Scientific Computing WS 2017/2018

Lecture 24

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Stability tests

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, then apply perfom discretization

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

$$\frac{u_i - u_{i-1}}{\tau_i} - \nabla \cdot \kappa \nabla u_\theta = f \quad \text{in } \Omega \times [0, T]$$

$$\kappa \nabla u_\theta \cdot \vec{n} + \alpha(u_\theta - g) = 0 \quad \text{on } \partial\Omega \times [0, T]$$

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

Time discretization: stability test

- Influence of
  - Forward/backward Euler
  - Mass lumping
  - Time vs space stepsize

The convection - diffusion equation

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

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

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

$$-\nabla \cdot (\kappa\nabla p) = 0$$

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

Finite volumes for convection diffusion

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

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

- Integrate time discrete equation over control volume

$$0 = \int_{\omega_k} \left(\frac{1}{\tau}(u - v) - \nabla \cdot \mathbf{j} \right) d\omega = \frac{1}{\tau} \int_{\omega_k} (u - v) d\omega - \int_{\partial\omega_k} \mathbf{j} \cdot \mathbf{n}_k d\gamma$$

$$= - \sum_{l \in \mathcal{N}_k} \int_{\sigma_{kl}} \mathbf{j} \cdot \mathbf{n}_{kl} d\gamma - \int_{\gamma_k} \mathbf{j} \cdot \mathbf{n} d\gamma - \frac{1}{\tau} \int_{\omega_k} (u - v) d\omega$$

$$\approx \underbrace{\frac{|\omega_k|}{\tau}(u_k - v_k)}_{\to M} + \sum_{l \in \mathcal{N}_k} \underbrace{\frac{|\sigma_{kl}|}{h_{kl}} g_{kl}(u_k, u_l)}_{\to A_0} + \underbrace{|\gamma_k| \alpha(u_k - g_k)}_{\to D}$$

- $\frac{1}{\tau} M u + A u = \frac{1}{\tau} M v$ where $A = A_0 + D$, $A_0 = (a_{kj})$

Central Difference Flux Approximation

- g_{kl} approximates normal convective-diffusive flux between control volumes ω_k, ω_l: $g_{kl}(u_k - u_l) \approx -(D\nabla u - u\mathbf{v}) \cdot n_{kl}$
- Let $v_{kl} = \frac{1}{|\sigma_{kl}|} \int \sigma_{kl} \mathbf{v} \cdot \mathbf{n}_{kl} d\gamma$ approximate the normal velocity $\mathbf{v} \cdot \mathbf{n}_{kl}$
- 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 $\mathbf{v}_{kl}$ is large compared to h_{kl}, the corresponding matrix (off-diagonal) entry may become positive
- Non-positive off-diagonal entries only guaranteed for $h \to 0$!
- Otherwise, 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

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

- 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 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!

Convection diffusion demo

- Influence of
  - upwinding

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

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

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 schem:
  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 demo

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!

Examination dates

Mon Feb 26 (not yet confirmed)
Mon March 5
Wed March 7
Mon March 12
Tue March 13
Wed March 14
Mon March 26
Tue March 27

Time: 10:00-13:00 (6 slots per examination date)

Room: MA 379

Please mark preferred dates in the list.