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Convection-Diffusion + Nonlinearities

Scientific Computing Winter 2016/2017

Lecture 24

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Examination dates

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20.2.
21.2. > 14:00
22.2.
24.2.

6.3.
7.3. >14:00
8.3. >14:00
9.3
13.3.
14.3.
15.3.
20.3.-24.3.
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Recap

Time dependent Robin boundary value problem

- Choose final time $T > 0$. Regard functions $(x, t) \to \mathbb{R}$.

$$
\begin{aligned}
\partial_t u - \nabla \cdot \kappa \nabla u &= f \quad \text{in } \Omega \times [0, T] \\
\kappa \nabla u \cdot \vec{n} + \alpha(u - g) &= 0 \quad \text{on } \partial\Omega \times [0, T] \\
u(x, 0) &= u_0(x) \quad \text{in}\Omega
\end{aligned}
$$

- This is an initial boundary value problem
- This problem has a weak formulation in the Sobolev space $L^2\left([0, T], H^1(\Omega)\right)$, which then allows for a Galerkin approximation in a corresponding subspace
- We will proceed in a simpler manner: first, perform a finite difference discretization in time, then perform a finite element (finite volume) discretization in space.
  - Rothe method: first discretize in time, then in space
  - Method of lines: first discretize in space, get a huge ODE system

Time discretization

- Choose time discretization points $0 = t_0 < t_1 \cdots < t_N = T$, let
  $\tau_i = t_i - t_{i-1}$
  For $i = 1 \dots N$, solve

$$\begin{aligned}
\frac{u_i - u_{i-1}}{\tau_i} - \nabla \cdot \kappa \nabla u_\theta = f \quad & \text{in } \Omega \times [0, T] \\
\kappa \nabla u_\theta \cdot \vec{n} + \alpha(u_\theta - g) = 0 \quad & \text{on } \partial\Omega \times [0, T]
\end{aligned}$$

  where $u_\theta = \theta u_i + (1 - \theta) u_{i-1}$
- $\theta = 1$: backward (implicit) Euler method
- $\theta = \frac{1}{2}$: Crank-Nicolson scheme
- $\theta = 0$: forward (explicit) Euler method
- Note that the explicit Euler method does not involve the solution of a PDE system. What do we have to pay for this ?

Weak formulation

- Weak formulation: search $u \in H^1(\Omega)$ such that

$$\frac{1}{\tau_i}\int_\Omega u_i v\, dx + \theta\left(\int_\Omega \kappa \nabla u_i \nabla v\, dx + \int_{\partial\Omega} \alpha u_i v\, ds\right) =$$
$$\frac{1}{\tau_i}\int_\Omega u_{i-1} v\, dx + (1-\theta)\left(\int_\Omega \kappa \nabla u_{i-1} \nabla v\, dx + \int_{\partial\Omega} \alpha u_{i-1} v\, ds\right)$$
$$+ \int_\Omega f v\, dx + \int_{\partial\Omega} \alpha g v\, ds \;\forall v \in H^1(\Omega)$$

- Matrix formulation (in case of constant coefficents, $A_i = A$)

$$\frac{1}{\tau_i} M u_i + \theta A_i u_i = \frac{1}{\tau_i} M u_{i-1} + (1-\theta) A_i u_{i-1} + F$$

- M: mass matrix, A: stiffness matrix

Mass matrix

- Mass matrix $M = (m_{ij})$:

$$m_{ij} = \int_\Omega \phi_i \phi_j \, dx$$

- Self-adjoint, coercive bilinear form $\Rightarrow$ M is symmetric, positiv definite
- For a family of quasi-uniform, shape-regular triangulations the condition number $\kappa(M)$ is bounded by a constant independent of h:

$$\kappa(M) \leq c$$

Mass matrix M-Property ?

- For P^1-finite elements, all integrals $m_{ij} = \int_\Omega \phi_i \phi_j \, dx$ are zero or positive, so we get positive off diagonal elements.
- No M-Property!

Stiffness matrix condition number + row sums

- Stiffness matrix $A = (a_{ij})$:

$$a_{ij} = a(\phi_i, \phi_j) = \int_\Omega \nabla\phi_i \nabla\phi_j \; dx$$

- bilinear form $a(\cdot, \cdot)$ is self-adjoint, therefore A is symmetric, positive definite
- Condition number estimate for P^1 finite elements on quasi-uniform triangulation:

$$\kappa(A) \leq ch^{-2}$$

- Row sums:

$$\begin{aligned}\sum_{j=1}^{N} a_{ij} &= \sum_{j=1}^{N} \int_\Omega \nabla\phi_i \nabla\phi_j \; dx = \int_\Omega \nabla\phi_i \nabla \left(\sum_{j=1}^{N} \phi_j \right) \; dx \\ &= \int_\Omega \nabla\phi_i \nabla (1) \; dx \\ &= 0\end{aligned}$$

Stiffness matrix entry signs

Local stiffness matrices

$$s_{ij} = \int_K \nabla\lambda_i \nabla\lambda_j \; dx = \frac{|K|}{2|K|^2} \left(y_{i+1} - y_{i+2}, x_{i+2} - x_{i+1}\right) \begin{pmatrix} y_{j+1} - y_{j+2} \\ x_{j+2} - x_{j+1} \end{pmatrix}$$

- Main diagonal entries must be positive
- Local contributions from element stiffness matrices: Scalar products of vectors orthogonal to edges. These are nonpositive if the angle between the edges are $\leq 90^\circ$
- *weakly acute triangulation*: all triangle angles are less than $\leq 90^\circ$
- in fact, for constant coefficients, in *2D*, Delaunay is sufficient!
- All rows sums are zero $\Rightarrow$ A is singular
- Matrix becomes irreducibly diagonally dominant if we add at least one positive value to the main diagonal, e.g. from Dirichlet BC or *lumped* mass matrix $\Rightarrow M - Matrix$
- Adding a mass matrix yields a positive definite matrix and thus nonsingularity, but *destroys* M-property

Back to time dependent problem

Assume M diagonal, $A = S + D$, where S is the stiffness matrix, and D is a nonnegative diagonal matrix. We have

$$
\begin{aligned}
(Su)_i = \sum_j s_{ij} u_j &= s_{ii} u_i + \sum_{i \neq j} s_{ij} u_j \\
&= (-\sum_{i \neq j} s_{ij}) u_i + \sum_{i \neq j} s_{ij} u_j \\
&= \sum_{i \neq j} -s_{ij}(u_i - u_j)
\end{aligned}
$$

Forward Euler

$$\frac{1}{\tau_i} M u_i = \frac{1}{\tau_i} M u_{i-1} + A_i u_{i-1}$$

$$u_i = u_{i-1} + \tau_i M^{-1} A_i u_{i-1} = (I + \tau M^{-1} D + \tau M^{-1} S) u_{i-1}$$

- Entries of $\tau M^{-1} A) u_{i-1}$ are of order $\frac{1}{h^2}$, and so we can expect stabilityonly if τ balances $\frac{1}{h^2}$, i.e.
$$\tau \leq Ch^2$$
- A more thorough stability estimate proves this situation

Backward Euler

$$\begin{aligned}
\frac{1}{\tau_i} M u_i + A u_i &= \frac{1}{\tau_i} M u_{i-1} \\
(I + \tau_i M^{-1} A) u_i &= u_{i-1} \\
u_i &= (I + \tau_i M^{-1} A)^{-1} u_{i-1}
\end{aligned}$$

But here, we can estimate that

$$||(I + \tau_i M^{-1} A)^{-1}||_\infty \leq 1$$

- We get this stability independent of the time step.
- Another theory is possible using L^2 estimates and positive definiteness

Discrete maximum principle

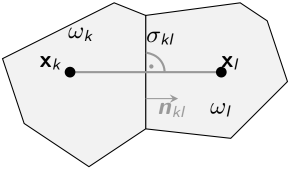
Assuming $v \geq 0$ we can conclude $u \geq 0$.

$$
\begin{aligned}
\frac{1}{\tau} Mu + (D+S)u &= \frac{1}{\tau} Mv \\
(\tau m_i + d_i)u_i + s_{ii} u_i &= \tau m_i v_i + \sum_{i \neq j} (-s_{ij}) u_j \\
u_i &= \frac{1}{\tau m_i + d_i + \sum_{i \neq j}(-s_{ij})} (\tau m_i v_i + \sum_{i \neq j} (-s_{ij}) u_j) \\
&\leq \frac{\tau m_i v_i + \sum_{i \neq j}(-s_{ij}) u_j}{\tau m_i + d_i + \sum_{i \neq j}(-s_{ij})} \max(\{v_i\} \cup \{u_j\}_{j \neq i}) \\
&\leq \max(\{v_i\} \cup \{u_j\}_{j \neq i})
\end{aligned}
$$

- Provided, the right hand side is zero, the solution in a given node is bounded by the value from the old timestep, and by the solution in the neigboring points.
- No new local maxima can appear during time evolution
- There is a continuous counterpart which can be derived from weak solution
- M-property is crucial for the proof.

The finite volume idea revisited

- Assume Ω is a polygon
- Subdivide the domain Ω into a finite number of **control volumes** :
  $\bar{\Omega} = \bigcup_{k \in \mathcal{N}} \bar{\omega}_k$
  such that
  - ω_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 ω_k, ω_l are neigbours
    - neigbours of ω_k: $\mathcal{N}_k = \{l \in \mathcal{N} : |\sigma_{kl}| > 0\}$
- To each control volume ω_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 σ_{kl}
  - if ω_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

Finite volumes for time dependent problem

Search function $u : \Omega \times [0, T] \to \mathbb{R}$ such that $u(x, 0) = u_0(x)$ and

$$\partial_t u - \nabla \cdot \lambda \nabla u = 0 \quad \text{in}\Omega \times [0, T]$$
$$\lambda \nabla u \cdot \mathbf{n} + \alpha(u - w) = 0 \quad \text{on}\Gamma \times [0, T]$$

- Given control volume ω_k, integrate equation over space-time control volume

$$0 = \int_{\omega_k} \left(\frac{1}{\tau}(u - v) - \nabla \cdot \lambda \nabla u \right) d\omega = - \int_{\partial \omega_k} \lambda \nabla u \cdot \mathbf{n}_k d\gamma + \frac{1}{\tau} \int_{\omega_k} (u - v) d\omega$$
$$= - \sum_{L \in \mathcal{N}_k} \int_{\sigma_{kl}} \lambda \nabla u \cdot \mathbf{n}_{kl} d\gamma - \int_{\gamma_k} \lambda \nabla u \cdot \mathbf{n} d\gamma - \frac{1}{\tau} \int_{\omega_k} (u - v) d\omega$$
$$\approx \frac{|\omega_k|}{\tau}(u_k - v_k) + \sum_{L \in \mathcal{N}_k} \frac{|\sigma_{kl}|}{h_{kl}}(u_k - u_l) + |\gamma_k|\alpha(u_k - w_k)$$

- Here, $u_k = u(\mathbf{x}_k)$, $w_k = w(\mathbf{x}_k)$, $f_k = f(\mathbf{x}_k)$
- $\frac{1}{\tau_i} M u_i + A u_i = \frac{1}{\tau_i} M u_{i-1}$

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Convection-Diffusion

The convection - diffusion equation

Search function $u : \Omega \times [0, T] \to \mathbb{R}$ such that $u(x, 0) = u_0(x)$ and

$$\begin{aligned} \partial_t u - \nabla(\cdot D \nabla u - u\mathbf{v}) &= 0 \quad \text{in}\Omega \times [0, T] \\ (D\nabla u - u\mathbf{v})n + \alpha(u - w) &= 0 \quad \text{on}\Gamma \times [0, T] \end{aligned}$$

- Here:
  - u: species concentration
  - D: diffusion coefficient
  - $\mathbf{v}$: velocity of medium (e.g. fluid)

$$\frac{|\omega_k|}{\tau}(u_k - v_k) + \sum_{L \in \mathcal{N}_k} \frac{|\sigma_{kl}|}{h_{kl}} g_{kl}(u_k, u_l) + |\gamma_k| \alpha(u_k - w_k) = f_k$$

Let $v_{kl} = \frac{1}{|\sigma_{kl}|} \int \sigma_{kl} \mathbf{v} \cdot \mathbf{n}_{kl} d\gamma$

Finite volumes for convection - diffusion II

- Central difference flux:

$$\begin{aligned} g_{kl}(u_k, u_l) &= D(u_k - u_l) - h_{kl}\frac{1}{2}(u_k + u_l)v_{kl} \\ &= (D - \frac{1}{2}h_{kl}v_{kl})u_k - (D + \frac{1}{2}h_{kl}v_{kl})xu_l \end{aligned}$$

  - M-Property (sign pattern) only guaranteed for $h \to 0$!
- Upwind flux:

$$\begin{aligned} g_{kl}(u_k, u_l) &= D(u_k - u_l) + \begin{cases} h_{kl}u_k v_{kl}, & v_{kl} < 0 \\ h_{kl}u_l v_{kl}, & v_{kl} > 0 \end{cases} \\ &= (D + \tilde{D})(u_k - u_l) - h_{kl}\frac{1}{2}(u_k + u_l)v_{kl} \end{aligned}$$

  - M-Property guaranteed unconditonally !
  - Artificial diffusion $\tilde{D} = \frac{1}{2}h_{kl}|v_{kl}|$

Finite volumes for convection - diffusion: exponential fitting

Project equation onto edge $x_K x_L$ of length $h = h_{kl}$, integrate once - $q = -v_{kl}$

$$
\begin{aligned}
c' + cq &= j \\
c|_0 &= c_K \\
c|_h &= c_L
\end{aligned}
$$

Solution of the homogeneus problem:

$$
\begin{aligned}
c' &= -cq \\
c'/c &= -q \\
\ln c &= c_0 - qx \\
c &= K \exp(-qx)
\end{aligned}
$$

Exponential fitting II

Solution of the inhomogeneous problem: set $K = K(x)$:

$$
\begin{aligned}
K' \exp(-qx) - qK \exp(-qx) + qK \exp(-qx) &= j \\
K' &= j \exp(qx) \\
K &= K_0 + \frac{1}{q} j \exp(qx)
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
c &= K_0 \exp(-qx) + \frac{1}{q} j \\
c_K &= K_0 + \frac{1}{q} j \\
c_L &= K_0 \exp(-qh) + \frac{1}{q} j
\end{aligned}
$$

Exponential fitting III

Use boundary conditions

$$
\begin{aligned}
K_0 =& \frac{c_K - c_L}{1 - \exp(-qh)} \\
c_K =& \frac{c_K - c_L}{1 - \exp(-qh)} + \frac{1}{q} j \\
j =& q c_K - \frac{q}{1 - \exp(-qh)}(c_K - c_L) \\
=& q(1 - \frac{1}{1 - \exp(-qh)}) c_K - \frac{q}{\exp(-qh) - 1} c_L \\
=& q(\frac{-\exp(-qh)}{1 - \exp(-qh)}) c_K - \frac{q}{\exp(-qh) - 1} c_L \\
=& \frac{-q}{\exp(qh) - 1} c_K - \frac{q}{\exp(-qh) - 1} c_L \\
=& \frac{B(-qh) c_L - B(qh) c_K}{h}
\end{aligned}
$$

where $B(\xi) = \frac{\xi}{\exp(\xi) - 1}$: Bernoulli function

Exponential fitting IV

- Upwind flux:

$$g_{kl}(u_k, u_l) = D(B(\frac{v_{kl}h_{kl}}{D})u_k - B(\frac{-v_{kl}h_{kl}}{D})u_l)$$

- Allen+Southwell 1955
- Scharfetter+Gummel 1969
- Ilin 1969
- Chang+Cooper 1970
- Guaranteed M property!

Exponential fitting: Artificial diffusion

- Difference of exponential fitting scheme and central scheme
- Use: $B(-x) = B(x) + x \Rightarrow$

$$B(x) + \frac{1}{2}x = B(-x) - \frac{1}{2}x = B(|x|) + \frac{1}{2}|x|$$

$$\begin{aligned}
D_{art}(u_k - u_l) =& D(B(\frac{vh}{D})u_k - B(\frac{-vh}{D})u_l) - D(u_k - u_l) + h\frac{1}{2}(u_k + u_l)v \\
=& D(\frac{vh}{2D} + B(\frac{vh}{D}))u_k - D(\frac{-vh}{2D} + B(\frac{-vh}{D})u_l) - D(u_k - u_l) \\
=& D(\frac{1}{2}|\frac{vh}{D}| + B(|\frac{vh}{D}|) - 1)(u_k - u_l)
\end{aligned}$$

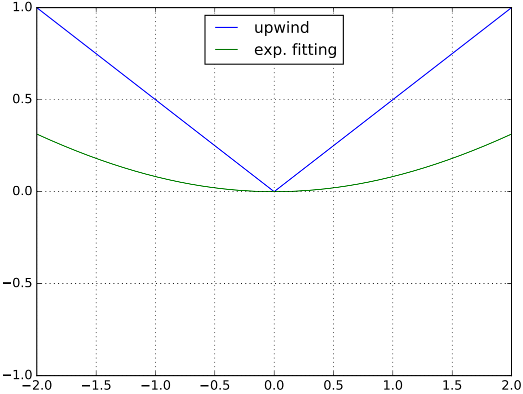
- Further, for $x > 0$:

$$\frac{1}{2}x \geq \frac{1}{2}x + B(x) - 1 \geq 0$$

- Therefore

$$\frac{|vh|}{2} \geq D_{art} \geq 0$$

Exponential fitting: Artificial diffusion II



Comparison of artificial diffusion functions $\frac{1}{2}|x|$ (upwind) and $\frac{1}{2}|x| + B(|x|) - 1$ (exp. fitting)

Convection-Diffusion implementation: central differences

```
F=0;
U=0;
for (int k=0, l=1;k<n-1;k++,l++)
{
  double g_kl=D - 0.5*(v*h);
  double g_lk=D + 0.5*(v*h);
  M(k,k)+=g_kl/h;
  M(k,l)-=g_kl/h;
  M(l,l)+=g_lk/h;
  M(l,k)-=g_lk/h;
}
M(0,0)+=1.0e30;
M(n-1,n-1)+=1.0e30;
F(n-1)=1.0e30;
```

Convection-Diffusion implementation: upwind scheme

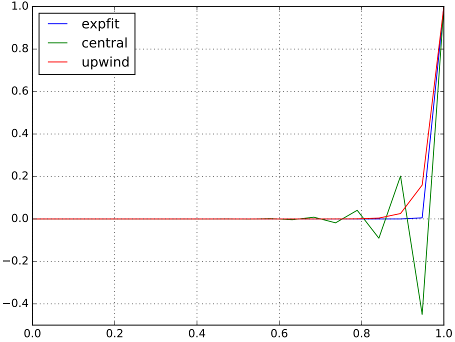
```
F=0;
U=0;
for (int k=0, l=1;k<n-1;k++,l++)
{
  double g_kl=D;
  double g_lk=D;
  if (v<0) g_kl-=v*h;
  else  g_lk+=v*h;

  M(k,k)+=g_kl/h;
  M(k,l)-=g_kl/h;
  M(l,l)+=g_lk/h;
  M(l,k)-=g_lk/h;
}

M(0,0)+=1.0e30;
M(n-1,n-1)+=1.0e30;
F(n-1)=1.0e30;
```

Convection-Diffusion implementation: exponential fitting scheme

```
  inline double B(double x)
  {
    if (std::fabs(x)<1.0e-10) return 1.0;
    return x/(std::exp(x)-1.0);
  }

...

    F=0;
    U=0;
    for (int k=0, l=1;k<n-1;k++,l++)
    {
      double g_kl=D* B(v*h/D);
      double g_lk=D* B(-v*h/D);
      M(k,k)+=g_kl/h;
      M(k,l)-=g_kl/h;
      M(l,l)+=g_lk/h;
      M(l,k)-=g_lk/h;
    }

    M(0,0)+=1.0e30;
    M(n-1,n-1)+=1.0e30;
    F(n-1)=1.0e30;
```

Convection-Diffusion test problem, N=20

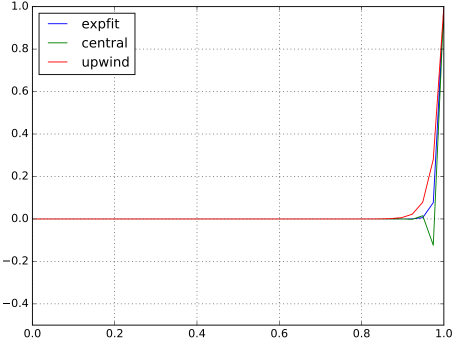
- $\Omega = (0,1)$, $-\nabla \cdot (D\nabla u + uv) = 0$, $u(0) = 0$, $u(1) = 1$
- $V = 1$, $D = 0.01$



- Exponential fitting: sharp boundary layer, for this problem it is exact
- Central differences: unphysical
- Upwind: larger boundary layer

Convection-Diffusion test problem, N=40

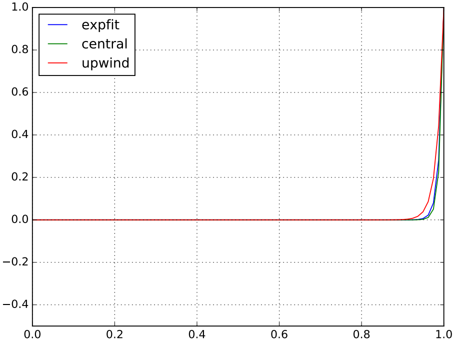
- $\Omega = (0,1)$, $-\nabla \cdot (D\nabla u + uv) = 0$, $u(0) = 0$, $u(1) = 1$
- $V = 1$, $D = 0.01$



- Exponential fitting: sharp boundary layer, for this problem it is exact
- Central differences: unphysical, but less ''wiggles"
- Upwind: larger boundary layer

Convection-Diffusion test problem, N=80

- $\Omega = (0,1)$, $-\nabla \cdot (D\nabla u + uv) = 0$, $u(0) = 0$, $u(1) = 1$
- $V = 1$, $D = 0.01$



- Exponential fitting: sharp boundary layer, for this problem it is exact
- Central differences: grid is fine enough to yield M-Matrix property, good approximation of boundary layer due to higher convergence order
- Upwind: "smearing" of boundary layer

1D convection diffusion summary

- upwinding and exponential fitting unconditionally yield the M-property of the discretization matrix
- exponential fitting for this case (zero right hand side, 1D) yields exact solution. It is anyway "less diffusive" as artificial diffusion is optimized
- central scheme has higher convergence order than upwind (and exponential fitting) but on coarse grid it may lead to unphysical oscillations
- for 2/3D problems, sufficiently fine grids to stabilize central scheme may be prohibitively expensive
- local grid refinement may help to offset artificial diffusion

Convection-diffusion and finite elements

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

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

- 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 $u - u_D \in H^1_0(\Omega)$ and $\forall w \in H^1_0(\Omega)$,

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

- 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

$\sim$

Nonlinear problems

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

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

with

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

where $\mathcal{D}(u) = \int_0^u D(\xi)\; d\xi$ (from 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.

- Fixed point iteration scheme:
  1. Choose initial value u_0, $i \leftarrow 0$
  2. For $i \geq 0$, solve $M(u_i)u_{i+1} = f$
  3. Set $i \leftarrow i + 1$
  4. Repeat from 2) until converged
- 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

- Let $u \in \mathbb{R}^n$.
- 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
  1. Choose initial value u_0, $i \leftarrow 0$
  2. Calculate residual $r_i = A(u_i) - f$
  3. Calculate Jacobi matrix $A'(u_i)$
  4. Solve update problem $A'(u_i)h_i = r_i$
  5. Update solution: $u_{i+1} = u_i - h_i$
  6. Set $i \leftarrow i + 1$
  7. Repeat from 2) until converged
- 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

Newton method II

- Remedies for small domain of convergence: damping
  1. Choose initial value u_0, $i \leftarrow 0$,
     damping parameter $d < 1$:
  2. Calculate residual $r_i = A(u_i) - f$
  3. Calculate Jacobi matrix $A'(u_i)$
  4. Solve update problem $A'(u_i)h_i = r_i$
  5. Update solution: $u_{i+1} = u_i - dh_i$
  6. Set $i \leftarrow i + 1$
  7. Repeat from 2) until converged
- Damping slows convergence
- Better way: increase damping parameter during iteration:
  1. Choose initial value u_0, $i \leftarrow 0$,
     damping parameter d_0,
     damping growth factor $\delta > 1$
  2. Calculate residual $r_i = A(u_i) - f$
  3. Calculate Jacobi matrix $A'(u_i)$
  4. Solve update problem $A'(u_i)h_i = r_i$
  5. Update solution: $u_{i+1} = u_i - d_i h_i$
  6. Update damping parameter: $d_{i+1} = \min(1, \delta d_i)$
     Set $i \leftarrow i + 1$
  7. Repeat from 2) until converged

Newton method III

- 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 IV

- 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:
  1. Solve $A(u_0, 0) = f$
     choose step size δ Set $\lambda = 0$
  2. Solve $A(u_{\lambda+\delta}, \lambda + \delta) = 0$ with initial value u_λ. Possibly decrease δ to achieve convergence
  3. Set $\lambda \leftarrow \lambda + \delta$
  4. Possibly increase δ
  5. Repeat from 2) until $\lambda = 1$
- Parameter embedding + damping + update based convergence control go a long way to solve even strongly nonlinear problems!