Numerical Simulation of Transport Processes in Porous Media

Classification of Partial Differential Equations

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Recapitulation: Groundwater Flow

- can be described by Darcy's Law $J_w = -K_s \nabla p_w$ and the continuity equation $\frac{\partial \theta(\vec{x})}{\partial t} + \nabla \cdot \vec{J}_w(\vec{x}) + r_w(\vec{x}) = 0$.
- gravity is included by $\frac{\partial \theta(\vec{x})}{\partial t} - \nabla \cdot \left[\bar{K}_s(\vec{x}) \cdot (\nabla p_w - \rho_w g \vec{e}_z) \right] + r_w(\vec{x}) = 0$
- heterogeneity is considered by different values of K_s at different positions of $\vec{x}$
- anisotropy is considered by using a tensor $\bar{K}_s$ instead of a scalar
- in steady state the flux equation is given by: $-\nabla \cdot \left[\bar{K}_s(\vec{x}) \cdot (\nabla p_w - \rho_w g \vec{e}_z) \right] + r_w(\vec{x}) = 0$

Partial Differential Equations

A partial differential equation

- determines a function $u(\vec{x})$ in $n \geq 2$ variables $\vec{x} = (x_1, \dots, x_n)^T$.
- is a functional relation between partial derivatives (to more than one variable) of u at *one* point.

In general:

$$F\left(\frac{\partial^m u}{\partial x_1^m}(\vec{x}), \frac{\partial^{m-1} u}{\partial x_1^{m-1}}(\vec{x}), \dots, \frac{\partial^m u}{\partial x_1^{m-1}\partial x_2}(\vec{x}), \dots, \frac{\partial^m u}{\partial x_n^m}(\vec{x}), \frac{\partial^{m-1} u}{\partial x_n^{m-1}}(\vec{x}), \dots, u(\vec{x}), \vec{x}\right) = 0 \quad \forall \vec{x} \in \Omega \tag{1}$$

Important:

- The highest derivative m determines the order of a PDE

Domains

PDE's are not posed on the whole $\mathbb{R}^n$ but on a subset of $\mathbb{R}^n$.

Definition (Domain)

$\Omega \subseteq \mathbb{R}^n$ is called domain if Ω is open and connected.

- open: For each $\vec{x} \in \Omega$ there exists a $B_\epsilon(\vec{x}) = \{\vec{y} \in \Omega \,|\, \|\vec{x} - \vec{y}\| < \epsilon\}$ such that $B_\epsilon(\vec{x}) \subseteq \Omega$ if ϵ is small enough.
- connected: if $\vec{x}, \vec{y} \in \Omega$, then there exists a steady curve $\vec{t}(s) : [0,1] \to \Omega$ with $\vec{t}(0) = \vec{x}$, $\vec{t}(1) = \vec{y}$, $\vec{t}(s) \in \Omega$.

$\overline{\Omega}$ designates the closure of Ω, i.e. Ω plus the limit values of all sequences, which can be generated from elements of Ω.
$\partial\Omega = \overline{\Omega} \setminus \Omega$ is the boundary of Ω. Often additional conditions on the smoothness of the boundary are necessary.
Finally $\vec{\nu}(\vec{x})$ is the outer unit normal at a point $\vec{x} \in \partial\Omega$. □

Solutions of PDE's

- $u : \Omega \rightarrow \mathbb{R}$ is called a solution of a PDE if it satisfies the PDE identically for every point $\vec{x} \in \Omega$
- Solutions of PDE's are usually not unique unless additional conditions are posed. Typically these are conditions for the function values (and/or derivatives) at the boundary
- A PDE is well posed if the solution
  - exists
  - is unique (with appropriate boundary conditions)
  - depends continuously on the data.

PDE Classification

Linear partial PDE's of second order are a case of specific interest. For 2 dimensions and order $m = 2$ the general equation is:

$$
\begin{aligned}
&a(x,y)\frac{\partial^2 u}{\partial x^2}(x,y) + 2b(x,y)\frac{\partial^2 u}{\partial x \partial y}(x,y) + c(x,y)\frac{\partial^2 u}{\partial y^2}(x,y) \\
&+d(x,y)\frac{\partial u}{\partial x}(x,y) + e(x,y)\frac{\partial u}{\partial y}(x,y) + f(x,y)u(x,y) \\
&+g(x,y) = 0
\end{aligned}
$$

At a point (x, y) a PDE can be classified according to the first three terms (main part) into

$$
\begin{aligned}
\text{elliptic} \quad & \text{if } \det \left(\begin{smallmatrix} a & b \\ b & c \end{smallmatrix}\right) = a(x,y)c(x,y) - b^2(x,y) > 0 \\
\text{hyperbolic} \quad & \text{if } \det \left(\begin{smallmatrix} a & b \\ b & c \end{smallmatrix}\right) = a(x,y)c(x,y) - b^2(x,y) < 0 \\
\text{parabolic} \quad & \text{if } \det \left(\begin{smallmatrix} a & b \\ b & c \end{smallmatrix}\right) = a(x,y)c(x,y) - b^2(x,y) = 0 \text{ and} \\
& \text{Rank} \begin{bmatrix} a & b & d \\ b & c & e \end{bmatrix} = 2 \text{ in } (x,y)
\end{aligned}
$$

PDE Classification in $n > 2$ space dimensions

The general linear PDE of 2nd order in n space dimensions is:

$$\underbrace{\sum_{i,j=1}^{n} a_{ij}(\vec{x})\partial_{x_i}\partial_{x_j} u}_{\text{main part}} + \sum_{i=1}^{n} a_i(\vec{x})\partial_{x_i} u + a_0(\vec{x})u = f(\vec{x}) \quad \text{in } \Omega.$$

without loss of generality one can set $a_{ij} = a_{ji}$. With $(A(\vec{x}))_{ij} = a_{ij}(\vec{x})$ the PDE is at a point $\vec{x}$

- **elliptic** if all eigenvalues of $A(\vec{x})$ have identical sign and no eigenvalue is zero.
- **hyperbolic** if $(n-1)$ eigenvalues have identical sign, one eigenvalue the opposite sign and no eigenvalue is zero.
- **parabolic** if one eigenvalue is zero, all other eigenvalues have identical sign and the $\text{Rank}[A(\vec{x}), a(\vec{x})] = n$.

□

Remarks on PDE Classification

- Why this classification? Different solution techniques are necessary for the different types of PDE's.
- The described classification is *complete* for linear PDE's with $n = m = 2$. In higher space dimensions the classification is no longer complete.
- The type is invariant under coordinate transformation $\xi = \xi(x, y)$, $\eta = \eta(x, y)$ and $u(x, y) = \tilde{u}(\xi(x, y), \eta(x, y))$, which yields a new PDE for $\tilde{u}(\xi, \eta)$ with the coefficients $\tilde{a}, \tilde{b}$, etc.. If the equation for u in (x, y) has the type t than $\tilde{u}$ in $(\xi(x, y), \eta(x, y))$ has the same type.
- The type *can* vary at different points (but not in our applications).
- The type is only determined by the main part of the PDE (except for parabolic equations).
- Pathological cases like $\frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial x} = 0; u(x, y) = 0$ are avoided.

Remarks on PDE Classification (cont.)

Definition

A linear PDE of 2nd order is called elliptic (hyperbolic, parabolic) in Ω if it is elliptic (hyperbolic, parabolic) for all points $(x, y) \in \Omega$. □

Classification for first-order PDE's

Definition

An equation of the form

$$d(x,y)\frac{\partial u}{\partial x}(x,y) + e(x,y)\frac{\partial u}{\partial y}(x,y) + f(x,y)u(x,y) + g(x,y) = 0$$

is called hyperbolic if $|d(x,y)| + |e(x,y)| > 0 \quad \forall (x,y) \in \Omega$ (else it is an ordinary differential equation). For $n \geq 2$ the equation $v(\vec{x}) \cdot \nabla u(\vec{x}) + f(\vec{x})u(\vec{x}) + g(\vec{x}) = 0$ is called hyperbolic. □

In this lecture we only cover scalar PDE's. Systems of PDE's contain several unknown functions $u_1, \ldots, u_n : \Omega \to \mathbb{R}$ and n PDE's. There is also a classification system for systems of PDE's.

Examples for PDE types: Poisson-Equation

$$\frac{\partial^2 u}{\partial x^2}(x,y) + \frac{\partial^2 u}{\partial y^2}(x,y) = f(x,y) \qquad \forall (x,y) \in \Omega \tag{2}$$

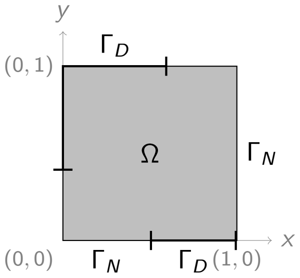
is called Poisson-Equation.
This is the prototype of an *elliptic* PDE. The solution of equation (2) is not unique. If $u(x,y)$ is a solution, then e.g. $u(x,y) + c_1 + c_2 x + c_3 y$ is also a solution for arbitrary values of c_1, c_2, c_3. To get a unique solution u values at the boundary have to be specified (we therefore call this a "boundary value problem").
Two types of boundary values are common:

1. $u(x,y) = g(x,y)$ for $(x,y) \in \Gamma_D \subseteq \partial\Omega$ (Dirichlet[1]),
2. $\frac{\partial u}{\partial \nu}(x,y) = h(x,y)$ for $(x,y) \in \Gamma_N \subset \partial\Omega$ (Neumann[2], flux),

and $\Gamma_D \cup \Gamma_N = \partial\Omega$. It is also important that $\Gamma_N \neq \partial\Omega$, as else the solution is only defined up to a constant.

[1] Peter Gustav Lejeune Dirichlet, 1805-1859, German Mathematician.
[2] John von Neumann, 1903-1957, Austro-Hungarian Mathematician

Examples for PDE types: Complete Poisson-Equation



$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f \text{ in } \Omega$$
$$u = g \text{ on } \Gamma_D \subseteq \partial\Omega$$
$$\frac{\partial u}{\partial \nu} = h \text{ on } \Gamma_N = \partial\Omega \setminus \Gamma_D \neq \partial\Omega$$

Generalisation to n space dimensions:

$$\sum_{i=1}^{n} \frac{\partial^2 u}{\partial x_i^2} =: \Delta u = f \text{ in } \Omega$$
$$u = g \text{ on } \Gamma_D \subseteq \partial\Omega$$
$$\nabla u \cdot \nu = h \text{ on } \Gamma_N = \partial\Omega \setminus \Gamma_D$$

This equation is also called elliptic. If $f \equiv 0$ it is called Laplace-Equation. □

Examples for PDE types: General Diffusion Equation

$K : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ is a map, which relates to each point $\vec{x} \in \Omega$ a $n \times n$ matrix $K(\vec{x})$. We demand also (for all $\vec{x} \in \Omega$) that $K(\vec{x})$

1. $K(\vec{x}) = K^\mathsf{T}(\vec{x})$ and $\xi^\mathsf{T} K(\vec{x})\xi > 0 \quad \forall \xi \in \mathbb{R}^n,\ \xi \neq 0$ (symmetric positive definite),
2. $C(\vec{x}) := \min \left\{ \xi^\mathsf{T} K(\vec{x})\xi \,\middle|\, \|\xi\| = 1 \right\} \geq C_0 > 0$ (uniform ellipticity).

$$\boxed{\begin{aligned} -\nabla \cdot \left\{ K(\vec{x}) \nabla u(\vec{x}) \right\} &= f \text{ in } \Omega \\ u &= g \text{ on } \Gamma_D \subseteq \partial\Omega \\ -\Big(K(\vec{x}) \nabla u(\vec{x}) \Big) \cdot \nu(\vec{x}) &= h \text{ on } \Gamma_N = \partial\Omega \setminus \Gamma_D \neq \partial\Omega \end{aligned}} \tag{3}$$

is then called General Diffusion Equation (e.g. groundwater flow equation).

For strongly varying K equation (3) can be very difficult to solve. □

Examples for PDE types: Wave-Equation

The prototype of a hyperbolic equation of second order is the Wave-Equation:

$$\frac{\partial^2 u}{\partial x^2}(x,y) - \frac{\partial^2 u}{\partial y^2}(x,y) = 0 \qquad \text{in } \Omega \quad . \tag{4}$$

Examples for PDE types: Wave-Equation

Possible boundary values for a domain $\Omega = (0,1)^2$ are e.g.:

$x \in [0,1]$:

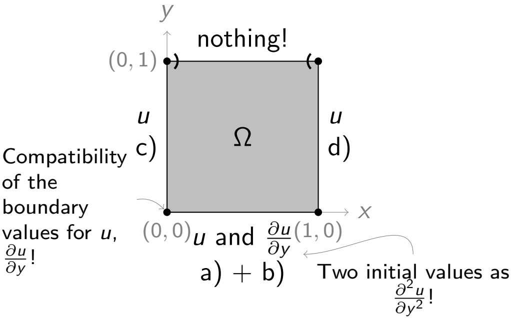
a) $u(x,0) = u_0(x)$

b) $\dfrac{\partial u}{\partial y}(x,0) = u_1(x)$

$y \in [0,1]$:

c) $u(0,y) = g_0(y)$

d) $u(1,y) = g_1(y)$

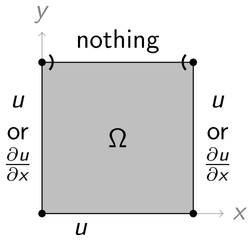


One direction (here y, usually the time) is special. a) + b) are called initial values and c) + d) boundary values (the boundary values can also be Neumann boundary conditions). It is not possible to prescribe values at the whole boundary (the future)! □

Examples for PDE types: Heat-Equation

The prototype of a parabolic equation is the heat equation:

$$\frac{\partial^2 u}{\partial x^2}(x,y) - \frac{\partial u}{\partial y}(x,y) = 0 \qquad \text{in } \Omega.$$



only one boundary value as PDE is first order in y

For a domain $\Omega = (0,1)^2$ typical boundary values are (with $x \in [0,1], y \in [0,1]$):

$$u(x,0) = u_0(x)$$

$$u(0,y) = g_0(y) \text{ or } \frac{\partial u}{\partial x}(0,y) = h_0(y)$$

$$u(1,y) = g_1(y) \text{ or } \frac{\partial u}{\partial x}(1,y) = h_1(y)$$

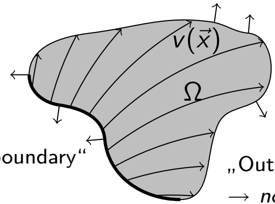
Examples for PDE types: Transport-Equation

If $\Omega \subset \mathbb{R}^n, v : \Omega \to \mathbb{R}^n$ is a given vector field, the equation

$$\nabla\cdot\{v(\vec{x})u(\vec{x})\} = f(\vec{x}) \qquad \text{in } \Omega$$

is called stationary transport equation and is a hyperbolic PDE of first order.
Possible boundary values are

$$u(\vec{x}) = g(\vec{x})$$



for $\vec{x} \in \partial\Omega$ with $v(\vec{x}) \cdot \nu(\vec{x}) < 0$ (Boundary value depends on the flux field)
$\frac{\partial u}{\partial t} + \nabla \cdot \{v(\vec{x}, t)u(\vec{x}, t)\} = f(\vec{x}, t)$ is also a hyperbolic PDE of first order. □

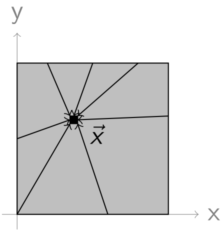
Sphere of Influence

Elliptic PDE

The type of a partial differential equation can also be illustrated with the following question:

> *Given $\vec{x} \in \Omega$. Which initial/boundary values influence the solution u at the point $\vec{x}$?*

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



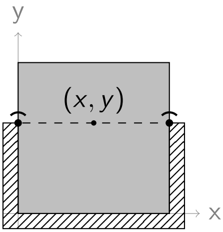
all boundary values influence $u(\vec{x})$, i.e. Change in $u(y), y \in \partial\Omega \Rightarrow$ Change in $u(\vec{x})$.

Sphere of Influence

Parabolic PDE

$u_{xx} - u_y = 0$

Note: The $-$ is crucial, $+$ is parabolic according to the definition *but* it is not well posed (stable)



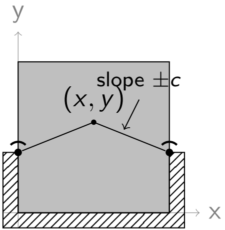
for (x, y) all (x', y') with $y' \leq y$ influence the value at $\vec{x}$.

„infinite velocity of propagation“

Sphere of Influence

Hyperbolic PDE (2nd order)

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



Solution at (x, y) is influenced by all boundary values below the cone

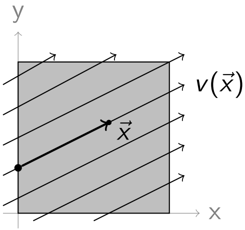
$$\{(x', y') \;|\; y' \leq (x' - x) \cdot c + y \;\wedge\; y' \leq (x - x') \cdot c + y\} \;\cap\; \partial\Omega$$

„finite velocity of propagation“

Sphere of Influence

Hyperbolic PDE (1st order)

$u_x + u_y = 0$



Only one boundary point influences the value.

The Steady-State Groundwater Flow Equation

- The steady-state groundwater flow equation $-\nabla \cdot \left[\bar{K}_s(\vec{x}) \cdot (\nabla p_w - \rho_w g \vec{e}_z)\right] + r_w(\vec{x}) = 0$ is an elliptic partial differential equation of second order.
- To get a well posed problem either Dirichlet boundary conditions (the pressure value is given) or Neumann boundary conditions (the flux is given) must be specified at each boundary point.
- At one point of the boundary a Dirichlet boundary condition should be specified (else the equation is only defined up to a constant).
- Each point in the domain is influenced by all boundary conditions.