tag{6.12}$$

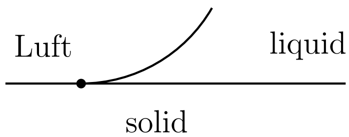
(6.12) holds on $\{h > 0\}$.

wanted: BCs on free boundary $\partial\{h > 0\}$.
Caution: in §6.1 the surface of the liquid was the free boundary, now it is the boundary of the liquid film.

(6.12) is parabolic eq. of 4th order with free boundary $\rightarrow$ 3 BCs at every $x \in \partial\{h > 0\}$ needed:

1) $h = 0$ on $\partial\{h > 0\}$
2) contact angle θ of the liquid at the intersection between fluid, der Flüssigkeit am Schnittpunkt zwischen Flüssigkeit, support, air $\rightarrow$ results from three surface tensions between two materials each (Young-Dupré law)
   a) $\theta \neq 0$ (e.g. water drops on plastic)
   b) $\theta = 0$ (e.g. water drops on very clean glass, wetting), $h_x = 0$ on $\partial\{h > 0\}$





3) Speed of propagation of contact line:

   First special case $n = 1$, $d = 1$ with BC 2b); hence

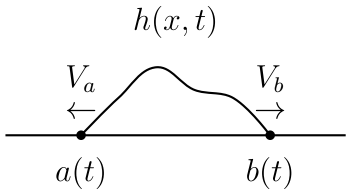
$$h_t + (h\,h_{xxx})_x = 0\,.$$

   Formally $V := h_{xxx}$ on $\partial\{h > 0\}$ is the speed of progation of the free boundary (compare linear transport equation $\rightarrow$ hyperbolic). Movement of contact line back and forth is possible.

Formulation as *free boundary value problem*:

$$\begin{cases} h_t + (h\,h_{xxx})_x = 0 & , \text{ in } \{h > 0\} \\ h = h_x = 0 & , \text{ on } \partial\{h > 0\} \\ V = h_{xxx} & , \text{ on } \partial\{h > 0\} \\ h(\,\cdot\,,0) = h_0 & \end{cases}$$

This is a coupled evolution system for $h(x,t)\big|_{\{h>0\}}$, $a(t)$, $b(t)$.



Deduction of $V = h_{xxx}$ for smooth solutions:

wlog let the (only) free boundary at $t = 0$ be at $x = 0$.
coordinate transformation

$$y := x - \int_0^t V(\tau)\, \mathrm{d}\tau \;\Rightarrow\; \text{ problem with fixed boundary for } \tilde{h}(y,t) := h(x,t) :$$

$$\begin{cases} \tilde{h}_t - \tilde{h}_y\, V(t) + (\tilde{h}\, \tilde{h}_{yyy})_y = 0 & , \quad \text{in } (0,\infty)^2 \qquad (6.13) \\ \tilde{h} = \tilde{h}_y = 0 & , \quad y = 0 \quad t > 0 \qquad (6.14) \\ \tilde{h}(\,\cdot\,, 0) = h_0 & \end{cases}$$

∂_y in (6.13):

$$\begin{aligned} \Rightarrow \quad 0 &= \tilde{h}_{yt} - \tilde{h}_{yy}\, V + (\tilde{h}\, \tilde{h}_{yyy})_{yy} \\ &= \tilde{h}_{yt} - \tilde{h}_{yy}\, V + \tilde{h}_{yy}\, \tilde{h}_{yyy} + 2\, \tilde{h}_y\, \partial_y^4\, \tilde{h} + \tilde{h}\, \partial_y^5\, \tilde{h} \end{aligned}$$

At $y = 0$ we have with (6.14): $\tilde{h}_{yy}(0,t) \Big[V(t) - \tilde{h}_{yyy}(0,t) \Big] = 0$
If $\tilde{h}_{yy}(0,t) \neq 0$, then $V = h_{xxx}$.

Generalisation to $d \in \mathbb{N}$, $n > 0$ (Proof: [GR] §9):

$$V(x_0) = \lim_{\substack{x \to x_0 \\ x \in \operatorname{supp}(h(\cdot,t))}} h^{n-1} \frac{\partial}{\partial \nu} \Delta h(x,t)\,, \quad x_0 \in \partial\{h > 0\}$$

References: [Kn] §1.1, §2.12

6.3 Positivity of the solution

Parabolic equations of 4th order in general have no maximum principle ($\rightarrow$ Exercises), but degenerateness of (6.12) "prevents" $h < 0$.

- technical aid: integral estimates

- multiply (6.12) by Δh; integration over $\mathbb{R}^d \times (0,T)$ formally gives

$$-\frac{1}{2}\int_0^T \partial_t \|\nabla h\|^2 \, \mathrm{d}t = \int_0^T \int_{\mathbb{R}^d} h^n \left|\nabla \Delta h\right|^2 \, \mathrm{d}x \, \mathrm{d}t$$

and hence the *energy estimate*:

$$\underbrace{\frac{1}{2}\int_{\mathbb{R}^d} \left|\nabla h\right|^2 (T) \, \mathrm{d}x}_{\substack{\text{energy of the linearised} \\ \text{surface tensions}}} + \underbrace{\int_0^T \int_{\mathbb{R}^d} h^n \left|\nabla \Delta h\right|^2 \, \mathrm{d}x \, \mathrm{d}t}_{\substack{\text{energy dissipation} \\ \text{through viscosity}}} = \frac{1}{2}\int_{\mathbb{R}^d} \left|\nabla h\right|^2 (0) \, \mathrm{d}x \tag{6.15}$$

$\Rightarrow$ energy $\searrow$ (if $\|\nabla h(0)\|_{L^2} < \infty$)

- "entropy" $\int_{\mathbb{R}^d} G(h) \, \mathrm{d}x$ defined using

$$G(s) := \int_A^s g(r) \, \mathrm{d}r \, , \quad g(s) := \int_A^s |r|^{-n} \, \mathrm{d}r \, , \qquad (A > 0; \text{ large enough})$$

Entropy ≥ 0 (see (6.20)).

- multiply (6.12) by $G'(h) = g(h)$; integration over $\mathbb{R}^d \times (0,T)$ *formally* gives

$$\int_{\mathbb{R}^d} \int_0^T \underbrace{h_t G'(h)}_{=\partial_t G(h)} \, \mathrm{d}t\mathrm{d}x = \int_0^T \int_{\mathbb{R}^d} (h^n \nabla \Delta h) \cdot \underbrace{\nabla g(h)}_{=h^{-n}\nabla h} \, \mathrm{d}x \, \mathrm{d}t$$

and hence the *entropy estimate*:

$$\int_{\mathbb{R}^d} G(h(T)) \, \mathrm{d}x + \int_0^T \int_{\mathbb{R}^d} (\Delta h)^2 \, \mathrm{d}x \, \mathrm{d}t = \int_{\mathbb{R}^d} G(h(0)) \, \mathrm{d}x \, . \tag{6.16}$$

$\Rightarrow$ entropy $\searrow$ (if $\int G(h(0)) \, \mathrm{d}x < \infty$)

Problem: the above calculations are only valid for "smooth solutions"!

For the following *rigorous* result consider with $1 < n < 4$:

$$\begin{cases} h_t = -(h^n \, h_{xxx})_x & ; \quad x \in \Omega = (-a, a) \, , \quad t > 0 \\ h_x = h_{xxx} = 0 & , \quad x = \pm a \\ h(\, . \, , 0) = h_0 \in H^1(-a, a) & \end{cases} \tag{6.17}$$

Theorem 6.1.

a) $\exists$ *"weak solution"* $h \in C([-a,a] \times [0,\infty))$ *(details in [BF] §3);*
(<u>Rem</u>: in general no uniqueness because weak formulation has "not enough" BCs. Subject largly unsettled.)

b) Additionally suppose $n \geq 2, h_0 \geq 0$ *and* $\int_\Omega |\ln h_0| \,\mathrm{d}x < \infty$ *(if* $n = 2$*) resp.* $\int_\Omega h_0^{2-n} \,\mathrm{d}x < \infty$ *(if* $2 < n < 4$*)* $(\to \int_\Omega G(h_0)\,\mathrm{d}x < \infty)$*.*

$\Rightarrow$ *solution from (a) satisfies* $h(x,t) \geq 0$*.*

Idea of proof:.

a) non-degenerate approximation problems:

$$\begin{cases} \partial_t h_\varepsilon = -\left(\left[\, |h_\varepsilon|^n + \varepsilon \,\right] \partial_x^3 h_\varepsilon \right)_x & , \quad \Omega \times (0,\infty) \\ \partial_x h_\varepsilon = \partial_x^3 h_\varepsilon = 0 & , \quad x = \pm a \\ h_\varepsilon(\,\cdot\,, 0) = h_{0\,\varepsilon} \in C^{4,\alpha}(\Omega) & \quad \text{(Hölder continuous)} \end{cases} \tag{6.18}$$

with $h_{0\,\varepsilon} \geq h_0\,,\quad h_{0\,\varepsilon} \stackrel{\varepsilon\to 0}{\longrightarrow} h_0$ in $H^1(\Omega)\,,\ \partial_x h_{0\,\varepsilon} = \partial_x^3 h_{0\,\varepsilon} = 0$ on $x = \pm a\,.$

$\Rightarrow$ (6.18) has unique classical solution h_ε; subsequence satisfies $h_\varepsilon \to h$ uniformly in $[-a,a] \times [0,T]$ $\forall T > 0$ (via a-priori estimates, compactness; details in [BF] §2-3). Sign of h_ε can change!

b) <u>Step 1</u>: deduction of 2 integral estimates for h_ε is rigorous.

Analogously to (6.15):

$$\frac{1}{2} \int_\Omega |\partial_x h_\varepsilon|^2 (T) \,\mathrm{d}x + \int_0^T \int_\Omega \left(|h_\varepsilon|^n + \varepsilon \right) \left|\partial_x^3 h_\varepsilon\right|^2 \,\mathrm{d}x\,\mathrm{d}t = \frac{1}{2} \int_\Omega |\partial_x h_\varepsilon|^2 (0) \,\mathrm{d}x$$

$$\Rightarrow \int_\Omega |h_{\varepsilon,x}|^2 (T) \,\mathrm{d}x \leq \int_\Omega |h_{0\,\varepsilon,x}|^2 \,\mathrm{d}x \leq 2 \int_\Omega |h_{0,x}|^2 \,\mathrm{d}x \quad \forall \varepsilon \leq \varepsilon_1 \quad (\text{from } H^1\text{-convergence}) \tag{6.19}$$

(6.18) is in divergence form $\quad\Rightarrow\quad \int_\Omega h_\varepsilon(T)\,\mathrm{d}x = \int_\Omega h_{0\,\varepsilon}\,\mathrm{d}x$

$\Rightarrow$ with Sobolev embedding, Poincaré, (6.19):

$$|h_\varepsilon(x,t)| \leq C\|h_\varepsilon(t)\|_{H^1} \leq C + C\|\partial_x h_\varepsilon(t)\|_{L^2} \leq: A \quad \forall x \in \Omega\,, \quad \forall t > 0\,, \quad \forall \varepsilon \leq \varepsilon_1\,.$$

Analogously zu (6.16):

$$\text{with} \quad g_\varepsilon(s) := -\int_s^A \frac{\mathrm{d}r}{|r|^n + \varepsilon} \leq 0\,, \quad G_\varepsilon(s) := -\int_s^A g_\varepsilon(r)\,\mathrm{d}r \geq 0 \quad (\text{für } s \leq A) \tag{6.20}$$

$$\int_\Omega G_\varepsilon(h_\varepsilon(T))\,\mathrm{d}x + \int_0^T\int_\Omega \left|\partial_x^2 h_\varepsilon\right|^2\,\mathrm{d}x\,\mathrm{d}t \;=\; \int_\Omega G_\varepsilon(h_{0\,\varepsilon})\,\mathrm{d}x$$
$$\le \int_\Omega G(h_{0\,\varepsilon})\,\mathrm{d}x \overset{\substack{G(s)\searrow \\ h_{0\varepsilon}\ge h_0}}{\le} \int_\Omega G(h_0)\,\mathrm{d}x < \infty \qquad (6.21)$$

Step 2: to show: $h(x,t)\ge 0$.

Assumption: let $h(x_0,t_0)<0$

$\Rightarrow$ (due to uniform convergence h_ε) $\exists\delta>0,\ \varepsilon_0>0$ with

$$h_\varepsilon(x,t_0) < -\delta \quad \text{for} \quad |x-x_0|<\delta\,,\quad x\in\Omega\,,\quad \varepsilon<\varepsilon_0\,.$$

For these x we have:

$$G_\varepsilon(h_\varepsilon(x,t_0)) = -\int_{h_\varepsilon(x,t_0)}^{A} \underbrace{g_\varepsilon(r)}_{\le 0}\,\mathrm{d}r \ge \underbrace{-\int_{-\delta}^{0} g_\varepsilon(r)\,\mathrm{d}r}_{<\infty} \xrightarrow{\varepsilon\to 0} -\int_{-\delta}^{0} g(r)\,\mathrm{d}r \overset{n\ge 2}{=} +\infty$$

$$\Rightarrow \quad \lim_{\varepsilon\to 0}\int_\Omega G_\varepsilon(h_\varepsilon(t_0))\,\mathrm{d}x = \infty \qquad \text{(contradiction to (6.21))}$$

■

Rem:

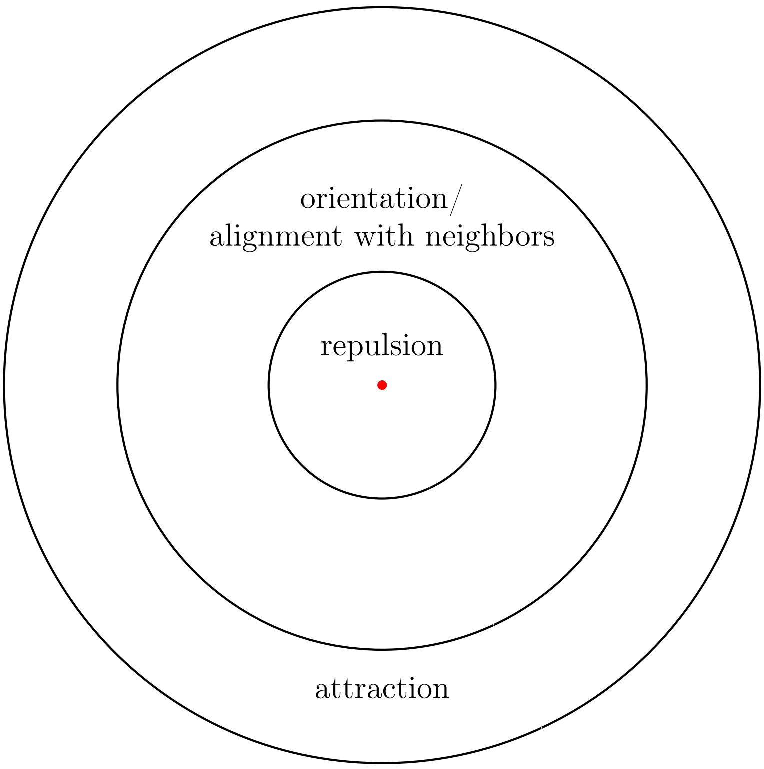
1) Discrete analoga of energy and entropy estimates are important for numerical schemes $\Rightarrow$ num. solution ≥ 0, (probably) uniqueness (subject still unsettled).
2) Film rupture (i.e. $h(x_0,t_0)=0$) for $n<\frac{1}{2}$ possible (rigorously proven) $\to$ no max-principle!
3) $h>0$ (i.e. prevention of film rupture) is of technological importance: oil lubrication, continuous coverage of paint.

References: [Be] §3, [BG] §2, [BF] §3, 4

7 Collective behaviour - kinetic equations

<u>Applications:</u> Many self-moving objects of similar size and shape (insects, fish, birds, pedestrians, many robots) often show complex global behaviour – despite simple individual rules of interaction.
The models described here are based on detailed observations of individual interactions (much more well-founded as with most applications of Turing instabilities).

For the interactions there often are 3 typical distances around a central object:



7.1 microscopic ODE-models

<u>Model 1</u> (2006)

$x_i \in \mathbb{R}^d;\ i = 1, ..., N$ positions of N objects
$v_i \in \mathbb{R}^d$ their velocities

Evolution in Newtonian Form:

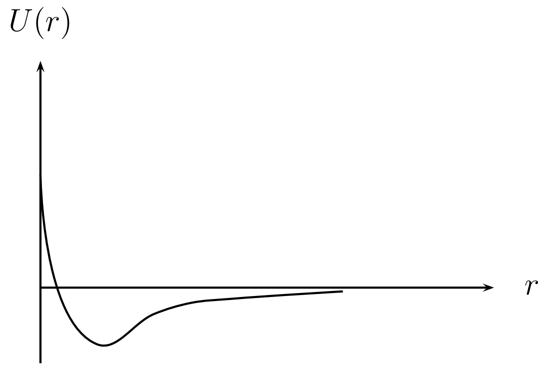
$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = v_i$$
$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = (\underbrace{\alpha}_{\text{propulsion}} \underbrace{-\beta|v_i|^2}_{\text{friction}})v_i \underbrace{-\frac{1}{N}\sum_{j\neq i}\nabla U(|x_i - x_j|)}_{\text{attraction/repulsion}} \tag{7.1}$$

$\rightarrow$ asymptotic speed $= \sqrt{\alpha/\beta}$

typical pair potentials (cf. Morse-, Lennard-Jones potentials in atomic physics):

$$U(r) = -C_A e^{-r/l_A} + C_R e^{-r/l_R}\ ,$$

with $C_R > C_A > 0$, $l_A > l_R > 0$, $\frac{l_A^2}{l_R^2} > \frac{C_R}{C_A}$.



Possible long-term effects in model (7.1): swarm formation (rotation); flock formation (translation $\forall\, i$: $v_i = \hat{v} \in \mathbb{R}^d$, $|\hat{v}| = \sqrt{\alpha/\beta}$)

<u>Cucker-Smale model</u> (2007)

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = v_i$$
$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = \underbrace{\sum_{j=1}^{N} a(|x_i - x_j|)\,(v_j - v_i)}_{\text{orientation}}\ , \tag{7.2}$$

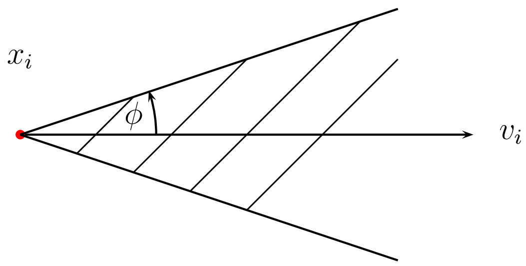
with $a(r) = \frac{1}{(1+r^2)^\gamma}$; $\gamma \geq 0$ ... rate of communication

Possible long-term effects in model (7.2): alignment of velocities, flock formation for $\gamma < \frac{1}{2}$:

Theorem 7.1 (Flock formation; [CS])**.** *Let* $d = 3$, $\gamma < \frac{1}{2}$. $\Rightarrow \exists \hat{X} \in \mathbb{R}^{3N\times 3N}$*:*
$\mathbb{R}^{3N\times 3N} \ni X(t) := \big(x_i(t) - x_j(t)\big)_{1\le i,j\le N} \overset{t\to\infty}{\longrightarrow} \hat{X}$ *(convergence of all pair distances);*
$\exists\, \hat{v} \in \mathbb{R}^3$*:* $v_i(t) \overset{t\to\infty}{\longrightarrow} \hat{v}\ \forall i$.

Model improvement: (e.g. for birds): alignment of velocities only in field of sight: replace sum in (7.2) by $\sum\limits_{j\in\sigma_i(t)}$ ... field of sight around own velocity vector, with

$$\sigma_i(t) := \Big\{ l \neq i \,\Big|\, \frac{(x_l - x_i)\cdot v_i}{|x_l - x_i|\,|v_i|} \ge \cos\phi \Big\} \quad \text{for some } \phi \in (0,\pi)\ .$$



7.2 mesoscopic PDE-models

For $N \gg 1$ it is often more practicable not to consider each individual "point" but only averaged models.

For $x,\, v \in \mathbb{R}^d$ consider the $x - v$–phase space with probability density $f(x,v,t)$; hence $f \ge 0$, $\int\int f(x,v,t)\,\mathrm{d}x\mathrm{d}v = 1\ \forall\, t$. $f(x,v)$ should decay "sufficiently" fast for $|x|$, $|v| \to \infty$.

Evolution of f according to *kinetic equation*:

$$\begin{aligned} f_t + v\cdot\nabla_x f + \mathrm{div}_v[(\alpha - \beta|v|^2)vf] - \mathrm{div}_v[(\nabla_x U(|x|) *_x \rho)f] &= 0\ , \quad t\ge 0\ , \\ f(x,v,0) &= f^0(x,v) \ge 0\ , \end{aligned} \tag{7.3}$$

with $\rho(x,t) := \int_{\mathbb{R}^d} f(x,v,t)\,\mathrm{d}v \ge 0$ ... position density (this is a *marginal density* and $\int \rho \mathrm{d}x = 1$).

This is a quadratically nonlinear Fokker-Planck-like equation (cf. plasma physics: for ion dynamics under electrostatic force).
Characteristics for the second and third term of (7.3): $\dot{X} = V$, $\dot{V} = (\alpha - \beta|V|^2)V$, cp. (7.1)

v–integration of (7.3) leads to continuity equation:

$$\rho_t + \mathrm{div}_x\, j = 0\,, \tag{7.4}$$

with flux $j(x,t) := \int_{\mathbb{R}^d} v f(x,v,t)\, dv$.

Total energy:

$$\mathcal{E}(t) := \frac{1}{2}\iint f(x,v,t)|v|^2\,\mathrm{d}x\mathrm{d}v + \frac{1}{2}\iint U(|x-y|)\rho(x,t)\rho(y,t)\,\mathrm{d}x\mathrm{d}y =: E_{kin} + E_{pot}\ .$$

Lemma 7.2.

$$\mathcal{E}(t) \le \max\{\mathcal{E}(0), C + \frac{\alpha}{2\beta}\},$$

with $C := \frac{1}{2}\sup|U|$. *(This implies* $E_{pot} \le C$, *as* $\int \rho \mathrm{d}x = 1$.*)*

Proof. For the kinetic energy of the second term of (7.3) we have:

$$-\frac{1}{2}\int\int v\cdot\nabla_x f|v|^2\,dxdv = -\frac{1}{2}\int\int \mathrm{div}_x(v|v|^2 f)\,dxdv = 0\ .$$

For the kinetic energy of the 4th term of (7.3) we have with 2x integration by parts and (7.4):

$$\begin{aligned}\frac{1}{2}\int\int |v|^2\,\mathrm{div}_v[(\nabla_x U(|x|)*\rho)f]\,dxdv &= -\int\int v\cdot(\nabla_x U(|x|)*\rho)f\,dxdv\\ = \int (U(|x|)*\rho)\ \mathrm{div}_x\Big(\int vf\,dv\Big)dx &= -\int (U(|x|)*\rho)\,\rho_t\,dx\end{aligned}$$

The last tem cancels with the time derivative of the potential energy:

$$\frac{dE_{pot}}{dt} = \frac{1}{2}\iint U(|x-y|)\big[\rho_t(x)\rho(y)+\rho(x)\rho_t(y)\big]\mathrm{d}x\mathrm{d}y = \iint U(|x-y|)\rho(y)\rho_t(x)\mathrm{d}y\mathrm{d}x$$

With $\iint f\,\mathrm{d}x\mathrm{d}v = 1$ we conclude:

$$\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} = \iint f[\alpha-\beta|v|^2]|v|^2\,\mathrm{d}x\mathrm{d}v \overset{\text{Hölder}}{\le} \alpha\iint f|v|^2\mathrm{d}x\mathrm{d}v - \beta\Big(\iint \underbrace{f|v|^2}_{=\sqrt{f}(\sqrt{f}|v|^2)}\ \mathrm{d}x\mathrm{d}v\Big)^2 \le 0\ ;$$

where the last inequality holds for $\iint f|v|^2\mathrm{d}x\mathrm{d}v \ge \frac{\alpha}{\beta}$.
Hence: $\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} \le 0$ for $\mathcal{E} \ge C + \frac{\alpha}{2\beta}$, as then $E_{kin} = \mathcal{E} - E_{pot} \ge C + \frac{\alpha}{2\beta} - C = \frac{\alpha}{2\beta}$. ■

This a-priori estimate on the energy is a crucial input for the global solvability of (7.3).

Relationship to ODE-Model (7.1):
(7.3) can be rigorously derived as "self-consistent" limit of (7.1) (cf. discrete vortex models). Conversely, (7.1) can be considered as numerical method (particle method) for (7.3); is also in use.

Definition 7.3. $\mathcal{M}(\mathbb{R})$ ... *signed* Radon measures *with finite mass (can also be negative; inner regular and locally finite); can be identified with* $C_0(\mathbb{R})'$ *(*C_0 *... continuous functions with compact support).*
$\mathcal{P}^1(\mathbb{R}) \subset \mathcal{M}(\mathbb{R})$ *... the subset of* probability measures *(which means* $\mu \geq 0$, $\int d\mu = 1$*).*

Let (x_i^0, v_i^0) be the IC of (7.1) and

$$f_N^0 := \sum_{j=1}^N m_j \delta_{(x_j^0, v_j^0)} \ \in \mathcal{P}^1(\mathbb{R}^{2d}) \ , \tag{7.5}$$

with $m_j = \frac{1}{N}$ be the corresponding *empirical measure* in $x - v$–phase space.
Idea:

$$f_N^0 \overset{N\to\infty}{\longrightarrow} f^0 \qquad \text{(weak * as measure, predual is } C_0(\mathbb{R}^{2d})). \tag{7.6}$$

Theorem 7.4 (From Newton to Fokker-Planck; "self-consistent" limit; cf. [BH, Ne, Do] for Vlasov equation)**.** *Let* $U \in C_b^2(\mathbb{R}_0^+)$ *with* $U'(0) = 0$*.*

a) *[N fixed] Let* $(x_i, v_i) \in C([0,T]; \mathbb{R}^{2d})$*;* $i = 1, ..., N$ *be solution of particle system* (7.1)*, for some* $T > 0$*.*

   $\Rightarrow$ *The probability measure*

$$f_N(t) := \sum_{j=1}^N m_j \delta_{(x_j(t), v_j(t))} \in \mathcal{P}^1(\mathbb{R}^{2d}) \ , \tag{7.7}$$

   with $\sum_{j=1}^N m_j = 1$ *(e.g.* $m_j = \frac{1}{N}$*) satisfies* $f_N \in C([0,T); \mathcal{P}^1(\mathbb{R}^{2d}))$ *(weak *) and solves* (7.3) *with IC* (7.5)*.*

b) *[*$N \to \infty$*] Let* $f^0 \geq 0$ *with* $|\mathcal{E}[f^0]| < \infty$*. Assume that an approximative sequence* $\{f_N^0\}_{N\in\mathbb{N}}$ *(of empirical measures) of the IC satisfies* (7.6)*, and that* $\mathcal{E}[f_N^0]$ *is uniformly bounded.*

   $\Rightarrow$ f_N *from* (7.7) *satisfies* $\forall T > 0$*:* $f_N \overset{N\to\infty}{\longrightarrow} f$ *in* $C([0,T]; \mathcal{P}^1(\mathbb{R}^{2d}))$ *(weak *), where* f *is the unique solution of* (7.3)*.*

Idea of proof. (only part a)
Step 1:
Let the "force field" $E(x,t)$ $[:= -\nabla_x U * \rho\,]$ be given.

Assumptions: let $E \in C(\mathbb{R}^d \times [0,T])$ be locally Lipschitz in x (uniformly in $t \in [0,T]$).

$$f_t + v \cdot \nabla_x f + \operatorname{div}_v[(\alpha - \beta|v|^2)vf] + \underbrace{E(x,t) \cdot \nabla_v f}_{=\operatorname{div}_v(Ef)} = 0 \ , \quad t \geq 0 \tag{7.8}$$

is a linear hyperbolic equation; corresponding characteristic equations:

$$\begin{aligned} \frac{\mathrm{d}X}{\mathrm{d}t} &= V \\ \frac{\mathrm{d}V}{\mathrm{d}t} &= E(X,t) + (\alpha - \beta|V|^2)V \end{aligned} \tag{7.9}$$

$\Rightarrow$ The measure transported by the flux of (7.9) solves (7.8) (in a weak sense).

Step 2:
For the particle density (actually a measure)

$$\rho_N(t) := \text{"} \int_{\mathbb{R}^d} f_N \, dv \text{"} = \sum_{j=1}^{N} m_j \delta_{x_j(t)} \in \mathcal{P}^1(\mathbb{R}^d)$$

we have

$$\Big(\nabla_x U(|.|) * \rho_N\Big)(x) = \sum_{j=1}^{N} m_j \nabla U(|x - x_j|) \ \in C_b^1(\mathbb{R}^d).$$

Hence the nonlinear term $(\nabla_x U(|x|) * \rho)f$ of (7.3) is also well-defined for empirical measures f_N, and the coefficient function $\nabla_x U(|x|) * \rho_N$ satisfies the assumptions of Step 1. ■

References: [CS], [BH, Ne, Do]

8 Nonlinear waves – Solitons

(only up to WS 2011/12)

- 1D wave equation: $u_{tt} - c^2 u_{xx} = 0, x \in \mathbb{R}, t \in \mathbb{R}$

  Solution: travelling waves $u(x,t) = f(x - ct) + g(x + ct)$ with const. velocity, not changing profile

  linear equation $\to$ superposition principle

- transport equation: $u_t + cu_x = 0$

  $\to$ wave propagation in only one dirction

- dispersive wave equation: $u_t + u_x + u_{xxx} = 0$

  harmonic wave solutions: $u(x,t) = e^{i(kx - \omega t)}$

  $\to$ *dispersion relation*: $\omega(k) = k - k^3$

  ω ... (angular)frequency

  k ... wave number

  $c = \frac{\omega}{k} = 1 - k^2$ ... speed of propagation (phase velocity)

  $\Rightarrow$ waves with different wave number are travel with different speeds $\to$ wave "disperses"; profile of wave is not preserved.

  $$\text{Superposition:} \quad u(x,t) = \int_{\mathbb{R}} \underbrace{A(k)}_{\text{Fourier-transform of } u(x,0)} e^{i(kx - \omega(k)t)} \mathrm{d}k$$

- inviscid Burgers' equation: $u_t + uu_x = 0$ develops shocks discontinuities ("shocks" $\to$ large wave numbers k in solution) in finite time.

  nonlinear equation $\to$ no superposition

- Korteweg - de Vries (KdV) equation: $u_t + uu_x + u_{xxx} = 0$

  Change of variables $u \mapsto \alpha u, t \mapsto \beta t, x \mapsto \gamma x$ $(\alpha, \beta, \gamma \in \mathbb{R} \setminus \{0\})$ gives general form of KdV:

  $$u_t + \frac{\alpha\beta}{\gamma} uu_x + \frac{\beta}{\gamma^3} u_{xxx} = 0$$

  Standard choice of parameters:

  $$u_t - 6uu_x + u_{xxx} = 0 \tag{8.1}$$

Smooth solution exists for $t \in \mathbb{R}$; "dispersive regularization" of Burgers' equation, i.e., wave components with large $|k|$ "travel away" more quickly. Dispersive term dampens large slopes; balance with nonlinearity.

(8.1) is invariant under the following *group of transformations*:

$$G_l, l \in \mathbb{R}\backslash\{0\} : X = lx, T = l^3 t, U = l^{-2} u$$

$\rightarrow$ suggests the existence of similarity solutions

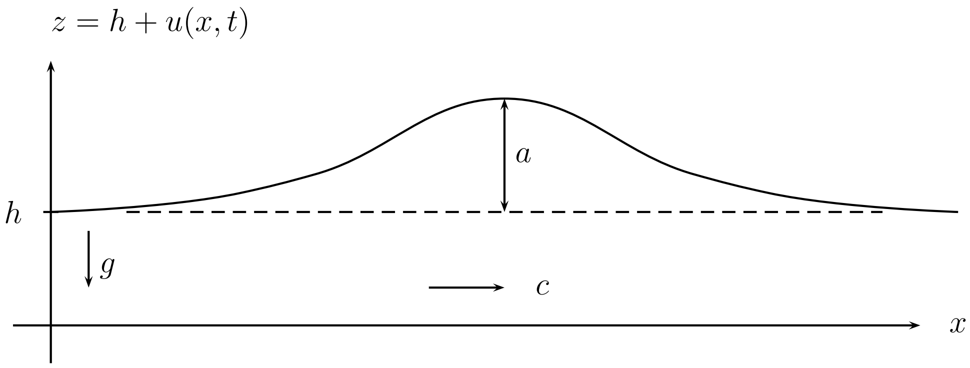
References: [DJ] §1

8.1 Applications of KdV

Long waves in a shallow canal can (seldom) have the form of solitons, i.e., do not change their shape:

$$u(x,t) = a \operatorname{sech}^2[b(x-ct)], \tag{8.2}$$

$$b^{-2} = 4h^2(h+a)/3a, c^2 = g(h+a)$$



u ... wave height over level at rest

$a > 0$ ... amplitude

h ... water depth

c ... speed of propagation (depending on amplitude!)

g ... gravitation constant

$\operatorname{sech} = 1/\cosh$ ... secans hyperbolikus

Assumption for "shallow water waves": wave length $\gg$ water depth

Figure 8.1: Imitation of Russel's soliton

Observed 1834 by J.S. Russel in Scotland (Fig. 8.1); is gavitational wave with constant mass transport in x-direction.

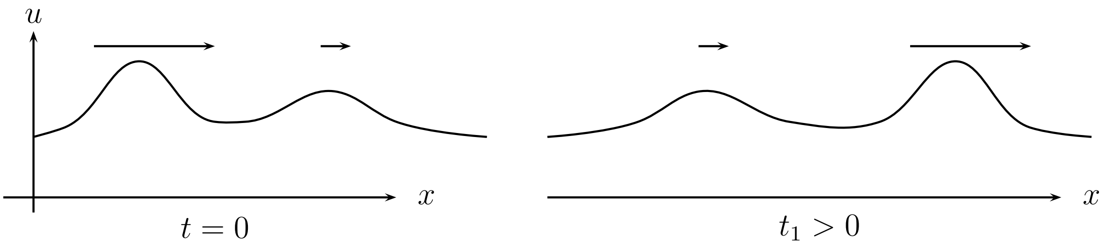
(8.2) satisfies KdV (with $\alpha\beta/\gamma = c/4b^2, \beta/\gamma^3 = 3bc/a$).

KdV can be derived for $\frac{a}{h} \ll 1$ from 2D incompressible, rotation-free, inviscid fluid equations (over horizontal plane with free surface) ([DJ] §1.2, [De] §9.3), or from 2D Euler equation ([Jo] §3.2.1).

(8.2) is gravitational wave, i.e. transport of mass.

further applications: (simple) tsunami-model.

Superimposition of solitons:



fast, high soliton "overtakes" slow, low soliton: short "interaction" (with phase shift) but *no* change of form (Fig. 8.2).

$\rightarrow$ almost a superposition principle, altough nonlinear equation$>$

Further *completely integrable systems* with soliton solutions:

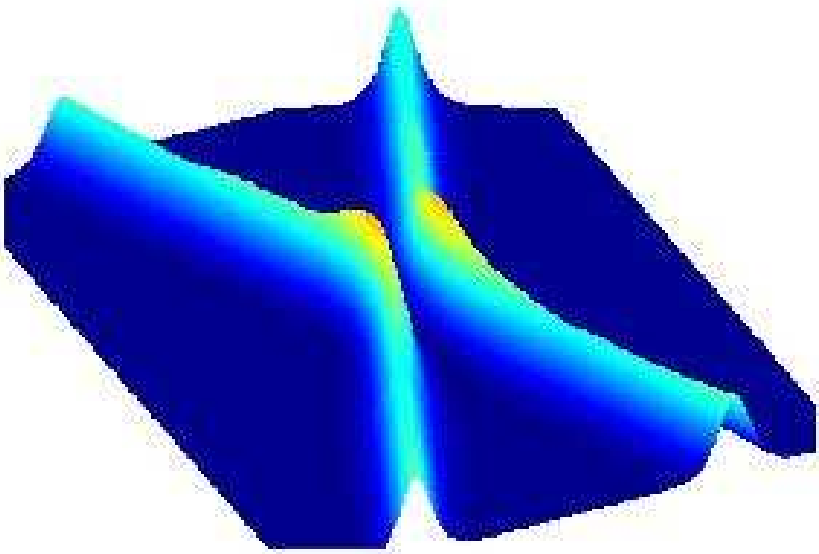


Figure 8.2: 2 interacting solitons as function of x, t: the interaction effects a local displacement of both solitons.

- kubic nonlinear Schrödinger equation

$$i\psi_t + \psi_{xx} \pm |\psi|^2\psi = 0, x \in \mathbb{R}, t > 0$$

Applications: nonlinear optics (disperson-free message transmission in fiber optic cables), Bose-Einstein condensate

- Sinus-Gordon equation

$$\frac{1}{c^2}\psi_{tt} - \psi_{xx} + \sin\psi = 0$$

Applications: differential geometry (for surfaces with constant negative Gauss curvature), displacements in a crystal with periodicity $\sin\psi$

<u>References</u>: [DJ] §1.2-4, §8.2, [TE]

8.2 Schrödinger scattering problems for KdV

Aim: Solution (resp. construction of solution) of IVP

$$\begin{cases} u_t - 6uu_x + u_{xxx} = 0, \quad x \in \mathbb{R}, t > 0 \\ u(x,0) = u_0(x), \quad x \in \mathbb{R} \end{cases} \tag{8.3}$$

Approach: transformation of (8.3) in family of linear eigenvalue problems (with parameter $t \geq 0$); $\psi \in \mathbb{C}$:

$$\left[-\frac{\partial^2}{\partial x^2} + u(x;t)\right]\psi(x;t) = \lambda(t)\psi(x;t).$$

Gives *stationäry Schrödinger* equation for (real) potential u.

"Miura-transformation"

$$u = v^2 + v_x \tag{8.4}$$

gives from (8.3):

$$(2v + \frac{\partial}{\partial x})\underbrace{(v_t - 6v^2 v_x + v_{xxx})}_{\text{modified KdV (mKdV)}} = 0.$$

Hence: if v solves mKdV then u solves KdV.

Solution of the *Riccati equation* (8.4) (for t fixed) with substitution

$$v = \psi_x/\psi \quad , \quad \psi(x;t) \neq 0 \tag{8.5}$$

$$\Rightarrow \psi_{xx} - u\psi = 0$$

KdV is *Galilei invariant*, i.e., invariant under transformations $\tilde{x} = x + 6\lambda t, \tilde{u} = u - \lambda$ for $\lambda \in \mathbb{R}$. Inserting into (8.4), (8.5) gives (t is only parameter!)

$$\psi_{xx} + (\lambda - u)\psi = 0 \tag{8.6}$$

Idea: 1) Solution of linear EVP (8.6) for $\psi(x;t), t \geq 0$.
2) (8.4), (8.5) then gives $u(x,t)$.
At first this sounds "weird" because u is given coefficient in (8.6), but we need the *scattering data S* (i.e. eigenvalues $\lambda(t)$, (generalized) eigenfunctions $\psi(x;t)$) only for $t = 0$, i.e. $u_0(x)$:

$$
\begin{tikzcd}
u_0(x) \arrow[rrr, "\text{scattering data}"] \arrow[d, dashed, "\text{KdV}"'] & & & S(0) \arrow[d, "\begin{array}{l}\text{simple}\\ \text{time evolution}\\ \text{(explicit}\\ \text{formula)}\end{array}"] \\
u(x,t) & & & S(t) \arrow[lll, "\text{inverse}", "\text{scattering problem}"']
\end{tikzcd}
$$

Spectral theory of $L = -\dfrac{\partial^2}{\partial x^2} + u$:

let $u = u(x;t)$ be bounded, smooth; rapidly decays for $|x| \to \infty$, because solution of KdV. $t \geq 0 \ldots$ parameter in operator L.

a) finitely many eigenvalues:

$$\lambda_n = -\kappa_n^2 < 0,\ \kappa_n > 0; \quad n = 1, 2, \ldots, N$$

asymptotic behaviour of real eigenfunctions (“bounded states”):

$$\psi_n(x;t) \sim c_n(t) e^{-\kappa_n x}, x \to \infty, \tag{8.7}$$

$c_n(t)$ from normalization $\|\psi_n\|_{L^2(\mathbb{R})} = 1$, $\psi_n(x;t)$ also decays exponentially for $x \to -\infty$.

b) continuous spectrum:

$\lambda = k^2 > 0$. Discussion here for $k > 0$; for $k < 0$ analogously:

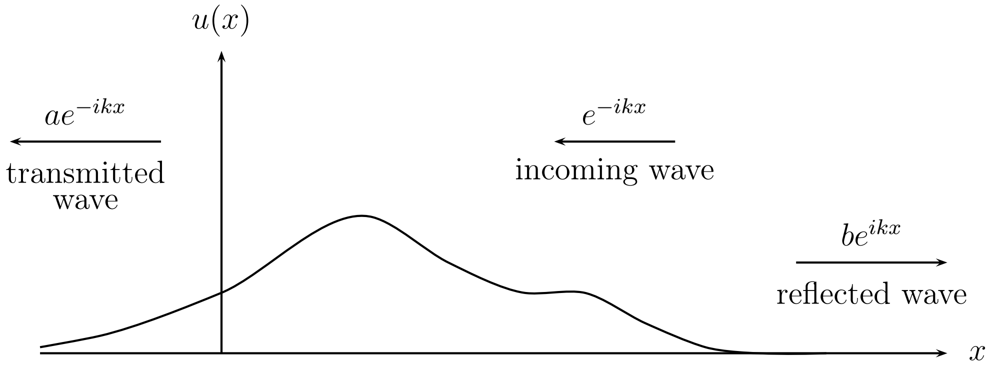
generalized eigenfunctions (“scattering states”; $\notin L^2$) oscillate for $|x| \to \infty$:

$$\psi(x;t) \sim \begin{cases} e^{-ikx} + b(k;t)e^{ikx} & , \quad x \to \infty \\ a(k;t)e^{-ikx} & , \quad x \to -\infty \end{cases} \tag{8.8}$$

$a \in \mathbb{C} \ldots$ transmission coefficient

$b \in \mathbb{C} \ldots$ reflection coefficient

We have: $|a|^2 + |b|^2 = 1$ (conservation of momentum resp. flow in scattering process)



Remark: (8.6) even has $\forall\, k = \sqrt{\lambda} \in \mathbb{C}$ solutions of the form (8.8), except in the upper half-plane for $k_n = i\kappa_n;\ n = 1, ..., N$.

If $u = u(x,t)$ solves KdV then also the scattering data of (8.6) have a simple t-dependence:

Theorem 8.1. *Let $u = u(x,t)$ be solution of* (8.3). $\Rightarrow$ *The "bounded states" satisfy (for $n = 1, \ldots, N; t \geq 0$):*

$$\begin{aligned} N &= \text{ const in } t; \\ \lambda_n(t) &= \lambda_n(0); \\ c_n(t) &= c_n(0)e^{4t\kappa_n^3}. \end{aligned} \tag{8.9}$$

Proof. Step 1: Differentiating (8.6) with respect to x resp. t:

$$\psi_{xxx} - u_x\psi + (\lambda - u)\psi_x = 0 \tag{8.10}$$

$$\psi_{xxt} + (\lambda_t - u_t)\psi + (\lambda - u)\psi_t = 0 \tag{8.11}$$

Define

$$R(x,t) := \psi_t + u_x\psi - 2(u + 2\lambda)\psi_x$$

$$\begin{aligned} &\Rightarrow \frac{\partial}{\partial x}(\psi_x R - \psi R_x) = \ldots = \psi_{xx}(\psi_t + u_x\psi - 2u\psi_x - 4\lambda\psi_x) \\ &\quad - \psi(\psi_{xxt} + u_{xxx}\psi - 3u_x\psi_{xx} - 2u\psi_{xxx} - 4\lambda\psi_{xxx}) \\ &[\psi_{xxx} \text{ and } \psi_{xxt} \text{ with (8.10), (8.11) eliminieren}] \\ &= \psi_{xx}(\psi_t - 2u\psi_x - 4\lambda\psi_x) - \psi(u_{xxx}\psi - 4u_x\psi_{xx}) \\ &\quad - \psi(u\psi_t - \lambda\psi_t - \lambda_t\psi + u_t\psi) + \psi(2u + 4\lambda)(u_x\psi - \lambda\psi_x + u\psi_x) \\ &\overset{(8.6)}{=} \psi^2(\lambda_t \underbrace{- u_t + 6uu_x - u_{xxx}}_{=0 \text{ with KdV}}) = \lambda_t\psi^2 \end{aligned} \tag{8.12}$$

Remark: (8.12) also holds for continuous spectrum $\lambda > 0$.

Let now $\lambda = \lambda_n = -\kappa_n^2 < 0, \psi = \psi_n, R = R[u, \psi_n] =: R_n$.

ψ_n, R_n decay exponentially for $|x| \to \infty$.

$\Rightarrow \int_{\mathbb{R}} \mathrm{d}x$–integral of (8.12):

$$0 = \psi_{n,x} R_n - \psi_n R_{n,x}\big|_{-\infty}^{\infty} = \lambda_{n,t} \int\limits_{\mathbb{R}} \underbrace{\psi_n^2}_{\in\mathbb{R}} \mathrm{d}x = \lambda_{n,t} \quad \checkmark$$

<u>Step 2:</u>

$\Rightarrow$ indefinite x-integral of (8.12) (i.e. $-\partial_x(\psi_{n,x} R_n - \psi_n R_{n,x}) = 0$, because $\lambda_{n,t} = 0$) gives:

$$\psi_n R_{n,x} - \psi_{n,x} R_n = g_n(t), \quad g_n(t) \ldots \text{arbitrary integration constant} \tag{8.13}$$

ψ_n, R_n decay for $|x| \to \infty \Rightarrow g_n = 0 \quad \forall t \geq 0$.

indefinite x-integral of (8.13) (i.e. $\frac{\psi_n R_{n,x} - \psi_{n,x} R_n}{\psi_n^2} = \partial_x \frac{R_n}{\psi_n} = 0$) :

$$\frac{R_n}{\psi_n} = h_n(t), \qquad h_n(t) \ldots \text{arbitrary integration constant} \tag{8.14}$$

Multiply by ψ_n^2, use (8.6):

$$R_n \psi_n = [\psi_t + u_x \psi - 2(u + 2\lambda)\psi_x]\,\psi = \frac{1}{2}(\psi_n^2)_t + (u\psi_n^2 - 2\psi_{n,x}^2 - 4\lambda\psi_n^2)_x = h_n(t)\psi_n^2$$

$\int_{\mathbb{R}} \mathrm{d}x$–integration:

$$0 = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\int\limits_{\mathbb{R}} \psi_n^2 \mathrm{d}x\right) = h_n(t) \underbrace{\int\limits_{\mathbb{R}} \psi_n^2 \mathrm{d}x}_{=1}$$

$\Rightarrow h_n(t) = 0, \forall t \geq 0$

(8.14), d.h. $R_n = 0$ gives evolution of $\psi_n(x;t)$:

$$\psi_{n,t} = -u_x \psi_n + 2(u + 2\lambda_n)\psi_{n,x}$$

use $u \overset{x\to\infty}{\longrightarrow} 0$, ψ_n—asymptotics (8.7):

$$\Rightarrow c_n'(t) - 4\kappa_n^3 c_n(t) = 0$$

$$\Rightarrow c_n(t) = c_n(0) e^{4t\kappa_n^3}. \quad \checkmark$$

■

Theorem 8.2. *Let $u = u(x, t)$ be solution of* (8.3). $\Rightarrow$ *The "scattering states" satisfy* ($\forall k > 0; t \geq 0$)*:*

$$a(k;t) = a(k;0), \quad b(k;t) = b(k;0)e^{8ik^3 t}. \tag{8.15}$$

Proof. Let $\lambda = k^2 > 0$ be fixed (i..e const in t, because continuous spectrum $(0, \infty)$ is t–indep.); ψ the corresponding generalized eigenfunction; $R = R[u, \psi]$.
Integrate (8.12) with respect to x (with $\lambda_t = 0$):

$$\psi_x R - \psi R_x = g(t;k) \ldots \text{arbitrary interation constant} \tag{8.16}$$

According to (8.8): $\psi(x; t, k) \sim a(k;t)e^{-ikx}, x \to -\infty$

$$\Rightarrow R(x, t; k) \sim \psi_t - 4\lambda\psi_x \sim \left(\frac{\mathrm{d}a}{\mathrm{d}t} + 4ik^3 a\right) e^{-ikx}, x \to -\infty$$

$$\Rightarrow \psi_x R - \psi R_x \overset{x \to -\infty}{\longrightarrow} 0 \quad \Rightarrow \quad g(t;k) = 0 \quad \forall t \geq 0$$

x–integration of (8.16):

$$\frac{R}{\psi} = h(t;k) \ldots \text{beliebig;} \quad R = h\psi \tag{8.17}$$

$x \to \infty$—asymptotics of ψ, R leads to:

$$\frac{\mathrm{d}a}{\mathrm{d}t} + 4ik^3 a = ha \tag{8.18}$$

analogous behaviour for $x \to \infty$:

$$R(x, t; k) \sim \frac{\mathrm{d}b}{\mathrm{d}t} e^{ikx} + 4ik^3(e^{-ikx} - be^{ikx}) \overset{(8.17),(8.8)}{=} h(e^{-ikx} + be^{ikx}) \sim h\psi$$

Because $e^{\pm ikx}$ is linearly independent (comparing coefficients):

$$\frac{\mathrm{d}b}{\mathrm{d}t} - 4ik^3 b = hb, \quad h(t;k) = 4ik^3$$

$\Rightarrow b(k;t) = b(k;0)e^{8ik^3 t}$,

$$a(k;t) = a(k;0) \quad \text{(from (8.18))}$$

■

Remark 8.3. In formulas (8.9), (8.15) the exact form of $u(x, t)$ does *not* enter. They give a lot of a-priori information for the KdV-evolution ("similar" to conserved quantity of evolution).

References: [De] §9.7, [DJ] §3.1-2,4.1-3, [Wh] §17.3

8.3 inverse scattering problem

Aim: Solution of nonlinear IVP

$$\begin{cases} u_t - 6uu_x + u_{xxx} = 0, & x \in \mathbb{R}, t > 0 \\ u(x,0) = u_0(x), & x \in \mathbb{R} \end{cases}$$

in 3 steps:

1) linear eigenvalue problem $\psi_{xx} + (\lambda - u_0(x))\psi = 0, x \in \mathbb{R} \to$ scattering data $S(0)$
2) explicit evolution of scattering data $S(t)$, $t \geq 0$ (according to Thm 8.1, 8.2)
3) inverse scattering problem: reconstruction of $u(x,t)$ from $S(t)$ with linear integral equation

$$\begin{tikzcd} u_0(x) \arrow[rr, "\text{scattering data"}] \arrow[d, dashed, "\text{KdV}"'] & & S(0) \arrow[d, "\substack{\text{explicit}\\ \text{time evolution}}"] \\ u(x,t) & & S(t) \arrow[ll, "\text{inverse}", "\text{scattering problem}"'] \end{tikzcd}$$

inverse scattering problem for t fixed:

$$\psi_{xx} + (k^2 - u(x))\psi = 0 \quad , \quad x \in \mathbb{R} \tag{8.19}$$

given: scattering data of (8.19) $S = S(t) := \{-\kappa_1^2, \dots, -\kappa_N^2; c_1, \dots, c_N; b(k), k \in \mathbb{R}\}$ (e.g. obtained using Thm. 8.1, 8.2 from $S(0)$)

wanted: potential $u(x) = u(x;t)$

Define for suitable decaying reflection coefficient $b(k)$:

$$F(\xi) := \sum_{n=1}^{N} c_n^2 e^{-\kappa_n \xi} + \underbrace{\frac{1}{2\pi} \int_{\mathbb{R}} b(k) e^{ik\xi} \mathrm{d}k}_{\text{inverse Fourier trans.}} \quad , \quad \xi \in \mathbb{R} \tag{8.20}$$

Theorem 8.4 (inverse scattering theorem)**.** *Let F be rapidly decaying.* $\Rightarrow$

$$u(x) = -2 \frac{\mathrm{d}}{\mathrm{d}x} K(x,x),$$

with: $K(x,z)$ *is the unique function on* $\mathbb{R}^2$ *such that* $K(x,z) = 0$ *for* $z < x$ *and satisfying the* linear Fredholm integral equation:

$$K(x,z) + F(x+z) + \int_x^\infty K(x,y)F(y+z)\mathrm{d}y = 0 \quad , -\infty < x < z$$

("Gelfand-Levitan-Marchenko" (GLM)-equation).

Idea of proof. First discussion of direct scattering problem (8.19); Deduction of GLM-equation:

Case 1: $L := -\frac{\partial^2}{\partial x^2} + u(x)$ has only continuou spectrum (e.g. for $u \geq 0$).
We are looking for solutions (for $k \in \mathbb{R}$ fixed) of the form Form ("Jost solutions")

$$\Phi_k(x) = e^{ikx} + \int_x^\infty K(x,z)e^{ikz}\mathrm{d}z, \tag{8.21}$$

$$\Phi_{-k}(x) = e^{-ikx} + \int_x^\infty K(x,z)e^{-ikz}\mathrm{d}z. \tag{8.22}$$

If K decays (suitably), then

$$\lim_{x\to\infty} \Phi_{\pm k}(x) = e^{\pm ikx}.$$

Aim: Find equation for K by inserting $\Phi_{\pm k}$ in (8.19):

$$\text{aus (8.21):} \quad \Phi_{kxx} = e^{ikx}\left[-k^2 - \frac{\mathrm{d}}{\mathrm{d}x}K(x,x) - ikK(x,x) - K_x(x,x)\right] + \int_x^\infty K_{xx}e^{ikz}\mathrm{d}z$$

$2\times$ integration by parts in (8.21):

$$\Phi_k = e^{ikx}\left[1 + \frac{iK(x,x)}{k} - \frac{K_z(x,x)}{k^2}\right] - \frac{1}{k^2}\int_x^\infty K_{zz}e^{ikz}\mathrm{d}z,$$

if $K(x,z), K_z(x,z) \overset{z\to\infty}{\longrightarrow} 0$ (such that the integrals exist):

$$\Rightarrow 0 \overset{(8.19)}{=} \Phi_{kxx} + (k^2 - u)\Phi_k =$$

$$= -e^{ikx}\left[u + 2\frac{\mathrm{d}}{\mathrm{d}x}K(x,x)\right] + \int_x^\infty (K_{xx} - K_{zz} - u(x)K)e^{ikz}\mathrm{d}z$$

This holds if

$$K_{xx} - K_{zz} - u(x)K = 0 \quad , z > x, \qquad \text{and}$$
$$u(x) = -2\frac{\mathrm{d}}{\mathrm{d}x}K(x,x) = -2[K_x(x,x) + K_z(x,x)]. \tag{8.23}$$

<u>next aim:</u> equation for K which only contains scattering data (but not u).

- $\Phi_{\pm k}(x)$ linearly independent $\Rightarrow$ are fundamental solutions of (8.19)
- generalized eigenfunctions according to (8.8):

$$\psi(x;t) \sim \begin{cases} e^{-ikx} + b(k;t)e^{ikx} & , \quad x \to \infty \\ a(k;t)e^{-ikx} & , \quad x \to -\infty \end{cases}$$

$\Rightarrow$ The particular solution with

$$\psi_k(x) \sim e^{-ikx} \quad \text{for } x \to -\infty, \quad \text{hence } \psi_k(x) = \frac{1}{a_k}\psi(x)$$

is:

$$\psi_k(x) = \frac{1}{a(k)} \underbrace{\Phi_{-k}(x)}_{\sim e^{-ikx},\, x\to\infty} + \frac{b(k)}{a(k)} \underbrace{\Phi_k(x)}_{\sim e^{ikx},\, x\to\infty} \tag{8.24}$$

$$\Rightarrow a(k)\psi_k(x) \overset{(8.21),(8.22)}{=} e^{-ikx} + \int_x^\infty K(x,z)e^{-ikz}\mathrm{d}z$$
$$+ b(k)\left[e^{ikx} + \int_x^\infty K(x,z)e^{ikz}\mathrm{d}z\right] \quad \forall\, x \in \mathbb{R};\ \forall\, k \in \mathbb{R} \text{ fixed.}$$

inverse Fourier-transformation ($k \to y$) gives for $y > x$:

$$\frac{1}{2\pi}\int_{\mathbb{R}} a(k)\psi_k(x)e^{iky}\mathrm{d}k \tag{8.25}$$
$$= \underbrace{\frac{1}{2\pi}\int_{\mathbb{R}} e^{ik(y-x)}\mathrm{d}k}_{=\delta(y-x)=0 \text{ as } y>x} + \int_x^\infty K(x,z)\underbrace{\left[\frac{1}{2\pi}\int_{\mathbb{R}} e^{ik(y-z)}\mathrm{d}k\right]}_{=\delta(y-z)}\mathrm{d}z$$
$$+ \underbrace{\frac{1}{2\pi}\int_{\mathbb{R}} b(k)e^{ik(x+y)}\mathrm{d}k}_{=:F(x+y) \text{ according to (8.20)}} + \int_x^\infty K(x,z)\left[\frac{1}{2\pi}\int_{\mathbb{R}} b(k)e^{ik(y+z)}\mathrm{d}k\right]\mathrm{d}z$$
$$= K(x,y) + F(x+y) + \int_x^\infty K(x,z)F(y+z)\mathrm{d}z,$$

because L has no discrete spectrum (by assumption).

Calculation of the integral (8.25) with residue theorem and complex contour integral:

$$\int_{\mathbb{R}} a(k)\psi_k(x)e^{iky}\mathrm{d}k = 0, \qquad \forall\, x, y \text{ fixed}$$

because $a(k), b(k), \psi_k$ are analytic in upper half-plane (details: [DJ], §3.3)

$\Rightarrow K$ satisfies (with $y \leftrightarrow z$):

$$K(x,z) + F(x+z) + \int_x^\infty K(x,y)F(y+z)\mathrm{d}y = 0, \quad -\infty < x < z. \tag{8.26}$$

inverse scattering problem:

F given by scattering data $\Rightarrow K(x,z)$ can be calculated from integral equation (8.26) $\Rightarrow$ u from (8.23).

case 2: L has $N \geq 1$ eigenvalues $\lambda_1, \ldots, \lambda_N$.

We have: $a(k), b(k)$ are meromorph in the upper half-plane with N simple poles at $k = i\kappa_n$ ($\kappa_n > 0, \lambda_n = -\kappa_n^2$)

Calculation of the integral (8.25):

With

$$\begin{aligned} \psi_{i\kappa_n}(x) &= c_{\kappa_n}\Phi_{i\kappa_n}(x) \quad \text{(cf. (8.24))} \\ &\overset{(8.21)}{=} c_{\kappa_n}\left(e^{-\kappa_n x} + \int_x^\infty K(x,z)e^{-\kappa_n z}\mathrm{d}z\right) \end{aligned}$$

one can show (details [DJ] §3.2-3):

$$\begin{aligned} \frac{1}{2\pi}\int_{\mathbb{R}} a(k)\psi_k(x)e^{iky}\mathrm{d}k &= -\sum_{n=1}^N c_{\kappa_n}\psi_{i\kappa_n}(x)e^{-\kappa_n y} \\ &= -\sum_{n=1}^N c_{\kappa_n}^2\left[e^{-\kappa_n(x+y)} + \int_x^\infty K(x,z)e^{-\kappa_n(y+z)}\mathrm{d}x\right] \end{aligned}$$

Inserting into (8.25) again gives (8.26).

Rem: (8.26) implies (as desired) $K_{xx} - K_{zz} - u(x)K = 0$, $z > x$ for $u(x) := -2\frac{d}{dx}K(x,x)$ (see Exercises). ■

Remark 8.5. 1) The Fredholm integral equation (8.26) can be written as fixed point iteration for $K \in C(\mathbb{R}^2)$ (or $\in C^\infty(\mathbb{R}^2)$):

$$K \mapsto K^*(x,z) := -F(x+z) - \int_x^\infty K(x,y)F(y+z)\mathrm{d}y. \tag{8.27}$$

Mapping (8.27) is Lipschitz with constant $\|F\|_{L^1(\mathbb{R})}$.

Let $\|F\|_{L^1} < 1 \Rightarrow$ GLM-equation has unique solution.

2) Special case: Let F be separable; i.e.,

$$F(x+z) = \sum_{n=1}^N X_n(x)Z_n(z) \quad , \quad N \in \mathbb{N} \text{ with } Z_n \text{ l.u.}$$

(e.g. for $b \equiv 0$, which means a reflection-free potential). $\Rightarrow$ GLM-equation becomes

$$K(x,z) + \sum_{n=1}^N X_n(x)Z_n(z) + \sum_{n=1}^N Z_n(z) \int_x^\infty K(x,y)X_n(y)\mathrm{d}y = 0$$

$\Rightarrow$ Ansatz for solution: $K(x,z) = \sum_{n=1}^N L_n(x)Z_n(z)$

$$\Rightarrow \quad L_n(x) + X_n(x) + \sum_{m=1}^N L_m(x) \underbrace{\int_x^\infty Z_m(y)X_n(y)\mathrm{d}y}_{=\text{known}} = 0; \quad n = 1,\dots,N$$

hence: N linear algebraic equations for N unknowns $L_n(x)$

3) We have: number of bounded states of operator L $(= N)$ = number of solitons a solution develops for $t \to \infty$.

Example 8.6 (Reflection coefficient with $N = 1$ pole)**.** Scattering data are given as

1) $b(k) = -\dfrac{\beta}{\beta + ik}$ (for some $0 < \beta = $ const), hence pole at $k = i\beta$, which means one eigenvalue $\lambda_1 = -\kappa_1^2 = -\beta^2$ of L.
2) $\psi_1(x) \sim \sqrt{\beta}e^{-\beta x}$ for $x \to \infty$; d.h. $c_1 = \sqrt{\beta}$

Aim: calculate corresponding potential u.

$$\to F(\xi) = \beta e^{-\beta\xi} - \frac{\beta}{2\pi} \int_{\mathbb{R}} \frac{e^{ik\xi}}{\beta + ik}\mathrm{d}k = \ldots = \beta e^{-\beta\xi} H(-\xi)$$

(with residue theorem; H …Heaviside function)

From GLM-equation (8.26): $K(x,z)=0$ for $x+z>0$.

GLM for $x+z<0$ (as $F(y+z)\neq 0$ only for $y+z<0$):

$$K(x,z)+\beta e^{-\beta(x+z)}+\beta\int_x^{-z}K(x,y)e^{-\beta(y+z)}\mathrm{d}y=0,\quad x<\min(z,-z).$$

(unique) solution: $K=-\beta$, hence

$$K(x,z)=\left\{\begin{array}{ccc}0 & , & x+z>0\\ -\beta & , & x+z<0\end{array}\right\}=-\beta H(-x-z)$$

$K(x,x)=-\beta H(-2x)=-\beta H(-x)$

$\Rightarrow u(x)=-2\frac{\mathrm{d}}{\mathrm{d}x}K(x,x)=-2\beta\delta(x)$.

Furthermore: initial profile $u_0=-2\beta\delta$ splits in one soliton

$$u(x,t)\sim 2\beta^2\,\mathrm{sech}^2\left[\beta(x-4\beta^2t+\frac{\ln 2}{2\beta})\right]$$

and a dispersive wave.

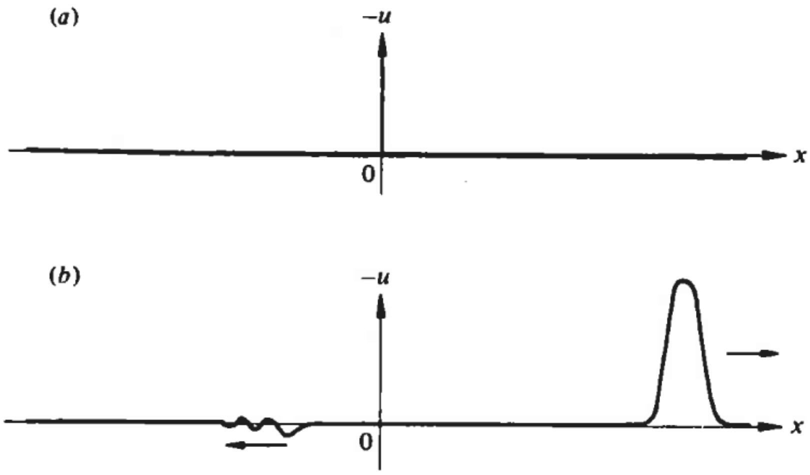


Figure 8.3: initial condition $u_0=-2\beta\delta$ (see (a)) splits in one soliton and a dispersive wave (siehe (b)) [DJ].

□

Rem: inverse (scattering) problems in many applications: e.g. computed tomography scan, acoustic exploration of soil geology

References: [De] §9.7, [DJ] §3.3, 4.4, [Wh] §17.3-5

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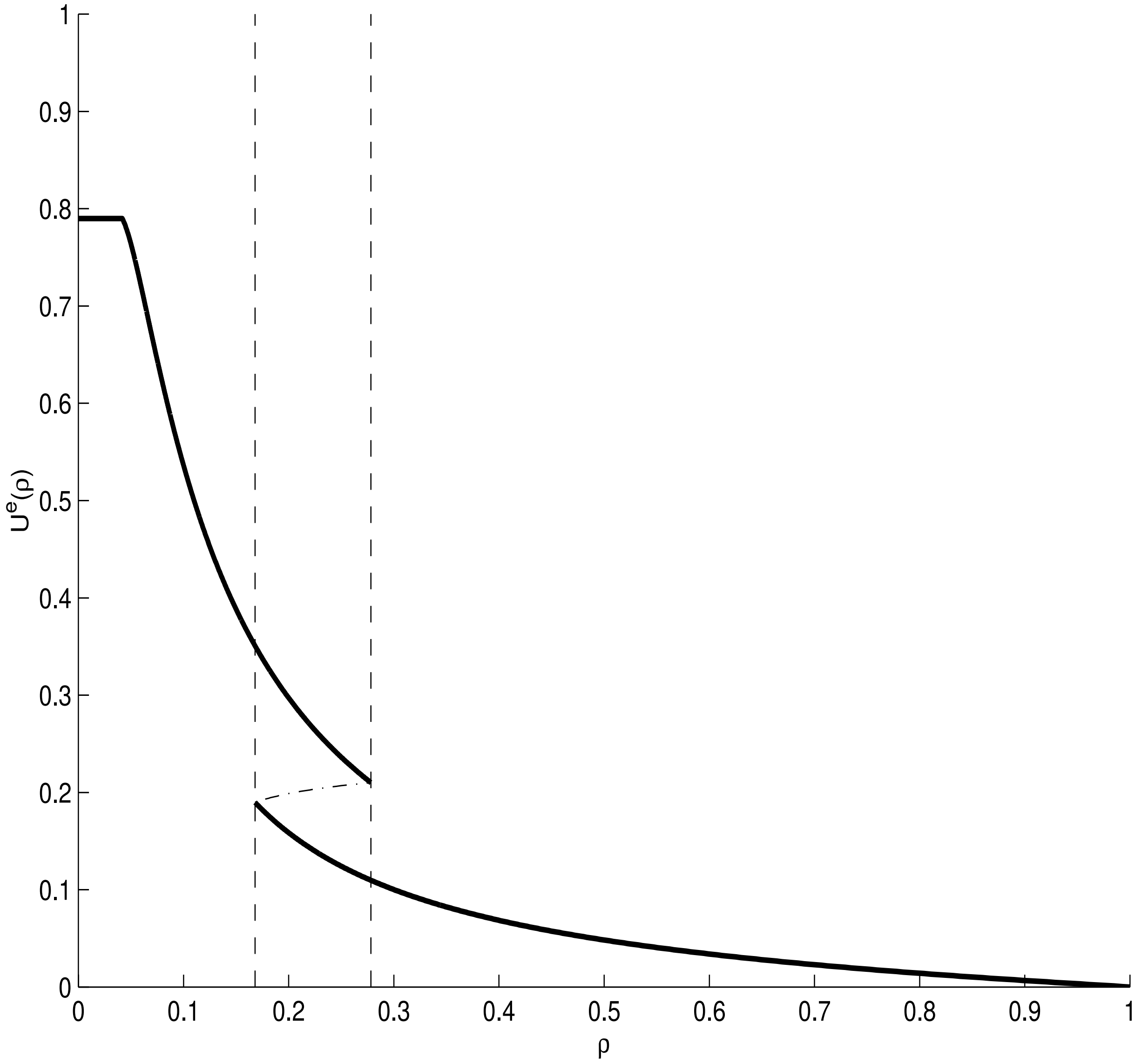
B Slides

Traffic flow diagram: velocity as multivalued function of density



Multivalued function $v(\rho)$ permits multiple stable traffic states; also hysteresis behaviour and "stop-and-go" possible. From [Günther-Klar-Materne-Wegner, SIAM J. Appl. Math. 2003].

Characteristics for traffic light example

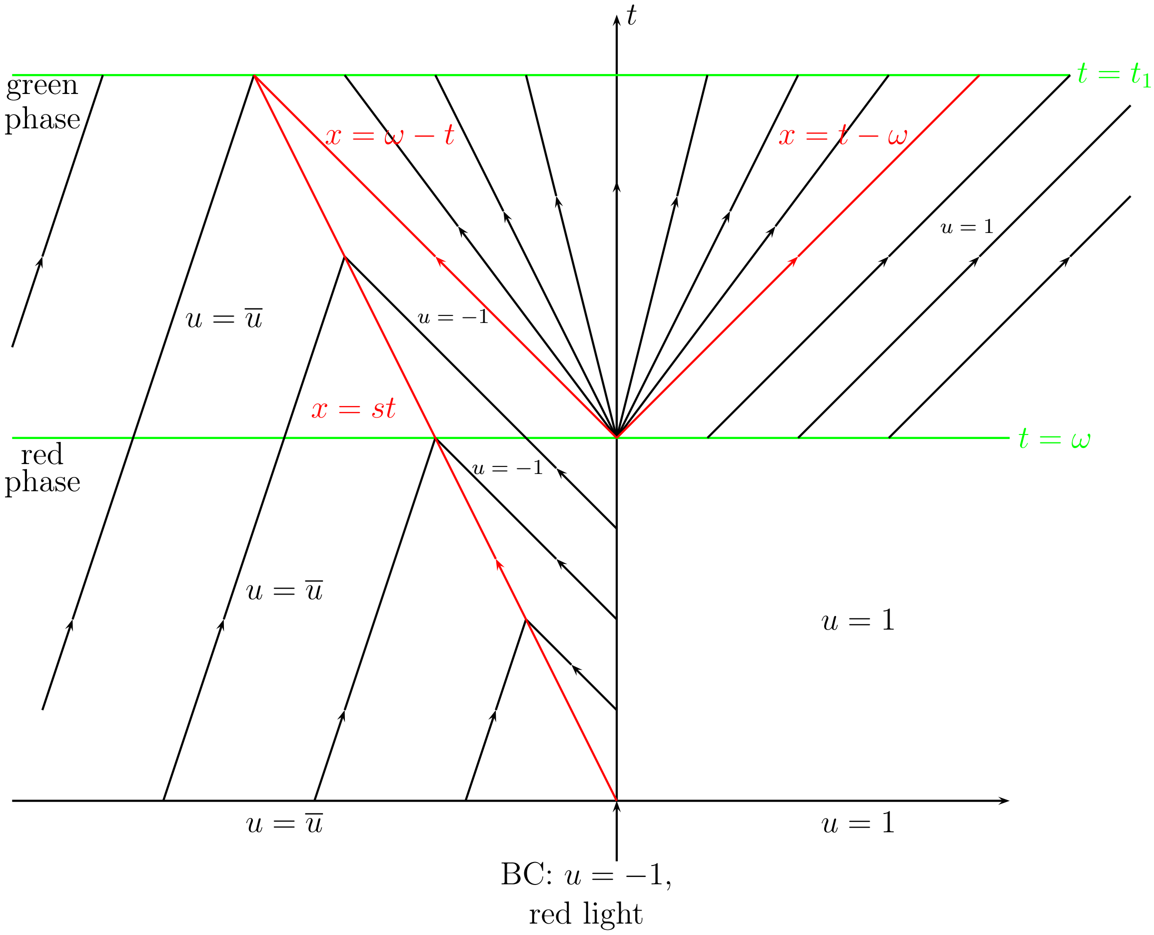
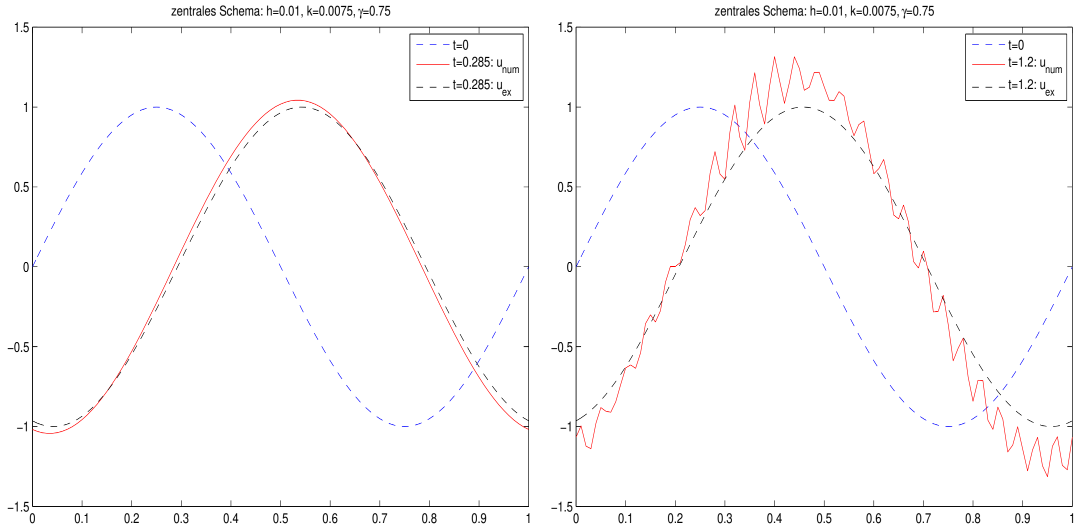


Figure B.1: Traffic light: red phase, 1st part of green phase

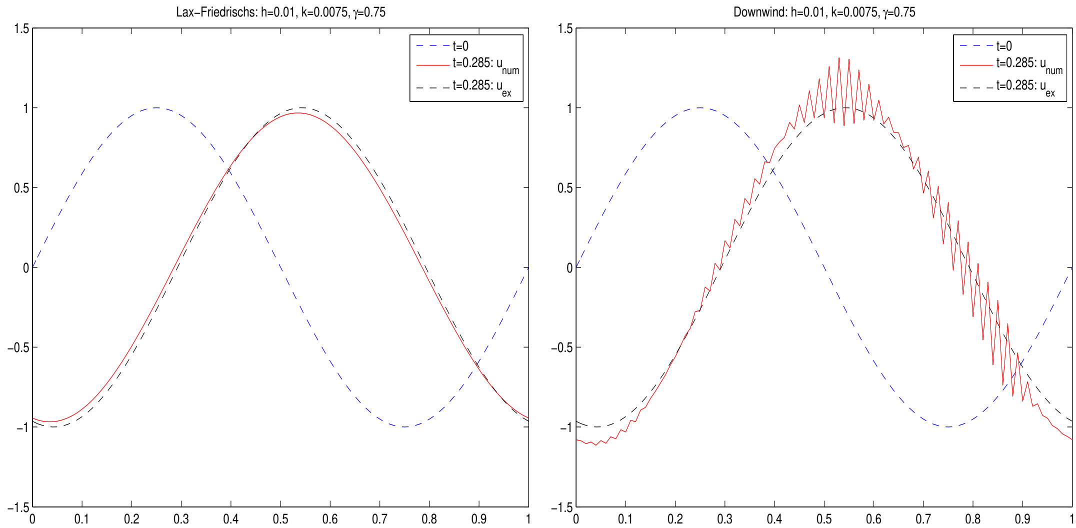
Numcerical methods for linear advection equation (smooth solutions 1)

$$\begin{aligned} u_t + u_x &= 0, \quad x \in \mathbb{R}, t > 0 \\ u_0(x) &= \sin(2\pi x) \end{aligned}$$

num. solution on $[0, 1]$ with periodic boundary conditions.



The central scheme is unstable.

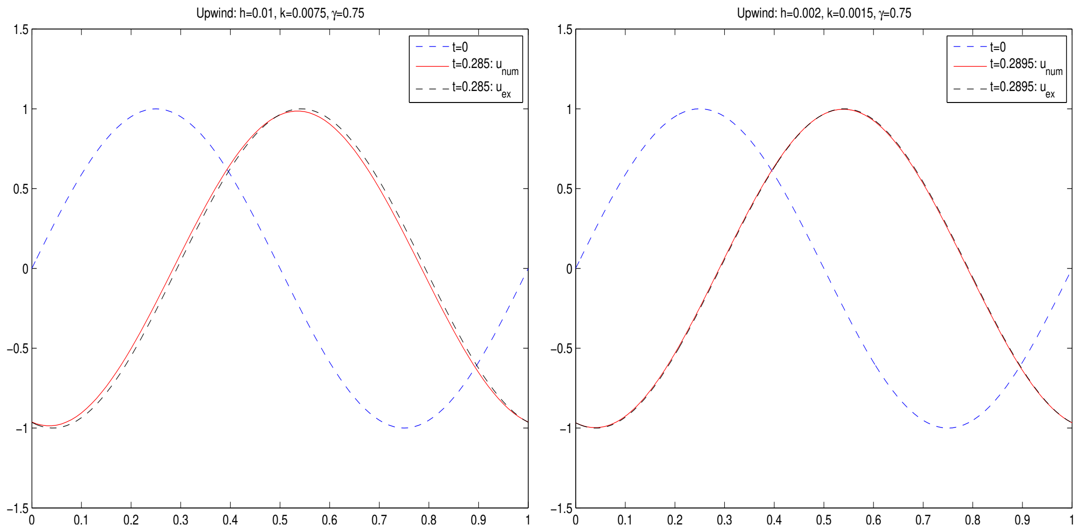


left: Lax-Friedrichs ist conditionally stable (for $\gamma := \frac{|a|k}{h} \leq 1$);
right: the downwind scheme is unstable.

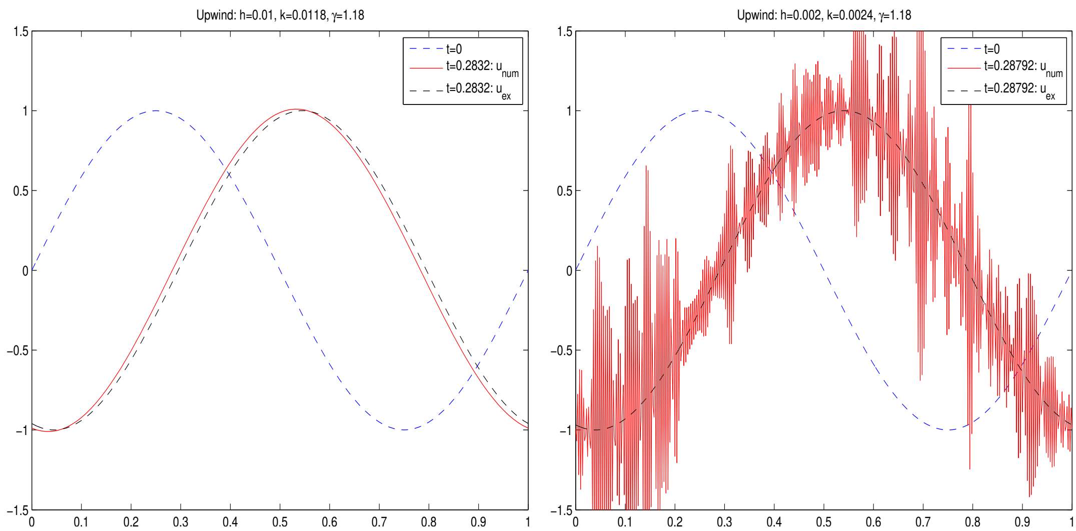
Numerical methods for linear advection equation (smooth solution 2)

$$
\begin{aligned}
u_t + u_x &= 0, \quad x \in \mathbb{R}, t > 0 \\
u_0(x) &= \sin(2\pi x)
\end{aligned}
$$

num. solution on $[0, 1]$ with periodic boundary conditions.



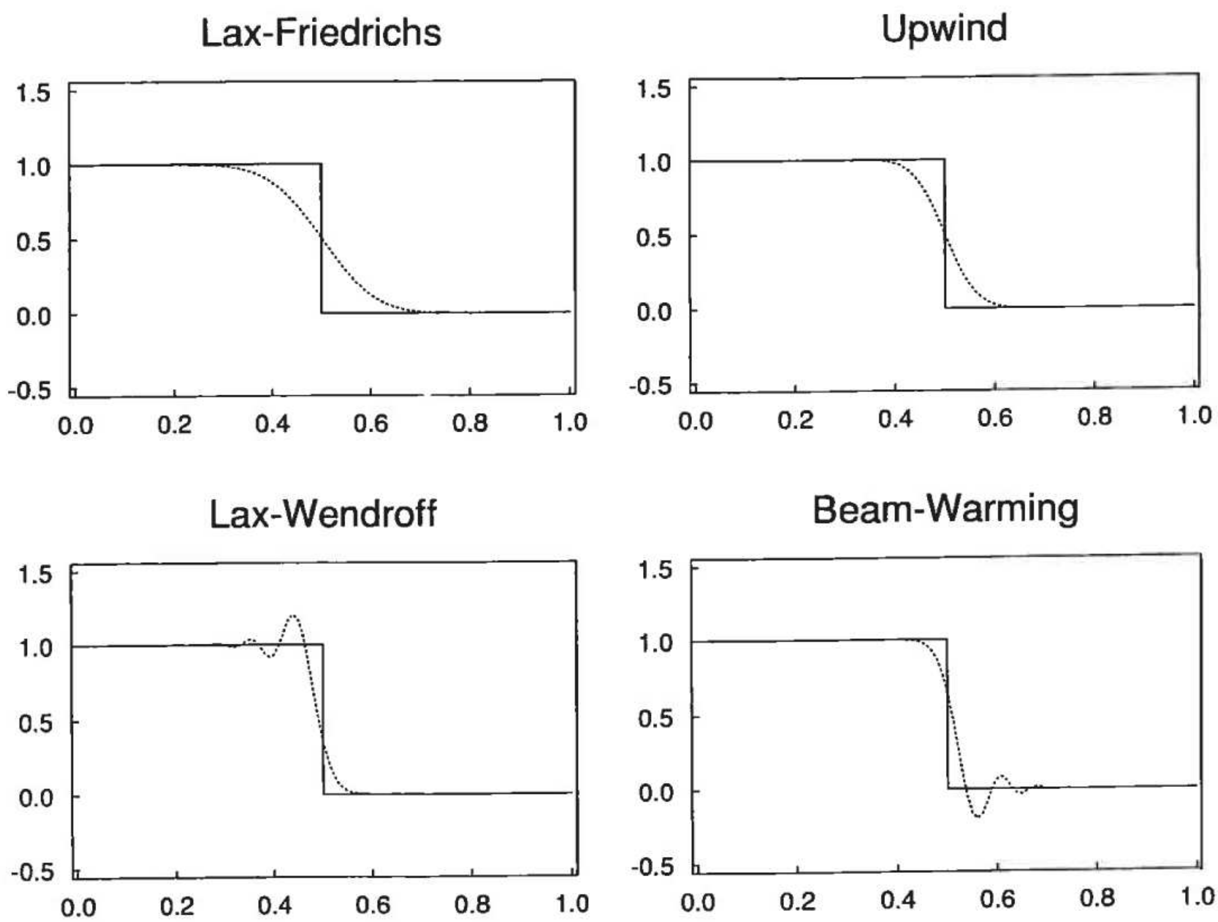
The upwind scheme is conditionally stable (for $0 \leq \gamma := \frac{ak}{h} \leq 1$); here $\gamma = 0.75$.



For $\gamma > 1$ the upwind scheme is unstable; here $\gamma = 1.18$.

Numerical methods for discontinuous solutions (1)

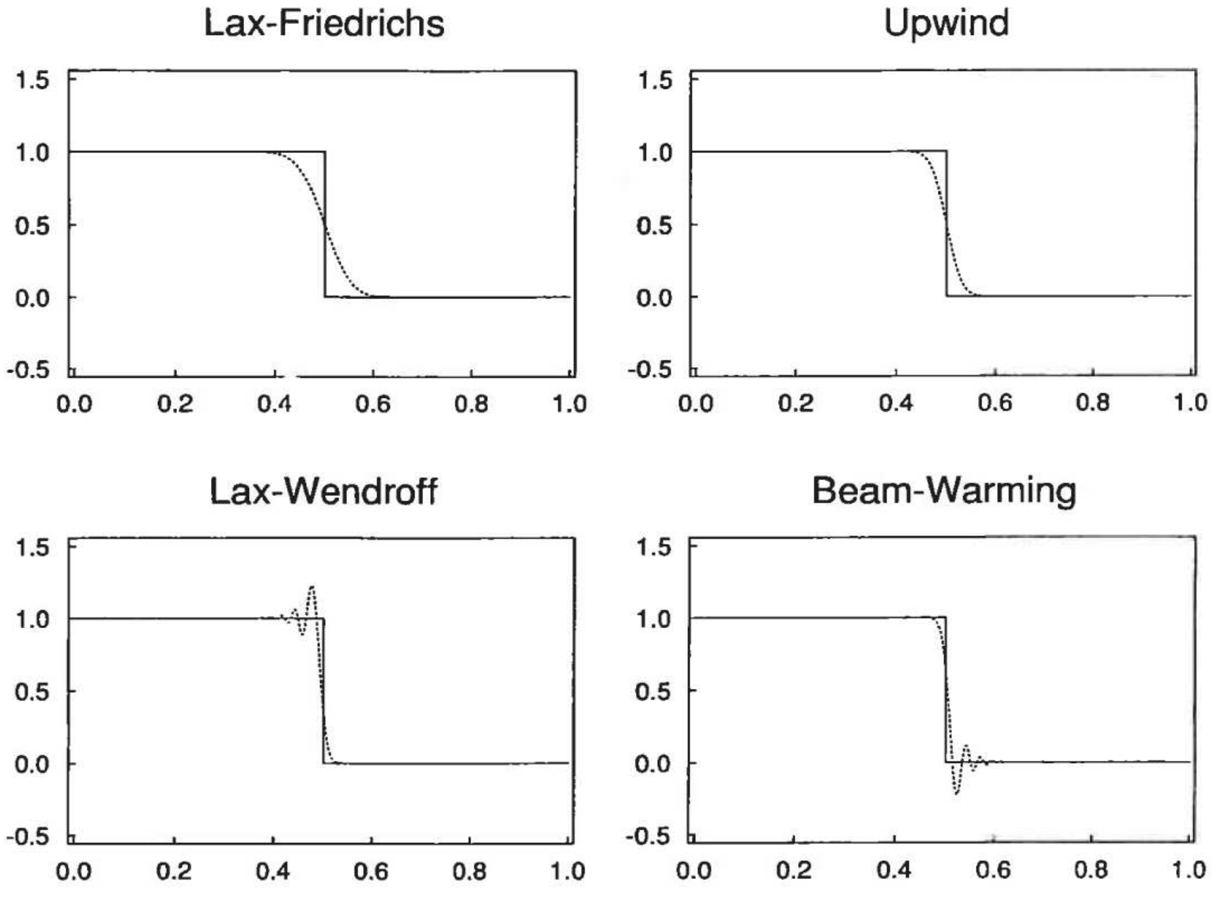
$$\begin{aligned} u_t + u_x &= 0, \quad x \in \mathbb{R}, t > 0 \\ u_0(x) &= \begin{cases} 1, & x < 0 \\ 0, & x > 0 \end{cases} \end{aligned}$$



exact solution (—) at $t = 0.5$ and numerical solution $(\cdots)$ with $h = 0.01$, $k/h = 0.5$ (from [LV])

Numerical methods for discontinuous solutions (2)

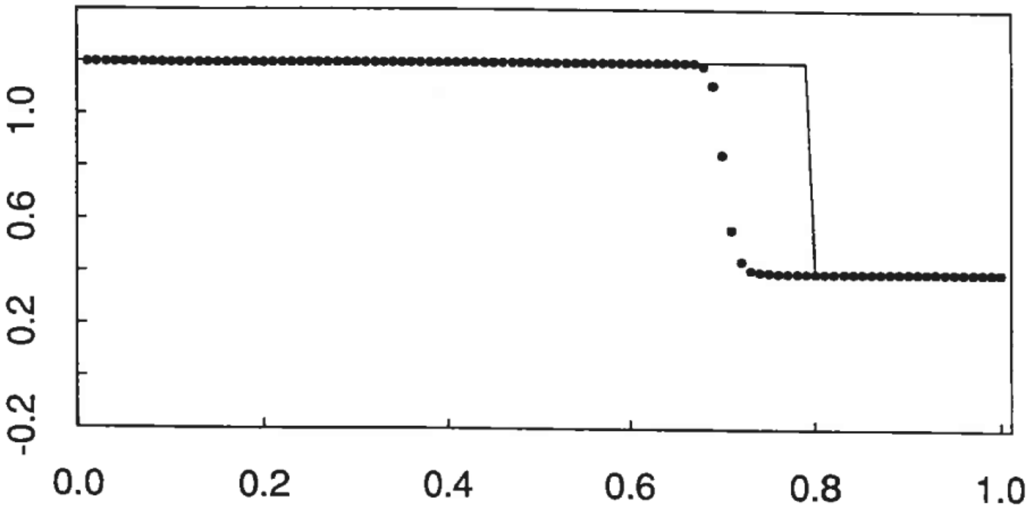
$$
\begin{aligned}
u_t + u_x &= 0, \quad x \in \mathbb{R}, t > 0 \\
u_0(x) &= \begin{cases} 1, & x < 0 \\ 0, & x > 0 \end{cases}
\end{aligned}
$$



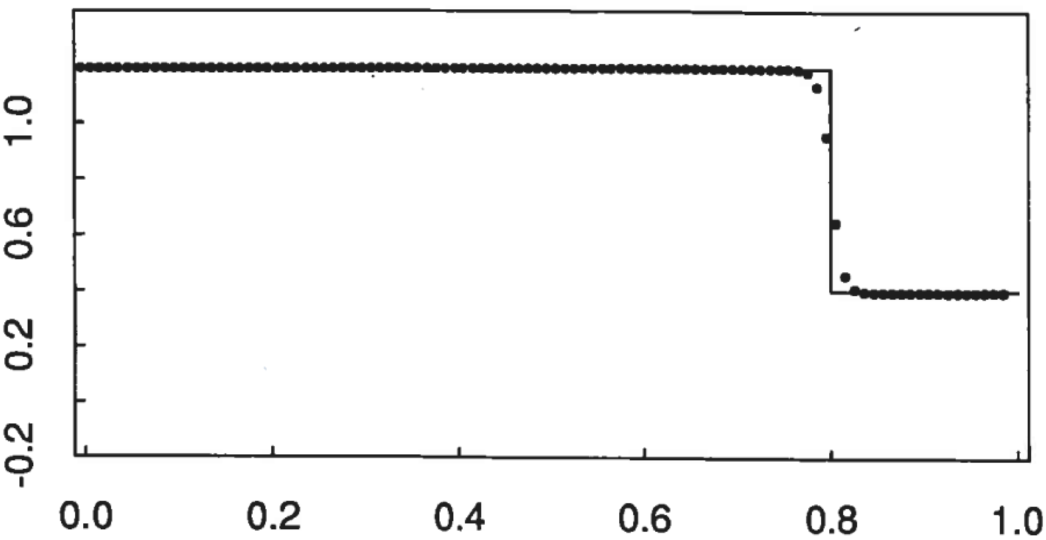
exact solution (—) at $t = 0.5$ and numerical solution $(\cdots)$ with $h = 0.0025$, $k/h = 0.5$. Order of convergence: 1/2 resp. 2/3 [LV]

Riemann-Problem for Burgers' equation

$$\begin{aligned} u_t + u\,u_x &= 0, \qquad x \in \mathbb{R}, t > 0 \\ u_l &= 1.2\,, \quad u_r = 0.4\,, \quad \to \text{ shock speed } s = 0.8 \end{aligned}$$



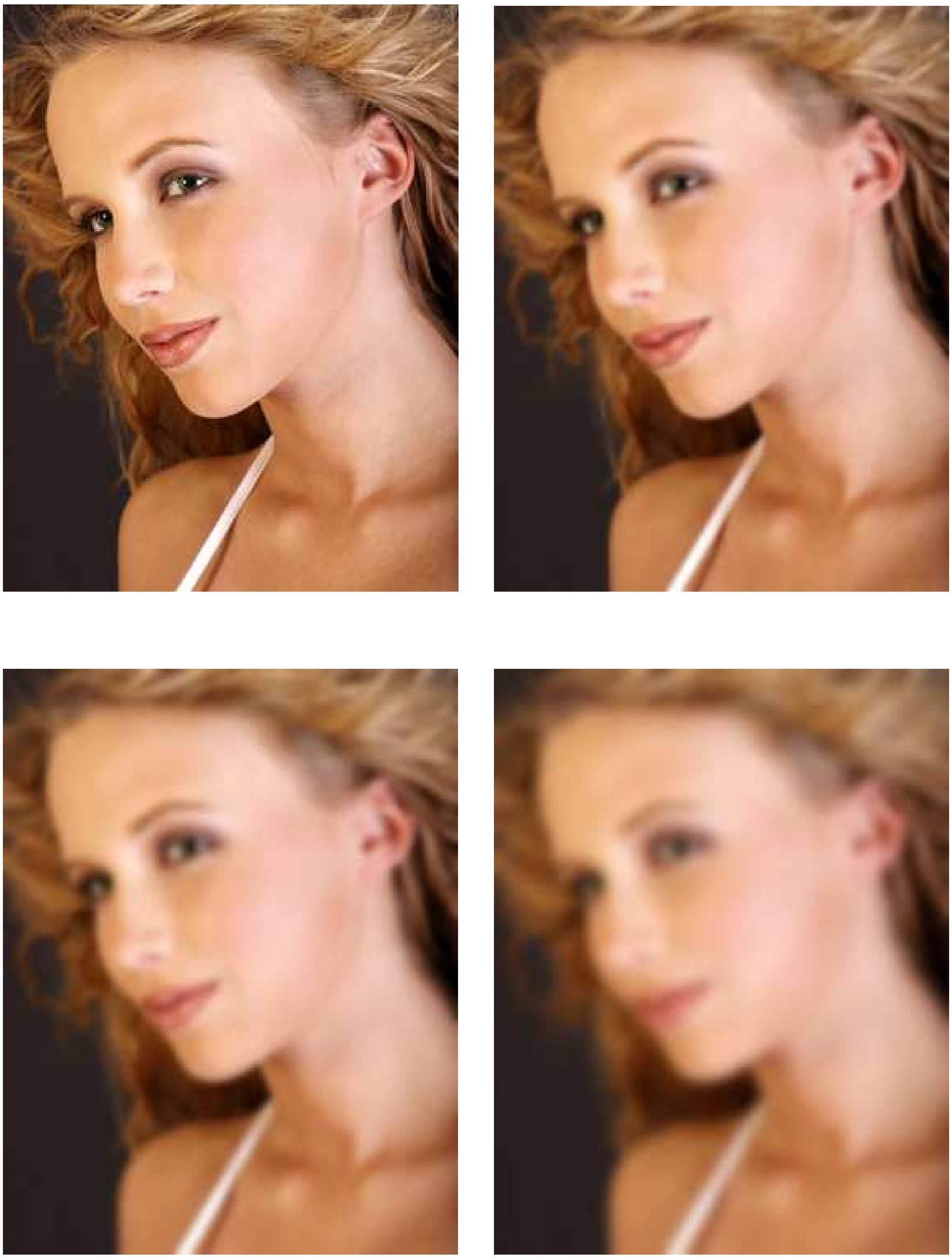
exact solution (—) at $t = 1$ and numerical solution $(\cdots)$ with non-conservative scheme:: $u_j^{n+1} = u_j^n - \frac{k}{h} u_j^n \left(u_j^n - u_{j-1}^n\right)$



num. solution with conservative upwind scheme (from [LV]):

$$u_j^{n+1} = u_j^n - \frac{k}{h}\left(\frac{1}{2}(u_j^n)^2 - \frac{1}{2}(u_{j-1}^n)^2\right)$$

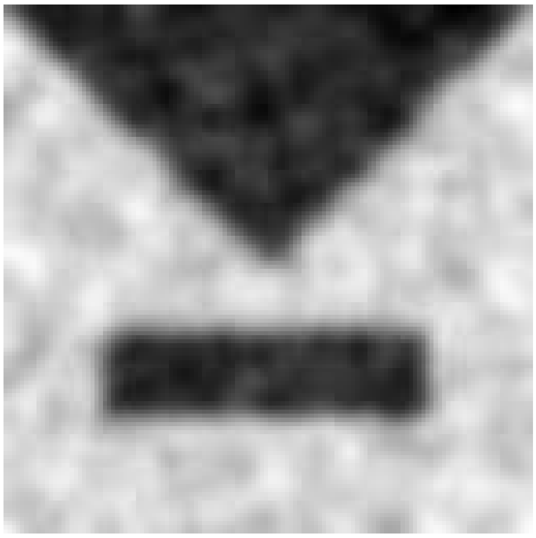
Linear Gaussian diffusion filter



original image f; diffusion filters $K_\sigma * f$ with growing "thickness" σ in (4.1) (created with *Photoshop*)

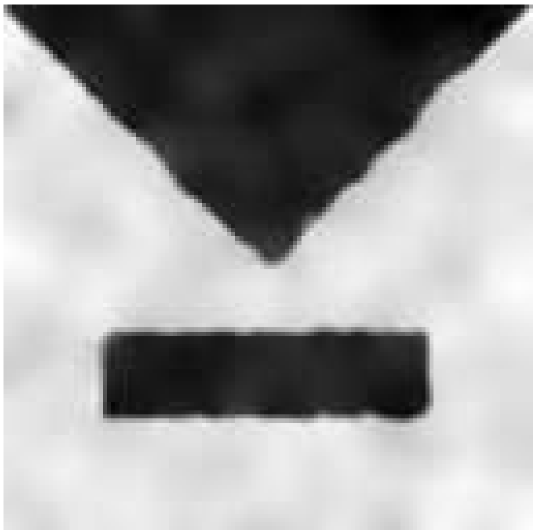
Diffusion filter (triangle and rectangle)

noisy input image



filtered with linear diffusion
(+ automatic stopping time)

filtered with isotropic nonlinear diffusion
[Perona-Malik equation] (+ automatic
stopping time)

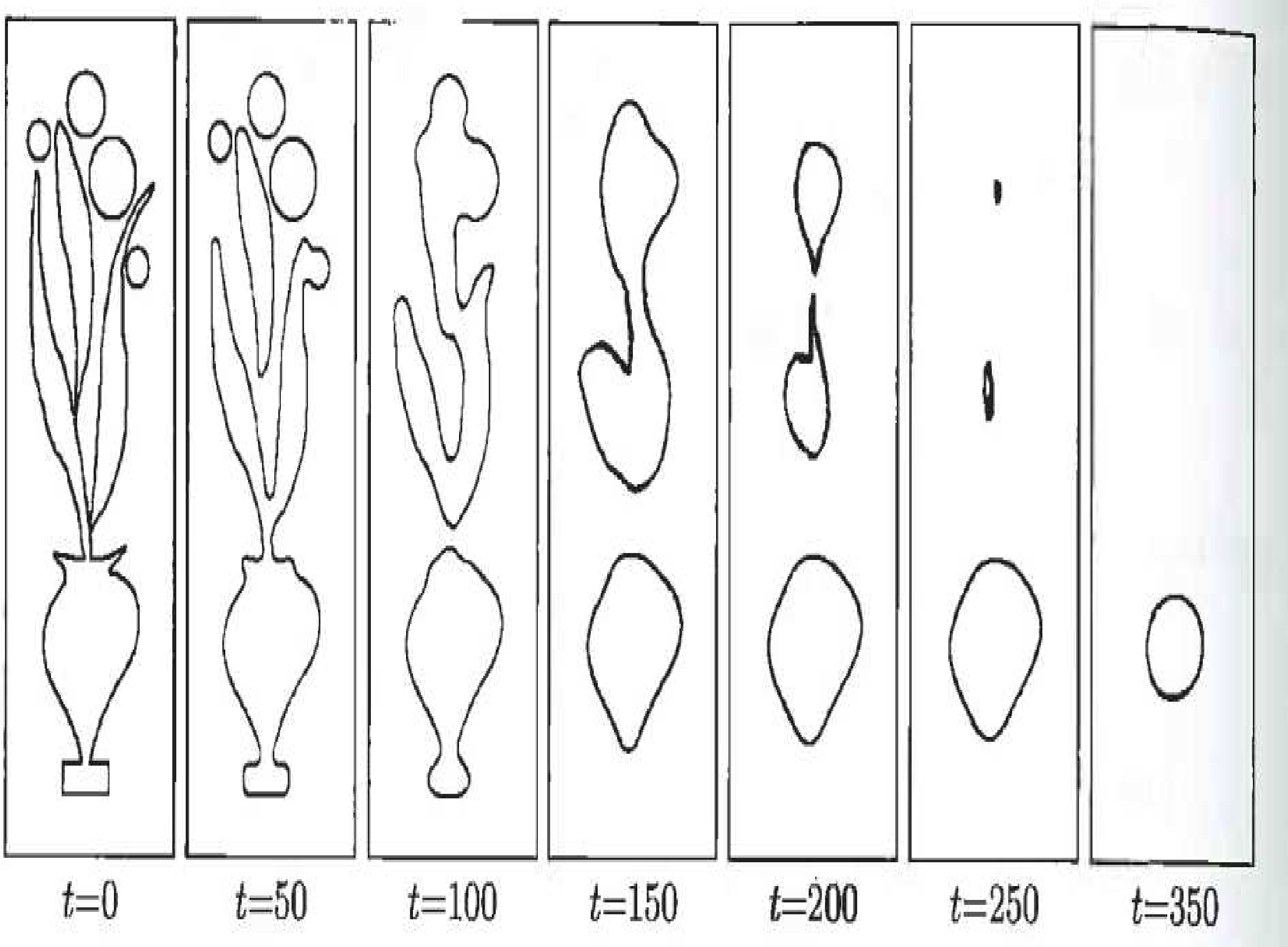


filtered with anisotropic nonlinear diffusion
(+ automatic stopping time)

from [Pavel Mrazek, Dissertation, Prag, 2001]

(mean) curvature equation

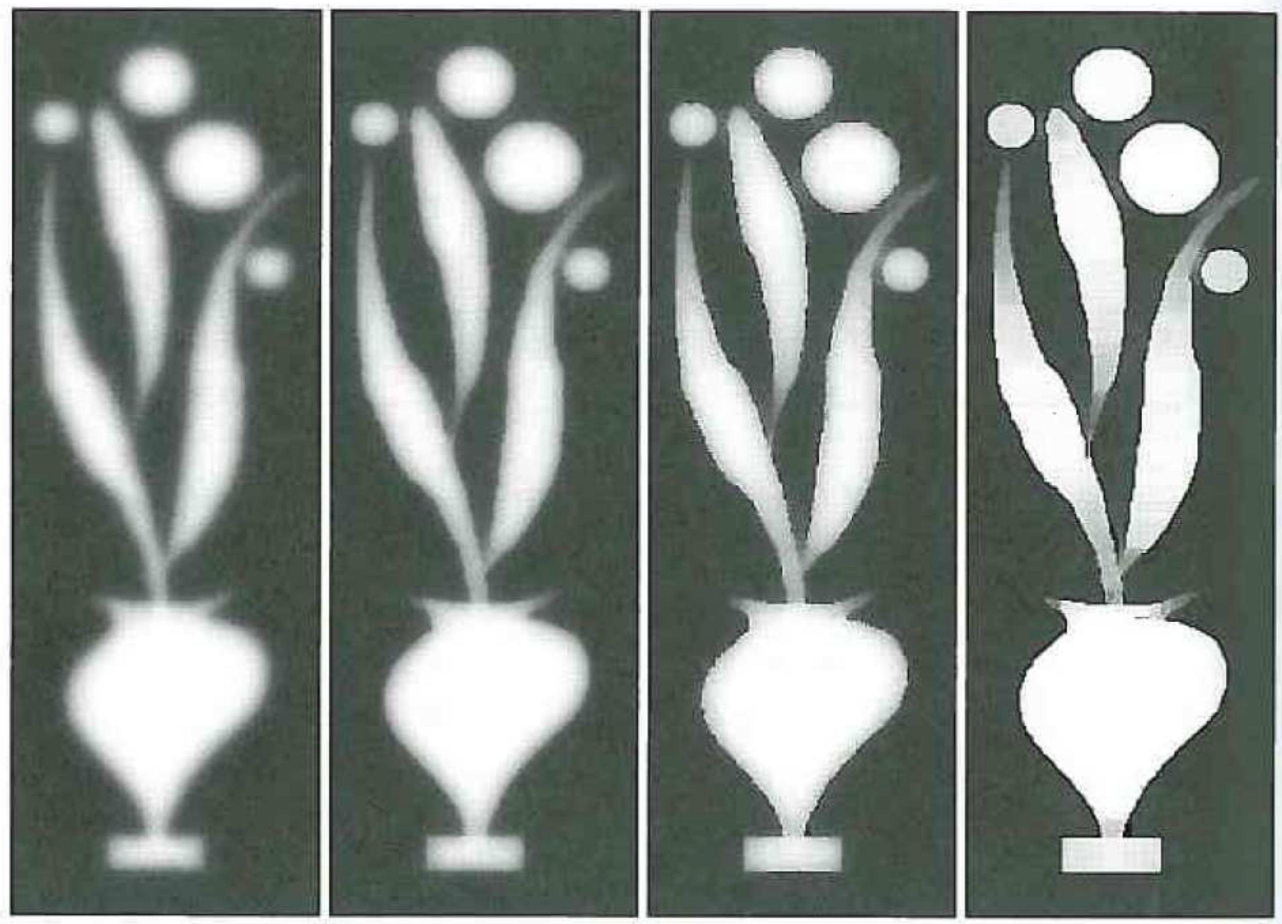
$$u_t = |\nabla u| \operatorname{div}\left(\frac{\nabla u}{|\nabla u|}\right)$$



Evolution of curves under (mean) evolution equation, [AK]. All closed curves asymptotically become circles and collapse in finite time.

Shock filter

$$u_t = -|\nabla u|\,\mathrm{sign}(\Delta u), \quad x \in \mathbb{R}^2,\ t > 0$$



t=0 t=2 t=4 t=10

Initial condition is Gauss-smoothened original image. Image reconstruction: convergence (in finite time) towards a step function (i.e. perfectly sharp image), [AK].

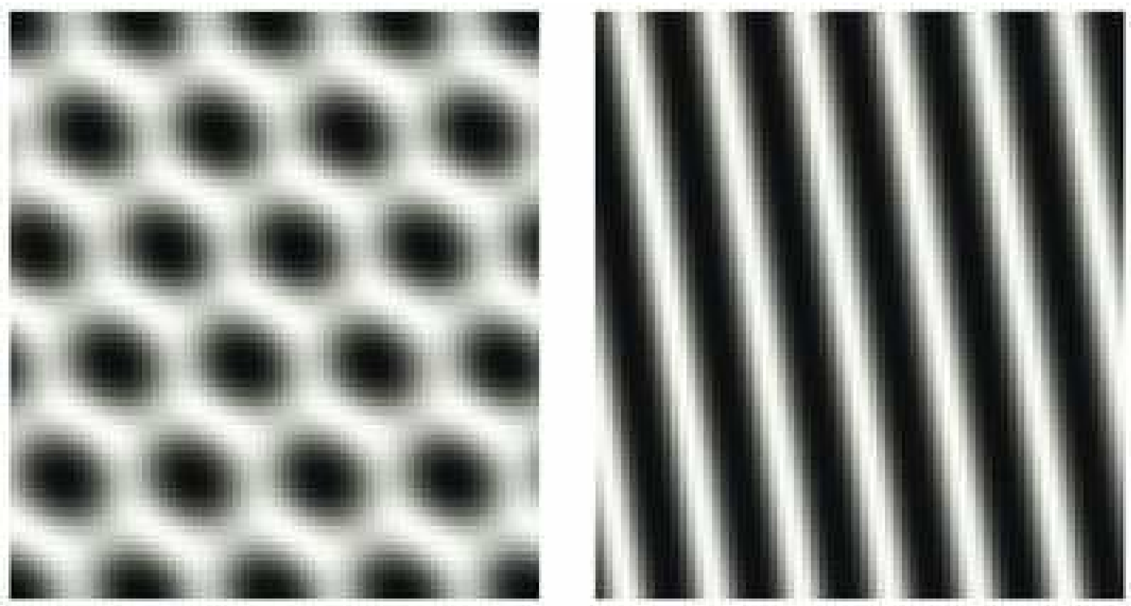
Brusselator (reaction-diffusion equation)

$$
\begin{aligned}
u_t &= a - (b+1)u + u^2 v + d_1 \Delta u \\
v_t &= bu - u^2 v + d_2 \Delta v
\end{aligned}
\tag{B.1}
$$

Model for autocatalytic, oscillating chemical reaction (i.e. a reaction product is also a reaction partner);
equation for 2 substances with densities $u(x,t)$, $v(x,t)$

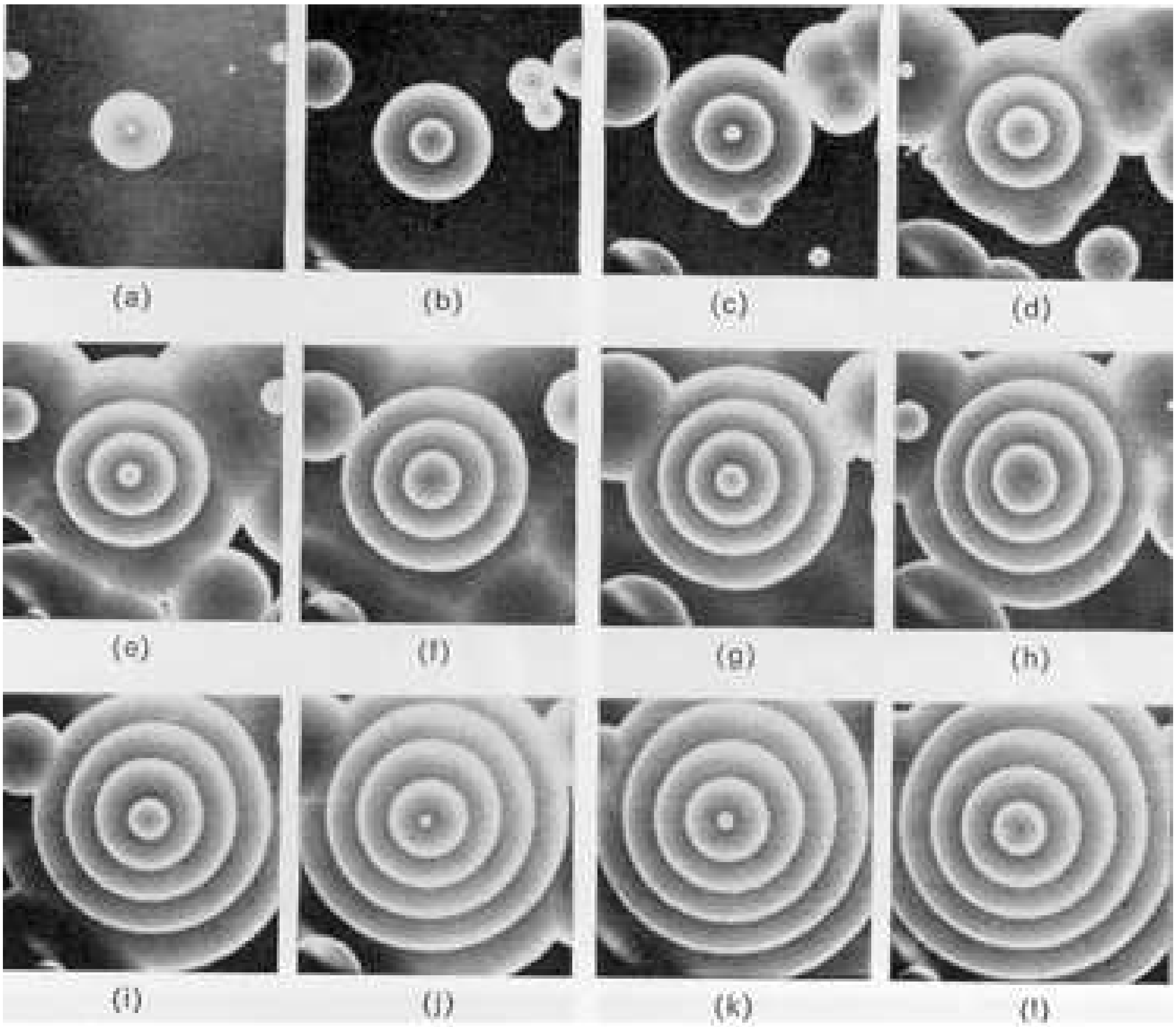
homogeneous stationary state $(u_0, v_0) = (a, b/a)$;
Turing instability for $b > (1 + a\sqrt{\frac{d_1}{d_2}})^2$ ... (= 2nd necessary condition)

2 numerical examples for spatially inhomogeneous stationary states $u_\infty(x) = \lim_{t\to\infty} u(x,t)$ (with same parameters a, b); are not unique!
stable, but not asymptotically stable.



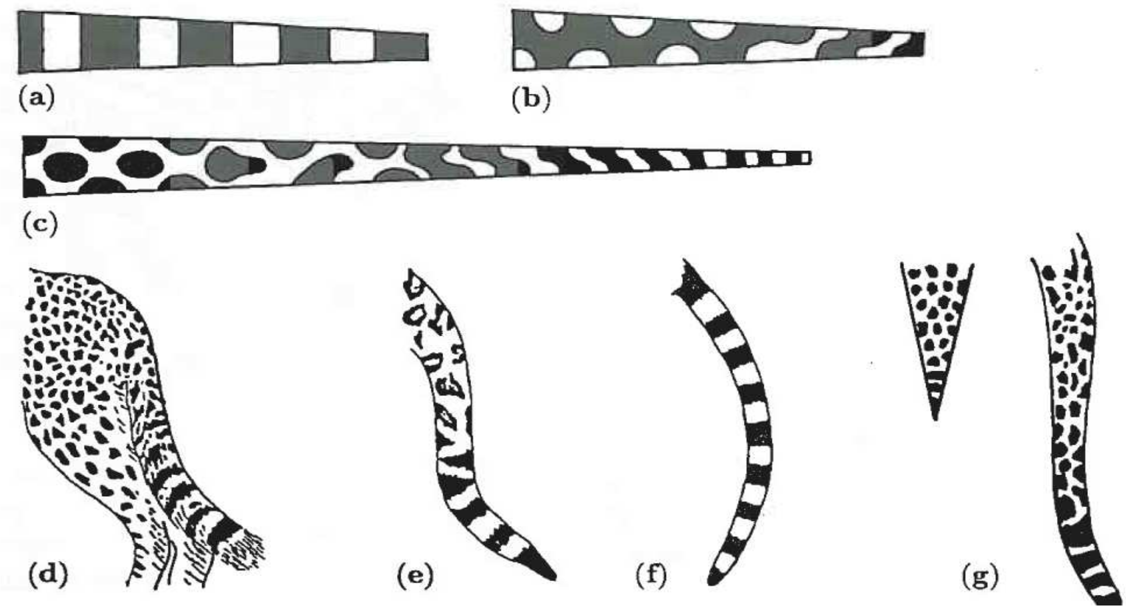
(B.1) is invariant under translations and rotations (modulo BC)

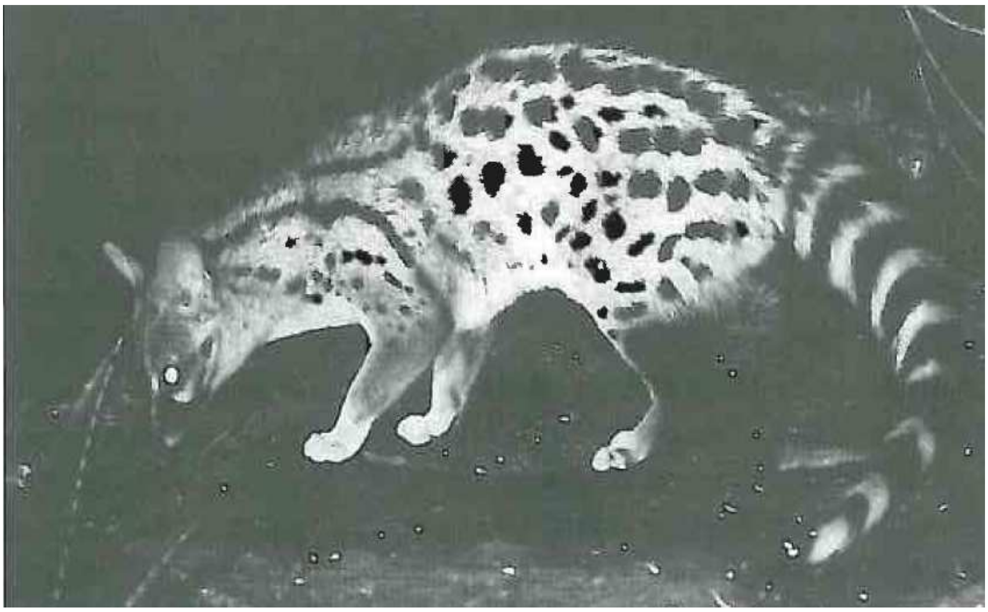
pattern formation in chemical process (experiment)



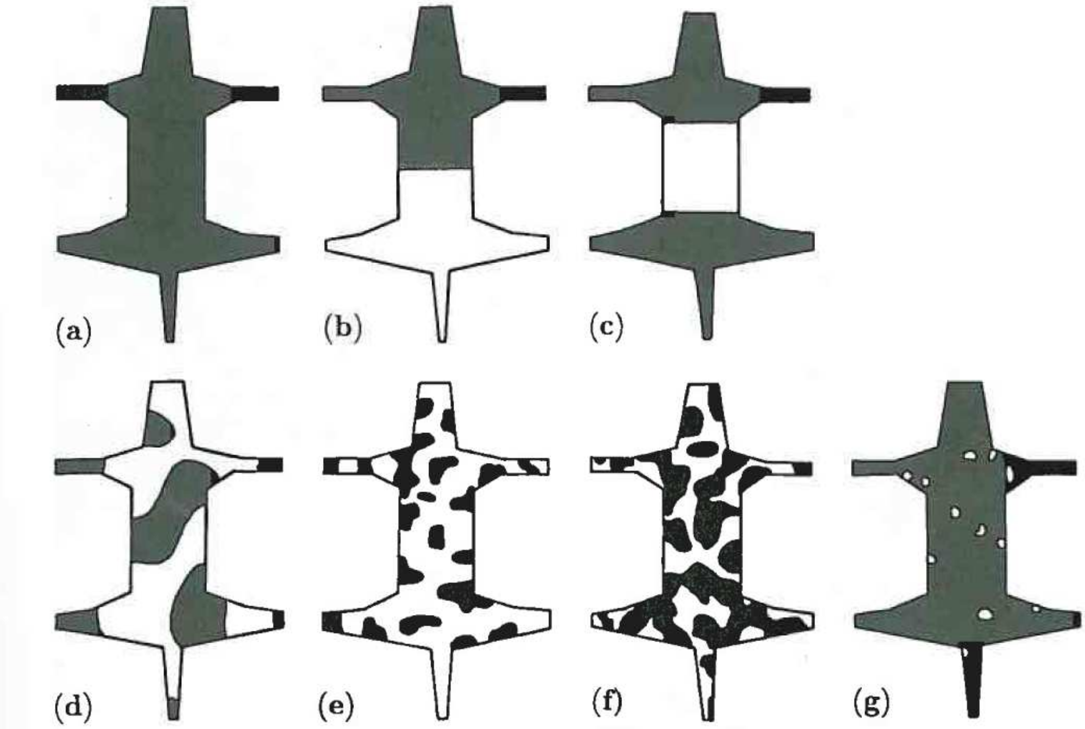
evolution of concentration waves in chemical reaction (Belousov-Zhabotinsky reaction)

Pattern formation with reaction-diffusion equations (1)

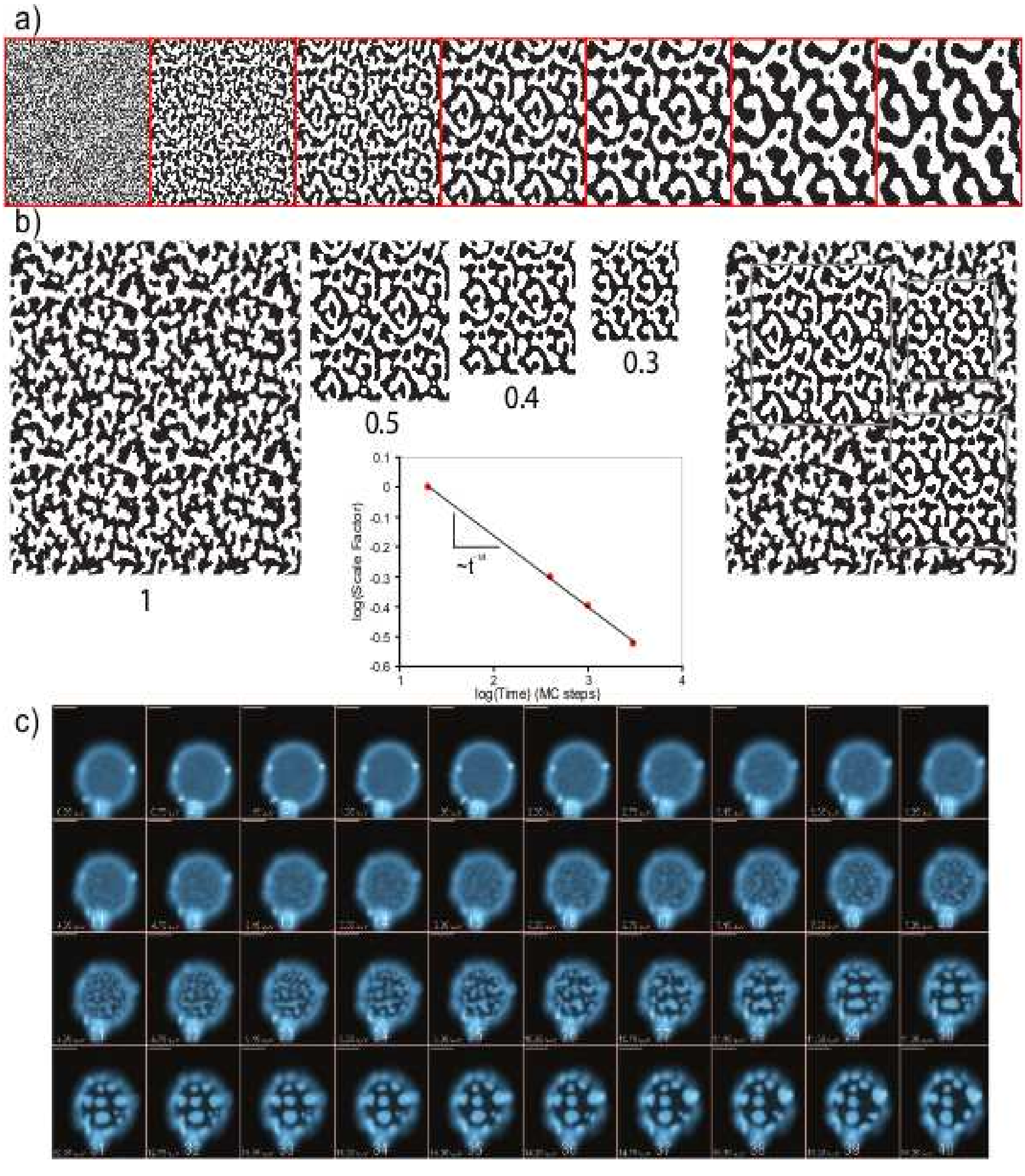




Pattern formation with reaction-diffusion equations (2)



Cahn-Hilliard: simulation / experiment



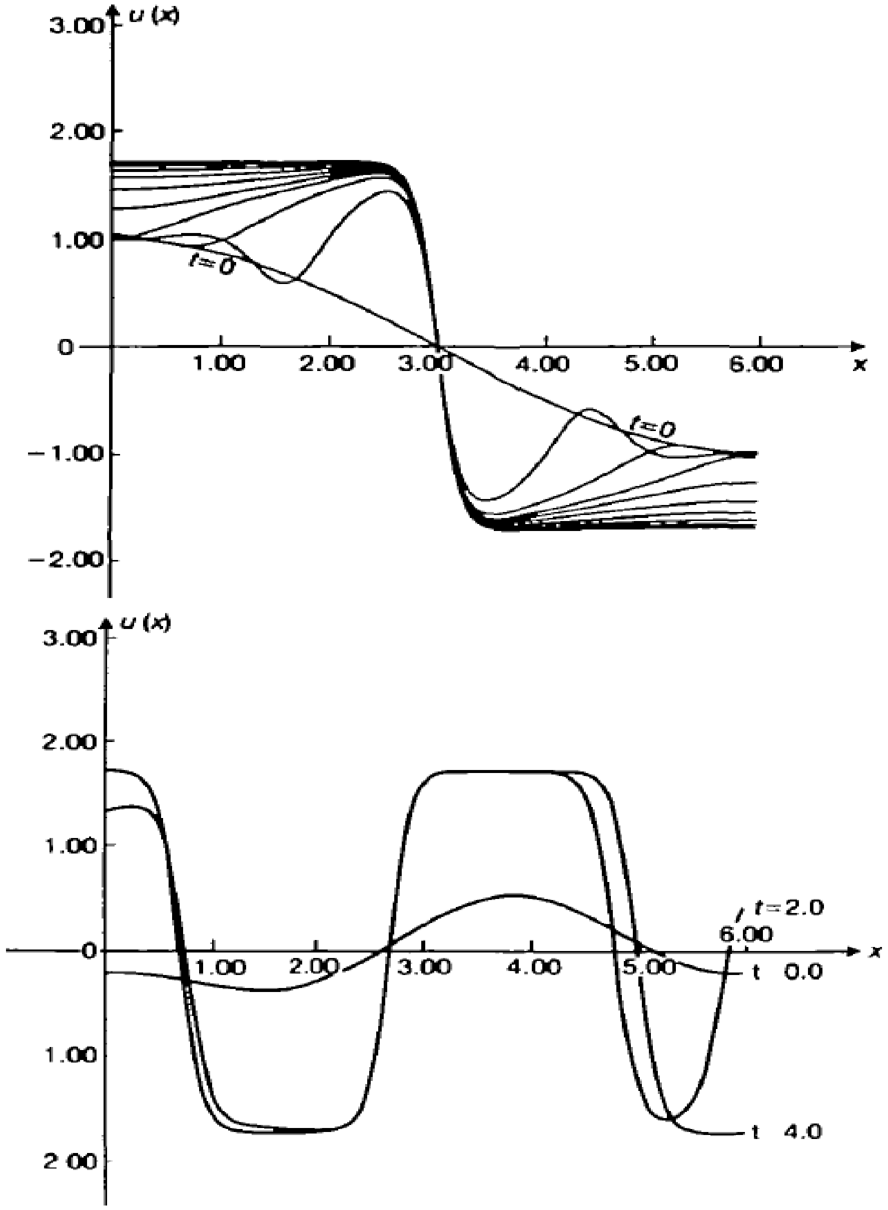
a) numerical simulation(Monte Carlo) of the Cahn-Hilliard Gleichung; t =0, 20, 100, 400, 1000, 3000, 5000

b) Magnification of t =20, 400, 1000, 3000 shows *scale invariance.*

c) Movie of experiment (fat bubbles) [T. Ursell, 2007]:
http://www.youtube.com/watch?v=kDsFP67_ZSE&NR=1

Cahn-Hilliard: simulation for $t \to \infty$

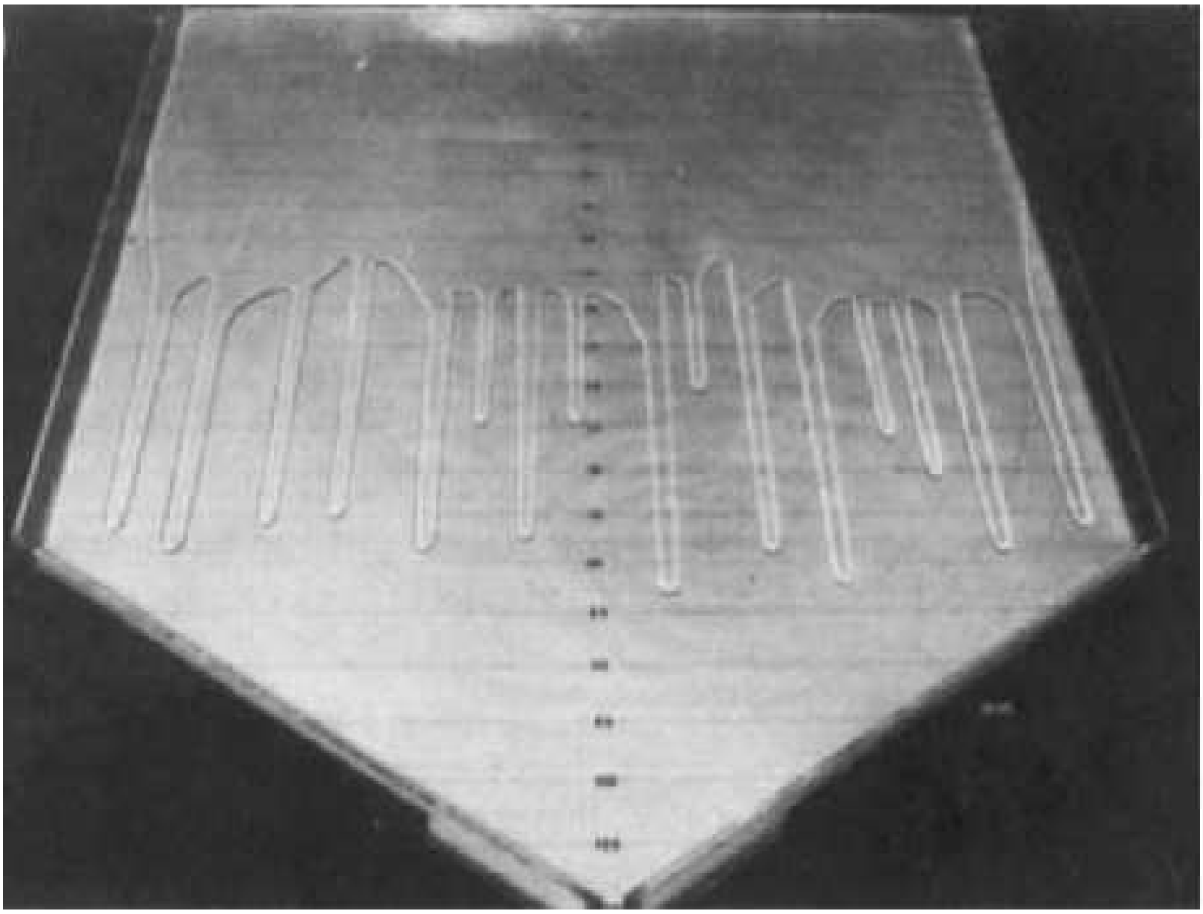
$f(c) := c^4/12 - c^2/2$; local minima at $c_m = \pm\sqrt{3}$
$\gamma = 0.03,\ L = 6$



FEM–simulation of Cahn-Hilliard equation [EF]:

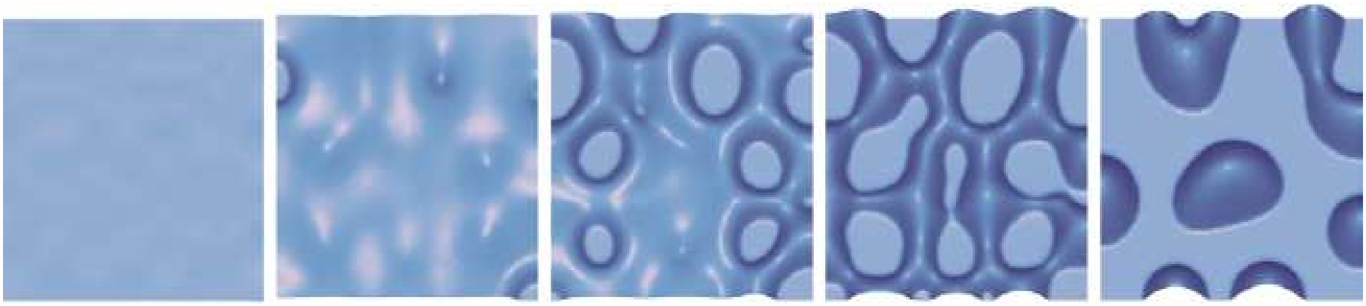
- solution converges towards c_∞
- c_∞ almost piecewise constant (values at $\pm\sqrt{3}$)
- still unclear, whether c_∞ stationary state or only *metastable*

thin films: “fingering”–instability of front



[Huppert, Nature, 1982]

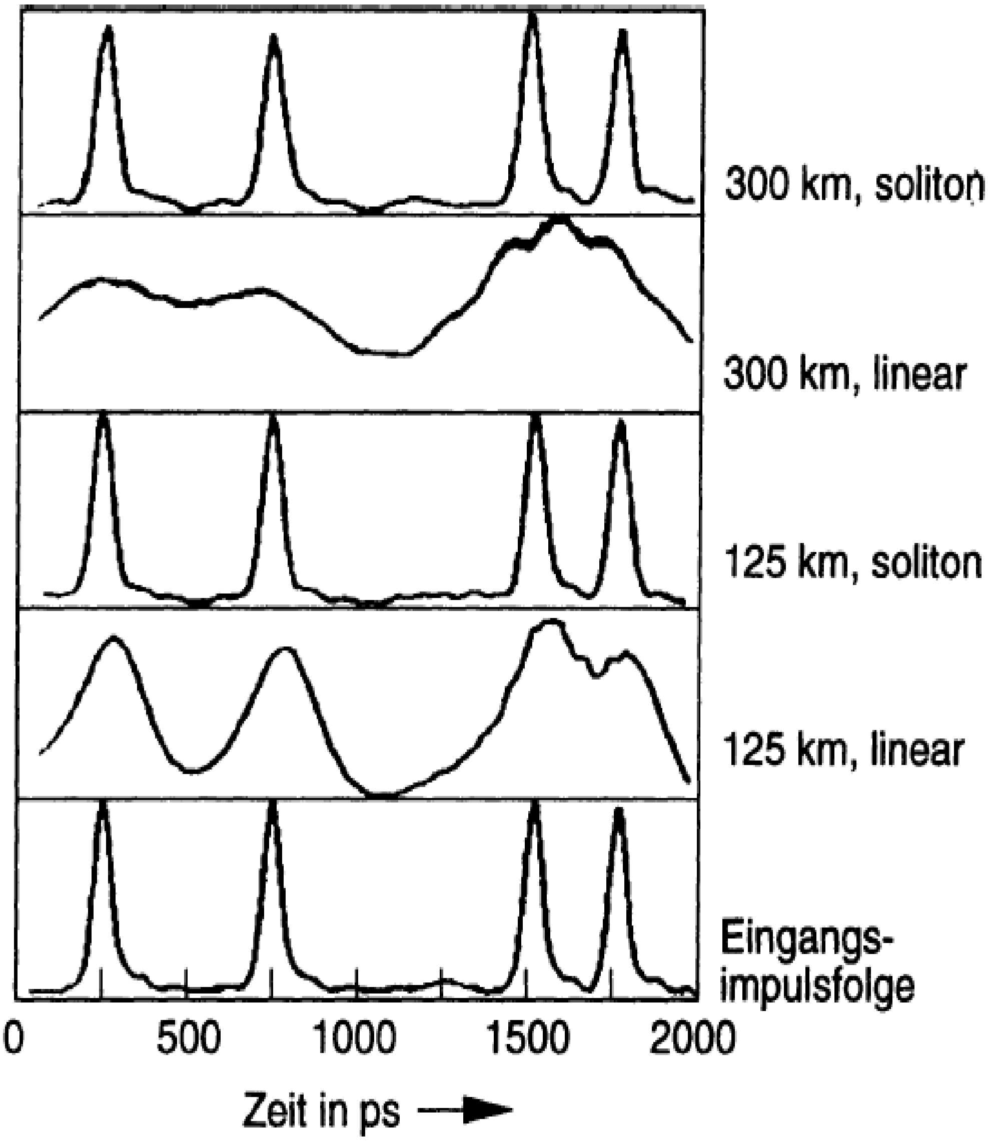
thin films: simulation



FEM–simulation of (extended) thin film equation [BG]:

- IC: homogeneous film with small disturbance
- film ruptures
- evolution to few large droplets

data transmission with solitons Datenübertragung mit Solitonen



- practical comparison for impulse transmission at 4 Gbit/s: soliton vs. linear
- at 300 km: signal cannot be recognized with linear transmission
- with soliton-transmission almost unchanged
- practical applications still in preparation