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Slide lecture 8

Jürgen Fuhrmann

juergen.fuhrmann@wias-berlin.de

Convection-Diffusion problems

The convection - diffusion equation

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

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

$$+ \text{ Boundary conditions}$$

- $u(x)$: species concentration, temperature
- $\vec{j} = D\vec{\nabla} u - u\vec{v}$: species flux
- D: diffusion coefficient
- $\vec{v}(x)$: velocity of medium (e.g. fluid)
    - Given analytically
    - Solution of free flow problem (Navier-Stokes equation)
    - Flow in porous medium (Darcy equation): $\vec{v} = -\kappa\vec{\nabla} p$ where

$$-\nabla \cdot (\kappa\vec{\nabla} p) = 0$$

- For constant density, the divergence conditon $\nabla \cdot \vec{v} = 0$ holds.

Finite volumes for convection diffusion

$$-\nabla \cdot \vec{j} = 0 \quad \text{in } \Omega$$
$$\vec{j} \cdot \vec{n} + \alpha u = g \quad \text{on } \Gamma = \partial\Omega$$

- Integrate equation over control volume

$$\begin{aligned}
0 &= -\int_{\omega_k} \nabla \cdot \vec{j} d\omega = -\int_{\partial\omega_k} \vec{j} \cdot \vec{n}_k d\gamma \\
&= -\sum_{l \in \mathcal{N}_k} \int_{\sigma_{kl}} \vec{j} \cdot \vec{n}_{kl} d\gamma - \int_{\gamma_k} \vec{j} \cdot \vec{n} d\gamma \\
&\approx \sum_{l \in \mathcal{N}_k} \underbrace{\frac{|\sigma_{kl}|}{h_{kl}} g_{kl}(u_k, u_l)}_{\to A_\Omega} + \underbrace{|\gamma_k| \alpha u_k}_{\to A_\Gamma} - |\gamma_k| g_k
\end{aligned}$$

- $A = A_\Omega + A_\Gamma$

Central Difference Flux Approximation

- g_{kl} approximates normal convective-diffusive flux between control volumes ω_k, ω_l: $g_{kl}(u_k - u_l) \approx -(D\vec{\nabla} u - u\vec{v}) \cdot n_{kl}$
- Let $\sigma_{kl} = \omega_k \cap \omega_l$
  Let $v_{kl} = \frac{1}{|\sigma_{kl}|} \int_{\sigma_{kl}} \vec{v} \cdot \vec{n}_{kl} d\gamma$ approximate the normal velocity $\vec{v} \cdot \vec{n}_{kl}$
- Central difference flux:

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

- if v_{kl} is large compared to h_{kl}, the corresponding matrix (off-diagonal) entry may become positive
- Non-positive off-diagonal entries only guaranteed for $h \to 0$!
- If all off-diagonal entries are non-positive, we can prove the discrete maximum principle

Simple upwind flux discretization

- Force correct sign of convective flux approximation by replacing central difference flux approximation $h_{kl}\frac{1}{2}(u_k + u_l)v_{kl}$ by

$$\left(\begin{cases} h_{kl}u_k v_{kl}, & v_{kl} < 0 \\ h_{kl}u_l v_{kl}, & v_{kl} > 0 \end{cases}\right) = h_{kl}\tfrac{1}{2}(u_k + u_l)v_{kl} + \underbrace{\frac{1}{2}h_{kl}|v_{kl}|}_{\text{Artificial Diffusion } \tilde{D}} (u_k - u_l)$$

- 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 introduces error: second order approximation replaced by first order approximation

Exponential fitting flux I

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

$$
\begin{aligned}
u' - uv &= j \\
u|_0 &= u_k \\
u|_h &= u_l
\end{aligned}
$$

- Linear ODE
- Solution of the homogeneus problem:

$$
\begin{aligned}
u' - uv &= 0 \\
u'/u &= v \\
\ln u &= u_0 + vx \\
u &= K \exp(vx)
\end{aligned}
$$

Exponential fitting II

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

$$K' \exp(vx) + vK \exp(vx) - vK \exp(vx) = -j$$
$$K' = -j \exp(-vx)$$
$$K = K_0 + \frac{1}{v} j \exp(-vx)$$

- Therefore,

$$u = K_0 \exp(vx) + \frac{1}{v} j$$
$$u_k = K_0 + \frac{1}{v} j$$
$$u_l = K_0 \exp(vh) + \frac{1}{v} j$$

Exponential fitting III

- Use boundary conditions

$$
\begin{aligned}
K_0 &= \frac{u_k - u_l}{1 - \exp(vh)} \\
u_k &= \frac{u_k - u_l}{1 - \exp(vh)} + \frac{1}{v} j \\
j =& \frac{v}{\exp(vh) - 1}(u_k - u_l) + v u_k \\
=& v \left(\frac{1}{\exp(vh) - 1} + 1 \right) u_k - \frac{v}{\exp(vh) - 1} u_l \\
=& v \left(\frac{\exp(vh)}{\exp(vh) - 1} \right) u_k - \frac{v}{\exp(vh) - 1} u_l \\
=& \frac{-v}{\exp(-vh) - 1} u_k - \frac{v}{\exp(vh) - 1} u_l \\
=& \frac{B(-vh) u_k - B(vh) u_l}{h}
\end{aligned}
$$

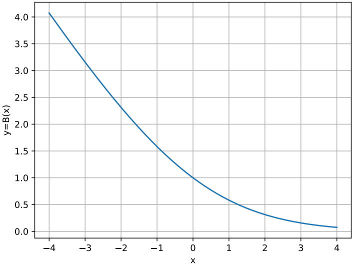
where $B(\xi) = \frac{\xi}{\exp(\xi) - 1}$: Bernoulli function

Exponential fitting IV

- General case: $Du' - uv = D(u' - u\frac{v}{D})$
- 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 sign pattern, M property!



Exponential fitting: Artificial diffusion

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

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

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

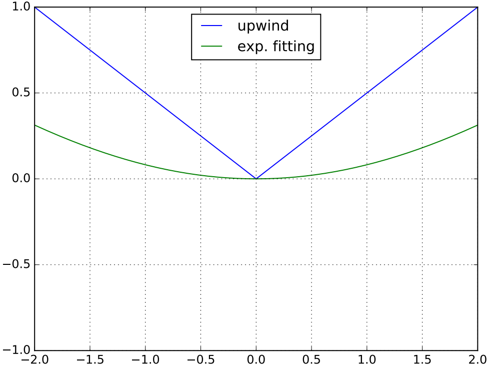
- Further, for $x > 0$:

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

- Therefore

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

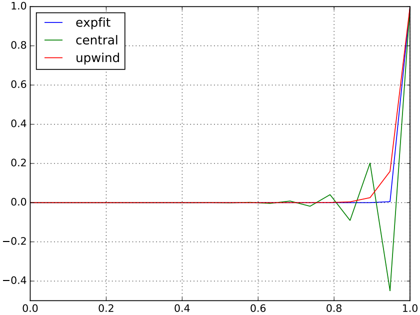
Exponential fitting: Artificial diffusion II



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

Convection-Diffusion test problem, N=20

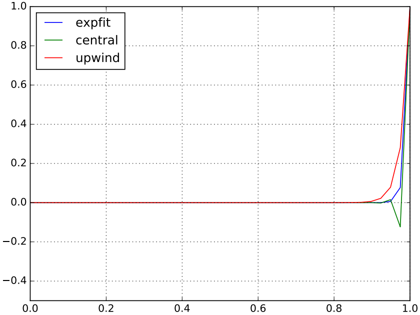
- $\Omega = (0,1)$, $-\nabla \cdot (D\vec{\nabla} u + uv) = 0$, $u(0) = 0$, $u(1) = 1$
- $V = 1$, $D = 0.01$



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

Convection-Diffusion test problem, N=40

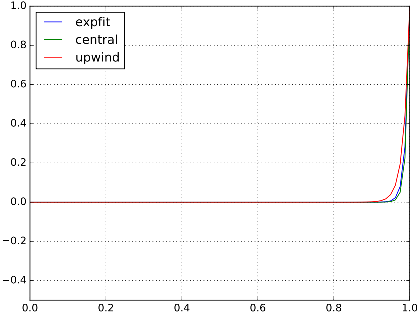
- $\Omega = (0, 1)$, $-\nabla \cdot (D\vec{\nabla} u + uv) = 0$, $u(0) = 0$, $u(1) = 1$
- $V = 1$, $D = 0.01$



- 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

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



- 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