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# PDEs and Finite Volume Discretizations

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Lecture 14

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Recap (CG)

# Conjugate gradients (Hestenes, Stiefel, 1952)

Given initial value $u_0$, spd matrix A, right hand side $b$.

$$
\begin{aligned}
d_0 &= r_0 = b - Au_0 \\
\alpha_i &= \frac{(r_i, r_i)}{(Ad_i, d_i)} \\
u_{i+1} &= u_i + \alpha_i d_i \\
r_{i+1} &= r_i - \alpha_i A d_i \\
\beta_{i+1} &= \frac{(r_{i+1}, r_{i+1})}{(r_i, r_i)} \\
d_{i+1} &= r_{i+1} + \beta_{i+1} d_i
\end{aligned}
$$

$r_i$: residual, $(r_i, r_j) = 0$ for $j < i$ $d_i$: search direction, $(d_i, d_j) = 0$ for $j < i$

**Theorem** The convergence rate of the method is

$$
||e_i||_A \leq 2 \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^i ||e_0||_A
$$

where $\kappa = \frac{\lambda_{max}(A)}{\lambda_{min}(A)}$ is the spectral condition number of $A$.

# Preconditioned CG

Assume $\tilde{r}_i = E^{-1} r_i$, $\tilde{d}_i = E^T d_i$, we get the equivalent algorithm

$$
\begin{aligned}
r_0 &= b - Au_0 \\
d_0 &= M^{-1} r_0 \\
\alpha_i &= \frac{(M^{-1} r_i, r_i)}{(Ad_i, d_i)} \\
u_{i+1} &= u_i + \alpha_i d_i \\
r_{i+1} &= r_i - \alpha_i A d_i \\
\beta_{i+1} &= \frac{(M^{-1} r_{i+1}, r_{i+1})}{(r_i, r_i)} \\
d_{i+1} &= M^{-1} r_{i+1} + \beta_{i+1} d_i
\end{aligned}
$$

It relies on the solution of the preconditioning system, the calculation of the matrix vector product and the calculation of the scalar product.

# Properties/issues

Usually we stop the iteration when the residual $r$ becomes small. However during the iteration, floating point errors occur which distort the calculations and lead to the fact that the accumulated residuals

$$r_{i+1} = r_i - \alpha_i A d_i$$

give a much more optimistic picture on the state of the iteration than the real residual

$$r_{i+1} = b - A u_{i+1}$$

# Unsymmetric problems

- By definition, CG is only applicable to symmetric problems.
- The biconjugate gradient (BICG) method provides a generalization:

Choose initial guess $x_0$, perform

$$
\begin{aligned}
r_0 &= b - A x_0 & \hat{r}_0 &= \hat{b} - \hat{x}_0 A^T \\
p_0 &= r_0 & \hat{p}_0 &= \hat{r}_0 \\
\alpha_i &= \frac{(\hat{r}_i, r_i)}{(\hat{p}_i, A p_i)} & & \\
x_{i+1} &= x_i + \alpha_i p_i & \hat{x}_{i+1} &= \hat{x}_i + \alpha_i \hat{p}_i \\
r_{i+1} &= r_i - \alpha_i A p_i & \hat{r}_{i+1} &= \hat{r}_i - \alpha_i \hat{p}_i A^T \\
\beta_i &= \frac{(\hat{r}_{i+1}, r_{i+1})}{(\hat{r}_i, r_i)} & & \\
p_{i+1} &= r_{i+1} + \beta_i p_i & \hat{p}_{i+1} &= \hat{r}_{i+1} + \beta_i \hat{p}_i
\end{aligned}
$$

The two sequences produced by the algorithm are biorthogonal, i.e., $(\hat{p}_i, A p_j) = (\hat{r}_i, r_j) = 0$ for $i \neq j$.

# Unsymmetric problems II

- BiCG is very unstable an additionally needs the transposed matrix vector product, it is seldomly used in practice
- There is as well a preconditioned variant of BiCG which also needs the transposed preconditioner.
- Main practical approaches to fix the situation:
  - "Stabilize" BiCG $\rightarrow$ BiCGstab
  - tweak CG $\rightarrow$ Conjugate gradients squared (CGS)
  - Error minimization in Krylov subspace $\rightarrow$ Generalized Minimum Residual (GMRES)
- Both CGS and BiCGstab can show rather erratic convergence behavior
- For GMRES one has to keep the full Krylov subspace, which is not possible in practice $\Rightarrow$ restart strategy.
- From my experience, BiCGstab is a good first guess

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# Recap (Meshing)

# Delaunay triangulations

- Given a finite point set $X \subset \mathbb{R}^d$. Then there exists simplicial a complex called *Delaunay triangulation* of this point set such that
  - $X$ is the set of vertices of the triangulation
  - The union of all its simplices is the convex hull of $X$.
  - (Delaunay property): For any given $d$-simplex $\Sigma \subset \Omega$ belonging to the triangulation, the interior of its circumsphere does not contain any vertex $x_k \in X$.
- Assume that the points of $X$ are in general position, i.e. no $n+2$ points lie on one sphere. Then the Delaunay triangulation is unique.

# Voronoi diagram

- Given a finite point set $X \subset \mathbb{R}^d$. Then the Voronoi diagram is a partition of $\mathbb{R}^d$ into convex nonoverlapping polygonal regions defined as

$$\mathbb{R}^d = \bigcup_{k=1}^{N_x} V_k$$

$$V_k = \{x \in \mathbb{R}^d : ||x - x_k|| < ||x - x_l|| \forall x_l \in X, l \neq k\}$$

# Voronoi - Delaunay duality

- Given a point set $X \subset \mathbb{R}^d$ in general position. Then its Delaunay triangulation and its Voronoi diagram are dual to each other:
  - Two Voronoi cells $V_k, V_l$ have a common facet if and only if $\overline{x_k x_l}$ is an edge of the triangulation.

# Boundary conforming Delaunay triangulations

- Domain $\Omega \subset \mathbb{R}^n$ (we will discuss only $n = 2$) with polygonal boundary $\partial\Omega$.
- Partition (triangulation) $\Omega = \bigcup_{s=1}^{N_\Sigma} \Sigma$ into non-overlapping simplices $\Sigma_s$ such that this partition represents a simplicial complex. Regard the set of nodes $X = \{x_1 \dots x_{N_x}\}$.
- It induces a partition of the boundary into lower dimensional simplices: $\partial\Omega = \bigcup_{t=1}^{N_\sigma} \sigma_t$. We assume that in 3D, the set $\{\sigma_t\}_{t=1}^{N_\sigma}$ includes all edges of surface triangles as well. For any given lower ($d-1$ or $d-2$) dimensional simplex $\sigma$, its *diametrical sphere* is defined as the smallest sphere containing all its vertices.
- *Boundary conforming Delaunay property*:
  - (Delaunay property): For any given $d$-simplex $\Sigma_s \subset \Omega$, the interior of its circumsphere does not contain any vertex $x_k \in X$.
  - (Gabriel property) For any simplex $\sigma_t \subset \partial\Omega$, the interior of its diametrical sphere does not contain any vertex $x_k \in X$.
- Equivalent formulation in 2D:
  - For any two triangles with a common edge, the sum of their respective angles opposite to that edge is less or equal to $180^\circ$.
  - For any triangle sharing an edge with $\partial\Omega$, its angle opposite to that edge is less or equal to $90^\circ$.

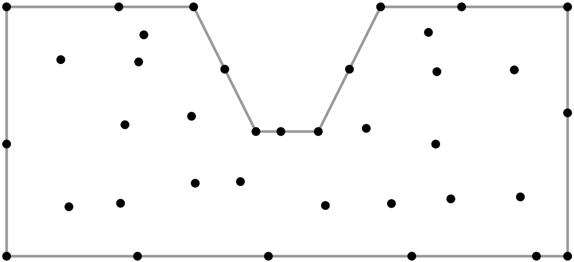
# Restricted Voronoi diagram

- Given a boundary conforming Delaunay discretization of $\Omega$, the *restricted Voronoi diagram* consists of the *restricted Voronoi cells* corresponding to the node set $X$ defined by

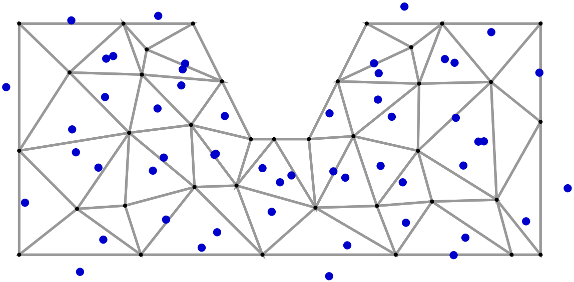
$$\omega_k = V_k \cap \Omega = \{x \in \Omega : ||x - x_k|| < ||x - x_l|| \forall x_l \in X, l \neq k\}$$

- These restricted Voronoi cells are used as control volumes in a finite volume discretization

# Piecewise linear description of computational domain with given point cloud

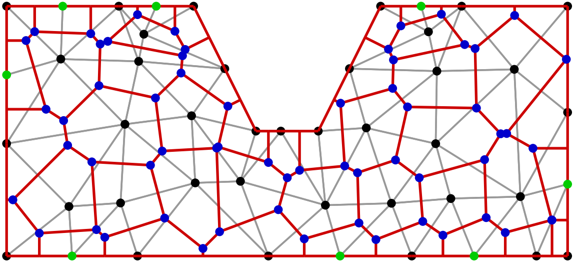


# Delaunay triangulation of domain and triangle circumcenters.



- Blue: triangle circumcenters
- Some boundary triangles have larger than $90^{\circ}$ angles opposite to the boundary $\Rightarrow$ their circumcenters are outside of the domain

# Boundary conforming Delaunay triangulation



- Automatically inserted additional points at the boundary (green dots)
- Restricted Voronoi cells (red).

# General approach to triangulations

- Obtain piecewise linear descriptiom of domain
- Call mesh generator (triangle, TetGen, NetGen ...) in order to obtain triangulation
- Performe finite volume or finite element discretization of the problem.

Alternative way:

- Construction "by hand" on regular structures

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# Partial Differential Equations

# DIfferential operators

- Bounded domain $\Omega \subset \mathbb{R}^d$, with piecewise smooth boundary
- Scalar function $u : \Omega \to \mathbb{R}$
- Vector function $\mathbf{v} : \Omega \to \mathbb{R}^d$
- Write $\partial_i u = \frac{\partial u}{x_i}$
- For a multindex $\alpha = (\alpha_1 \dots \alpha_d)$, write $|\alpha| = \alpha_1 + \dots + \alpha_d$ and define $\partial^\alpha u = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdot \dots \cdot \partial x_d^{\alpha_d}}$
- Gradient $\mathrm{grad} = \nabla$: $u \mapsto \nabla u = \begin{pmatrix} \partial_1 u \\ \vdots \\ \partial_d u \end{pmatrix}$
- Divergence $\mathrm{div} = \nabla \cdot$ : $\mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} \mapsto \nabla \cdot \mathbf{v} = \partial_1 v_1 + \dots + \partial_d v_d$
- Laplace operator $\Delta = \mathrm{div} \cdot \mathrm{grad} = \nabla \cdot \nabla$: $u \mapsto \Delta u = \partial_{11} u + \dots + \partial_{dd} u$

# Matrices from PDE revisited

Given:

- Domain $\Omega = (0, X) \times (0, Y) \subset \mathbb{R}^2$ with boundary $\Gamma = \partial\Omega$, outer normal $\mathbf{n}$
- Right hand side $f : \Omega \to \mathbb{R}$
- "Conductivity" $\lambda$
- Boundary value $v : \Gamma \to \mathbb{R}$
- Transfer coefficient $\alpha$

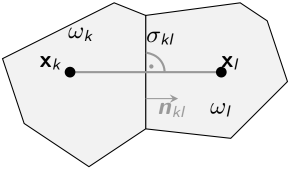
Search function $u : \Omega \to \mathbb{R}$ such that

$$\begin{aligned} -\nabla \cdot \lambda \nabla u &= f \quad \text{in}\Omega \\ -\lambda \nabla u \cdot \mathbf{n} + \alpha(u - v) &= 0 \quad \text{on}\Gamma \end{aligned}$$

- Example: heat conduction:
  - $u$: temperature
  - $f$: volume heat source
  - $\lambda$: heat conduction coefficient
  - $v$: Ambient temperature
  - $\alpha$: Heat transfer coefficient

# The finite volume idea revisited

- Assume $\Omega$ is a polygon
- Subdivide the domain $\Omega$ into a finite number of **control volumes** :
  $\bar{\Omega} = \bigcup_{k\in\mathcal{N}} \bar{\omega}_k$
  such that
  - $\omega_k$ are open (not containing their boundary) convex domains
  - $\omega_k \cap \omega_l = \emptyset$ if $\omega_k \neq \omega_l$
  - $\sigma_{kl} = \bar{\omega}_k \cap \bar{\omega}_l$ are either empty, points or straight lines
    - we will write $|\sigma_{kl}|$ for the length
    - if $|\sigma_{kl}| > 0$ we say that $\omega_k$, $\omega_l$ are neigbours
    - neigbours of $\omega_k$: $\mathcal{N}_k = \{l \in \mathcal{N} : |\sigma_{kl}| > 0\}$
- To each control volume $\omega_k$ assign a **collocation point**: $\mathbf{x}_k \in \bar{\omega}_k$ such that
  - **admissibility condition**: if $l \in \mathcal{N}_k$ then the line $\mathbf{x}_k\mathbf{x}_l$ is orthogonal to $\sigma_{kl}$
  - if $\omega_k$ is situated at the boundary, i.e. $\gamma_k = \partial\omega_k \cap \partial\Omega \neq \emptyset$, then $\mathbf{x}_k \in \partial\Omega$




- Now, we know how to construct this partition
  - obtain a boundary conforming Delaunay triangulation
  - construct restricted Voronoi cells

# Discretization ansatz

- Given control volume $\omega_k$, integrate equation over control volume

$$
\begin{aligned}
0 &= \int_{\omega_k} \left(-\nabla \cdot \lambda \nabla u - f\right) d\omega \\
&= -\int_{\partial\omega_k} \lambda \nabla u \cdot \mathbf{n}_k d\gamma - \int_{\omega_k} f d\omega && \text{(Gauss)} \\
&= -\sum_{L \in \mathcal{N}_k} \int_{\sigma_{kl}} \lambda \nabla u \cdot \mathbf{n}_{kl} d\gamma - \int_{\gamma_k} \lambda \nabla u \cdot \mathbf{n} d\gamma - \int_{\omega_k} f d\omega \\
&\approx \sum_{L \in \mathcal{N}_k} \frac{\sigma_{kl}}{h_{kl}} (u_k - u_l) + |\gamma_k| \alpha (u_k - v_k) - |\omega_k| f_k
\end{aligned}
$$

- Here,
  - $u_k = u(\mathbf{x}_k)$
  - $v_k = v(\mathbf{x}_k)$
  - $f_k = f(\mathbf{x}_k)$

# Solvability of discrete problem

- $N = |\mathcal{N}|$ equations (one for each control volume)
- $N = |\mathcal{N}|$ unknowns (one in each collocation point $\equiv$ control volume)
- Graph of discretzation matrix $\equiv$ edge graph of triangulation $\Rightarrow$ matrix is irreducible
- Matrix is symmetric
- Main diagonal entries are positive, off diagonal entries are non-positive
- The matrix is diagonally dominant
- For positive heat transfer coefficients, the matrix becomes irreducibly diagonally dominant

$\Rightarrow$ the discretization matrix has the $M$-property.

# Note on matrix $M$ property and discretization methods

- Finite volume methods on boundary conforming Delaunay triangulations can be *practically* constructed on large classes of 2D and 3D polygonal domains using *provable* algorithms
  - Results mostly by J. Shewchuk (triangle) and H. Si (TetGen)
- Later we will discuss the finite element method. It has a significantly simpler convergence theory than the finite volume method.
  - For constant heat conduction coefficients, in 2D it yields the same discretization matrix as the finite volume method.
  - However this is *not true* in 3D.
  - Consequence: there is no provable mesh construction algorithm which leads to the $M$-Propertiy of the finite element discretization matrix in 3D.

# Convergence theory

For an excurse into convergence theory, we need to recall a number of concepts from functional analysis.

See e.g. Appendix of the book of Ern/Guermond.

# Lebesgue integral, $L^1(\Omega)$ I

- Let $\Omega$ have a boundary which can be represented by continuous, piecewiese smooth functions in local coordinate systems, without cusps and other+ degeneracies (more precisely: Lipschitz domain).
  - Polygonal domains are Lipschitz.
- Let $C_c(\Omega)$ be the set of continuous functions $f : \Omega \to \mathbb{R}$ with compact support.
- For these functions, the Riemann integral $\int_\Omega f(x)dx$ is well defined, and $||f|| := \int_\Omega |f(x)|dx$ provides a norm, and induces a metric
- 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:

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

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

# Lebesgue integral, $L^1(\Omega)$ II

- Let $L^1(\Omega)$ be the completion of $C_c(\Omega)$ with respect to the metric defined by the integral norm, i.e. "include" all limites of Cauchy sequences
- Defined via sequences, $\int_\Omega |f(x)|dx$ is defined for all functions in $L^1(\Omega)$.
- 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".
- Examples for Lebesgue integrable (measurable) functions:
  - Step functions
  - Bounded functions continuous except in a finite number of points

# Spaces of integrable functions

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

$$\int_\Omega |f(x)|^p dx < \infty$$

equipped with the norm

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

- 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

$$(f, g) = \int_\Omega f(x) g(x) dx.$$

# Green's theorem

- Green's theorem for *smooth* functions: Let $u, v \in C^1(\overline{\Omega})$ (continuously differentiable). Then for $\mathbf{n} = (n_1 \ldots n_d)$ being the outward normal to $\Omega$,

$$\int_\Omega u \partial_i v dx = \int_{\partial\Omega} u v n_i ds - \int_\Omega v \partial_i u dx$$

In particular, if $v = 0$ on $\partial\Omega$ one has

$$\int_\Omega u \partial_i v dx = - \int_\Omega v \partial_i u dx$$

# Weak derivative

- Let $L^1_{loc}(\Omega)$ 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

$$\int_\Omega v \partial_i u dx = -\int_\Omega u \partial_i v dx \quad \forall v \in C_0^\infty(\Omega)$$

and $\partial^\alpha u$ by

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

*if these integrals exist*.

# 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 $C^\infty$ in the norm $||u||_{W^{k,p}(\Omega)}$
- $W_0^{k,p}(\Omega)$ is the completion of $C_0^\infty$ in the norm $||u||_{W^{k,p}(\Omega)}$
- The Sobolev spaces are Banach spaces.

## Fractional Sobolev spaces and traces

- For $0 < s < 1$ define the *fractional Sobolev space*

$$W^{s,p}(\Omega) = \left\{ u \in L^p(\Omega) : \frac{u(x) - u(y)}{||x - y||^{s + \frac{d}{p}}} \in L^p(\Omega \times \Omega) \right\}$$

- Let $H^{\frac{1}{2}}(\Omega) = W^{\frac{1}{2},2}(\Omega)$
- A priori it is hard to say what the value of a function from $L^p$ on the boundary is like.
- For Lipschitz domains there exists unique continuous *trace mapping* $\gamma_0 : W^{1,p}(\Omega) \to L^p(\partial\Omega)$ where $\frac{1}{p} + \frac{1}{p'} = 1$ such that
  - $\mathrm{Im}\gamma_0 = W^{\frac{1}{p'},p}(\partial\Omega)$
  - $\mathrm{Ker}\gamma_0 = W_0^{1,p}(\Omega)$

# Sobolev spaces of square integrable functions

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

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

  is a Hilbert space.
- $H^k(\Omega)_0 = W_0^{k,2}(\Omega)$ with the scalar product

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

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

# Heat conduction revisited: Derivation of weak formulation

- Sobolev space theory provides the necessary framework to formulate existence and uniqueness of solutions of PDEs.
- Heat conduction equation with homogeneous Dirichlet boundary conditions:

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

Multiply and integrate with an arbitrary *test function* from $C_0^\infty(\Omega)$:

$$
\begin{aligned}
-\int_\Omega \nabla \cdot \lambda \nabla u v \, dx &= \int_\Omega f v \, dx \\
\int_\Omega \lambda \nabla u \nabla v \, dx &= \int_\Omega f v \, dx
\end{aligned}
$$

# Weak formulation of homogeneous Dirichlet problem

- Search $u \in H_0^1(\Omega)$ such that

$$\int_\Omega \lambda \nabla u \nabla v \, dx = \int_\Omega fv \, dx \; \forall v \in H_0^1(\Omega)$$

- Then,

$$a(u, v) := \int_\Omega \lambda \nabla u \nabla v \, dx$$

is a self-adjoint bilinear form defined on the Hilbert space $H_0^1(\Omega)$

- $f(v) = \int_\Omega fv \, dx$ 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

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

# Heat conduction revisited

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

$$\int_\Omega \lambda \nabla u \nabla v \, dx = \int_\Omega fv \, dx \; \forall v \in H_0^1(\Omega)$$

has an unique solution.