Advanced Topics from Scientific Computing
TU Berlin Winter 2022/23
Notebook 12
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Partial Differential Equations

Notations

Given: domain $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3 \dots$)

- Dot product: for $\vec{x}, \vec{y} \in \mathbb{R}^d$, $\vec{x} \cdot \vec{y} = \sum_{i=1}^d x_i y_i$
- Bounded domain $\Omega \subset \mathbb{R}^d$, with piecewise smooth boundary
- Scalar function $u : \Omega \to \mathbb{R}$
- Vector function $\vec{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} : \Omega \to \mathbb{R}^d$
- Partial derivative $\partial_i u = \frac{\partial u}{\partial x_i}$
- Second partial derivative $\partial_{ij} u = \frac{\partial^2 u}{\partial x_i x_j}$

- *Gradient* of scalar function $u : \Omega \to \mathbb{R}$:

$$\mathrm{grad} = \vec{\nabla} = \begin{pmatrix} \partial_1 \\ \vdots \\ \partial_d \end{pmatrix} : u \mapsto \vec{\nabla} u = \begin{pmatrix} \partial_1 u \\ \vdots \\ \partial_d u \end{pmatrix}$$

- *Divergence* of vector function $\vec{v} = \Omega \to \mathbb{R}^d$:

$$\mathrm{div} = \nabla \cdot : \vec{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} \mapsto \nabla \cdot \ \vec{v} = \partial_1 v_1 + \cdots + \partial_d v_d$$

- *Laplace operator* of scalar function $u : \Omega \to \mathbb{R}$

$$\begin{aligned} \mathrm{div} \cdot \mathrm{grad} &= \nabla \cdot \vec{\nabla} \\ &= \Delta : u \mapsto \Delta u = \partial_{11} u + \cdots + \partial_{dd} u \end{aligned}$$

Lipschitz domains

Definition: A connected open subset $\Omega \subset \mathbb{R}^d$ is called *domain*. If Ω is a bounded set, the domain is called *bounded*.

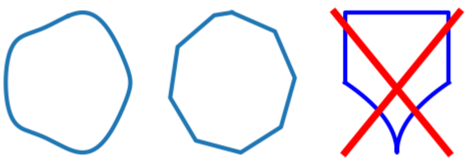
Definition:

- Let $D \subset \mathbb{R}^n$. A function $f : D \to \mathbb{R}^m$ is called *Lipschitz continuous* if there exists $c > 0$ such that $||f(x) - f(y)|| \leq c||x - y||$ for any $x, y \in D$
- A hypersurface in $\mathbb{R}^n$ is a *graph* if for some k it can be represented on some domain $D \subset \mathbb{R}^{n-1}$ as

$$x_k = f(x_1, \dots, x_{k-1}, x_{k+1}, \dots, x_n)$$

- A domain $\Omega \subset \mathbb{R}^n$ is a *Lipschitz domain* if for all $x \in \partial\Omega$, there exists a neigborhood of x on $\partial\Omega$ which can be represented as the graph of a Lipschitz continuous function.

Standard PDE calculus happens in Lipschitz domains



- Boundaries of Lipschitz domains are continuous
- Polygonal domains are Lipschitz
- Boundaries of Lipschitz domains have no cusps (e.g. the graph of $y = \sqrt{|x|}$ has a cusp at $x = 0$)

Divergence theorem (Gauss' theorem)

Theorem: Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain and $\vec{v} : \Omega \to \mathbb{R}^d$ be a continuously differentiable vector function. Let $\vec{n}$ be the outward normal to Ω. Then,

$$\int_\Omega \nabla \cdot \vec{v}\, d\vec{x} = \int_{\partial\Omega} \vec{v} \cdot \vec{n}\, ds.$$

This is a generalization of the Newton-Leibniz rule of calculus:

Let $d = 1$, $\Omega = (a, b)$. Then:

- $n_a = (-1)$
- $n_b = (1)$
- $\nabla \cdot v = v'$

$$\int_\Omega \nabla \cdot \vec{v}\, d\vec{x} = \int_a^b v'(x)\, dx = v(b) - v(a) = v(a)n_a + v(b)n_b$$

Species evolution in a domain Ω

Let

- Ω: domain, $(0, T)$: time evolution interval
- $u(\vec{x}, t) : \Omega \times [0, T] \to \mathbb{R}$: time dependent *local amount of species* (aka species concentration)
- $f(\vec{x}, t) : \Omega \times [0, T] \to \mathbb{R}$: species *sources/sinks*
- $\vec{j}(\vec{x}, t) : \Omega \times [0, T] \to \mathbb{R}^d$: vector field of the species *flux*

Representative Elementary Volume (REV)

Let $\omega \subset \Omega$: be a *representative elementary volume (REV)* Define averages:

- $J(t) = \int_{\partial\omega} \vec{j}(\vec{x}, t) \cdot \vec{n}\; ds$: flux of species trough $\partial\omega$ at moment t
- $U(t) = \int_\omega u(\vec{x}, t)\; d\vec{x}$: amount of species in ω at moment t
- $F(t) = \int_\omega f(\vec{x}, t)\; d\vec{x}$: rate of creation/destruction at moment t

Species conservation

Let $(t_0, t_1) \subset (0, T)$. The Change of the amount of species in ω during (t_0, t_1) is proportional to the sum of the amount transported through boundary and the amount created/destroyed

$$U(t_1) - U(t_0) + \int_{t_0}^{t_1} J(t)\; dt = \int_{t_0}^{t_1} F(t)\; dt$$

Using the definitions of U,F,J, we get

$$\int_\omega (u(\vec{x}, t_1) - u(\vec{x}, t_0))\, d\vec{x} + \int_{t_0}^{t_1} \int_{\partial\omega} \vec{j}(\vec{x}, t) \cdot \vec{n}\, ds\, dt = \int_{t_0}^{t_1} \int_\omega f(\vec{x}, t)\, ds$$

Gauss' theorem gives

$$\int_{t_0}^{t_1} \int_\omega \partial_t u(\vec{x}, t)\, d\vec{x}\, dt + \int_{t_0}^{t_1} \int_\omega \nabla \cdot \vec{j}(\vec{x}, t)\, d\vec{x}\, dt = \int_{t_0}^{t_1} \int_\omega f(\vec{x}, t)\, ds$$

Continuity equation

The above is true for all $\omega \subset \Omega$, $(t_0, t_1) \subset (0, T) \Rightarrow$

$$\partial_t u(\vec{x}, t) + \nabla \cdot \vec{j}(\vec{x}, t) = f(\vec{x}, t) \quad \text{in } \Omega \times [0, T]$$

- While this sounds obvious, mathematical reasoning about this is more complex
- Whenever one encounters the divergence operator, chances are that it describes a conservation law for certain species. This physical meaning is very concrete and, if possible should be preserved during the process of discretizing PDEs.

Flux expressions

As a rule, species flux is proportional to the negative gradient of the species concentration: $\vec{j}(\vec{x}, t) \sim -\vec{\nabla} u(\vec{x}, t)$. This corresponds to the direction of steepest descend.

Therefore we set $\vec{j} = -\delta \vec{\nabla} u$, where $\delta > 0$ can be constant, space/time dependent or even depend on u. For simplicity, we assume δ to be constant, unless stated otherwise.

Heat conduction

- $u = T$: temperature
- $\delta = \lambda$: heat conduction coefficient
- f: heat source
- $\vec{j} = -\lambda \vec{\nabla} T$: *Fourier law*

Diffusion of molecules in a given medium (for low concentrations)

- $u = c$: concentration
- $\delta = D$: diffusion coefficient
- f: species source (e.g due to reactions)
- $\vec{j} = -D\vec{\nabla}c$: *Fick's law*

Flow in a saturated porous medium:

- $u = p$: pressure
- $\delta = k$: permeability
- $\vec{j} = -k\vec{\nabla}p$: *Darcy's law*

Electrical conduction

- $u = \varphi$: electric potential
- $\delta = \sigma$: electric conductivity
- $\vec{j} = -\sigma\vec{\nabla}\varphi \equiv$ current density: *Ohms's law*

Electrostatics in a constant magnetic field:

- $u = \varphi$: electric potential
- $\delta = \varepsilon$: dielectric permittivity
- $\vec{E} = \vec{\nabla}\phi$: electric field
- $\vec{j} = \vec{D} = \varepsilon\vec{E} = \varepsilon\vec{\nabla}\varphi$: electric displacement field: *Gauss's Law*
- $f = \rho$: charge density

Second order partial differential equations (PDEs)

Combine continuity equation with flux expression:

$$\partial_t u - \nabla \cdot (\delta \nabla u) = f.$$

This type of PDEs is called *parabolic*.

Assuming stationarity - i.e. independence of time results in $\partial_t u = 0$ and the *elliptic* PDE

$$-\nabla \cdot (\delta \nabla u) = f.$$

Boundary conditions

So far, we cared about the species balance of an REV in the interior of the domain. How about the species balance between Ω and its exterior ? This is described by *boundary conditions*.

Assume $\partial\Omega = \cup_{i=1}^{N_\Gamma}\Gamma_i$ is the union of a finite number of non-intersecting subsets Γ_i which are locally Lipschitz.

Define boundary conditions on each of Γ_i

Dirichlet boundary conditions

Let $g_i : \Gamma_i \to \mathbb{R}$.

$$u(\vec{x}, t) = g_i(\vec{x}, t) \quad \text{for } \vec{x} \in \Gamma_i$$

- fixed solution at the boundary
- also called *boundary condition of first kind*
- called *homogeneous* for $g_i = 0$

Neumann boundary conditions

Let $g_i : \Gamma_i \to \mathbb{R}$.

$$-\vec{j}(\vec{x}, t) \cdot \vec{n} = g_i(\vec{x}, t) \quad \text{for } \vec{x} \in \Gamma_i$$

- fixed boundary normal flux
- also called *boundary condition of second kind*
- called *homogeneous* for $g_i = 0$

Robin boundary conditions

let $\alpha_i > 0, g_i : \Gamma_i \to \mathbb{R}$

$$-\vec{j}(\vec{x},t)\cdot\vec{n} + \alpha_i(\vec{x},t)u(\vec{x},t) = g_i(\vec{x},t) \quad \text{for } \vec{x} \in \Gamma_i$$

- Boundary flux proportional to solution
- also called *third kind boundary condition*

Generalizations

- δ may depend on $\vec{x}$, u, $|\vec{\nabla}u|$ $\dots \Rightarrow$ equations become nonlinear
- Coefficients can depend on other processes
  - temperature can influence conductvity
  - source terms can describe chemical reactions between different species
  - chemical reactions can generate/consume heat
  - Electric current generates heat (``Joule heating'')
  - $\dots$

  $\Rightarrow$ coupled PDEs
- Convective terms: $\vec{j} = -\delta\vec{\nabla}u + u\vec{v}$ where $\vec{v}$ is a convective velocity
- PDEs for vector unknowns
  - Momentum balance $\Rightarrow$ Navier-Stokes equations for fluid dynamics
  - Elasticity
  - Maxwell's electromagnetic field equations

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