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Lecture 20

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Nonlinear problems: motivation

- Assume nonlinear dependency of some coefficients of the equation on the solution. E.g. nonlinear diffusion problem

$$
\begin{aligned}
-\nabla(\cdot D(u)\nabla u) &= f \quad \text{in } \Omega \\
u &= u_D \text{on} \partial\Omega
\end{aligned}
$$

- FE+FV discretization methods lead to large nonlinear systems of equations

Nonlinear problems: caution!

This is a significantly more complex world:

- Possibly multiple solution branches
- Weak formulations in L^p spaces
- No direct solution methods
- Narrow domains of definition (e.g. only for positive solutions)

Finite element discretization for nonlinear diffusion

- Find $u_h \in V_h$ such that for all $w_h \in V_h$:

$$\int_\Omega D(u_h)\nabla u_h \cdot \nabla w_h \; dx = \int_\Omega f w_h \; dx$$

- Use appropriate quadrature rules for the nonlinear integrals
- Discrete system

$$A(u_h) = F(u_h)$$

Finite volume discretization for nonlinear diffusion

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

with

$$
g_{kl}(u_k, u_l) = \begin{cases} D(\frac{1}{2}(u_k + u_l))(u_k - u_l) \\ \text{or} \quad \mathcal{D}(u_k) - \mathcal{D}(u_l) \end{cases}
$$

where $\mathcal{D}(u) = \int_0^u D(\xi)\, d\xi$ (exact solution ansatz at discretization edge)

- Discrete system

$$A(u_h) = F(u_h)$$

Iterative solution methods: fixed point iteration

- Let $u \in \mathbb{R}^n$.
- Problem: $A(u) = f$:
- Assume $A(u) = M(u)u$, where for each u, $M(u) : \mathbb{R}^n \to \mathbb{R}^n$ is a linear operator.
- Iteration scheme:

  Choose u_0, $i \leftarrow 0$;
  while *not converged* **do**
      Solve $M(u_i)u_{i+1} = f$;
      $i \leftarrow i + 1$;
  end
- Convergence criteria:
  - residual based: $||A(u) - f|| < \varepsilon$
  - update based $||u_{i+1} - u_i|| < \varepsilon$
- Large domain of convergence
- Convergence may be slow
- Smooth coefficients not necessary

Iterative solution methods: Newton method

- Solve

$$A(u) = \begin{pmatrix} A_1(u_1 \dots u_n) \\ A_2(u_1 \dots u_n) \\ \vdots \\ A_n(u_1 \dots u_n) \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix} = f$$

- Jacobi matrix (Frechet derivative) for given u: $A'(u) = (a_{kl})$ with

$$a_{kl} = \frac{\partial}{\partial u_l} A_k(u_1 \dots u_n)$$

- Iteration scheme:

Choose u_0, $i \leftarrow 0$;
while *not converged* **do**
  Calculate residual $r_i = A(u_i) - f$;
  Calculate Jacobi matrix $A'(u_i)$;
  Solve update problem $A'(u_i)h_i = r_i$;
  Update solution: $u_{i+1} = u_i - h_i$;
  $i \leftarrow i + 1$;
end

Newton method II

- Convergence criteria: - residual based: $||r_i|| < \varepsilon$ - update based $||h_i|| < \varepsilon$
- Limited domain of convergence
- Slow initial convergence
- Fast (quadratic) convergence close to solution

Damped Newton method

- Remedy for small domain of convergence: damping

  Choose u_0, $i \leftarrow 0$, damping parameter $d < 1$;
  while *not converged* **do**
  Calculate residual $r_i = A(u_i) - f$;
  Calculate Jacobi matrix $A'(u_i)$;
  Solve update problem $A'(u_i)h_i = r_i$;
  Update solution: $u_{i+1} = u_i - dh_i$;
  $i \leftarrow i + 1$;
  end

- Damping slows convergence down from quadratic to linear
- Better way: increase damping parameter during iteration:

  Choose u_0, $i \leftarrow 0$,damping $d < 1$, growth factor $\delta > 1$;
  while *not converged* **do**
  Calculate residual $r_i = A(u_i) - f$;
  Calculate Jacobi matrix $A'(u_i)$;
  Solve update problem $A'(u_i)h_i = r_i$;
  Update solution: $u_{i+1} = u_i - dh_i$;
  Update damping parameter: $d_{i+1} = \min(1, \delta d_i)$;
  $i \leftarrow i + 1$;
  end

Newton method: further issues

- Even if it converges, in each iteration step we have to solve linear system of equations
  - Can be done iteratively, e.g. with the LU factorization of the Jacobi matrix from first solution step
  - Iterative solution accuracy my be relaxed, but this may diminuish quadratic convergence
- Quadratic convergence yields very accurate solution with no large additional effort: once we are in the quadratic convergence region, convergence is very fast
- Monotonicity test: check if residual grows, this is often an sign that the iteration will diverge anyway.

Newton method: embedding

- Embedding method for parameter dependent problems.
- Solve $A(u_\lambda, \lambda) = f$ for $\lambda = 1$.
- Assume $A(u_0, 0)$ can be easily solved.
- Parameter embedding method:

  Solve $A(u_0, 0) = f$;
  Choose initial step size δ;
  Set $\lambda = 0$;
  while $\lambda < 1$ **do**
      Solve $A(u_{\lambda+\delta}, \lambda + \delta) = 0$ with initial value1 u_λ;
      $\lambda \leftarrow \lambda + \delta$;
  end

- Possibly decrease stepsize if Newton's method does not converge, increase it later
- Parameter embedding + damping + update based convergence control go a long way to solve even strongly nonlinear problems!

Inhomogeneous Dirichlet problem: strong formulation

$$-\nabla \cdot \lambda \nabla u = f \text{ in } \Omega$$
$$u = g \text{ on } \partial\Omega$$

- What can we say about minimum and maximum of the solution ?
- u has local local extremum in $x_0 \in \Omega$ if
  - x_0 is a critical point: $\nabla_u|_{x_0} = 0$
  - The matrix of second derivatives in x_0 is definite
  - This is linked to the sign of the right hand side: if $f = 0$ the main diagonal entries have different signs (as their sum is zero), so perhaps we would get a saddle point

Inhomogeneous Dirichlet problem: weak formulation

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

$$u = u_g + \phi$$

$$\int_\Omega \lambda \nabla \phi \nabla v \, d\mathbf{x} = \int_\Omega f v \, d\mathbf{x} - \int_\Omega \lambda \nabla u_g \nabla v \quad \forall v \in H^1_0(\Omega)$$

Here, necessarily, $\phi \in H^1_0(\Omega)$ and we can apply the theory for the homogeneous Dirichlet problem.

- if u is a solution, we also have

$$\int_\Omega \lambda \nabla u \nabla v \, d\mathbf{x} = \int_\Omega f v \, d\mathbf{x} \quad \forall v \in H^1_0(\Omega)$$

as we can add $\int_\Omega \lambda \nabla u_g \nabla v$ on left and right side

Inhomogeneous Dirichlet problem: minimum principle

- Let $f \geq 0$.
- Let $g^\flat = \inf_{\partial\Omega} g$.
- Let $w = (u - g^\flat)^- = \min\{u - g^\flat, 0\} \in H_0^1(\Omega)$
- Consequently, $w \leq 0$
- As $\nabla u = \nabla(u - g^\flat)$ and $\nabla w = 0$ where $w \neq u - g^\flat$, one has

$$0 \geq \int_\Omega fw \, d\mathbf{x} = \int_\Omega \lambda \nabla u \nabla w \, d\mathbf{x}$$
$$= \int_\Omega \lambda \nabla w \nabla w \, d\mathbf{x} \geq 0$$

- Therefore: $(u - g^\flat)^- = 0$ and $u \geq g^\flat$

Inhomogeneous Dirichlet problem: maximum principle

- Let $f \leq 0$.
- Let $g^\sharp = \sup_{\partial\Omega} g$.
- Let $w = (u - g^\sharp)^+ = \max\{u - g^\sharp, 0\} \in H_0^1(\Omega)$
- Consequently, $w \geq 0$
- As $\nabla u = \nabla(u - g^\sharp)$ and $\nabla w = 0$ where $w \neq u - g^\sharp$, one has

$$
\begin{aligned}
0 \geq \int_\Omega fw \, d\mathbf{x} &= \int_\Omega \lambda \nabla u \nabla w \, d\mathbf{x} \\
&= \int_\Omega \lambda \nabla w \nabla w \, d\mathbf{x} \geq 0
\end{aligned}
$$

- Therefore: $(u - g^\sharp)^- = 0$ and $u \leq g^\sharp$

Inhomogeneous Dirichlet problem: minmax principle

Theorem: The weak solution of the inhomogeneous Dirichlet problem

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

fulfills the global minimax principle: it attains its maximum at the boundary if $f \leq 0$ and attains its minimum at the boundary if $f \geq 0$.

Corollary: If $f = 0$ then u attains both its minimum and its maximum at the boundary.

Corolloary: Local minimax principle: This is true of any subdomain $\omega \subset \Omega$.

Convection-Diffusion problem

Green's theorem: If $w = 0$ on $\partial\Omega$:

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

Let $\nabla \cdot \mathbf{v} = 0$. Search function $u : \Omega \to \mathbb{R}$ such that

$$\begin{aligned} -\nabla \cdot (D\nabla u - u\mathbf{v}) &= f \quad \text{in } \Omega \\ u &= g \quad \text{on } \partial\Omega \end{aligned}$$

From weak formulation (with Dirichlet lifting trick):

$$\int_\Omega (D\nabla u - u\mathbf{v}) \cdot \nabla w \, d\mathbf{x} = \int_\Omega f w \, d\mathbf{x} \quad \forall w \in H_0^1(\Omega)$$

Coercivity of bilinear form

Regard the convection contribution to the coercivity estimate:

$$
\begin{aligned}
-\int_\Omega u\mathbf{v}\cdot\nabla u\,d\mathbf{x} &= \int u\nabla\cdot(u\mathbf{v})\,d\mathbf{x} \quad \text{Green's theorem}\\
\int_\Omega u^2\nabla\cdot\mathbf{v}\,d\mathbf{x} + \int_\Omega u\mathbf{v}\cdot\nabla u\,d\mathbf{x} &= \int u\nabla\cdot(u\mathbf{v})\,d\mathbf{x} \quad \text{Product rule}\\
\int_\Omega u^2\nabla\cdot\mathbf{v}\,d\mathbf{x} + 2\int_\Omega u\mathbf{v}\cdot\nabla u\,d\mathbf{x} &= 0 \quad \text{Equation difference}\\
\int_\Omega u\mathbf{v}\cdot\nabla u\,d\mathbf{x} &= 0 \quad \text{Divergence condition}\nabla\cdot\mathbf{v}=0
\end{aligned}
$$

Then

$$
\int_\Omega (D\nabla u - u\mathbf{v})\cdot\nabla u\,d\mathbf{x} = \int_\Omega D\nabla u\cdot\nabla u\,d\mathbf{x} \geq C||u||_{H_0^1(\Omega)}
$$

One could allow for fixed sign of $\nabla\cdot\mathbf{v}$.

Convection diffusion problem: maximum principle

- Let $f \leq 0$, $\nabla \cdot \mathbf{v} = 0$
- Let $g^\sharp = \sup_{\partial\Omega} g$.
- Let $w = (u - g^\sharp)^+ = \max\{u - g^\sharp, 0\} \in H_0^1(\Omega)$
- Consequently, $w \geq 0$
- As $\nabla u = \nabla(u - g^\sharp)$ and $\nabla w = 0$ where $w \neq u - g^\sharp$, one has

$$
\begin{aligned}
0 \geq \int_\Omega f w \, d\mathbf{x} &= \int_\Omega D(\nabla u - u\mathbf{v})\nabla w \, d\mathbf{x} \\
&= \int_\Omega D(\nabla w - w\mathbf{v})\nabla w \, d\mathbf{x} - Dg^\sharp \int_\Omega \mathbf{v} \cdot \nabla w \, d\mathbf{x} \\
&= \int_\Omega D\nabla w \cdot \nabla w \, d\mathbf{x} + Dg^\sharp \int_\Omega w \nabla \cdot \mathbf{v} \, d\mathbf{x} \\
&\geq C||w||_{H_0^1(\Omega)}
\end{aligned}
$$

- Therefore: $w = (u - g^\sharp)^- = 0$ and $u \leq g^\sharp$
- Similar for minimum part

Mimimax for convection-diffusion

Theorem: If $\nabla \cdot \mathbf{v} = 0$, the weak solution of the inhomogeneous Dirichlet problem

$$\begin{aligned} -\nabla \cdot (D\nabla u - u\mathbf{v}) &= f \quad \text{in } \Omega \\ u &= g \quad \text{on } \partial\Omega \end{aligned}$$

fulfills the global minimax principle: it attains its maximum at the boundary if $f \leq 0$ and attains its minimum at the boundary if $f \geq 0$.

Corollary: If $f = 0$ then u attains both its minimum and its maximum at the boundary.

Corolloary: Local minimax principle: This is true of any subdomain $\omega \subset \Omega$.

Interpretation of minimax principle

- Positive right hand side $\Rightarrow$ "production" of heat, matter ...
- No local minimum in the interior of domain if matter is produced.
- Also, positivity/nonnegativity of solutions if boundary conditions are positive/nonnegative
- Negative right hand side $\Rightarrow$ "consumption" of heat, matter ...
- No local maximum in the interior of domain if matter is consumed.
- Basic physical principle !

Discrete minimax principle

- $Au = f$
- A: matrix from diffusion or convection- diffusion
- A irreducibly diagonally dominant, positive main diagonal entries, negative off diagonal entries

$$a_{ii}u_i = \sum_{j\neq i} -a_{ij}u_j + f_i$$

$$u_i = \sum_{j\neq i, a_{ij}\neq 0} -\frac{a_{ij}}{a_{ii}}u_j + f_i$$

- For interior points,, $a_{ii} = -\sum_{j\neq i} a_{ij}$
- Assume i is interior point. Assume $f_i \geq 0 \Rightarrow$

$$u_i \geq \min_{j\neq i, a_{ij}\neq 0} u_j \sum_{j\neq i, a_{ij}\neq 0} -\frac{a_{ij}}{a_{ii}} = \min_{j\neq i, a_{ij}\neq 0} u_j$$

- Assume i is interior point. Assume $f_i \leq 0 \Rightarrow$

$$u_i \leq \max_{j\neq i, a_{ij}\neq 0} u_j \sum_{j\neq i, a_{ij}\neq 0} -\frac{a_{ij}}{a_{ii}} = \max_{j\neq i, a_{ij}\neq 0} u_j$$

Discussion of discrete minimax principle I

- P1 finite elements, Voronoi finite volumes: matrix graph $\equiv$ triangulation of domain
- The set $\{j \neq i, a_{ij} \neq 0\}$ is exactly the set of neigbor nodes
- Solution in point x_i estimated by solution in neigborhood
- The estimate can be propagated to the boundary of the domain

Discussion of discrete minimax principle II

- Minimax principle + positivity/nonnegativity of solutions can be seen as an important qualitative property of the physical process
- Along with good approximation quality, its preservation in the discretization process may be necessary
- Guaranteed for irreducibly diagonally dominant matrices
- Nonnegativity for nonnegative right hand sides guaranteed by M-Property
- Finite volume method may be preferred as it can guarantee these properties for boundary conforming Delaunay grids.

Convection-diffusion and finite elements

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

$$-\nabla(\cdot D\nabla u - u\mathbf{v}) = f \quad \text{in } \Omega$$
$$u = u_D \quad \text{on } \partial\Omega$$

- Assume v is divergence-free, i.e. $\nabla \cdot v = 0$.
- Then the main part of the equation can be reformulated as

  $$-\nabla(\cdot D\nabla u) + v \cdot \nabla u = 0 \quad \text{in } \Omega$$

  yielding a weak formulation: find $u \in H^1(\Omega)$ such that $u - u_D \in H_0^1(\Omega)$ and $\forall w \in H_0^1(\Omega)$,

  $$\int_\Omega D\nabla u \cdot \nabla w \; dx + \int_\Omega \mathbf{v} \cdot \nabla u \; w \; dx = \int_\Omega fw \; dx$$

- Galerkin formulation: find $u_h \in V_h$ with bc. such that $\forall w_h \in V_h$

  $$\int_\Omega D\nabla u_h \cdot \nabla w_h \; dx + \int_\Omega \mathbf{v} \cdot \nabla u_h \; w_h \; dx = \int_\Omega fw_h \; dx$$

Convection-diffusion and finite elements II

- Galerkin ansatz has similar problems as central difference ansatz in the finite volume/finite difference case $\Rightarrow$ stabilization ?
- Most popular: streamline upwind Petrov-Galerkin

$$\int_\Omega D\nabla u_h \cdot \nabla w_h \; dx + \int_\Omega \mathbf{v} \cdot \nabla u_h \; w_h \; dx + S(u_h, w_h) = \int_\Omega f w_h \; dx$$

with

$$S(u_h, w_h) = \sum_K \int_K (-\nabla(\cdot D\nabla u_h - u_h \mathbf{v}) - f)\delta_K v \cdot w_h \; dx$$

where $\delta_K = \frac{h_K^v}{2|\mathbf{v}|}\xi(\frac{|\mathbf{v}|h_K^v}{D})$ with $\xi(\alpha) = coth(\alpha) - \frac{1}{\alpha}$ and h_K^v is the size of element K in the direction of $\mathbf{v}$.

Convection-diffusion and finite elements III

- Many methods to stabilize, *none* guarantees M-Property even on weakly acute meshes ! (V. John, P. Knobloch, Computer Methods in Applied Mechanics and Engineering, 2007)
- Comparison paper:

  M. Augustin, A. Caiazzo, A. Fiebach, J. Fuhrmann, V. John, A. Linke, and R. Umla, "An assessment of discretizations for convection-dominated convection-diffusion equations," Comp. Meth. Appl. Mech. Engrg., vol. 200, pp. 3395–3409, 2011:

  - if it is necessary to compute solutions without spurious oscillations: use FVM, taking care on the construction of an appropriate grid might be essential for reducing the smearing of the layers,
  - if sharpness and position of layers are important and spurious oscillations can be tolerated: often the SUPG method is a good choice.

- Topic of ongoing research