Scientific Computing WS 2017/2018

Lecture 21

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Species balance over an REV

- Let $u(\mathbf{x}, t) : \Omega \times [0, T] \to \mathbb{R}$ be the local amount of some species.
- Assume representative elementary volume $\omega \subset \Omega$
- Subinterval in time $(t_0, t1) \subset (0, T)$
- $-\delta \nabla u \cdot \mathbf{n}$ describes the flux of these species trough $\partial\omega$, where δ is some transfer coefficient
- Let $f(\mathbf{x}, t)$ be some local source of species. Then the flux through the boundary is balanced by the change of the amount of species in ω and the source strength.

$$\begin{aligned} 0 &= \int_\omega (u(\mathbf{x}, t_1) - u(\mathbf{x}, t_0))\, d\mathbf{x} - \int_{t_0}^{t_1} \int_{\partial\omega} \delta \nabla u \cdot \mathbf{n}\, ds\, dt - \int_{t_0}^{t_1} \int_\omega f(\mathbf{x}, t)\, ds \\ &= \int_{t_0}^{t_1} \int_\omega \partial_t u(\mathbf{x}, t)\, d\mathbf{x}\, dt - \int_{t_0}^{t_1} \int_\omega \nabla \cdot (\delta \nabla u)\, d\mathbf{x}\, dt - \int_{t_0}^{t_1} \int_\omega f(\mathbf{x}, t)\, ds \end{aligned}$$

- True for all $\omega \subset \Omega$, $(t_0, t1) \subset (0, T) \Rightarrow$ parabolic second order PDE

$$\partial_t u(x, t) - \nabla \cdot (\delta \nabla u(x, t)) = f(x, t)$$

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

$$\begin{aligned}\frac{u_i - u_{i-1}}{\tau_i} - \nabla \cdot \kappa \nabla u_\theta = f \quad & \text{in } \Omega \times [0, T] \\ \kappa \nabla u_\theta \cdot \vec{n} + \alpha(u_\theta - g) = 0 \quad & \text{on } \partial\Omega \times [0, T]\end{aligned}$$

  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 $\forall v \in H^1(\Omega)$

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

- 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:

$$\begin{aligned}\sum_{j=1}^{N} a_{ij} &= \sum_{j=1}^{N} \int_\Omega \nabla\phi_i \nabla\phi_j \, dx = \int_\Omega \nabla\phi_i \nabla \left(\sum_{j=1}^{N} \phi_j \right) \, dx \\ &= \int_\Omega \nabla\phi_i \nabla\left(1\right) \, dx \\ &= 0\end{aligned}$$

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

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

- 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

$$\begin{aligned}\frac{1}{\tau_i}Mu_i + Au_i &= \frac{1}{\tau_i}Mu_{i-1}\\ (I+\tau_i M^{-1}A)u_i &= u_{i-1}\\ u_i &= (I+\tau_i M^{-1}A)^{-1}u_{i-1}\end{aligned}$$

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

More general problems: linear reaction-diffusion

- Assume additional process in each REV which produces or destroys species depending on the amount of species present with given rate r.

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

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

- $\Rightarrow$ additional, time step independent term in mass matrix
- Be careful about coercivity (guaranteed for $R > 0$ which means species destruction)

More general problems: convection-diffusion

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

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

- Here:
  - u: species concentration
  - D: diffusion coefficient
  - $\mathbf{v}$: velocity of medium (e.g. fluid)

Tentative examination dates

Tue Feb 27
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: t.b.a. (MA, third floor)

Finite volumes for convection-diffusion

$$\frac{|\omega_k|}{\tau}(u_k - v_k) + \sum_{l \in \mathcal{N}_k} \frac{|\sigma_{kl}|}{h_{kl}} g(u_k, u_l) + |\gamma_k| \alpha (u_k - w_k)$$

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:

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

  - M-Property (sign pattern) only guaranteed for $h \to 0$!
- Upwind flux:

$$
\begin{aligned}
g(u_k, u_l) &= D(u_k - u_l) + \begin{cases} h_{kl}u_k v_{kl}, & v_{kl} < 0 \\ h_{kl}u_l v_{kl}, & v_{kl} > 0 \end{cases} \\
&= (D + \tilde{D})(u_k - u_l) - h_{kl}\frac{1}{2}(u_k + u_l)v_{kl}
\end{aligned}
$$

  - 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 $K = K(x)$:

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

Therefore,

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

Exponential fitting III

Use boundary conditions

$$
\begin{aligned}
K_0 &= \frac{c_K - c_L}{1-\exp(-qh)}\\
c_K &= \frac{c_K - c_L}{1-\exp(-qh)} + \frac{1}{q}j\\
j =& qc_K - \frac{q}{1-\exp(-qh)}(c_K - c_L)\\
=& q(1-\frac{1}{1-\exp(-qh)})c_K - \frac{q}{\exp(-qh)-1}c_L\\
=& q(\frac{-\exp(-qh)}{1-\exp(-qh)})c_K - \frac{q}{\exp(-qh)-1}c_L\\
=& \frac{-q}{\exp(qh)-1}c_K - \frac{q}{\exp(-qh)-1}c_L\\
=& \frac{B(-qh)c_L - B(qh)c_K}{h}
\end{aligned}
$$

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

Exponential fitting IV

- Upwind flux:

$$g(u_k, u_l) = D\frac{B(\frac{-v_{kl}h_{kl}}{D})u_k - B(\frac{v_{kl}h_{kl}}{D})u_l}{h}$$

- Allen+Southell 1955
- Scharfetter+Gummel 1969
- Ilin 1969
- Chang+Cooper 1970
- Guaranteed M property!