PhD Course on Numerical Modeling of Geological Processes Lecture title: Numerical methods for the saturation equation

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Saturation Equation

Let's consider a two-phase flow and the global pressure formulation. For a given total velocity $\mathbf{u}$ the equation for the saturation reads:

$$\begin{cases} \Phi \frac{\partial}{\partial t} S_w + \nabla \cdot \mathbf{u}_w = q_w \\ \mathbf{u}_w = f_w \mathbf{u} + \lambda_n(S_w) f_w(S_w) \mathbf{K} \left[p_c'(S_w) \nabla S_w + (\rho_n - \rho_w) \mathbf{e}_z \right] \end{cases} \tag{1}$$

(of course we can consider the analogous equation for S_n instead).

Numerical issues

We need a method that is able to

- Treat the hyperbolic (transport) term (which is normally the dominant one) appropriately, without spurious oscillations.
- Be locally conservative: if $q_w = 0$ by applying divergence theorem on a volume $V \subset \Omega$ we have $d/dt \int_V \Phi S_w = -\int_{\partial V} \mathbf{u}_w \cdot \mathbf{n}$. In a local conservative scheme this relation holds true at elemental level (of course the time derivatives will be replaced by appropriate finite differences).
- Be able to handle boundary conditions appropriately (even in the degenerate case).

If we neglect gravity and capillary pressure and assume that $\mathbf{u}$ is constant and that the fractional flow depend on saturation only, we have the multidimensional Buckley-Leverett equation.

$$\Phi \frac{\partial}{\partial t} S_w + \nabla \cdot \mathbf{F}_w(S_w) = 0 \quad \text{in } \Omega,\ t > 0 \tag{2}$$

with $\mathbf{F}_w(S_w) = f_w(S_w)\mathbf{u}$. Boundary conditions, typically of Dirichlet type, have to be imposed only on the inflow boundary. Rigorously, the inflow boundary should be defined as

$$\Gamma^- = \{\mathbf{x} \in \partial\Omega :\ \frac{d\mathbf{F}_w}{dS_w} \cdot \mathbf{n} > 0\}$$

Yet, in many practical code it is approximated as

$$\Gamma^- = \{\mathbf{x} \in \partial\Omega :\ \mathbf{u}_w \cdot \mathbf{n} > 0\}$$

which is fine as long as $df_w/dS_w > 0$.

The major difficulties

Let consider the one dimensional case

$$\Phi \frac{\partial}{\partial t} S_w + \frac{\partial}{\partial x} F_w(S_w) = 0 \quad \text{in } (0, L) \tag{3}$$

We have a non-linear hyperbolic equation.

The theory for such type of equations is very well established when flux function F_w is strictly convex, i.e. $F_w{}'' \neq 0$ for $0 < S_w < 1$.
Unfortunately, this is not our case!

A simpler problem

To understand the issue we first consider a more classical problem, a model of flow of cars in a motorway, described by

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x} F(q) = 0, \quad x \in \mathbb{R}, \ t > 0$$

with $F(q) = u_m q(1-q)$, $q \in [0,1]$ being the density of cars and $u_m > 0$ the maximal speed.

The problem is complemented by an initial condition $q = q_0$ at $t = 0$. We do not have boundary conditions since, for the sake of simplicity, we have set the problem in the whole real axis.

This problem is an example of non-linear conservation law. In this example $F(q)$ is a convex function.

Quasi-linear form

Even if the conservation form is most fundamental, many properties of the solution are found by looking at the quasi-linear form

$$\frac{\partial q}{\partial t} + F'(q)\frac{\partial}{\partial x}q = 0, \quad x \in \mathbb{R}, \ t > 0$$

where $F'(q) = dF(q)/dq = u_m(1-2q)$ is the so-called transport velocity.

Characteristic lines

It is immediate to see that a smooth solution q of the given problem is constant along the curves $y(t)$ in the (x, t) planes that satisfy the ordinary differential equation

$$\frac{dy}{dt}(t) = F'(q(y(t)))$$

Therefore, those curves are in fact straight lines, and are called characteristic lines.

Note: in the linear case F' is constant and the solution is simply $q(x, t) = q_0(x - F't)$.

Discontinuities

An important characteristic of non-linear hyperbolic equations is that the solution may develop discontinuities in the derivatives and in the solution itself even if the initial data (and the boundary data) are smooth!

Indeed, to treat irregular solutions we need to "interpret" the differential equation in a weak sense (otherwise we cannot give meaning to the derivatives!), but we will not go into this matter here. The interested reader can consult any good book on PDEs.

We will describe what happens in a particular case, when the initial data is discontinuous.

The Riemann problem

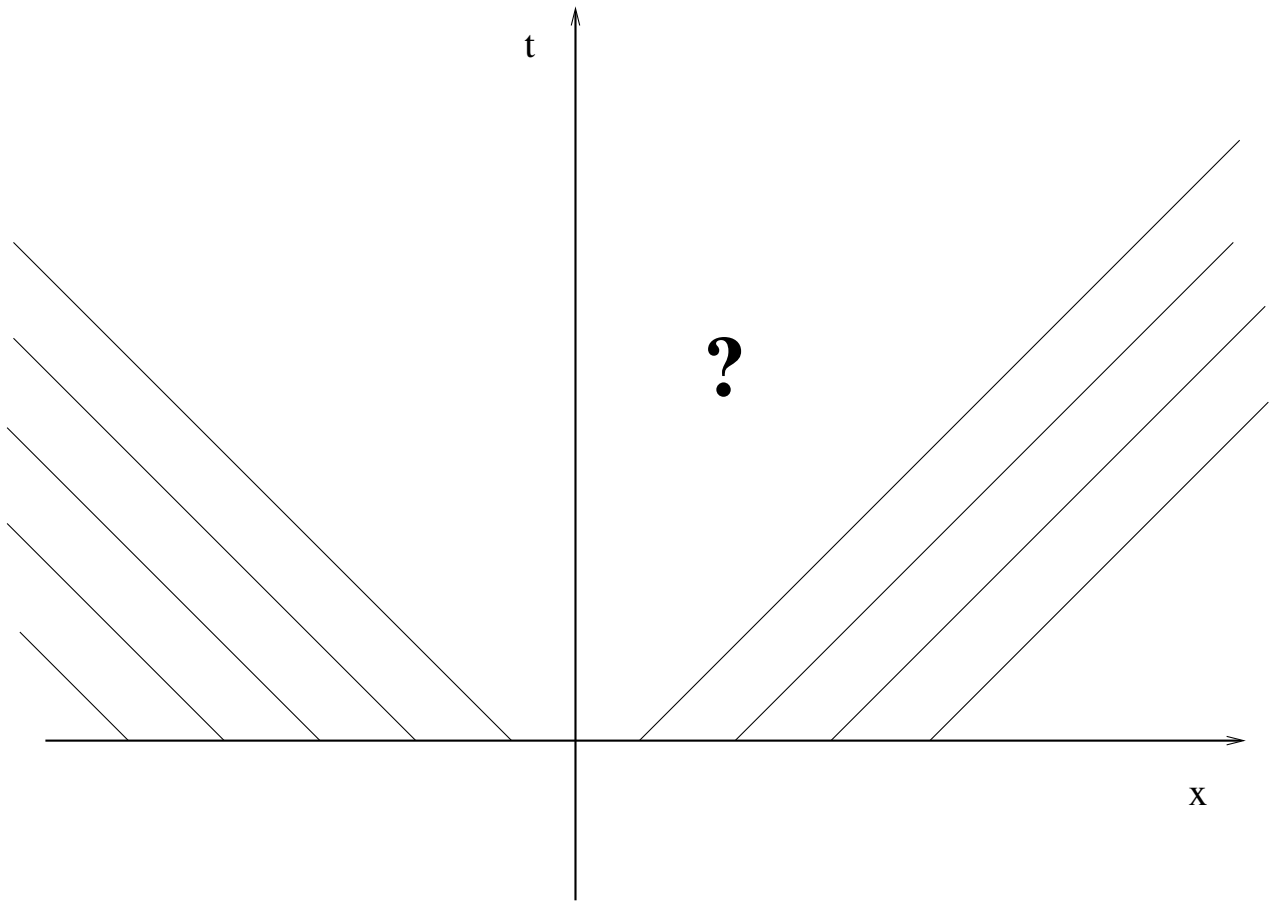
The following problem, called Riemann problem, plays an important role both in understanding the properties of the solution and in the development of numerical schemes. We look for the solution of our problem when

$$q_0(x) = \begin{cases} q_l & \text{for } x < 0 \\ q_r & \text{for } x \geq 0 \end{cases}$$

What happens?. Let's have a look at the characteristic lines.

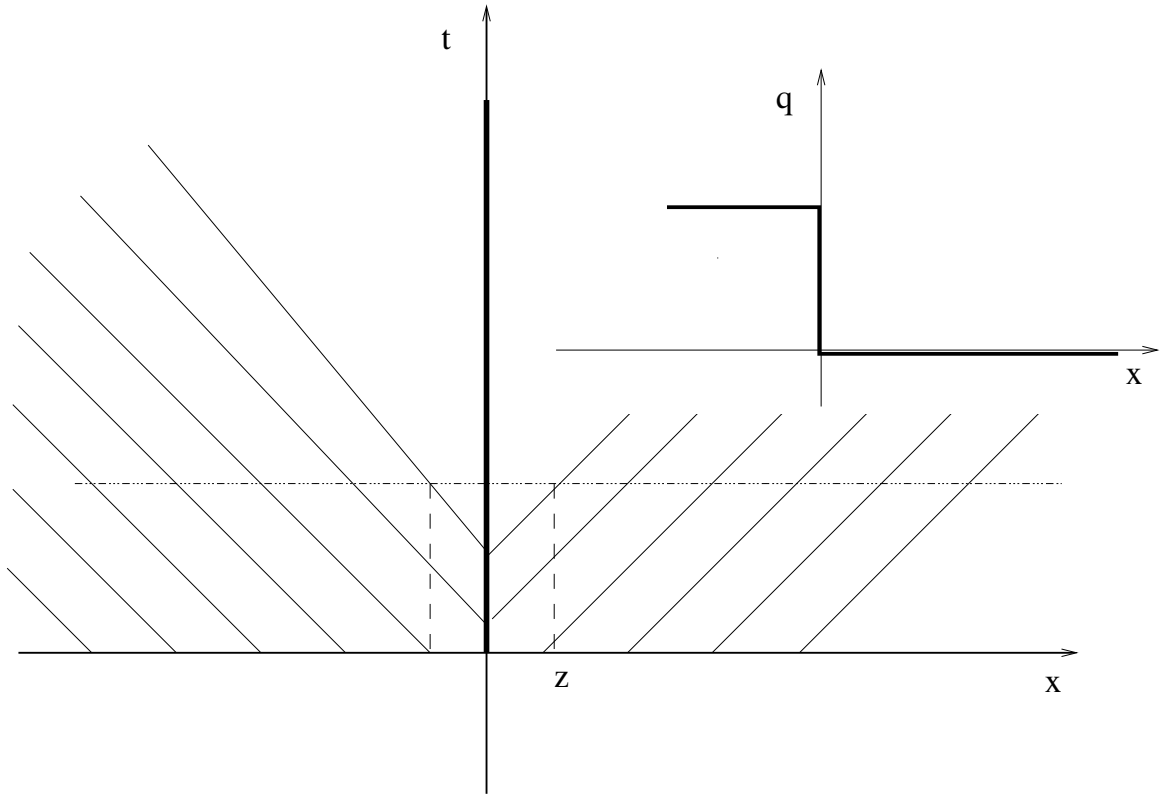
The case $q_l > q_r$

Take $q_l = 1$ and $q_r = 0$ (queue at the traffic light).



For $x < -u_m t$ the solution remains $q = 0$, for $x > u_m t$ we have $q = 1$. What happens in between?.

An unphysical solution



A possibility is a shock (i.e. a discontinuity) traveling at speed $s = \frac{F(q_l)-F(q_r)}{q_l-q_r}$ (Rankine-Hugoniot relation) and linking the states q_l and q_r. In this particular case $s = 0$ so the shock is stationary. This solution satisfies the equation (in the weak sense) but is unphysical since it does not satisfy the entropy condition.

An entropy condition for strictly convex scalar conservation laws

Lax Condition: a discontinuity propagating with speed s given by the Rankine-Hugoniot expression satisfies the Lax entropy condition if

$$F'(q_l) > s > F'(q_r)$$

Oleinik condition for scalar conservation laws

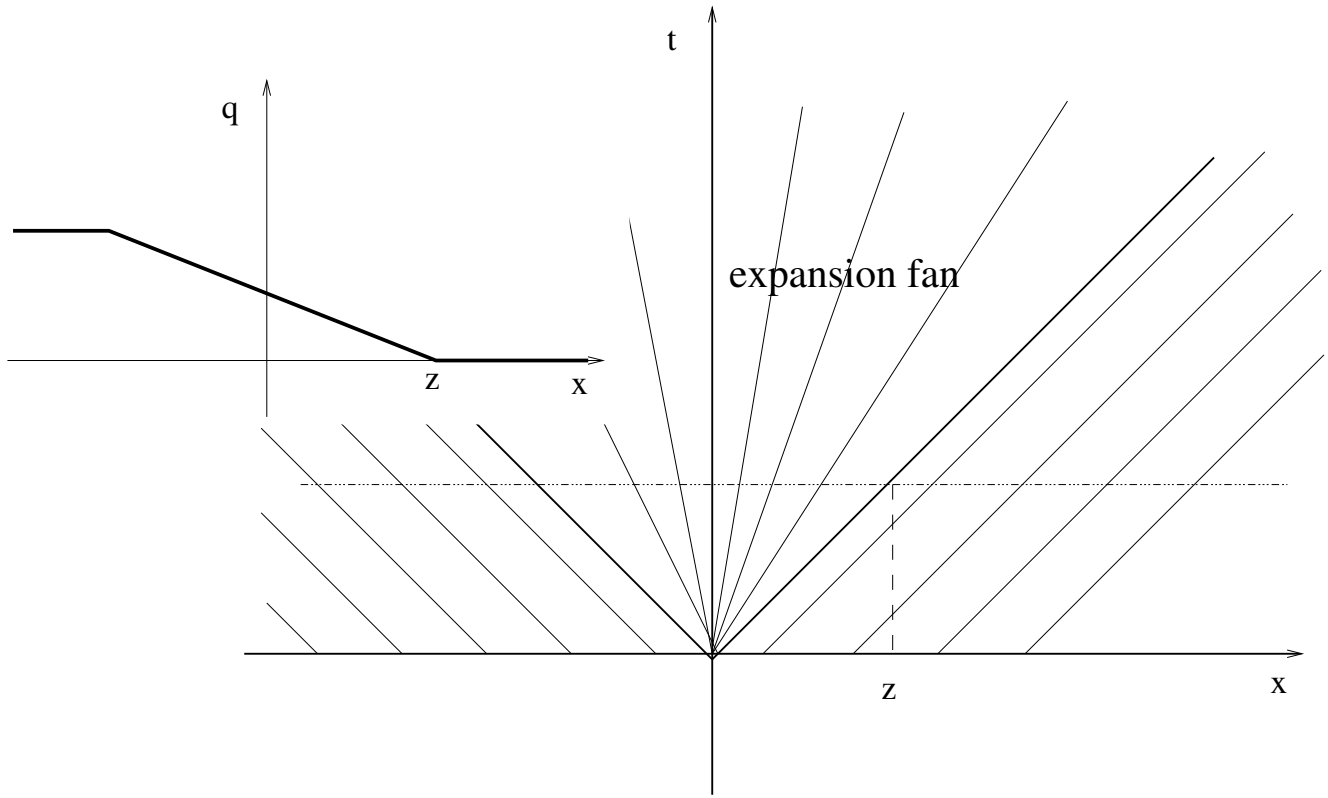
This condition extends to scalar conservation laws with non convex flux function. Is related to "vanishing viscosity solutions" and in the case of a strictly convex flux it reduces to the Lax Condition.

A weak solution $q(x,t)$ is the vanishing-viscosity solution of a scalar conservation law if all the discontinuities have the property that

$$\frac{F(q)-F(q_l)}{q-q_l} \geq s \geq \frac{F(q)-F(q_r)}{q-q_r}.$$

s being given by the Rankine-Hugoniot condition.

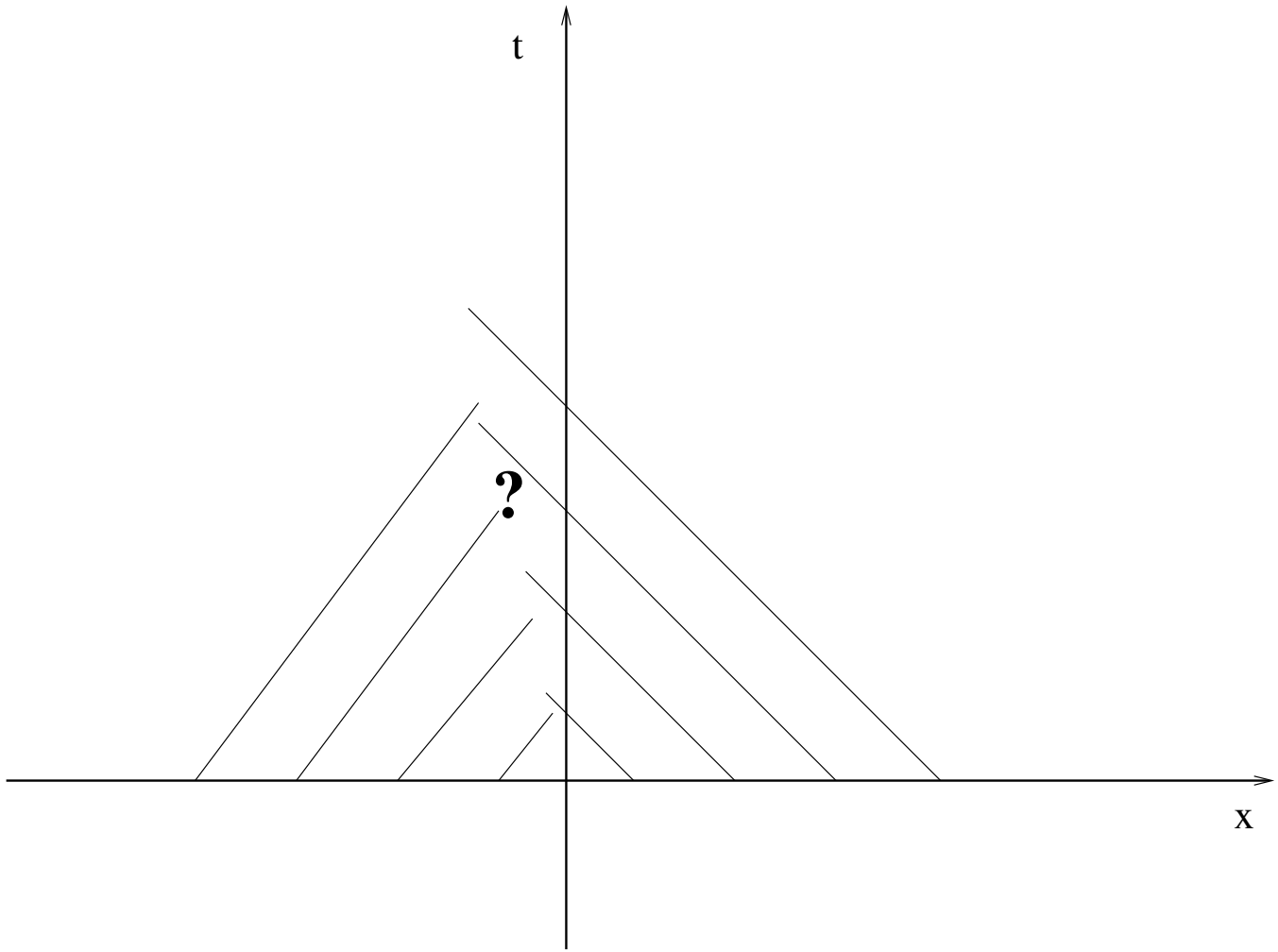
The correct solution for $q_l > q_r$



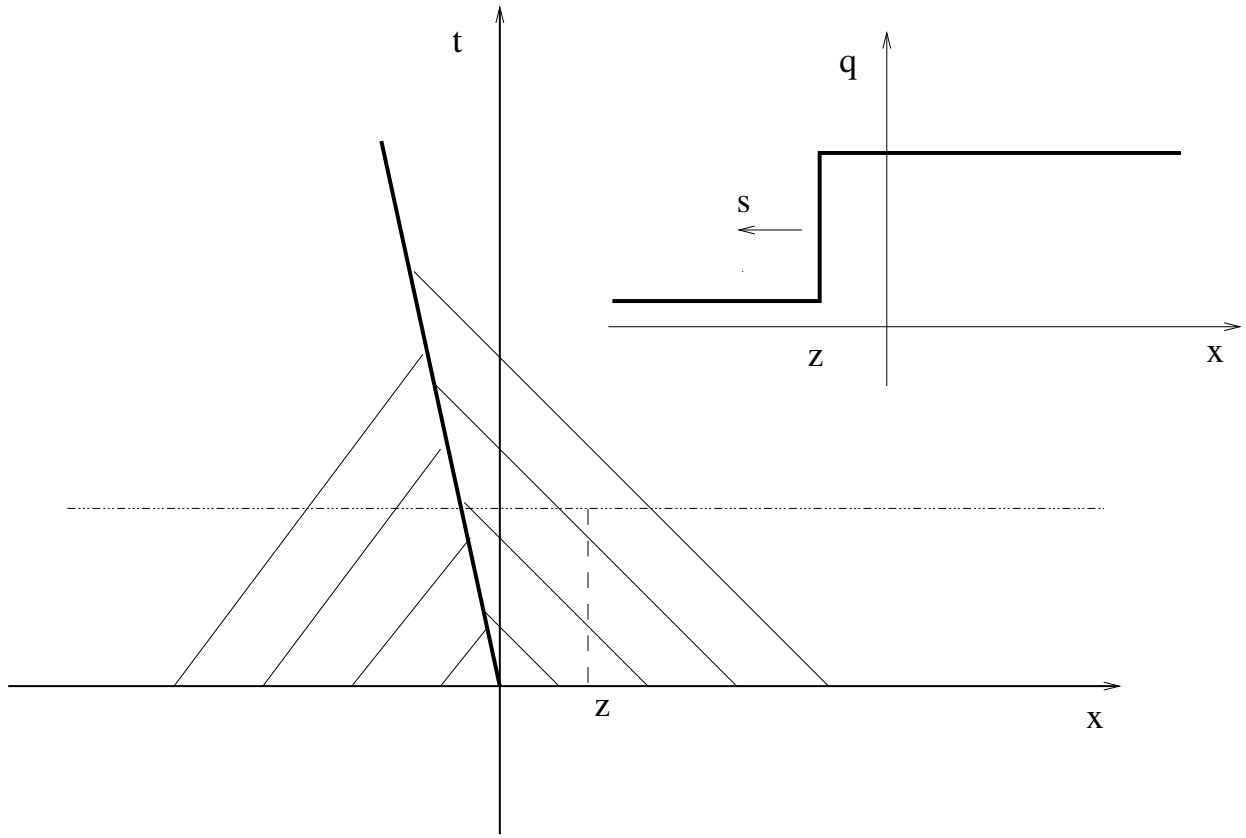
The correct solution is a rarefaction wave. It is continuous and the characteristics in $x = 0$ form an expansion fan. The curve that connects the states $q_l = 1$ and $q_r = 0$ is, in this particular case, a line. In general, in a rarefaction wave $q(x, t) = r(x/t)$, with $r = (F')^{-1}$.

The case $q_r > q_l$

We take $q_l = 1/8$ and $q_r = 1$ (cars approaching a traffic jam). We note that the characteristic lines starting from the left and the right of $x = 0$ must necessarily meet after a finite time.



The case $q_r > q_l$



The solution is here a shock traveling backward at speed $s = \frac{F(q_l)-F(q_r)}{q_l-q_r} = -u_m/8$.

This shock is physical, i.e. it satisfies the entropy condition.

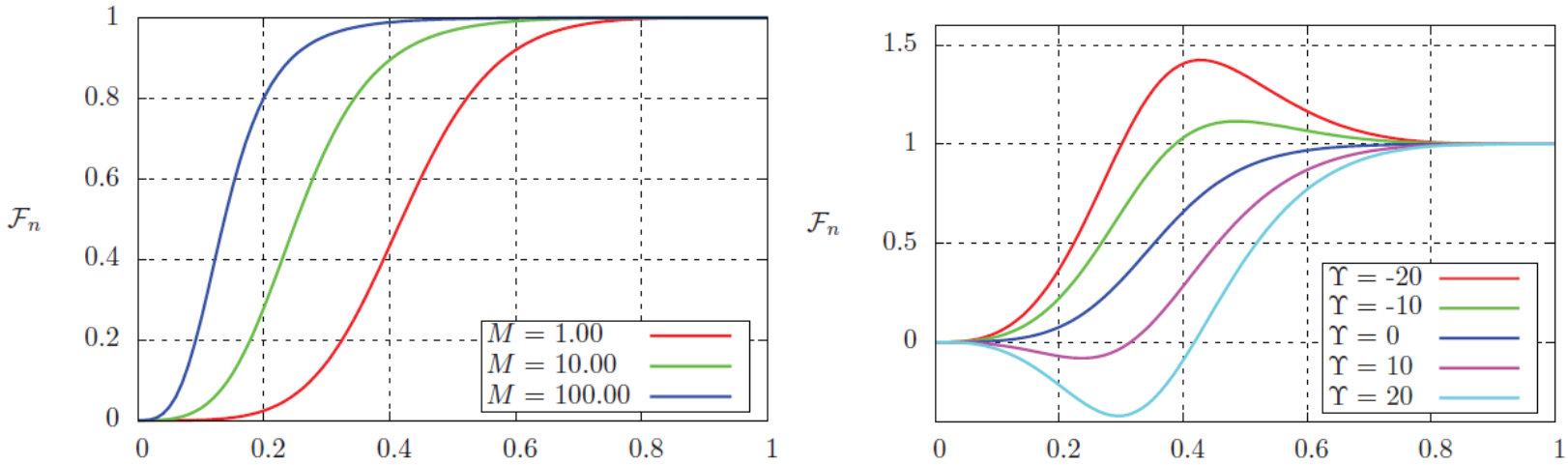
Back to the Backley-Leverett

It would be nice if our saturation system behaved like the traffic problem.

It would mean that injecting water in a porous media filled of oil a solution similar to that of the previous slide would form, pushing the oil out.
In a finite time all the oil would be extracted.

Unfortunately, this is not true.

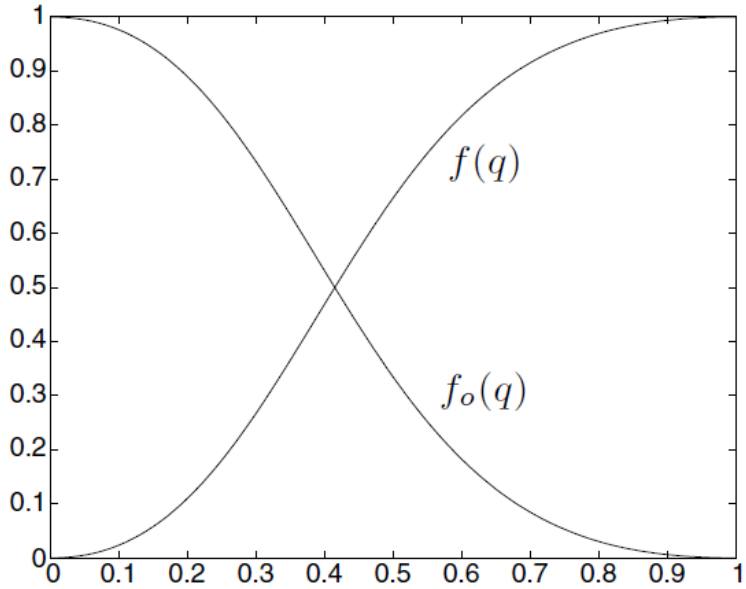
A typical profile for the saturation fluxes

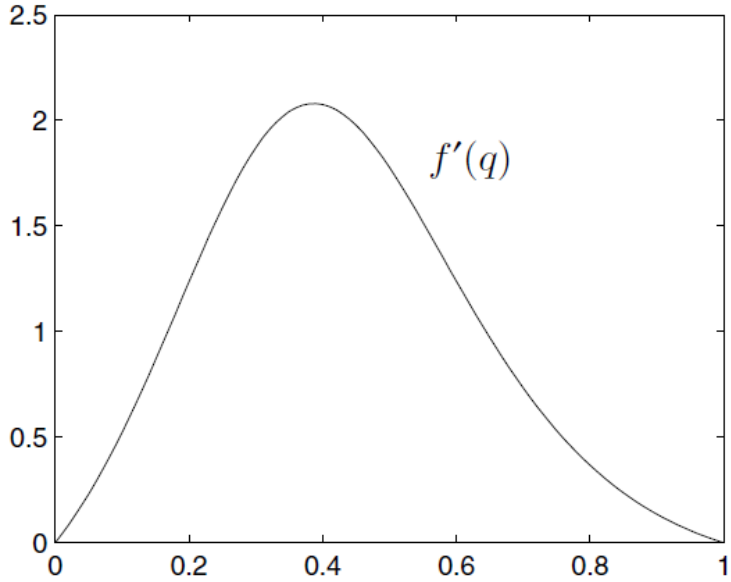


We show typical curves for the saturation fluxes. At the left for different values of the mobility ratio, at the left varying the importance of gravity effects.

An important thing to note is that they are not convex functions!. Moreover gravity induces a change of sign of F'.

Why it matters?

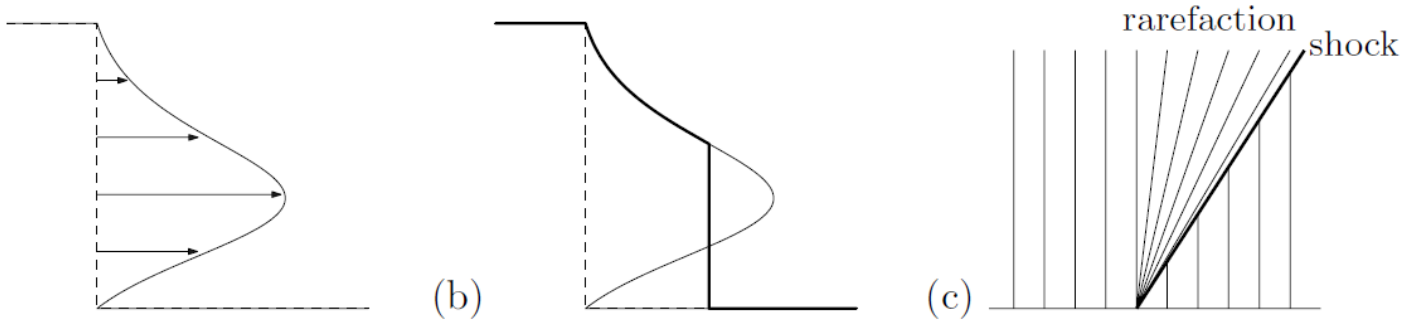




Lets consider this situation. The subscript o here refers to the non-wetting phase, f is the flux, f' its derivative.
Lets consider a Riemann problem with initial values across the inflection point.

Shock and rarefaction wave at the same point

The situation is depicted in the picture (taken from LeVeque, Finite Volume Methods for Conservation Laws). In figure (b) the profile of q after a certain (small) time. In (c) the characteristic lines.



We have a discontinuity followed by an expansion wave!!

As a consequence: we cannot extract all the non-wetting phase in a finite time.

Possible numerical schemes

Characteristics based schemes

They are based in identifying the convective and diffusive part of the fluxes:

$$\mathbf{F} = f_w \mathbf{u} + \lambda_n f_w (\rho_n - \rho_w)\mathbf{K}\mathbf{g} \quad \mathbf{D} = \lambda_n f_w \mathbf{K} p_c' \nabla S_w$$

rewriting the equation in the semi-linear form

$$\Phi \frac{\partial S_w}{\partial_t} + \frac{d\mathbf{F}}{dS_w} \cdot \nabla S_w + \nabla \cdot \mathbf{D} = q_w$$

The transport term is then interpreted as total derivative

$$\Phi \frac{\partial S_w}{\partial_t} + \frac{d\mathbf{F}}{dS_w} \cdot \nabla S_w = \Phi \frac{DS_w}{Dt}$$

Possible numerical schemes

Here $\frac{DS_w}{Dt}$ is the derivative along the characteristic line defined by the differential equation

$$\frac{d\mathbf{y}(t)}{dt} = \Phi^{-1}\frac{d\mathbf{F}}{dS_w}(\mathbf{y}(t), t)$$

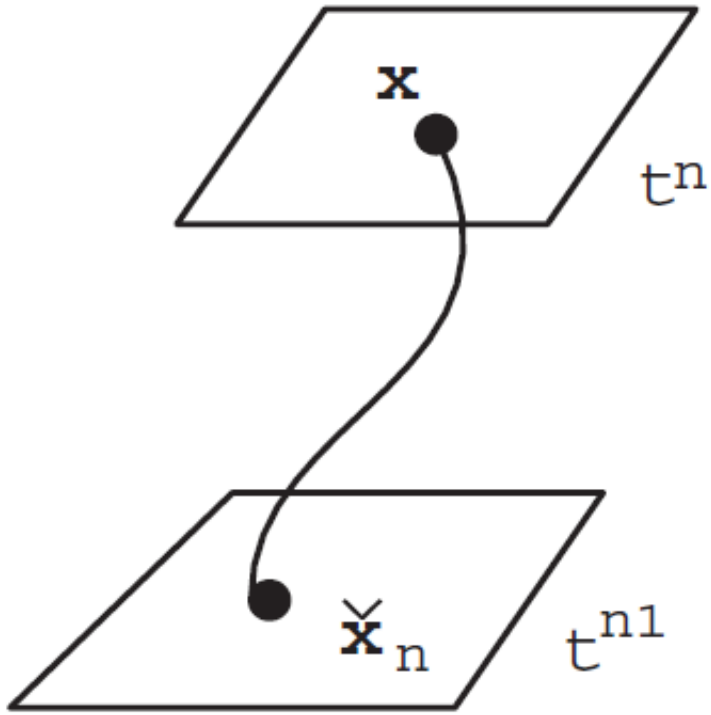
A possible treatment of the characteristic derivative is to find at each time step (t^n, t^{n+1}) and for any grid point $\mathbf{x}$ the foot of the characteristic line ending in $(\mathbf{x}, t^{n+1})$, for instance by using Euler differentiation:

$$\check{\mathbf{x}} = \mathbf{x} - \Delta t \Phi^{-1}(\mathbf{x})\frac{d\mathbf{F}}{dS_w}(\mathbf{x}, t^n)$$

and then setting

$$\Phi(\mathbf{x})\frac{DS_w}{Dt}(\mathbf{x}, t^{n+1}) \simeq \Phi(\mathbf{x})(\Delta t)^{-1}\left[S_w(\mathbf{x}, t^{n+1}) - S_w(\check{\mathbf{x}}, t^n)\right]$$

The foot of the characteristic line



For each node (or quadrature point) we need to compute the foot of the characteristic line passing through $(\mathbf{x}, t^{n+1})$. This is a costly, yet trivially parallel, operation.

Diffusive term is treated in a standard way by finite elements of finite volumes.

Characteristic based scheme

Characteristic based schemes enjoy good stability properties, but it is difficult to satisfy conservation at discrete level and also the application of boundary conditions is tricky (what happens if a characteristic line exits the domain?). So various variants have been proposed in the literature
In the context of porous media flow two characteristic based schemes are most common

- The modified method of characteristics (MMOC), Duoglas and Russel (1982) and Pironneau (1982).
- The Eulerian Lagrangian localized adjoint problem (ELLAM) (Wang, Ewing, Russel 1990). Based on a space-time formulation.

Both methods suffers difficulties in handling general boundary conditions and are rather expensive computationally.

The methods that are more commonly used in practical codes are finite volume methods, which we are going to describe.

Let's consider the pure hyperbolic problem

$$\Phi \frac{\partial S}{\partial t} + \nabla \cdot \mathbf{F}(S) = 0$$

where we also assume that $\partial \Phi / \partial t = 0$.
The first step is to create a grid τ_h and integrate the equation on each element $E \in \tau_h$, and apply the divergence theorem to get

$$\frac{d}{dt} \int_E \Phi S + \int_{\partial E} \mathbf{F}(S) \cdot \mathbf{n} = \int_E q$$

The degrees of freedom of the semi-discrete problem are the values of S on each element, we also compute an elemental characteristic value of the porosity such that $\Phi_E S_E(t) \simeq |E|^{-1} \int_E \Phi S d\Omega$. Then

$$\frac{d}{dt} \int_E \Phi S \simeq \Phi_E |E| \frac{d}{dt} S_E$$

The finite volume method

We now integrate in time over the generic time step (t^n, t^{n+1}). We obtain

$$\Phi_E |E| \left(S_E^{n+1} - S_E^n\right) = - \int_{t^n}^{t^{n+1}} \int_{\partial E} \mathbf{F} \cdot \mathbf{n}$$

If $e \in \partial E$ is an element facet at the boundary between elements E and E_e^+ we approximate the last integral as

$$\Delta t \sum_{e \in \partial E} |e| H_e(S_E^n, S_{E_e^+}^n)$$

The quantity H is called numeric flux.

Note: we are considering here an explicit time integration scheme.

Basic properties of a numeric flux

If S is constant

$$H_e(S, S) = \mathbf{F}(S) \cdot \mathbf{n} \quad \text{Consistency}$$

and

$$H_e(S, W) = -H_e(W, S) \quad \text{Conservation}$$

The simplest numerical flux

$$H_e(S_1, S_2) = \frac{\mathbf{F}(S_1) + \mathbf{F}(S_2)}{2} \cdot \mathbf{n}$$

does not work since it gives rise to an unstable numerical scheme.

Upwinding

It is well known that you need to add some "upwinding" to the numerical flux, to account for the propagation direction of the solution, governed by $d\mathbf{F}/dS$.

We also want that the numerical scheme does not create spurious oscillations in the numerical solution. This is normally obtained by looking for monotonicity preserving schemes, whose definition is more simply given for a 1D problem. If $\ldots, x_{i-1}, x_i m \ldots$ are the mesh nodes in a monotonicity preserving scheme if

$$S_i^n \geq S_{i+1}^n, \quad \forall i$$

then

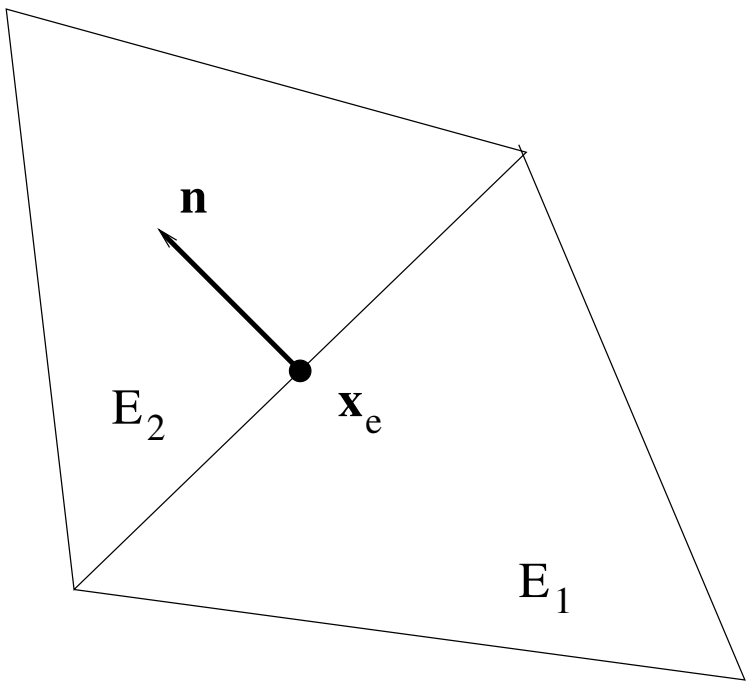
$$S_i^{n+1} \geq S_{i+1}^{n+1}, \quad \forall i$$

We will present a first order method which is monotonicity preserving, the Godonov scheme.

On each facet between E_1 and E_2 we consider the 1D Riemann problem along the line $\mathbf{x} = \mathbf{x}_e + y\mathbf{n}$ ($\mathbf{n}$ is pointing from E_1 to E_2) and given by the solution of the problem

$$S = \begin{cases} S_1 & y \leq 0 \\ S_2 & y > 0 \end{cases}$$

(here $S_1 = S_{E_1}$ etc.)



Note that the problem has been reduced to a one-dimensional problem governed by the projected flux $\mathcal{F}_e = \mathbf{F} \cdot \mathbf{n}$.

The solution to the Riemann problem may often be computed exactly, sometimes approximately (in that case we have an approximate Riemann solver)

We set $\mathcal{F}_e = \mathbf{F} \cdot \mathbf{n}$ and define

$$H_e(S_1, S_s) = \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} \mathcal{F}_e(S^+(S_1, S_2))dt$$

where S^+ is the solution of the Riemann problem at $y = 0$ (which for the homogeneous case is a constant!).

Godonov flux

If $\mathbf{F}(S)$ is Lipschitz continuous the Godonov numerical flux may be build explicitly as

$$H_e(S_1, S_2) = \begin{cases} \min\limits_{\theta \in [S_2, S_1]} \mathcal{F}_e(\theta) & \text{if } S_2 < S_1 \\ \max\limits_{\theta \in [S_1, S_2]} \mathcal{F}_e(\theta) & \text{if } S_2 \geq S_1 \end{cases}$$

However, if the material properties are discontinuous across the element, this formula is not valid.

Godonov fluxes for discontinuous coefficients

We need to distinguish between $\mathcal{F}_1 = \mathcal{F}_e|_{E_1}$ and $\mathcal{F}_2 = \mathcal{F}_e|_{E_2}$ (we assume that the fluxes are continuous within each element). Under some mild assumptions (Adimurthi et al. 2004, S. Mishra et al, 2010) it can be shown that in this case is still possible to build exact Godonov fluxes, by first computing

$$H_e = \min(\mathcal{F}_1(\min(S_1, \theta_1)), \mathcal{F}_2(\max(S_2, \theta_2)))$$

where $\theta_{1,2} = \text{argmax}_{S \in [0,1]} \mathcal{F}_{1,2}(S)$

Upstream mobility flux

An alternative to Godonov scheme very used in practical code is upstream mobility.
In practice one computes the flux using mobilities chosen according to the sign of $\mathbf{u}_w \cdot \mathbf{n}$ (or $\mathbf{u}_n \cdot \mathbf{n}$ if we are solving for the non-wetting phase saturation).
We have

$$H_e^{UM}(S_1, S_2) = \frac{\lambda_w^*}{\lambda_n^* + \lambda_w^*} (\mathbf{u}_e + \lambda_n^*(\rho_w - \rho_n)\mathbf{K}\mathbf{g}) \cdot \mathbf{n}$$

where

$$\lambda_\alpha^* = \begin{cases} \lambda_{1,\alpha} & \text{if } \mathbf{u}_{e,\alpha} \cdot \mathbf{n} > 0 \\ \lambda_{2,\alpha} & \text{if } \mathbf{u}_{e,\alpha} \cdot \mathbf{n} \leq 0 \end{cases} \qquad \alpha \in \{w, n\}$$

This scheme works well in practice if the flux is "dominated" by the Darcy velocity. It may however give unphysical solutions if the jump of mobilities is high or if there is a strong gravity effect.

Application of boundary conditions

We recall that (if we neglect capillary effects) we can apply boundary conditions only at the inflow boundary Γ^-. Let $e \in \Gamma^-$. In the calculation of the fluxes we will set S_2^n equal to the given boundary values at $t = t^n$.

Let $e \in \Gamma^+$. In this case we still need to compute the numerical flux H_e which requires the knowledge of S_2^n. We then build this value by extrapolation, for instance constant extrapolation: $S_2^2 = S_1^n$.

The CFL condition

A necessary condition for the (strong) stability of an explicit scheme for hyperbolic conservation laws is the satisfaction of the Courant-Friedrichs-Lewy condition (CFL). The CFL number σ is defined as

$$\sigma = \Delta t \max_{E \in \tau_h} \max_{e \in \partial E} \frac{|\mathcal{F}_e|}{h_E},$$

where h_E is the diameter of element E.
For CFL condition states

$$\sigma \leq C$$

For a constant C that depends on the scheme. In the schemes we have presented $C = 1$.

Explicit or implicit treatment of the diffusive term?

In the case we do not neglect capillary pressure we need to treat also the diffusive term. It is better to treat it implicitly since the explicit treatment will induce a parabolic-type stability condition of the form

$$\Delta t \leq C \min h_E^{-2}$$

which is more restrictive in general than the CFL condition.

Source term

A possible treatment of the source term is to add

$$\Delta t \int_E q^* d\Omega$$

to the general scheme, where q^* may be either computed at time step t^n (explicit) or t^{n+1} (implicit).

Note however that this can lead to inaccuracies because the Riemann solution is modified by the presence of the source term. So also the computation of the numerical fluxes should be in principle modified.
The explicit treatment may induce instability.