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Slide lecture 9

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Time dependent Robin boundary value problem

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

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

- This is an initial boundary value problem
- We will proceed in a simpler manner: first, perform a finite difference discretization in time, then perform discretization in space.
  - *Rothe method:* first discretize in time, then in space
  - *Method of lines:* first discretize in space, get a huge ODE system, then apply perfom discretization

Time discretization

- Choose time discretization points $0 = t^0 < t^1 \cdots < t^N = T$
- let $\tau^n = t^n - t^{n-1}$
  For $i = 1 \dots N$, solve

$$\frac{u^n - u^{n-1}}{\tau^n} - \nabla \cdot D\vec{\nabla} u^\theta = f \quad \text{in } \Omega \times [0, T]$$
$$D\vec{\nabla} u_\theta \cdot \vec{n} + \alpha u^\theta = g \quad \text{on } \partial\Omega \times [0, T]$$

  where $u^\theta = \theta u^n + (1-\theta)u^{n-1}$
- $\theta = 1$: backward (implicit) Euler method
  Solve PDE problem in each timestep. First order accuracy in time.
- $\theta = \frac{1}{2}$: Crank-Nicolson scheme
  Solve PDE problem in each timestep. Second order accuracy in time.
- $\theta = 0$: forward (explicit) Euler method
  First order accurate in time. This does not involve the solution of a PDE problem $\Rightarrow$ Cheap? What do we have to pay for this ?

Finite volumes for time dependent hom. Neumann problem

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

$$\begin{aligned} \partial_t u - \nabla \cdot D\vec{\nabla} u &= 0 \quad \text{in}\Omega \times [0, T] \\ D\vec{\nabla} u \cdot \vec{n} &= 0 \quad \text{on}\Gamma \times [0, T] \end{aligned}$$

- Given control volume ω_k, integrate equation over space-time control volume $\omega_k \times (t^{n-1}, t^n)$, divide by τ^n:

$$\begin{aligned} 0 &= \int\limits_{\omega_k} \left(\frac{1}{\tau^n}(u^n - u^{n-1}) - \nabla \cdot D\vec{\nabla} u^\theta \right) d\omega \\ &= \frac{1}{\tau}^n \int\limits_{\omega_k} (u^n - u^{n-1}) d\omega - \int\limits_{\partial\omega_k} D\vec{\nabla} u^\theta \cdot \vec{n}_k d\gamma \\ &= -\sum_{l \in \mathcal{N}_k} \int\limits_{\sigma_{kl}} D\vec{\nabla} u^\theta \cdot \vec{n}_{kl} d\gamma - \int\limits_{\gamma_k} D\vec{\nabla} u^\theta \cdot \vec{n} d\gamma - \frac{1}{\tau}^n \int\limits_{\omega_k} (u^n - u^{n-1}) d\omega \\ &\approx \underbrace{\frac{|\omega_k|}{\tau^n}(u_k^n - u_k^{n-1})}_{\to M} + \underbrace{\sum_{l \in \mathcal{N}_k} \frac{|\sigma_{kl}|}{h_{kl}}(u_k^\theta - u_l^\theta)}_{\to A} \end{aligned}$$

Matrix equation

- Resulting matrix equation:

$$\frac{1}{\tau^n}\left(Mu^n - Mu^{n-1}\right) + Au^\theta = 0$$

$$\frac{1}{\tau^n}Mu^n + \theta Au^n = \frac{1}{\tau^n}Mu^{n-1} + (\theta-1)Au^{n-1}$$

$$u^n + \tau^n M^{-1}\theta Au^n = u^{n-1} + \tau^n M^{-1}(\theta-1)Au^{n-1}$$

- $M = (m_{kl})$, $A = (a_{kl})$ with

$$a_{kl} = \begin{cases} \sum_{l'\in\mathcal{N}_k} D\frac{|\sigma_{kl'}|}{h_{kl'}} & l = k \\ -D\frac{\sigma_{kl}}{h_{kl}}, & l \in \mathcal{N}_k \\ 0, & else \end{cases}$$

$$m_{kl} = \begin{cases} |\omega_k| & l = k \\ 0, & else \end{cases}$$

- $\Rightarrow \theta A + M$ is strictly diagonally dominant!

A matrix norm estimate

Lemma: Assume A has positive main diagonal entries, nonpositive off-diagonal entries and row sum zero. Then, $||(I+A)^{-1}||_\infty \leq 1$

Proof: Assume that $||(I+A)^{-1}||_\infty > 1$. $I+A$ is a irreducible M-matrix, thus $(I+A)^{-1}$ has positive entries. Then for α_{ij} being the entries of $(I+A)^{-1}$,

$$\max_{i=1}^{n} \sum_{j=1}^{n} \alpha_{ij} > 1.$$

Let k be a row where the maximum is reached. Let $e = (1\dots 1)^T$. Then for $v = (I+A)^{-1}e$ we have that $v > 0$, $v_k > 1$ and $v_k \geq v_j$ for all $j \neq k$. The kth equation of $e = (I+A)v$ then looks like

$$\begin{aligned} 1 &= v_k + v_k \sum_{j\neq k} |a_{kj}| - \sum_{j\neq k} |a_{kj}| v_j \\ &\geq v_k + v_k \sum_{j\neq k} |a_{kj}| - \sum_{j\neq k} |a_{kj}| v_k \\ &= v_k \\ &> 1 \end{aligned}$$

Stability estimate

- Matrix equation again:

$$u^n + \tau^n M^{-1}\theta A u^n = u^{n-1} + \tau^n M^{-1}(\theta - 1)Au^{n-1} =: B^n u^{n-1}$$

$$u^n = (I + \tau^n M^{-1}\theta A)^{-1} B^n u^{n-1}$$

- From the lemma we have $||(I + \tau^n M^{-1}\theta A)^n||_\infty \leq 1$
  $\Rightarrow ||u^n||_\infty \leq ||B^n u^{n-1}||_\infty$.
- For the entries b^n_{kl} of B^n, we have

$$b^n_{kl} = \begin{cases} 1 + \frac{\tau^n}{m_{kk}}(\theta - 1)a_{kk}, & k = l \\ \frac{\tau^n}{m_{kk}}(\theta - 1)a_{kl}, & else \end{cases}$$

- In any case, $b_{kl} \geq 0$ for $k \neq l$.
  If $b_{kk} \geq 0$, one estimates $||B||_\infty = \max_{k=1}^N \sum_{l=1}^N b_{kl}$.
- But

$$\sum_{l=1}^N b_{kl} = 1 + (\theta - 1)\frac{\tau^n}{m_{kk}}\left(a_{kk} + \sum_{l \in \mathcal{N}_k} a_{kl}\right) = 1 \quad \Rightarrow ||B||_\infty = 1.$$

Stability conditions

- For a shape regular triangulation in $\mathbb{R}^d$, we can assume that $m_{kk} = |\omega_k| \sim h^d$, and $a_{kl} = \frac{|\sigma_{kl}|}{h_{kl}} \sim \frac{h^{d-1}}{h} = h^{d-2}$, thus $\frac{a_{kk}}{m_{kk}} \leq \frac{1}{Ch^2}$
- $b_{kk} \geq 0$ gives

$$(1-\theta)\frac{\tau^n}{m_{kk}} a_{kk} \leq 1$$

- A sufficient condition is that for some $C > 0$,

$$(1-\theta)\frac{\tau^n}{Ch^2} \leq 1$$
$$(1-\theta)\tau^n \leq Ch^2$$

- Method stability:
  - Implicit Euler: $\theta = 1 \Rightarrow$ unconditional stability !
  - Explicit Euler: $\theta = 0 \Rightarrow$ CFL condition $\tau \leq Ch^2$
  - Crank-Nicolson: $\theta = \frac{1}{2} \Rightarrow$ CFL condition $\tau \leq 2Ch^2$
    Tradeoff stability vs. accuracy.

Stability discussion

- $\tau \leq Ch^2$ CFL == "Courant-Friedrichs-Levy"
- Explicit (forward) Euler method can be applied on very fast systems (GPU), with small time step comes a high accuracy in time.
- Implicit Euler: unconditional stability – helpful when stability is of utmost importance, and accuracy in time is less important
- For hyperbolic systems (pure convection without diffusion), the CFL conditions is $\tau \leq Ch$, thus in this case explicit computations are ubiquitous
- Comparison for a fixed size of the time interval. Assume for implicit Euler, time accuracy is less important, and the number of time steps is independent of the size of the space discretization.

	1D	2D	3D
# unknowns	$N = O(h^{-1})$	$N = O(h^{-2})$	$N = O(h^{-3})$
# steps	$M = O(N^2)$	$M = O(N)$	$M = O(N^{2/3})$
complexity	$M = O(N^3)$	$M = O(N^2)$	$M = O(N^{5/3})$

Backward Euler: discrete maximum principle

$$\frac{1}{\tau^n}Mu^n + Au^n = \frac{1}{\tau}Mu^{n-1}$$

$$\frac{1}{\tau^n}m_{kk}u_k^n + a_{kk}u_k^n = \frac{1}{\tau^n}m_{kk}u_k^{n-1} + \sum_{k\neq l}(-a_{kl})u_l^n$$

$$u_k^n = \frac{1}{\frac{1}{\tau^n}m_{kk} + \sum_{l\neq k}(-a_{kl})}\left(\frac{1}{\tau^n}m_{kk}u_k^{n-1} + \sum_{l\neq k}(-a_{kl})u_l^n\right)$$

$$\leq \frac{\frac{1}{\tau^n}m_{kk} + \sum_{l\neq k}(-a_{kl})}{\frac{1}{\tau^n}m_{kk} + \sum_{l\neq k}(-a_{kl})}\max(\{u_k^{n-1}\} \cup \{u_l^n\}_{l\in\mathcal{N}_k})$$

$$\leq \max(\{u_k^{n-1}\} \cup \{u_l^n\}_{l\in\mathcal{N}_k})$$

- 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
- Sign pattern is crucial for the proof.

Backward Euler: Nonnegativity

$$
\begin{aligned}
u^n + \tau^n M^{-1} A u^n &= u^{n-1} \\
u^n &= (I + \tau^n M^{-1} A)^{-1} u^{n-1}
\end{aligned}
$$

- $(I + \tau^n M^{-1} A)$ is an M-Matrix
- If $u_0 > 0$, then $u^n > 0 \ \forall n > 0$

Mass conservation

- Equivalent of $\int_\Omega \nabla \cdot D\vec{\nabla} u d\vec{x} = \int_{\partial\Omega} D\vec{\nabla} u \cdot \vec{n} d\gamma = 0$:

$$\sum_{k=1}^{N} \left(a_{kk} u_k + \sum_{l \in \mathcal{N}_k} a_{kl} u_l \right) = \sum_{k=1}^{N} \sum_{l=1, l \neq k}^{N} a_{kl}(u_l - u_k)$$
$$= \sum_{k=1}^{N} \sum_{l=1, l < k}^{N} (a_{kl}(u_l - u_k) + a_{lk}(u_k - u_l))$$
$$= 0$$

- $\Rightarrow$ Equivalent of $\int_\Omega u^n d\vec{x} = \int_\Omega u^{n-1} d\vec{x}$:
  - $\sum_{k=1}^{N} m_{kk} u_k^n = \sum_{k=1}^{N} m_{kk} u_k^{n-1}$

Weak formulation of time step problem

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

$$\frac{1}{\tau^n}\int_\Omega u^n v\,dx + \theta\int_\Omega D\vec{\nabla}u^n\vec{\nabla}v\,dx = \frac{1}{\tau^n}\int_\Omega u^{n-1}v\,dx + (1-\theta)\int_\Omega D\vec{\nabla}u^{n-1}\vec{\nabla}v\,dx$$

- Matrix formulation

$$\frac{1}{\tau^n}Mu^n + \theta Au^n = \frac{1}{\tau^n}Mu^{n-1} + (1-\theta)Au^{n-1}$$

- M: mass matrix, A: stiffness matrix.