# 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)

$$S_0 p_t = \mathrm{div}(K \nabla p) + f$$

$p$: pressure

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

$K = (K_1, K_2, K_3) : \Omega \to \mathbb{R}^{3,3}$: hydraulic permeability

$f = \rho g \mathrm{div} K_3 + gF$: gravity and source terms

# Darcy's and Poisson's Equation

Darcy's equation:

$S_0 = 0$: pressure-stable granular structure

$$-\mathrm{div}(K\nabla p) = f$$

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Poisson's equation:

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

transformation of variables: $p(x) \hookrightarrow p(Kx) =: u(x)$

$$-\Delta u = f$$

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)

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

boundary conditions (BC):

| | | |
|---|---|---|
| $u = g$ | pressure BC | (Dirichlet BC, 1. kind) |
| $\alpha u + \beta \frac{\partial}{\partial n} u = g$ | transmission BC | (Robin BC, 3. kind) |

Theorem (well-posedness)

Assumption: $\Omega$, $f$, $g$ sufficiently smooth.

Assertion: There exists a unique solution $u \in C^2(\Omega) \cap C(\overline{\Omega})$ and $u$ depends continuously on $f$, $g$.

# Ill-Posed Problems

flux boundary conditions:

$\frac{\partial}{\partial n}u = g$ outflow BC (Neumann BC, 2. kind)

no uniqueness: $u$ solution $\Longrightarrow$ $u + c$ 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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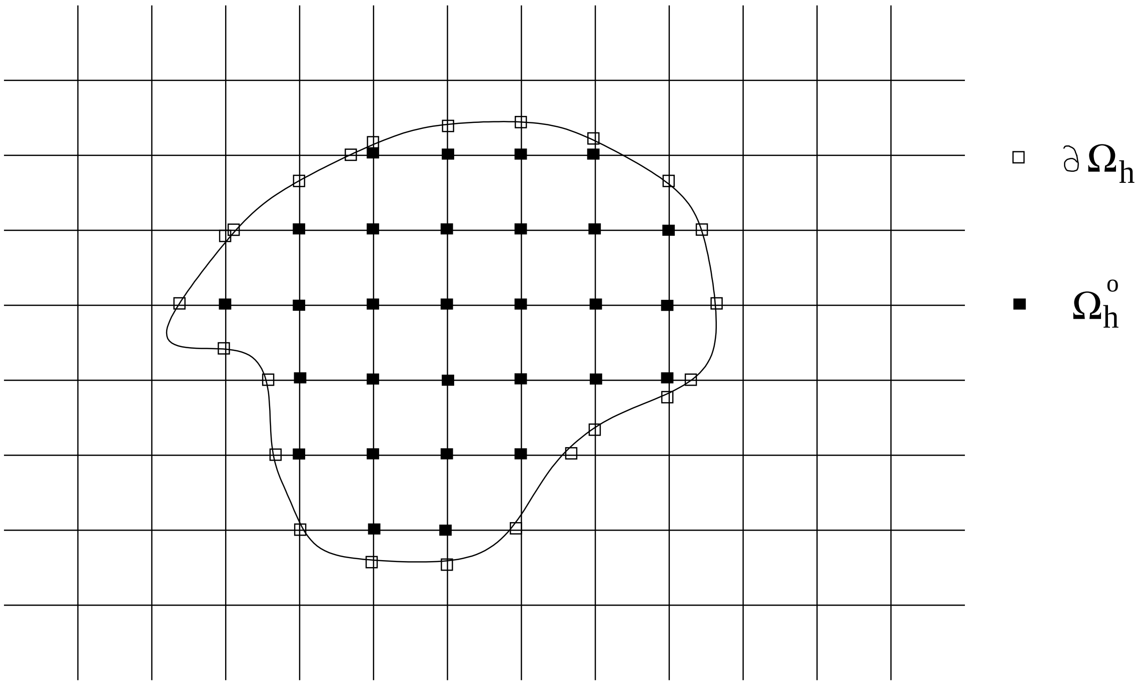
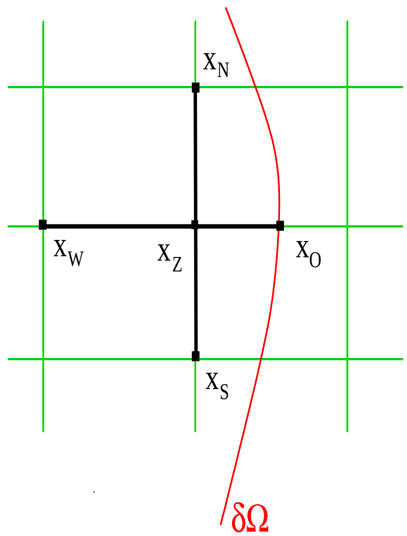
Caution: $\Gamma_D$ too small, e.g. $\Gamma_D = \{x_0, x_1, .., x_m\}$, $\Rightarrow$ no uniqueness!!

# 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:

$$-\Delta_h U = f \quad \text{on } \Omega_h^\circ, \qquad U(x) = g \quad \text{on } \partial\Omega_h$$

linear system: $A^{\mathrm{FD}}\overline{U} = b$

Theorem (Convergence):

Assumption: $u \in C^3(\overline{\Omega})$.

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

# 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: $\operatorname{div}(K \nabla u) = f$ on $\Omega$

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- 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:

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

Darcy's equation:

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

# Finite Volumes

finite dimensional ansatz space: $\mathcal{S}_h$, dim $\mathcal{S}_h = n$, $v|_{\partial\Omega} = 0 \quad \forall v \in \mathcal{S}_h$

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

finite volume discretization:

$$u_h \in \mathcal{S}_h : \quad -\int_{\partial\Omega_i} K \frac{\partial}{\partial n} u_h \, d\sigma = \int_{\Omega_i} f \, dx \quad \forall i = 1, \ldots, n$$

linear system:

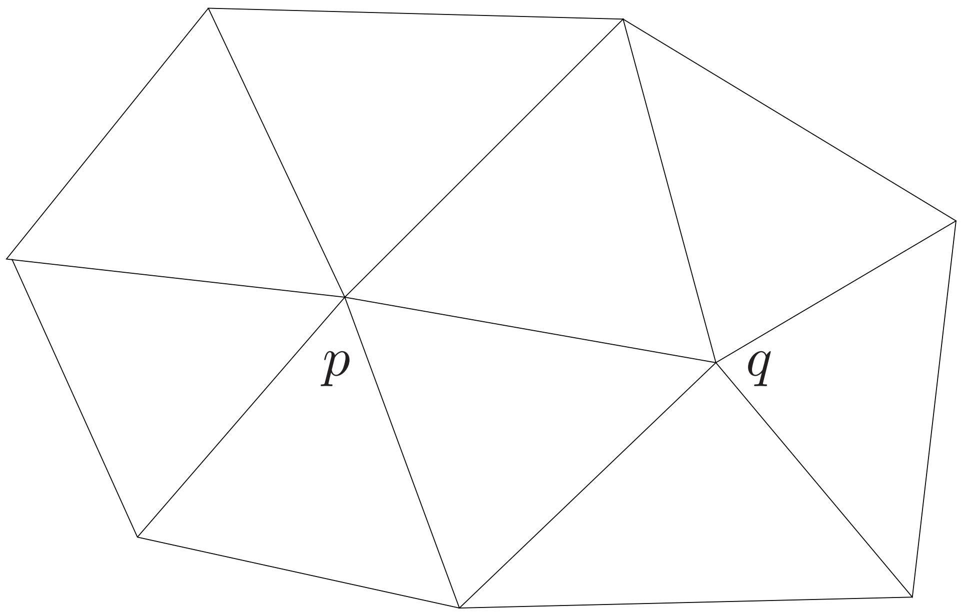
choice of basis: $\mathcal{S}_h = \text{span}\{\varphi_i \mid i = 1, \ldots, n\}$

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

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

# Choice of Ansatz Space

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

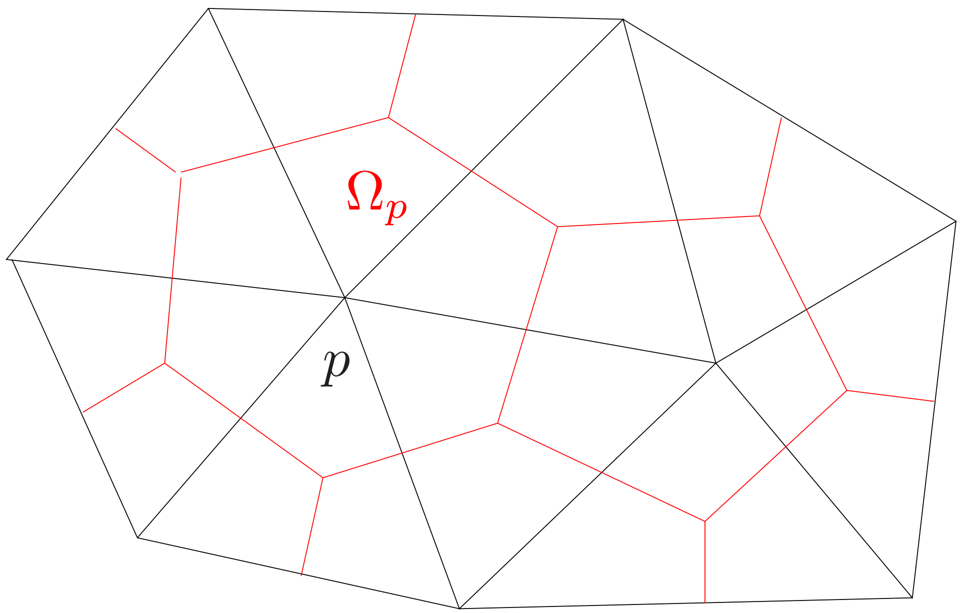



linear finite elements: $\mathcal{S}_h := \{v \in C(\overline{\Omega}) \mid v|_T \text{ linear } \forall T \in \mathcal{T}_h,\ v|_{\partial\Omega} = 0\}$

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

# Vertex-Centered Finite Volumes

control volumes: linear connection of barycenters




linear system:

$$A^{\mathrm{FV}}\overline{u}_h = b^{\mathrm{FV}}, \qquad u_h = \sum_{p\in\mathcal{N}_h} u_p\lambda_p$$

# Principle of Minimal Energy

quadratic energy functional:

$$\mathcal{J}(v) = \tfrac{1}{2}a(v,v) - \ell(v), \qquad a(v,w) = \int_\Omega K \nabla v \nabla w \; dx, \quad \ell(v) = \int_\Omega f v \; dx$$

minimization problem:

$$u \in H_0^1(\Omega): \quad \mathcal{J}(u) \leq \mathcal{J}(v) \quad \forall v \in H_0^1(\Omega)$$

variational formulation:

$$u \in H_0^1(\Omega): \quad \mathcal{J}'(u)(v) = a(u,v) - \ell(v) = 0 \quad \forall v \in H_0^1(\Omega)$$

weak solution $u \in H_0^1(\Omega)$ (Sobolev space)

# Weak Versus Classical Solution

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

Green's formula:

$$0 = a(u,v) - \ell(v) = -\int_\Omega (\operatorname{div}(K\nabla u) + f)v \, dx + \int_{\partial\Omega} \left(K\tfrac{\partial}{\partial n}u\right) v \, d\sigma$$

suitable choice of test functions $v \in C_0^1(\overline{\Omega})$:

$$-\operatorname{div}(K\nabla u) = f \qquad \text{on } \Omega$$

# Ritz-Galerkin Method

finite dimensional ansatz space: $\mathcal{S}_h \subset H_0^1(\Omega)$, dim $\mathcal{S}_h = n$

Ritz-Galerkin method

$$u_h \in \mathcal{S}_h : \quad \mathcal{J}'(u_h)(v) = a(u_h, v) - \ell(v) = 0 \quad \forall v \in \mathcal{S}_h$$

linear system:

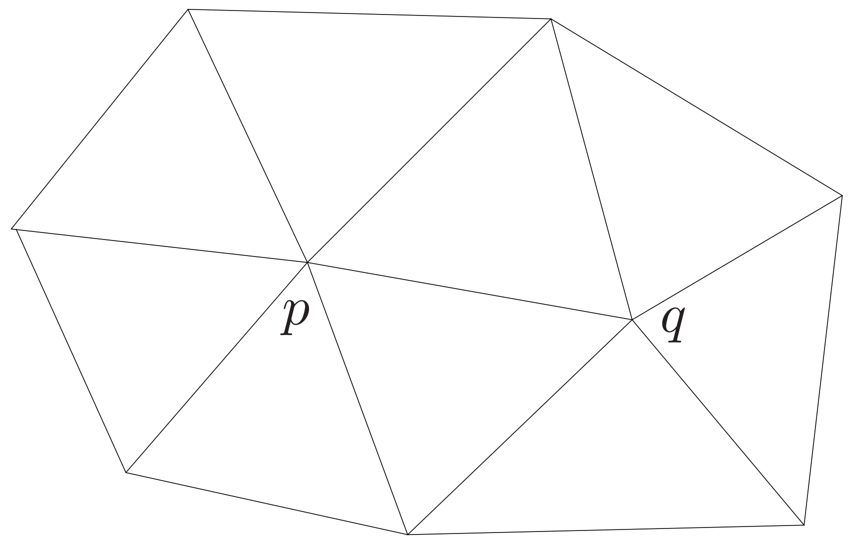
choice of basis: $\mathcal{S}_h = \text{span}\{\varphi_i \mid i = 1, \dots, n\}$

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

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

nodal basis: $\lambda_p(q) = \delta_{p,q}, \quad p, q \in \mathcal{N}_h$ linear system: $A^{\mathrm{FE}} \overline{u}_h = b^{\mathrm{FE}}$

# Finite Elements Versus Finite Volumes

Theorem (Hackbusch 89)

$$A^{\mathrm{FV}} = A^{\mathrm{FE}}, \qquad |b^{\mathrm{FV}} - b^{\mathrm{FE}}|_{-1} = \mathcal{O}(h^2)$$

Corollary:

$$\|u_h^{\mathrm{FV}} - u_h^{\mathrm{FE}}\|_1 = \mathcal{O}(h^2), \qquad \|v\|_1^2 = \int_\Omega v^2 + |\nabla v|^2 \, dx$$

in general:

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

# Stability

maximum principle:

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

$$f_1 \geq f_2 \quad \Longrightarrow \quad u_1 \geq u_2$$

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$$f_1 \geq f_2 \quad \Longrightarrow \quad u_1 \geq u_2$$

no discrete maximum principle:

$$A^{\mathrm{FE}}\overline{u}_1 = b_1^{\mathrm{FE}}, \quad A^{\mathrm{FE}}\overline{u}_2 = b_2^{\mathrm{FE}}$$

$$b_1^{\mathrm{FE}} \geq b_2^{\mathrm{FE}} \quad \not\Longrightarrow \quad \overline{u}_1 \geq \overline{u}_2$$

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"bad" angles of triangles might cause oscillations!

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"bad" angles of triangles might cause oscillations!

remedy: Delaunay triangulation $\mathcal{T}_h$

# Discretization Error

Galerkin orthogonality: $a(u - u_h, v) = 0 \quad \forall v \in \mathcal{S}$

optimal error estimate:

$$\|u - u_h\| = \inf_{v \in \mathcal{S}_h} \|u - v\|, \qquad \|v\|^2 = a(v, v) \quad \text{(energy norm)}$$

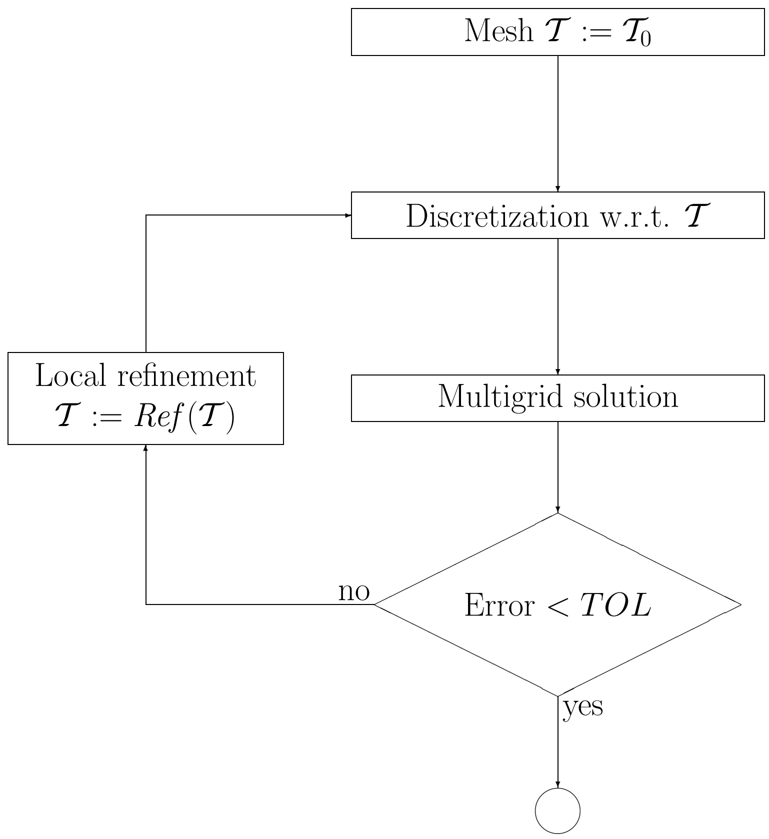
ellipticity: $\alpha \|v\|_1 \le \|v\| \le \beta \|v\|_1, \quad \alpha, \beta > 0, \quad \forall v \in H_0^1(\Omega)$

quasioptimal error estimate: $\|u - u_h\|_1 \le \frac{\beta}{\alpha} \inf_{v \in \mathcal{S}_h} \|u - v\|_1$

estimate of the discretization error

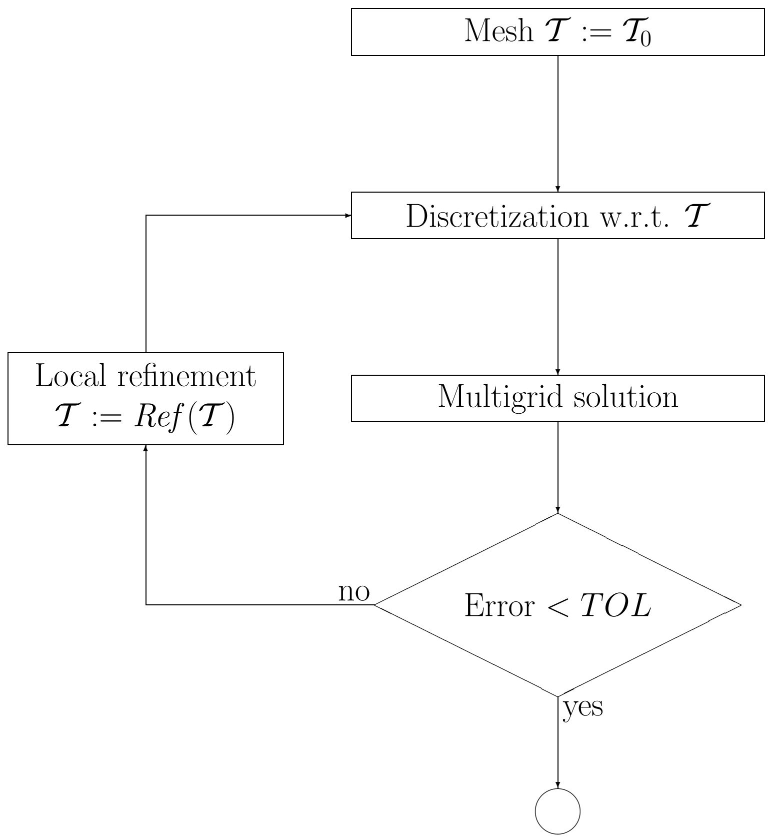
$$\inf_{v \in \mathcal{S}_h} \|u - v\|_1 \le c \|u\|_2 h = \mathcal{O}(h), \qquad c = c(\mathcal{T}_h)$$

# Adaptive Multilevel Methods




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

# Adaptive Multilevel Methods




- coarse grid generator
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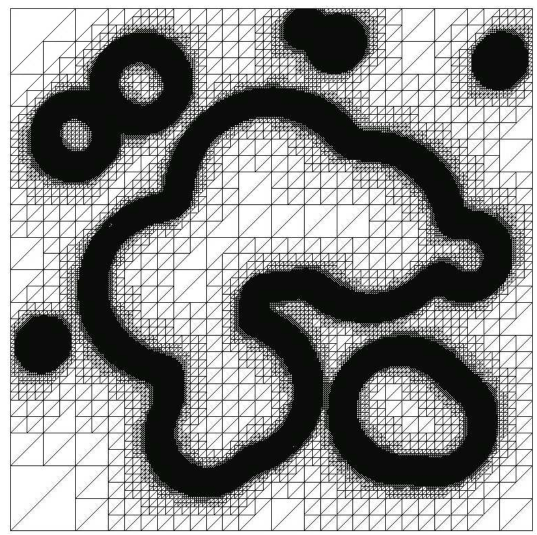
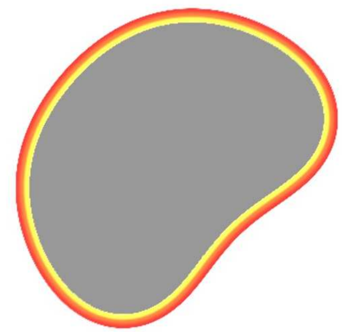
quasioptimal error estimate: $\|u - u_j\|_1 \leq c n_j^{-1/d}$

# Phase Transition





# Hierarchical A Posteriori Error Estimators

extended ansatz space: $\mathcal{Q}_h = \mathcal{S} \oplus \mathcal{V}_h$

(hopefully) better discretization: $u_h^{\mathcal{Q}} \in \mathcal{Q}_h: \quad a(u_h^{\mathcal{Q}}, v) = \ell(v) \quad \forall v \in \mathcal{Q}_h$

basic idea: $\|u_h^{\mathcal{Q}} - u_h\|_1 \approx \|u - u_h\|_1$

algorithmic realization:

basis of $\mathcal{V}_h$: $\mathcal{V}_h = \text{span}\{\mu_e \mid e \in \mathcal{E}_h\}$ (quadratic bubbles)

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

Theorem (Deuflhard, Leinen & Yserentant 88)

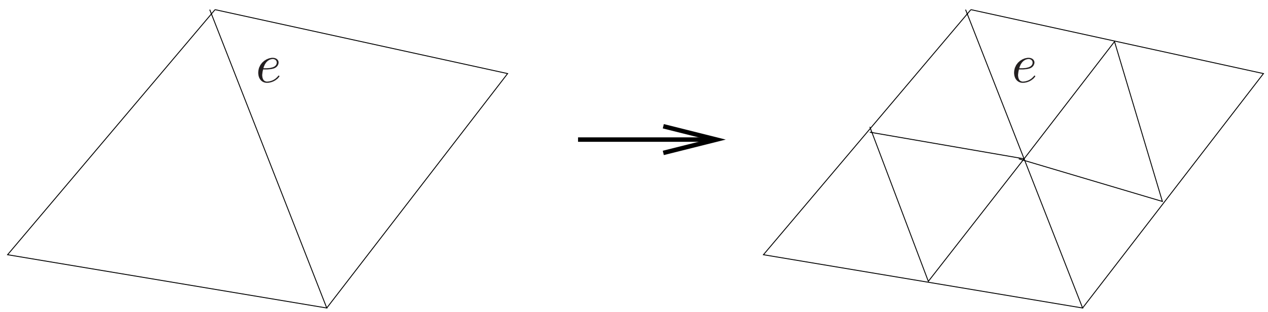
The saturation assumption: $\|u - u_h^{\mathcal{Q}}\|_1 \leq q\|u - u_h\|_1, \quad q < 1,$

implies the error bounds: $c\eta \leq \|u - u_h\|_1 \leq C\eta, \qquad \eta = \sum_{e \in \mathcal{E}_h} \eta_e$

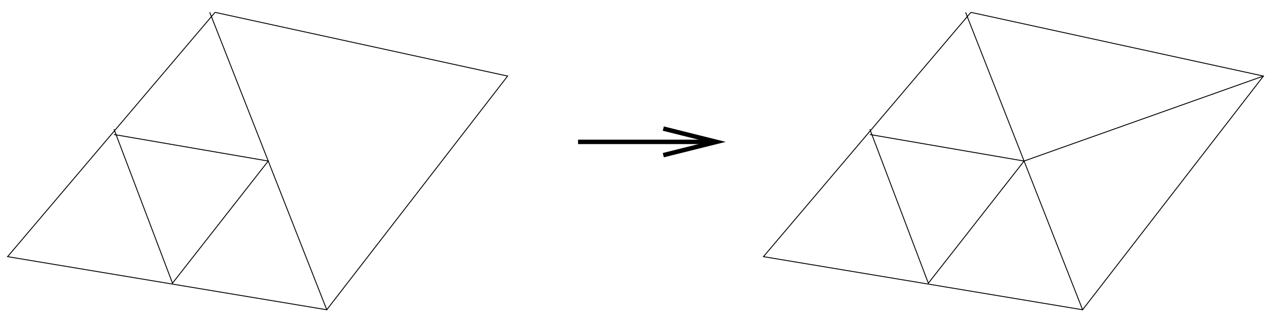
# Adaptive Refinement Strategy

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

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

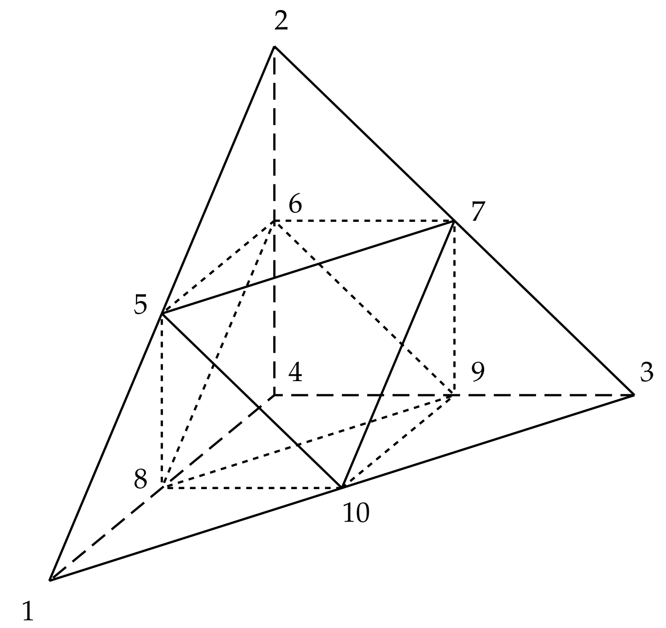



'green' closures:



# Stable Refinement in 3D

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



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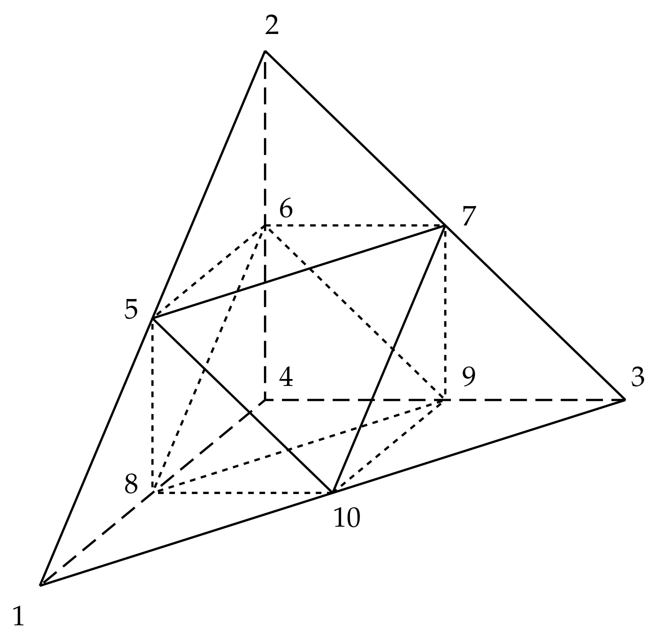



Learn from crystallography (Bey 91)!

# Linear Algebraic Solvers

stiffness matrix $A = (a(\lambda_p, \lambda_q))_{p,q \in \mathcal{N}_h}$

$A$ is symmetric, positive definite and sparse

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

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

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

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

error estimate:

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

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

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

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

error estimate:

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

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

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

# Subspace Correction Methods

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

subspace decomposition: $\mathcal{S}_h = \mathcal{V}_0 + \mathcal{V}_1 + \cdots + \mathcal{V}_m$

Algorithm (sucessive subspace correction) Xu 92

$$w_{-1} = u^k$$

$$v_l \in \mathcal{V}_l : \quad a(v_l, v) = \ell(v) - a(w_{l-1}, v) \quad \forall v \in \mathcal{V}_l \qquad w_l = w_{l-1} + v_l$$

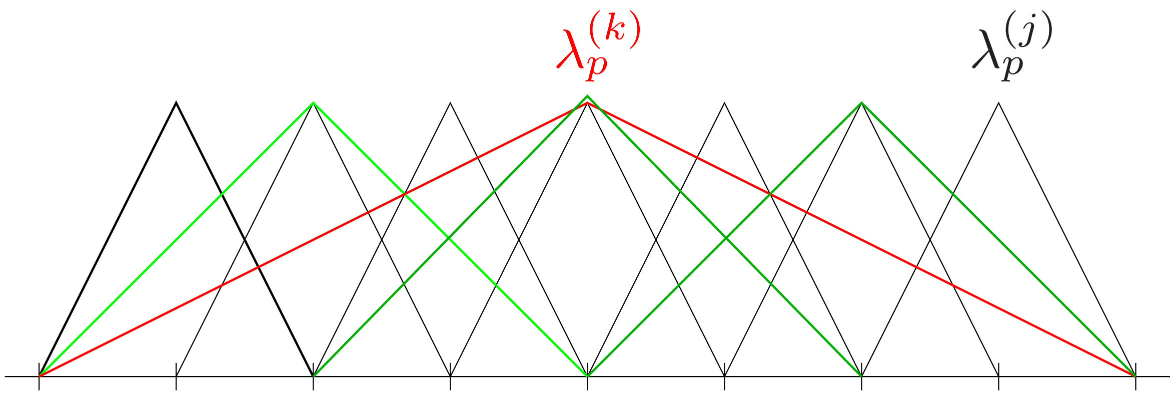
$$u^{k+1} = w_m$$

- Gauß-Seidel iteration: $\mathcal{V}_p = \text{span}\{\lambda_p\}$ $\qquad \rho_h = 1 - \mathcal{O}(h^{-2})$
- Jacobi-iteration: parallel subspace correction $\qquad \rho_h = 1 - \mathcal{O}(h^{-2})$
- domain decomposition, multigrid, . . . $\qquad \rho_h \leq \rho < 1$ 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: $\mathcal{S}_0 \subset \mathcal{S}_1 \subset \cdots \subset \mathcal{S}_j = \mathcal{S}_h$

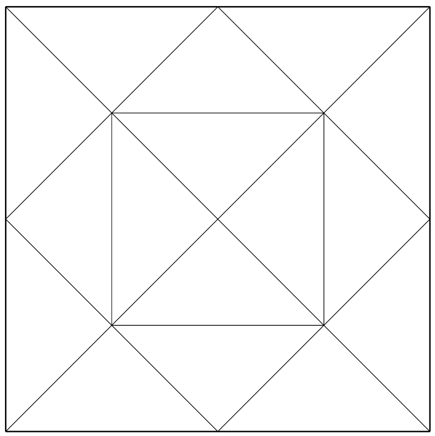



multilevel decomposition: $\mathcal{S}_h = \sum_{k=0}^{j} \sum_{p \in \mathcal{N}_k} \mathcal{V}_p^{(k)}, \qquad \mathcal{V}_p^{(k)} = \text{span}\{\lambda_p^{(k)}\}$

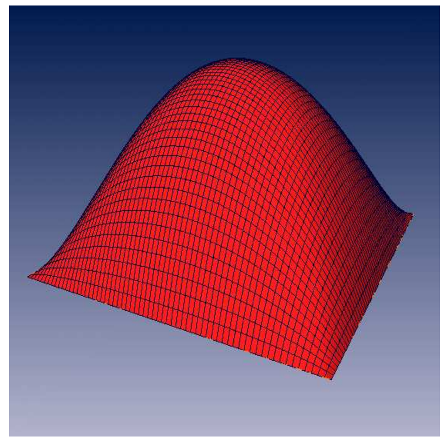
multigrid method with Gauß-Seidel smoothing and Galerkin restriction

# Poisson's Equation on the Unit Square

$\Omega = (0,1) \times (0,1)$, $f \equiv 1$, $V(1,0)$ cycle, symmetric Gauß-Seidel smoother



coarse grid $\mathcal{T}_0$



approximate solution

convergence rates:

| | j=2 | j=3 | j=4 | j=5 | j=6 | j=7 |
|---|---|---|---|---|---|---|
| $\rho_j$ | 0.28 | 0.30 | 0.31 | 0.32 | 0.33 | 0.33 |

# Approximation History (L-Shaped Domain)

| levels | nodes | iterations | est. error | est. error$/n_j^{-1/2}$ |
|---:|---:|:---:|:---:|:---:|
| 0 | 8 | — | 0.34985 | 0.989 |
| 1 | 21 | 2 | 0.21165 | 0.969 |
| 2 | 65 | 2 | 0.11978 | 0.965 |
| 3 | 225 | 2 | 0.06441 | 0.966 |
| 4 | 833 | 2 | 0.03427 | 0.989 |
| 5 | 2.359 | 2 | 0.02185 | 1.061 |
| 6 | 3.320 | 2 | 0.01672 | 0.963 |
| 7 | 4.118 | 2 | 0.01505 | 0.966 |
| 8 | 10.032 | 2 | 0.01002 | 1.003 |
| 9 | 13.377 | 2 | 0.00805 | 0.931 |
| 10 | 16.369 | 2 | 0.00742 | 0.950 |
| 11 | 40.035 | 2 | 0.00494 | 0.989 |
| 12 | 53.188 | 2 | 0.00399 | 0.921 |
| 13 | 64.647 | 2 | 0.00371 | 0.943 |
| 14 | 159.064 | 2 | 0.00247 | 0.986 |

# Uncertain Data

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

- by lack of sufficiently accurate measurements
- by external sources

random Darcy equation:

$$S_0 p_t(t,x,\theta) = \operatorname{div}(K(x,\theta)\nabla p(t,x,\theta)) + f(x,\theta), \qquad \theta \in \Theta,$$

probability space $(\Theta, \mathcal{A}, P)$.

# Random Partial Differential Equations

random Darcy equation:

$$S_0 p_t(t,x,\theta) = \mathrm{div}(K(x,\theta)\nabla p(t,x,\theta)) + f(x,\theta)$$

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 $\theta_1$,. . . ,$\theta_N$.

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

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

advantage: always feasible and simple
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Multilevel Monte Carlo methods:
solve random PDEs with almost deterministic computational cost!