Numerical Solution I
Stationary Flow

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Summerschool “Modelling of mass and energy transport in porous media with practical applications”
October 8 - 12, 2018
Schedule

• Classical Solutions (Finite Differences)

• The Conservation Principle (Finite Volumes)

• Principle of Minimal Energy (Finite Elements)

• Adaptive Finite Elements

• (Fast) Solvers for Linear Systems

• Random Partial Differential Equations
Saturated Groundwater Flow (Darcy Equation)

\[ S_0 p_t = \text{div}(K \nabla p) + f \]

\( p: \) pressure

\[ S_0 = \rho g \frac{\partial n}{\partial p} \geq 0: \] specific storage coefficient

\[ K = (K_1, K_2, K_3) : \Omega \rightarrow \mathbb{R}^{3,3}: \] hydraulic permeability

\[ f = \rho g \text{div} K_3 + gF: \] gravity and source terms
Darcy’s and Poisson’s Equation

Darcy’s equation:

\[ S_0 = 0: \text{ pressure-stable granular structure} \]

\[ -\text{div}(K \nabla p) = f \]
Darcy’s and Poisson’s Equation

Darcy’s equation:

\[ S_0 = 0: \] pressure-stable granular structure
\[ -\text{div}(K \nabla p) = f \]

Poisson’s equation:

homogeneous soil: \( K \in \mathbb{R}^{3,3} \quad \Rightarrow \quad K \nabla p(x) = \nabla p(Kx) \)

transformation of variables: \( p(x) \leftrightarrow p(Kx) =: u(x) \)
\[ -\Delta u = f \]

Laplace operator: \( \Delta u = \sum_{i=1}^{3} u_{x_i x_i} = u_{x_1 x_1} + u_{x_2 x_2} + u_{x_3 x_3} \)
Classical Solution of Poisson’s Equation

Poisson’s equation: \( \Omega \subset \mathbb{R}^d \) (bounded domain)

\[-\Delta u = f \quad \text{on } \Omega \quad + \quad \text{boundary conditions on } \partial \Omega\]

boundary conditions (BC):

\[u = g\] pressure BC \quad (Dirichlet BC, 1. kind)

\[\alpha u + \beta \frac{\partial}{\partial n} u = g\] transmission BC \quad (Robin BC, 3. kind)

Theorem (well-posedness)

Assumption: \( \Omega, f, g \) sufficiently smooth.

Assertion: There exists a unique solution \( u \in C^2(\Omega) \cap C(\Omega) \) and \( u \) depends continuously on \( f, g \).
Ill-Posed Problems

flux boundary conditions:

\[ \frac{\partial u}{\partial n} = g \quad \text{outflow BC (Neumann BC, 2. kind)} \]

no uniqueness: \( u \) solution \( \Rightarrow u + c \) solution for all \( c \in \mathbb{R} \)

necessary for existence: \( \int_{\Omega} f \, dx + \int_{\partial\Omega} g \, d\sigma = 0 \) \ (Green’s formula)
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different BCs on disjoint subsets \( \Gamma_D \cup \Gamma_N \cup \Gamma_R = \partial\Omega \) allowed
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different BCs on disjoint subsets \( \Gamma_D \cup \Gamma_N \cup \Gamma_R = \partial \Omega \) allowed

Caution: \( \Gamma_D \) too small, e.g. \( \Gamma_D = \{x_0, x_1, .., x_m\} \), \( \Rightarrow \) no uniqueness!!
Finite Differences

rectangular mesh with mesh size $h$: 
Finite Difference Approximations

1. order forward and backward:

\[ D_1^+ U(x_Z) = \frac{U(x_O) - U(x_Z)}{|x_O - x_Z|} \]

\[ D_1^- U(x_Z) = \frac{U(x_Z) - U(x_W)}{|x_Z - x_W|} \]

2. order central finite differences:

\[ D_{11} U(x_Z) = \frac{2}{|x_O - x_W|} \left( D_1^+ U(x_Z) - D_1^- U(x_Z) \right) \]
Finite Difference Discretization (Shortley/Weller)

discrete Laplacian: \( \Delta_h U(x) = D_{11} U(x) + D_{22} U(x) \)

discrete problem:

\[ -\Delta_h U = f \quad \text{on} \quad \Omega_h, \quad U(x) = g \quad \text{on} \quad \partial\Omega_h \]

linear system: \( A^{FD} \overline{U} = b \)

Theorem (Convergence):

Assumption: \( u \in C^3(\Omega). \)

Assertion: \( \max_{x \in \Omega_h} |U(x) - u(x)| = O(h) \)
Heterogeneous Media

piecewise constant permeabilities:

\[ K = \begin{cases} 
  k_1 & x \in \Omega_1 \\
  k_2 & x \in \Omega_2 
\end{cases} \quad \Omega = \Omega_1 \cup \Omega_2 \cup \Gamma \]

no classical solution of: \( \text{div}(K\nabla u) = f \) on \( \Omega \)
Heterogeneous Media

piecewise constant permeabilities:

\[ K = \begin{cases} k_1 & x \in \Omega_1 \\ k_2 & x \in \Omega_2 \end{cases} \quad \Omega = \Omega_1 \cup \Omega_2 \cup \Gamma \]

no classical solution of: \( \text{div}(K \nabla u) = f \) on \( \Omega \)

- finite difference discretizations lead to interface problems
- interface problems require finite difference approximations of flux across the interface
Conservation Principle

conservation of mass in $\Omega' \subset \Omega$:

$$\int_{\partial\Omega'} K(x) \frac{\partial}{\partial n} u(x) \, d\sigma + \int_{\Omega'} f(x) \, dx = 0$$

regularity condition: $K \nabla u \in C^1(\overline{\Omega})^d$

Green’s formula:

$$\int_{\partial\Omega'} K(x) \frac{\partial}{\partial n} u(x) \, d\sigma = \int_{\Omega'} \operatorname{div}(K(x) \nabla u(x)) \cdot 1 \, dx + \int_{\Omega'} K(x) \nabla u(x) \cdot \nabla 1 \, dx$$

Darcy’s equation:

$$\int_{\Omega'} \operatorname{div}(K(x) \nabla u(x)) + f(x) \, dx = 0 \quad \forall \Omega' \subset \Omega$$
Finite Volumes

finite dimensional ansatz space: \( S_h, \dim S_h = n, \ v|_{\partial \Omega} = 0 \quad \forall v \in S_h \)

finite decomposition of \( \Omega \) into control volumes \( \Omega_i \): \( \Omega = \bigcup_{i=1}^{n} \Omega_i \)

finite volume discretization:

\[
\begin{align*}
   u_h \in S_h : & \quad - \int_{\partial \Omega_i} K \frac{\partial}{\partial n} u_h \, d\sigma = \int_{\Omega_i} f \, dx \quad \forall i = 1, \ldots, n
\end{align*}
\]

linear system:

choice of basis: \( S_h = \text{span}\{ \varphi_i \mid i = 1, \ldots, n\} \)

\[
A \overline{u}_h = b, \quad a_{ij} = \int_{\partial \Omega_i} K \frac{\partial}{\partial n} \varphi_j \, d\sigma, \quad b_i = \int_{\Omega_i} f \, dx
\]

solution: \( u_h = \sum_{i=1}^{n} u_i \varphi_i, \quad \overline{u}_h = (u_i) \)
Choice of Ansatz Space

triangulation: \( \mathcal{T}_h = \{ T \mid T \text{ triangle} \} \), \( \Omega = \bigcup_{T \in \mathcal{T}_h} T \)

linear finite elements: \( S_h := \{ v \in C(\overline{\Omega}) \mid v|_T \text{ linear } \forall T \in \mathcal{T}_h, \ v|_{\partial\Omega} = 0 \} \)

nodal basis: \( \lambda_p(q) = \delta_{p,q}, \quad p, q \in N_h \)
Vertex-Centered Finite Volumes

control volumes: linear connection of barycenters

linear system:

$$A^{FV} u_h = b^{FV}, \quad u_h = \sum_{p \in \mathcal{N}_h} u_p \lambda_p$$
Principle of Minimal Energy

quadratic energy functional:

\[ \mathcal{J}(v) = \frac{1}{2} a(v, v) - \ell(v), \quad a(v, w) = \int_{\Omega} K \nabla v \nabla w \, dx, \quad \ell(v) = \int_{\Omega} f v \, dx \]

minimization problem:

\[ u \in H^1_0(\Omega) : \quad \mathcal{J}(u) \leq \mathcal{J}(v) \quad \forall v \in H^1_0(\Omega) \]

variational formulation:

\[ u \in H^1_0(\Omega) : \quad \mathcal{J}'(u)(v) = a(u, v) - \ell(v) = 0 \quad \forall v \in H^1_0(\Omega) \]

weak solution \( u \in H^1_0(\Omega) \) (Sobolev space)
Weak Versus Classical Solution

regularity condition: \( K \nabla u \in C^1(\overline{\Omega})^d \)

Green’s formula:

\[
0 = a(u, v) - \ell(v) = -\int_{\Omega} (\text{div}(K \nabla u) + f) v \, dx + \int_{\partial \Omega} (K \frac{\partial}{\partial n} u) v \, d\sigma
\]

suitable choice of test functions \( v \in C^1_0(\overline{\Omega}) \):

\[
-\text{div}(K \nabla u) = f \quad \text{on} \ \Omega
\]
Ritz-Galerkin Method

finite dimensional ansatz space: $S_h \subset H^1_0(\Omega)$, $\dim S_h = n$

Ritz-Galerkin method

$$u_h \in S_h : \quad J'(u_h)(v) = a(u_h, v) - \ell(v) = 0 \quad \forall v \in S_h$$

linear system:

choice of basis: $S_h = \text{span}\{\varphi_i \mid i = 1, \ldots, n\}$

$$A \overline{u}_h = b, \quad a_{ij} = a(\varphi_j, \varphi_i), \quad b_i = \ell(\varphi_i)$$

solution: $u_h = \sum_{i=1}^{n} u_i \varphi_i, \quad \overline{u}_h = (u_i)$
Finite Element Discretization

triangulation: \( \mathcal{T}_h = \{T \mid T \text{ triangle}\}, \quad \Omega = \bigcup_{T \in \mathcal{T}_h} T \)

linear finite elements: \( S_h := \{v \in C(\overline{\Omega}) \mid v|_T \text{ linear } \forall T \in \mathcal{T}_h, \ v|_{\partial \Omega} = 0\} \)

nodal basis: \( \lambda_p(q) = \delta_{p,q}, \quad p, q \in \mathcal{N}_h \)

linear system: \( A^{\text{FE}} \overline{u}_h = b^{\text{FE}} \)
Finite Elements Versus Finite Volumes

Theorem (Hackbusch 89)

\[ A^{\text{FV}} = A^{\text{FE}}, \quad |b^{\text{FV}} - b^{\text{FE}}|_{-1} = \mathcal{O}(h^2) \]

Corollary:

\[ \|u^{\text{FV}}_h - u^{\text{FE}}_h\|_1 = \mathcal{O}(h^2), \quad \|v\|_1^2 = \int_{\Omega} v^2 + |\nabla v|^2 \, dx \]

in general:

- finite volumes: finite element discretization with suitable test functions
- finite elements: finite volume discretization with suitable numerical flux
Stability

maximum principle:

\[-\Delta u_1 = f_1, \quad -\Delta u_2 = f_2 \quad \text{on } \Omega, \quad u_1 = u_2 = 0 \quad \text{on } \partial \Omega\]

\[f_1 \geq f_2 \quad \implies \quad u_1 \geq u_2\]

"bad" angles of triangles might cause oscillations!

remedy: Delaunay triangulation
Stability

maximum principle:

\[-\Delta u_1 = f_1, \quad -\Delta u_2 = f_2 \quad \text{on } \Omega, \quad u_1 = u_2 = 0 \quad \text{on } \partial \Omega\]

\[f_1 \geq f_2 \implies u_1 \geq u_2\]

no discrete maximum principle:

\[A^{FE}u_1 = b_1^{FE}, \quad A^{FE}u_2 = b_2^{FE}\]

\[b_1^{FE} \geq b_2^{FE} \implies \overline{u}_1 \geq \overline{u}_2\]

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Stability

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\[b_1^{FE} \geq b_2^{FE} \implies \overline{u}_1 \geq \overline{u}_2\]

"bad" angles of triangles might cause oscillations!

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Stability

maximum principle:

\[-\Delta u_1 = f_1, \quad -\Delta u_2 = f_2 \quad \text{on } \Omega, \quad u_1 = u_2 = 0 \quad \text{on } \partial \Omega\]

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no discrete maximum principle:

\[A^{FE}u_1 = b_1^{FE}, \quad A^{FE}u_2 = b_2^{FE}\]

\[b_1^{FE} \geq b_2^{FE} \quad \implies \quad \bar{u}_1 \not\geq \bar{u}_2\]

"bad" angles of triangles might cause oscillations!

remedy: Delaunay triangulation \( \mathcal{T}_h \)
Discretization Error

Galerkin orthogonality: \( a(u - u_h, v) = 0 \) \( \forall \ v \in S \)

optimal error estimate:
\[
\|u - u_h\| = \inf_{v \in S_h} \|u - v\|,
\quad \|v\|^2 = a(v, v) \quad \text{(energy norm)}
\]

ellipticity: \( \alpha \|v\|_1 \leq \|v\| \leq \beta \|v\|_1, \quad \alpha, \beta > 0, \quad \forall \ v \in H^1_0(\Omega) \)

quasioptimal error estimate: \( \|u - u_h\|_1 \leq \frac{\beta}{\alpha} \inf_{v \in S_h} \|u - v\|_1 \)

estimate of the discretization error
\[
\inf_{v \in S_h} \|u - v\|_1 \leq c\|u\|_{2h} = \mathcal{O}(h), \quad c = c(T_h)
\]
Adaptive Multilevel Methods

Mesh $T := T_0$

Discretization w.r.t. $T$

Local refinement $T := Ref(T)$

Multigrid solution

- coarse grid generator
- finite element discretisation
- (iterative) algebraic solver
- a posteriori error estimate
- local refinement indicators
- local marking and refinement strategy

$\text{Error} < TOL$
Adaptive Multilevel Methods

- coarse grid generator
- finite element discretisation
- (iterative) algebraic solver
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- local refinement indicators
- local marking and refinement strategy

quasioptimal error estimate:

\[ \|u - u_j\|_1 \leq cn_j^{-1/d} \]
Phase Transition
Hierarchical A Posteriori Error Estimators

extended ansatz space: \( Q_h = S \oplus V_h \)

(hopefully) better discretization: \( u_Q^h \in Q_h : \quad a(u_Q^h, v) = \ell(v) \quad \forall v \in Q_h \)

basic idea: \( \| u_Q^h - u_h \|_1 \approx \| u - u_h \|_1 \)

algorithmic realization:

basis of \( V_h \): \( V_h = \text{span}\{\mu_e \mid e \in E_h\} \) (quadratic bubbles)

weighted residuals: \( \eta_e = \frac{r(\mu_e)}{a(\mu_e, \mu_e)}, \quad r(\mu_e) = \ell(\mu_e) - a(\mu_e, \mu_e), \quad e \in E_h \)

Theorem (Deuflhard, Leinen & Yserentant 88)

The saturation assumption: \( \| u - u_Q^h \|_1 \leq q \| u - u_h \|_1, \quad q < 1 \)

implies the error bounds: \( c\eta \leq \| u - u_h \|_1 \leq C\eta, \quad \eta = \sum_{e \in E_h} \eta_e \)
Adaptive Refinement Strategy

Local errors have local origin (wrong for transport equations!):

\[ \eta_e \geq \theta \implies \text{mark all } T \text{ with } T \cap e \neq \emptyset \text{ for 'red' refinement!} \]

'green' closures:
Stable Refinement in 3D

'red' refinement: What to do with the remaining octahedron?
Stable Refinement in 3D

’red’ refinement: What to do with the remaining octahedron?

Learn from crystallography (Bey 91)!
Linear Algebraic Solvers

stiffness matrix \( A = (a(\lambda_p, \lambda_q))_{p,q \in N_h} \)

\( A \) is symmetric, positive definite and sparse

condition number: \( \frac{1}{\mathcal{O}(1)} \leq \kappa(A) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} \leq \mathcal{O}(h^{-2}) \)

\( A \) is arbitrarily ill-conditioned for \( h \to 0 \)

Corollary:

Use iterative solvers for small \( h \) or, equivalently, large \( n \) \((n \geq 20 \ 000 - 50 \ 000)\)
Conjugate Gradient (CG) Iteration

Underlying idea: inductive construction of an $A$-orthogonal basis of $\mathbb{R}^n$

Algorithm (Hestenes und Stiefel, 1952)

initialization: $U^0 \in \mathbb{R}^n$, $r_0 = b - AU^0$, $e_0 = r_0$

iteration: $U^{k+1} = U^k + \alpha_k e_k$, $\alpha_k = \frac{\langle r_k, r_k \rangle}{\langle e_k, Ae_k \rangle}$

update: $r_k \rightarrow r_{k+1}$, $e_k \rightarrow e_{k+1}$

error estimate:

$$\|U - U^k\| \leq 2\rho^k \|U - U^0\|, \quad \rho = \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1}$$

Corollary: Slow convergence for $\kappa(A) \gg 1$
Preconditioned Conjugate Gradient (CG) Iteration

Underlying idea: inductive construction of an $A$-orthogonal basis of $\mathbb{R}_n$

Algorithm (Hestenes und Stiefel 1952)

initialization: $U^0 \in \mathbb{R}^n$, $r_0 = B(b - AU^0)$, $e_0 = r_0$

iteration: $U^{k+1} = U^k + \alpha_k e_k$, $\alpha_k = \frac{\langle r_k, Br_k \rangle}{\langle e_k, Ae_k \rangle}$

update: $r_k \rightarrow r_{k+1}$, $e_k \rightarrow e_{k+1}$

error estimate:

$$\|U - U^k\| \leq 2\rho^k \|U - U^0\|,$$

$$\rho = \frac{\sqrt{\kappa(BA)} - 1}{\sqrt{\kappa(BA)} + 1}$$

Corollary: Fast convergence for $\kappa(BA) \approx 1$

preconditioner $B$: optimal complexity $O(n_j)$ and $B \approx A^{-1}$
Subspace Correction Methods

basic idea: solve many small problems instead of one large problem

subspace decomposition: \( S_h = V_0 + V_1 + \cdots + V_m \)

Algorithm (successive subspace correction) Xu 92

\[
\begin{align*}
w_{-1} &= u^k \\
v_l &\in V_l : \quad a(v_l, v) = \ell(v) - a(w_{l-1}, v) \quad \forall v \in V_l \quad w_l = w_{l-1} + v_l \\
u^{k+1} &= w_m
\end{align*}
\]

- Gauß-Seidel iteration: \( V_p = \text{span}\{\lambda_p\} \) \quad \rho_h = 1 - O(h^{-2})

- Jacobi-iteration: parallel subspace correction \quad \rho_h = 1 - O(h^{-2})

- domain decomposition, multigrid, \ldots \quad \rho_h \leq \rho < 1 \quad \text{BPXW 93}
Multigrid Methods

hierarchy of grids (adaptive refinement!): $\mathcal{T}_0 \subset \mathcal{T}_1 \subset \cdots \subset \mathcal{T}_j = \mathcal{T}_h$

hierarchy of frequencies: $\mathcal{S}_0 \subset \mathcal{S}_1 \subset \cdots \subset \mathcal{S}_j = \mathcal{S}_h$

multilevel decomposition: $\mathcal{S}_h = \sum_{k=0}^{j} \sum_{p \in \mathcal{N}_k} \mathcal{V}_p^{(k)}$, $\mathcal{V}_p^{(k)} = \text{span}\{\lambda_p^{(k)}\}$

multigrid method with Gauß-Seidel smoothing and Galerkin restriction
Poisson’s Equation on the Unit Square

\[ \Omega = (0, 1) \times (0, 1), \quad f \equiv 1, \quad V(1, 0) \text{ cycle, symmetric Gauß-Seidel smoother} \]

coarse grid \( T_0 \)

approximate solution

convergence rates:

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<th>( \rho_j )</th>
<th>( j=2 )</th>
<th>( j=3 )</th>
<th>( j=4 )</th>
<th>( j=5 )</th>
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### Approximation History (L-Shaped Domain)

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Uncertain Data

uncertainty of permeability, source terms, boundary conditions, ...

• by lack of sufficiently accurate measurements

• by external sources

random Darcy equation:

\[ S_0 p_t(t, x, \theta) = \text{div}(K(x, \theta) \nabla p(t, x, \theta)) + f(x, \theta), \quad \theta \in \Theta, \]

probability space \((\Theta, \mathcal{A}, P)\).
Random Partial Differential Equations

random Darcy equation:

\[ S_0 p_t(t, x, \theta) = \text{div}(K(x, \theta)\nabla p(t, x, \theta)) + f(x, \theta) \]

desired statistics of solutions:

- expectation value \( E[p] := \int_{\Theta} p \, dP \)
- variance \( E[(p - E[p])^2] \)
- probability of particular events \( P[\int_{\Omega} p(t, x, \theta) \, dx < 0 \text{ for } t < 1] \)
Numerical Approximation of Random PDEs

Monte-Carlo Method:

(i) generate $N$ independent, $P$-equidistributed samples $\theta_1, \ldots, \theta_N$.

(ii) compute approximations of the $N$ solutions for the samples $\theta_1, \ldots, \theta_N$.

(iii) compute the corresponding expectation value, variance, ....

advantage: always feasible and simple
disadvantage: convergence rate $\frac{1}{\sqrt{N}} \implies N$ has to be very large
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Multilevel Monte Carlo methods:
solve random PDEs with almost deterministic computational cost!