Scientific Computing WS 2017/2018

Lecture 22

Jürgen Fuhrmann

juergen.fuhrmann@wias-berlin.de

Convergence + stability tests

P1 FEM, homogeneous Dirichlet

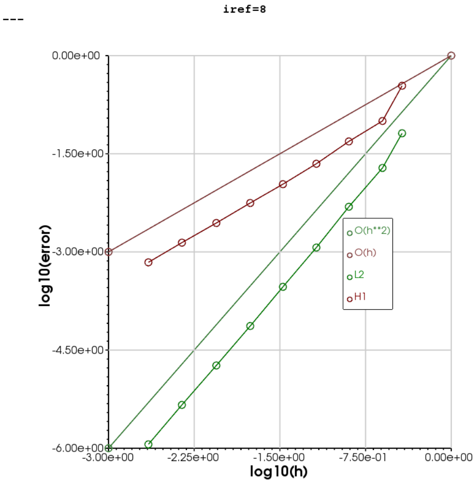
- Problem:

$$
\begin{aligned}
-\Delta u &= f \text{ in } \Omega \\
u &= 0 \text{ on } \partial\Omega
\end{aligned}
$$

- Exact solution + rhs:

$$
\begin{aligned}
u(x,y) &= \sin(\pi x)\sin(\pi y) \\
f(x,y) &= 2\pi \sin(\pi x)\sin(\pi y)
\end{aligned}
$$

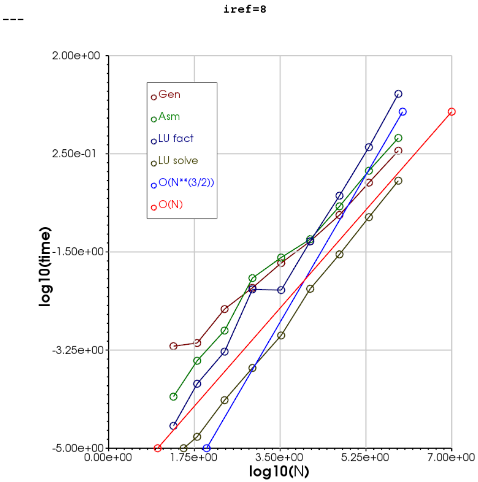
P1 FEM: error plot



- As expected:

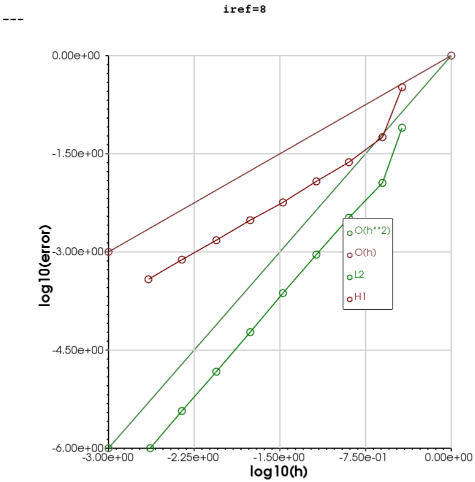
$$||u - u_h||_{L^2} \leq Ch^2$$
$$||u - u_h||_{H^1} \leq Ch$$

P1 FEM:timing plot



asm:	Assembly
gen:	Mesh generation
luf:	LU factorization
lus:	LU solution
- For large problems, $t_{luf} > t_{asm} > t_{gen} > t_{lus}$
- $t_{luf} = O(N^{\frac{3}{2}})$

FVM: error plot



- As with P1 FEM

$$||u - u_h||_{L^2} \leq Ch^2$$
$$||u - u_h||_{H^1} \leq Ch$$

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 ?

Weak formulation of time step problem

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

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

- 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, $A = A_0 + D$, A_0: stiffness matrix, D: boundary contribution

Mass matrix properties

- 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, for every eigenvalue μ one has the estimate

$$c_1 h^d \leq \mu \leq c_2 h^d$$

  T $\Rightarrow$ condition number $\kappa(M)$ bounded by constant independent of h:

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

- How to see this ? Let $u_h = \sum_{i=1}^N U_i \phi_i$, and μ an eigenvalue (positive,real!) Then

$$||u_h||_0^2 = (U, MU)_{\mathbb{R}^N} = \mu(U, U)_{\mathbb{R}^N} = \mu||U||_{\mathbb{R}^N}^2$$

  From quasi-uniformity we obtain

$$c_1 h^d ||U||_{\mathbb{R}^N}^2 \leq ||u_h||_0^2 \leq c_2 h^d ||U||_{\mathbb{R}^N}^2$$

  and conclude

Mass matrix M-Property (P1 FEM) ?

- 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!

Mass matrix lumping (P1 FEM)

- Local mass matrix for P1 FEM on element K
  (calculated by 2nd order exact edge midpoint quadrature rule):

$$M_K = |K| \begin{pmatrix} \frac{1}{6} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{6} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{6} \end{pmatrix}$$

- Lumping: sum up off diagonal elements to main diagonal, set off diagonal entries to zero

$$\tilde{M}_K = |K| \begin{pmatrix} \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} \end{pmatrix}$$

- Interpretation as change of quadrature rule to first order exact vertex based quadrature rule
- Loss of accuracy, gain of stability

Stiffness matrix condition number + row sums (FEM)

- Stiffness matrix $A_0 = (a_{ij})$:

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

- bilinear form $a(\cdot, \cdot)$ is self-adjoint, therefore A_0 is symmetric, positive definite
- Condition number estimate for P^1 finite elements on quasi-uniform triangulation:

$$\kappa(A_0) \leq ch^{-2}$$

- 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 (P1 FEM)

Local stiffness matrix S_K

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

- Main diagonal entries are 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 row sums are zero $\Rightarrow A_0$ 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 $\Rightarrow A = A_0 + D$: M-Matrix
- Adding a mass matrix which is not lumped yields a positive definite matrix and thus nonsingularity, but *destroys M*-property unless the absolute values of its off diagonal entries are less than those of A_0.

Back to time dependent problem

Assume M diagonal, $A = A_0 + D$ where A_0 is the stiffness matrix, and D is a nonnegative diagonal matrix. We have

$$
\begin{aligned}
(A_0 u)_i &= \sum_j a_{ij} u_j = a_{ii} u_i + \sum_{i \neq j} a_{ij} u_j \\
&= (-\sum_{i \neq j} a_{ij}) u_i + \sum_{i \neq j} a_{ij} u_j \\
&= \sum_{i \neq j} -a_{ij} (u_i - u_j)
\end{aligned}
$$

Forward Euler

$$\frac{1}{\tau_i} M u_i = \frac{1}{\tau_i} M u_{i-1} + A_i u_{i-1}$$
$$u_i = u_{i-1} + \tau_i M^{-1} A_i u_{i-1} = (I + \tau M^{-1} D + \tau M^{-1} A_0) u_{i-1}$$

- Entries of $\tau M^{-1} A$ are of order $\frac{1}{h^2}$, and so we can expect an h independent estimate of u_i via u_{i-1} resp. u_0 only if τ balances $\frac{1}{h^2}$, i.e.

$$\tau \leq Ch^2$$

- This is the CFL (Courant-Friedrichs-Lewy) condition

Backward Euler

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

$$(I + \tau_i M^{-1} A) u_i = u_{i-1}$$

$$u_i = (I + \tau_i M^{-1} A)^{-1} u_{i-1}$$

But here, we can estimate that

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

Backward Euler Estimate

Theorem: Assume $A_0 = (a_{ij})$ has the sign pattern of an M-Matrix with row sum zero, and D is a nonnegative diagonal matrix. Then $||(I + D + A_0)^{-1}||_\infty \leq 1$

Proof: Assume that $||(I + A_0)^{-1}||_\infty > 1$. We know that $(I + A_0)^{-1}$ has positive entries. Then for α_{ij} being the entries of $(I + A_0)^{-1}$,

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

Let k be a row where the maximum is reached. Let $e = (1 \dots 1)^T$. Then for $v = (I + A_0)^{-1} e$ we have that $v > 0$, $v_k > 1$ and $v_k \geq v_j$ for all $j \neq k$. The kth equation of $e = (I + A_0)v$ then looks like

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

This contradiction enforces $||(I + A_0)^{-1}||_\infty \leq 1$.

Backward Euler Estimate II

$$
\begin{aligned}
I + A =& I + D + A_0\\
=&(I + D)(I + D)^{-1}(I + D + A_0)\\
=&(I + D)(I + A_{D0})
\end{aligned}
$$

with $A_{D0} = (I + D)^{-1}A_0$ has row sum zero Thus

$$
\begin{aligned}
||(I + A)^{-1}||_\infty =& ||(I + A_{D0})^{-1}(I + D)^{-1}||_\infty\\
\leq& ||(I + D)^{-1}||_\infty\\
\leq& 1,
\end{aligned}
$$

because all main diagonal entries of $I + D$ are greater or equal to 1. $\square$

Backward Euler Estimate III

We can estimate that

$$I + \tau_i M^{-1} A = I + \tau_i M^{-1} D + \tau_i M^{-1} A_0$$

and obtain

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

- We get this stability independent of the time step.
- Another theory is possible using L^2 estimates and positive definiteness
- Assuming $v \geq 0$ we can conclude $u \geq 0$.

Discrete maximum principle

$$\frac{1}{\tau}Mu + (D + A_0)u = \frac{1}{\tau}Mv$$

$$(\frac{1}{\tau}m_i + d_i)u_i + a_{ii}u_i = \frac{1}{\tau}m_i v_i + \sum_{i \neq j}(-a_{ij})u_j$$

$$u_i = \frac{1}{\frac{1}{\tau}m_i + d_i + \sum_{i \neq j}(-a_{ij})}(\frac{1}{\tau}m_i v_i + \sum_{i \neq j}(-a_{ij})u_j)$$

$$\leq \frac{\frac{1}{\tau}m_i v_i + \sum_{i \neq j}(-a_{ij})u_j}{\frac{1}{\tau}m_i + d_i + \sum_{i \neq j}(-a_{ij})} \max(\{v_i\} \cup \{u_j\}_{j \neq i})$$

$$\leq \max(\{v_i\} \cup \{u_j\}_{j \neq i})$$

- 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.

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

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

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

$$\begin{aligned} 0 &= \int_{\omega_k} \left(\frac{1}{\tau}(u - v) - \nabla \cdot \lambda \nabla u \right) d\omega = \frac{1}{\tau} \int_{\omega_k} (u - v) d\omega - \int_{\partial \omega_k} \lambda \nabla u \cdot \mathbf{n}_k d\gamma \\ &= - \sum_{l \in \mathcal{N}_k} \int_{\sigma_{kl}} \lambda \nabla u \cdot \mathbf{n}_{kl} d\gamma - \int_{\gamma_k} \lambda \nabla u \cdot \mathbf{n} d\gamma - \frac{1}{\tau} \int_{\omega_k} (u - v) d\omega \\ &\approx \underbrace{\frac{|\omega_k|}{\tau}(u_k - v_k)}_{\to M} + \underbrace{\sum_{l \in \mathcal{N}_k} \frac{|\sigma_{kl}|}{h_{kl}}(u_k - u_l)}_{\to A_0} + \underbrace{|\gamma_k| \alpha(u_k - g_k)}_{\to D} \end{aligned}$$

- Here, $u_k = u(\mathbf{x}_k)$, $g_k = g(\mathbf{x}_k)$, $f_k = f(\mathbf{x}_k)$
- $\frac{1}{\tau_i} M u_i + A u_i = \frac{1}{\tau_i} M u_{i-1}$ where $A = A_0 + D$

Finite volumes for time dependent problem II

- The finite volume method provides the M-Property of the stiffness matrix and immediately to a diagonal mass matrix M.
- $\Rightarrow$ Unconditional stability of the implicit Euler method
- CFL condition for time step size for explicit Euler