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Examples

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Lecture 25

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Recap

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 $K = K(x)$:

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

Therefore,

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

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: $B(-x) = B(x) + x \Rightarrow$

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

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

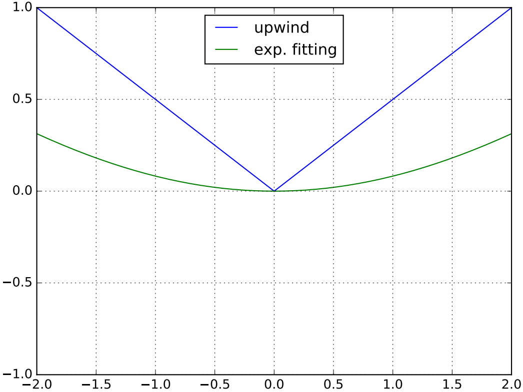
- Further, for $x > 0$:

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

- 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

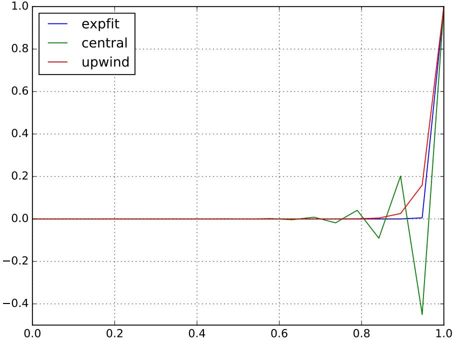
```
F=0;
U=0;
for (int k=0, l=1;k<n-1;k++,l++)
{
  double g_kl=D;
  double g_lk=D;
  if (v<0) g_kl-=v*h;
  else  g_lk+=v*h;

  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

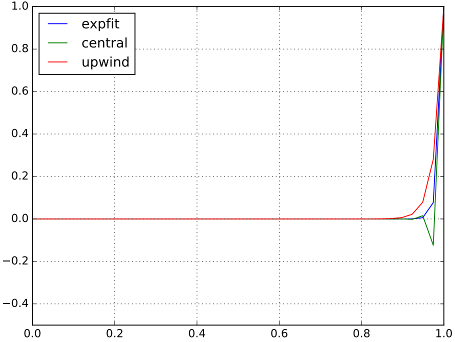
- $\Omega = (0,1)$, $-\nabla \cdot (D\nabla u + uv) = 0$, $u(0) = 0$, $u(1) = 1$
- $V = 1$, $D = 0.01$



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

Convection-Diffusion test problem, N=40

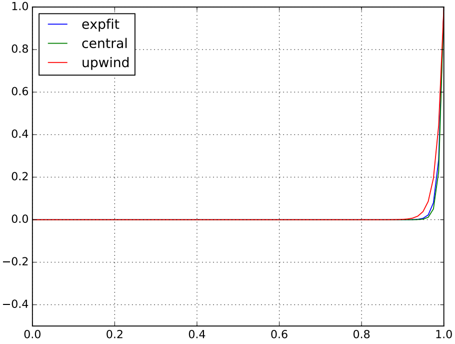
- $\Omega = (0, 1)$, $-\nabla \cdot (D\nabla u + uv) = 0$, $u(0) = 0$, $u(1) = 1$
- $V = 1$, $D = 0.01$



- 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 $u - u_D \in H_0^1(\Omega)$ 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

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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!

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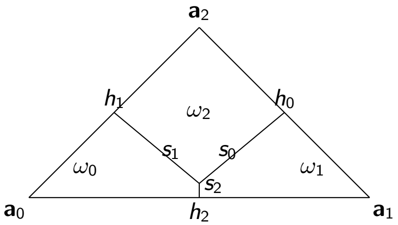
Finite volume local stiffness matrix calculation

Finite volume local stiffness matrix calculation

$a_0 = (x_0, y_0) \dots a_d = (x_2, y_2)$: vertices of the simplex K Calculate the contribution from triangle to $\frac{\sigma_{kl}}{h_{kl}}$ in the finite volume discretization



Let $h_i = ||a_{i+1} - a_{i+2}||$ (i counting modulo 2) be the lengths of the discretization edges. Let A be the area of the triangle. Then for the contribution from the triangle to the form factor one has

$$\frac{|s_i|}{h_i} = \frac{1}{8A}(h_{i+1}^2 + h_{i+2}^2 - h_i^2)$$

$$|\omega_i| = (|s_{i+1}|h_{i+1} + |s_{i+2}|h_{i+2})/4$$