Scientific Computing WS 2017/2018

Lecture 14

Jürgen Fuhrmann

juergen.fuhrmann@wias-berlin.de

Homework

- Now due Dec. 15
- Another correction . . .

1D heat conduction

- v_L, v_R: ambient temperatures, α: heat transfer coefficient
- Second order boundary value problem in $\Omega = [0, 1]$:

$$
\begin{aligned}
-u''(x) &= f(x) && \text{in}\Omega \\
-u'(0) + \alpha(u(0) - v_L) &= 0 \\
u'(1) + \alpha(u(1) - v_R) &= 0
\end{aligned}
$$

- Let $h = \frac{1}{n-1}$, $x_i = x_0 + (i-1)h \; i = 1 \dots n$ be discretization points, let u_i approximations for $u(x_i)$ and $f_i = f(x_i)$
- Finite difference approximation:

$$
\begin{aligned}
-u'(0) + \alpha(u(0) - v_L) &\approx \frac{1}{h}(u_0 - u_1) + \alpha(u_0 - v_L) \\
-u''(x_i) - f(x_i) &\approx \frac{1}{h^2}(-u_{i+1} + 2u_i - u_{i-1}) - f_i \quad (i = 2 \dots n-1) \\
u'(1) + \alpha(u(1) - v_R) &\approx \frac{1}{h}(u_n - u_{n-1}) + \alpha(u_n - v_R)
\end{aligned}
$$

numcxx availability

- Please report any problem with UNIX pool
- A virtual machine (tested for VirtualBox) is now available via the course homepage

Differential operators: notations

Given: domain $\Omega \subset \mathbb{R}^d$.

- Dot product: for $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, $\mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^d x_i y_i$
- Bounded domain $\Omega \subset \mathbb{R}^d$, with piecewise smooth boundary
- Scalar function $u : \Omega \to \mathbb{R}$
- Vector function $\mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} : \Omega \to \mathbb{R}^d$
- Write $\partial_i u = \frac{\partial u}{\partial x_i}$
- For a multindex $\alpha = (\alpha_1 \dots \alpha_d)$, write $|\alpha| = \alpha_1 + \dots + \alpha_d$ and define $\partial^\alpha u = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdot \dots \cdot \partial x_d^{\alpha_d}}$

Basic Differential operators

- Gradient
$$\mathrm{grad} = \nabla = \begin{pmatrix} \partial_1 \\ \vdots \\ \partial_d \end{pmatrix} \colon\ u \mapsto \nabla u = \begin{pmatrix} \partial_1 u \\ \vdots \\ \partial_d u \end{pmatrix}$$
- Divergence
$$\mathrm{div} = \nabla \cdot :\ \mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} \mapsto \nabla \cdot \mathbf{v} = \partial_1 v_1 + \cdots + \partial_d v_d$$
- Laplace operator
$$\Delta = \mathrm{div} \cdot \mathrm{grad} = \nabla \cdot \nabla \colon\ u \mapsto \Delta u = \partial_{11} u + \cdots + \partial_{dd} u$$

Lipschitz domains

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 $\|f(x) - f(y)\| \leq c\|x - y\|$
- A hypersurface in $\mathbb{R}^n$ is a *graph* if for some k it can be represented as

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

  defined on some domain $D \subset \mathbb{R}^{n-1}$
- 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 continous function.

Corollaries

- Boundaries of Lipschitz domains are continuous
- Boundaries of Lipschitz domains have no cusps
- Polygonal domains are Lipschitz

Divergence theorem (Gauss' theorem)

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

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

□

Species balance over an REV

- Let $u(\mathbf{x}, t) : \Omega \times [0, T] \to \mathbb{R}$ be the local amount of some species.
- Assume representative elementary volume $\omega \subset \Omega$
- Subinterval in time $(t_0, t1) \subset (0, T)$
- $-\delta \nabla u \cdot \mathbf{n}$ describes the flux of these species trough $\partial\omega$, where δ is some transfer coefficient
- Let $f(\mathbf{x}, t)$ be some local source of species. Then the flux through the boundary is balanced by the change of the amount of species in ω and the source strength.

$$\begin{aligned} 0 &= \int_\omega (u(\mathbf{x}, t_1) - u(\mathbf{x}, t_0))\, d\mathbf{x} - \int_{t_0}^{t_1} \int_{\partial\omega} \delta \nabla u \cdot \mathbf{n}\, ds\, dt - \int_{t_0}^{t_1} \int_\omega f(\mathbf{x}, t)\, ds \\ &= \int_{t_0}^{t_1} \int_\omega \partial_t u(\mathbf{x}, t)\, d\mathbf{x}\, dt - \int_{t_0}^{t_1} \int_\omega \nabla \cdot (\delta \nabla u)\, d\mathbf{x}\, dt - \int_{t_0}^{t_1} \int_\omega f(\mathbf{x}, t)\, ds \end{aligned}$$

- True for all $\omega \subset \Omega$, $(t_0, t1) \subset (0, T) \Rightarrow$ parabolic second order PDE

$$\partial_t u(x, t) - \nabla \cdot (\delta \nabla u(x, t)) = f(x, t)$$

PDE examples

- Heat conduction:
  u: temperature, δ: heat conduction coefficient, f: heat source
  flux$=-\delta\nabla u$: "Fourier law"
- Diffusion:
  u: concentration, δ: diffusion coefficient, f: species source
  flux$=-\delta\nabla u$: "Fick's law"

Second order *elliptic* PDE describes stationary case:

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

- Incompressible flow in saturated porous media
  u: pressure, δ: permeability,
  flux$=-\delta\nabla u$: "Darcy's law"
- Electrical conduction:
  u: electrostatic potential, δ: conductivity
  flux$=-\delta\nabla u$= current density: "Ohms's law"
- Poisson equation (electrostatics in a constant magnetic field):
  u: electrostatic potential,∇u: electric field, δ: dielectric permittivity,
  f: charge density

PDEs: boundary conditions, generalizations

- Given bounded domain Ω, combine PDE in the interior with boundary conditions specifiying u or $\nabla u \cdot \mathbf{n}$
- δ may depend on $\mathbf{x}$, u, $|\nabla u|$ ... $\Rightarrow$ equations become nonlinear
- Coupled equations:
  - temperature can influence conductvity
  - source terms can describe chemical reactions between different species
  - chemical reactions can generate/consume heat
  - Electric current generate heat ("Joule heating")
  - ...

Problems with “strong formulation”

Writing the PDE with divergence and gradient assumes smoothness of coefficients and at least second derivatives for the solution.

- δ may not be continuous – what is then $\nabla \cdot (\delta u)$?
- In FEM we want to approximate u e.g. by piecewise linear functions – once again: what does $\nabla \cdot (\delta u)$ mean in this case ?
- The structure of the space of continuously differentiable functions is not very convenient
  - they can be equipped with norms $\Rightarrow$ Banach spaces
  - no scalar product $\Rightarrow$ no Hilbert space
  - Not complete: Cauchy sequences of functions may not converge

Cauchy sequences of functions

- Regard sequences of functions on a given domain
- A *Cauchy sequence* is a sequence f_n of functions where the norm of the difference between two elements can be made arbitrarily small by increasing the element numbers:

$$\forall \varepsilon > 0 \; \exists n_0 \in \mathbb{N} : \forall m, n > n_0, ||f_n - f_m|| < \varepsilon$$

- All convergent sequences of functions are Cauchy sequences
- A metric space is *complete* if all Cauchy sequences of its elements have a limit within this space

Riemann integral $\rightarrow$ Lebesgue integral

- Let Ω be a Lipschitz domain, let $C_c(\Omega)$ be the set of continuous functions $f : \Omega \rightarrow \mathbb{R}$ with compact support. ($\Rightarrow$ they vanish on $\partial\Omega$)
- For these functions, the Riemann integral $\int_\Omega f(x)d\mathbf{x}$ is well defined, and $\|f\|_{L^1} := \int_\Omega |f(x)|d\mathbf{x}$ provides a norm, and induces a metric.
- Let $L^1(\Omega)$ be the completion of $C_c(\Omega)$ with respect to the metric defined by the norm $\|\cdot\|_{L^1}$. That means that $L^1(\Omega)$ consists of all elements of $C_c(\Omega)$, and of all limites of Cauchy sequences of elements of $C_c(\Omega)$. Such functions are called *measurable*.
- For any measurable $f = \lim_{n\rightarrow\infty} f_n \in L^1(\Omega)$ with $f_n \in C_c(\Omega)$, define the *Lebesque integral*

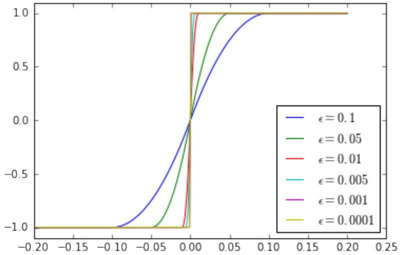
$$\int_\Omega f(x)\, d\mathbf{x} := \lim_{n\rightarrow\infty} \int_\Omega f_n(x)\, d\mathbf{x}$$

as the limit of a sequence of Riemann integrals of continuous functions

Examples for Lebesgue integrable (measurable) functions

- Bounded functions continuous except in a finite number of points
- Step functions

$$f_\epsilon(x) = \begin{cases} 1, & x \geq \epsilon \\ -(\frac{x-\epsilon}{\epsilon})^2 + 1, & 0 \leq x < \epsilon \\ (\frac{x+\epsilon}{\epsilon})^2 - 1, & -\epsilon \leq x < 0 \\ -1, & x < -\epsilon \end{cases} \xrightarrow{\epsilon \to 0} f(x) = \begin{cases} 1, & x \geq 0 \\ -1, & \text{else} \end{cases}$$



- Equality of L^1 functions is elusive as they are not necessarily continuous: best what we can say is that they are equal "almost everywhere". In particular, L^1 functions whose values differ in a finite number of points are equal almost everywhere.

Spaces of integrable functions

- For $1 \leq p \leq \infty$, let $L^p(\Omega)$ be the space of measureable functions such that

$$\int_\Omega |f(x)|^p d\mathbf{x} < \infty$$

equipped with the norm

$$||f||_p = \left(\int_\Omega |f(x)|^p d\mathbf{x}\right)^{\frac{1}{p}}$$

- These spaces are *Banach spaces*, i.e. complete, normed vector spaces.
- The space $L^2(\Omega)$ is a *Hilbert space*, i.e. a Banach space equipped with a scalar product $(\cdot, \cdot)$ whose norm is induced by that scalar product, i.e. $||u|| = \sqrt{(u, u)}$. The scalar product in L^2 is

$$(f, g) = \int_\Omega f(x)g(x)d\mathbf{x}.$$

Green's theorem for smooth functions

Theorem Let $u, v \in C^1(\overline{\Omega})$ (continuously differentiable). Then for $\mathbf{n} = (n_1 \dots n_d)$ being the outward normal to Ω,

$$\int_\Omega u \partial_i v \, d\mathbf{x} = \int_{\partial\Omega} uvn_i \, ds - \int_\Omega v \partial_i u \, d\mathbf{x}$$

Corollaries

- Let $\mathbf{u} = (u_1 \dots u_d)$. Then

$$\int_\Omega (\sum_{i=1}^{d} u_i \partial_i v) \, d\mathbf{x} = \int_{\partial\Omega} v \sum_{i=1}^{d} (u_i n_i) \, ds - \int_\Omega v \sum_{i=1}^{d} (\partial_i u_i) \, d\mathbf{x}$$

$$\int_\Omega \mathbf{u} \cdot \nabla v \, d\mathbf{x} = \int_{\partial\Omega} v \mathbf{u} \cdot \mathbf{n} \, ds - \int_\Omega v \nabla \cdot \mathbf{u} \, d\mathbf{x}$$

- If $v = 0$ on $\partial\Omega$:

$$\int_\Omega u \partial_i v \, d\mathbf{x} = - \int_\Omega v \partial_i u \, d\mathbf{x}$$

$$\int_\Omega \mathbf{u} \cdot \nabla v \, d\mathbf{x} = - \int_\Omega v \nabla \cdot \mathbf{u} \, d\mathbf{x}$$

Weak derivative

- Let $L^1_{loc}(\Omega)$ be the set of functions which are Lebesgue integrable on every compact subset $K \subset \Omega$. Let $C_0^\infty(\Omega)$ be the set of functions infinitely differentiable with zero values on the boundary.
- For $u \in L^1_{loc}(\Omega)$ we *define* $\partial_i u$ by

$$\int_\Omega v \partial_i u d\mathbf{x} = -\int_\Omega u \partial_i v d\mathbf{x} \quad \forall v \in C_0^\infty(\Omega)$$

  and $\partial^\alpha u$ by

$$\int_\Omega v \partial^\alpha u d\mathbf{x} = (-1)^{|\alpha|} \int_\Omega u \partial_i v d\mathbf{x} \quad \forall v \in C_0^\infty(\Omega)$$

  if these integrals exist.
- For smooth functions, weak derivatives coincide with with the usual derivative

Sobolev spaces

- For $k \geq 0$ and $1 \leq p < \infty$, the *Sobolev space* $W^{k,p}(\Omega)$ is the space functions where all up to the k-th derivatives are in L^p:

$$W^{k,p}(\Omega) = \{u \in L^p(\Omega) : \partial^\alpha u \in L^p(\Omega) \ \forall |\alpha| \leq k\}$$

with then norm

$$||u||_{W^{k,p}(\Omega)} = \left(\sum_{|\alpha| \leq k} ||\partial^\alpha u||^p_{L^p(\Omega)} \right)^{\frac{1}{p}}$$

- Alternatively, they can be defined as the completion of C^∞ in the norm $||u||_{W^{k,p}(\Omega)}$
- $W_0^{k,p}(\Omega)$ is the completion of C_0^∞ in the norm $||u||_{W^{k,p}(\Omega)}$
- The Sobolev spaces are Banach spaces.

Sobolev spaces of square integrable functions

- $H^k(\Omega) = W^{k,2}(\Omega)$ with the scalar product

$$(u, v)_{H^k(\Omega)} = \sum_{|\alpha| \leq k} \int_\Omega \partial^\alpha u \partial^\alpha v \, d\mathbf{x}$$

  is a Hilbert space.
- $H_0^k(\Omega) = W_0^{k,2}(\Omega)$ with the scalar product

$$(u, v)_{H_0^k(\Omega)} = \sum_{|\alpha| = k} \int_\Omega \partial^\alpha u \partial^\alpha v \, d\mathbf{x}$$

  is a Hilbert space as well.
- The initally most important:
  - $L^2(\Omega)$, scalar product $(u, v)_{L^2(\Omega)} = (u, v)_{0,\Omega} = \int_\Omega uv \, d\mathbf{x}$
  - $H^1(\Omega)$, scalar product $(u, v)_{H^1(\Omega)} = (u, v)_{1,\Omega} = \int_\Omega (uv + \nabla u \cdot \nabla v) \, d\mathbf{x}$
  - $H_0^1(\Omega)$, scalar product $(u, v)_{H_0^1(\Omega)} = \int_\Omega (\nabla u \cdot \nabla v) \, d\mathbf{x}$
- Inequalities:

$$|(u, v)|^2 \leq (u, u)(v, v) \quad \text{Cauchy-Schwarz}$$
$$||u + v|| \leq ||u|| + ||v|| \quad \text{Triangle inequality}$$

A trace theorem

The notion of function values on the boundary initially is only well defined for continouos functions. So we need an extension of this notion to functions from Sobolev spaces.

Theorem: Let Ω be a bounded Lipschitz domain. Then there exists a bounded linear mapping

$$\mathrm{tr} : H^1(\Omega) \to L^2(\partial\Omega)$$

such that

(i) $\exists c > 0$ such that $\|\mathrm{tr}\, u\|_{0,\partial\Omega} \leq c\|u\|_{1,\Omega}$
(ii) $\forall u \in C^1(\bar{\Omega})$, $\mathrm{tr}\, u = u|_{\partial\Omega}$

□

Derivation of weak formulation

- Sobolev space theory provides a convenient framework to formulate existence and uniqueness of solutions of PDEs.
- Stationary heat conduction equation with homogeneous Dirichlet boundary conditions:

$$
\begin{aligned}
-\nabla \cdot \lambda \nabla u(x) &= f(x) \text{ in } \Omega \\
u &= 0 \text{ on } \partial\Omega
\end{aligned}
$$

Multiply and integrate with an arbitrary *test function* $v \in C_0^\infty(\Omega)$ and apply Green's theorem using $v = 0$ on $\partial\Omega$

$$
\begin{aligned}
-\int_\Omega (\nabla \cdot \lambda \nabla u) v \, d\mathbf{x} &= \int_\Omega f v \, d\mathbf{x} \\
\int_\Omega \lambda \nabla u \nabla v \, d\mathbf{x} &= \int_\Omega f v \, d\mathbf{x}
\end{aligned}
$$

Weak formulation of homogeneous Dirichlet problem

- Search $u \in H_0^1(\Omega)$ (here, $\operatorname{tr} u = 0$) such that

$$\int_\Omega \lambda \nabla u \nabla v \, d\mathbf{x} = \int_\Omega fv \, d\mathbf{x} \; \forall v \in H_0^1(\Omega)$$

- Then,

$$a(u, v) := \int_\Omega \lambda \nabla u \nabla v \, d\mathbf{x}$$

  is a self-adjoint bilinear form defined on the Hilbert space $H_0^1(\Omega)$.
- It is bounded due to Cauchy-Schwarz:

$$|a(u, v)| = |\lambda| \cdot |\int_\Omega \nabla u \nabla v \, d\mathbf{x}| \leq ||u||_{H_0^1(\Omega)} \cdot ||v||_{H_0^1(\Omega)}$$

- $f(v) = \int_\Omega fv \, d\mathbf{x}$ is a linear functional on $H_0^1(\Omega)$. For Hilbert spaces V the dual space V' (the space of linear functionals) can be identified with the space itself.

The Lax-Milgram lemma

Let V be a Hilbert space. Let $a : V \times V \to \mathbb{R}$ be a self-adjoint bilinear form, and f a linear functional on V. Assume a is coercive, i.e.

$$\exists \alpha > 0 : \forall u \in V, a(u,u) \geq \alpha ||u||_V^2.$$

Then the problem: find $u \in V$ such that

$$a(u,v) = f(v) \; \forall v \in V$$

admits one and only one solution with an a priori estimate

$$||u||_V \leq \frac{1}{\alpha} ||f||_{V'}$$

Coercivity of weak formulation

Theorem: Assume $\lambda > 0$. Then the weak formulation of the heat conduction problem: search $u \in H_0^1(\Omega)$ such that

$$\int_\Omega \lambda \nabla u \nabla v \, d\mathbf{x} = \int_\Omega fv \, d\mathbf{x} \; \forall v \in H_0^1(\Omega)$$

has an unique solution.

Proof: $a(u, v)$ is cocercive:

$$a(u, v) = \int_\Omega \lambda \nabla u \nabla u \, d\mathbf{x} = \lambda ||u||^2_{H_0^1(\Omega)}$$

□