Numerical Solution II
Instationary Flow and Trasport

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Summerschool
"Modelling of mass and energy transport in porous media with practical applications"

Schedule

Instationary diffusion

- Method of lines: stability
- Finite differences: consistency, stability, and convergence

Instationary diffusion and convection

- Finite differences: stability and artificial viscosity

Unsaturated ground water flow: Richards equation

- Nonlinear algebraic systems
- Monotone multigrid

Instationary Diffusion

Instationary Darcy flow

$$S_0 p_t = \operatorname{div}(K \nabla p) + f, \qquad \text{specific storage coefficient } S_0 = \rho g \tfrac{\partial n}{\partial p} > 0$$

Heat equation

$$u_t = \operatorname{div}(D_T \nabla u), \quad D_T = \tfrac{\lambda}{c\rho} \quad \text{in } \Omega$$

Boundary conditions $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_R$

$$u|_{\Gamma_D} = g_D, \quad D_T \tfrac{\partial}{\partial n} u|_{\Gamma_N} = g_N, \quad \alpha u + \beta \tfrac{\partial}{\partial n} u|_{\Gamma_R} = g_R,$$

Initial conditions

$$u(x,0) = u_0(x) \quad \text{in } \Omega$$

Method of Lines

Weak formulation

Find $u \in H = C([0,T], L^2(\Omega)) \cap L^2((0,T), H_0^1(\Omega))$:

$$\frac{d}{dt}(u,v) + a(u,v) = \ell(v) \quad \forall v \in H_0^1(\Omega)$$

Theorem

If u_0, f are sufficiently smooth, then there is a unique solution u.

Semi-discretization in space

Let $\mathcal{S}_h \subset H_0^1(\Omega)$. Find $u_h \in C^1([0,T], \mathcal{S}_h)$:

$$\frac{d}{dt}(u_h,v) + a(u_h,v) = \ell(v) \quad \forall v \in \mathcal{S}_h$$

Theorem

If $\mathcal{S}_h$ is the space of piecewise linear finite elements, then

$$u \in C^1([0,T], H_0^1(\Omega) \cap H^2(\Omega)) \quad \Longrightarrow \quad \max_{t \in [0,T]} \|u(t) - u_h(t)\| = \mathcal{O}(h)$$

System of Ordinary Differential Equations

Select a basis

$$\mathcal{S}_h = \{\text{span}\{\varphi_p \mid p \in \mathcal{N}_h\}, \qquad u_h(t) = \sum_{p \in \mathcal{N}_h} u_p(t)\varphi_p$$

Insert basis representation

$$M^* U'(t) + AU(t) = b, \qquad U(t) = (u_p(t))_{p \in \mathcal{N}_h}$$

- stiffness matrix: $A = (a(\varphi_p, \varphi_q))_{p,q \in \mathcal{N}_h}$
- mass matrix: $M^* = ((\varphi_p, \varphi_q))_{p,q \in \mathcal{N}_h}$
- lumping: $M^* \to M = (m_{p,q})_{p,q \in \mathcal{N}_h}$ (diagonal matrix)

$$m_{pq} = \tfrac{1}{3} \sum_{Tr \in \mathcal{T}_h} \sum_{s \in Tr} \varphi_p(s)\varphi_q(s)|Tr| = \begin{cases} \int_\Omega \varphi_p \, dx, & p = q \\ 0 & \text{else} \end{cases}$$

Diagonalization

$$U'(t) = -BU(t) + b, \qquad B = M^{-1}A \quad \text{symmetric, positive definite}$$

Matrix T of eigenvectors

$$T^T BT = D, \qquad D = \mathsf{diag}(\lambda_1(B), \ldots, \lambda_n(B))$$

Diagonalized system

$$V'(t) = -DV(t) + d, \qquad V = T^T U, \quad d = T^T b$$

Decoupled problems

$$v_i'(t) = -\lambda_i(B)v_i(t) + d_i, \quad \lambda_i(B) > 0, \qquad i = 1, \ldots, n$$

Dahlquist's Test Equation

$$v'(t) = -\lambda v(t), \quad v(0) = v_0, \qquad \lambda > 0$$

Unique solution

$$v(t) = v_0 e^{-\lambda t}$$

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$$v(t) = v_0 e^{-\lambda t} \qquad v(t) \to 0 \quad \text{for } t \to \infty$$

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Discretization

$$\tfrac{1}{\Delta t}(v_{j+1} - v_j) = -\lambda(\theta v_{j+1} + (1-\theta)v_j)$$

- implicit Euler scheme: $\theta = 1$
- Crank-Nicolson scheme: $\theta = \frac{1}{2}$
- explicit Euler scheme: $\theta = 0$

Truncation error

$$\tfrac{1}{\Delta t}(v(t_{j+1}) - v(t_j)) + \lambda(\theta v(t_{j+1}) + (1-\theta)v(t_j)) = \begin{cases} \mathcal{O}(\Delta t), & \theta \neq \frac{1}{2} \\ \mathcal{O}(\Delta t^2), & \theta = \frac{1}{2} \end{cases}$$

Stability

Discrete solution

$$v_j = \left(\frac{1 - (1-\theta)\Delta t \lambda}{1 + \theta \Delta t \lambda} \right)^j v_0, \qquad j = 1, \ldots$$

Proper decay (strongly stable):

$$v_j \to 0 \quad \text{for } j \to 0 \quad \Longleftrightarrow \quad R(\Delta t \lambda) = \left| \frac{1 - (1-\theta)\Delta t \lambda}{1 + \theta \Delta t \lambda} \right| < 1$$

- implicit Euler: $R(\Delta t \lambda) = (1 + \Delta t \lambda)^{-1}$ strongly stable
- explicit Euler: time step restriction $\Delta t < \frac{2}{\lambda}$
- Crank-Nicolson: strongly stable, but $R(\Delta t \lambda) \to 1$ for $\lambda \to \infty$

Implications for the Heat Equation

$$U' = -BU + b, \qquad B = M^{-1}A \quad \text{symmetric, positive definite}$$

Eigenvalues

$$1/o(1) \leq \lambda_{\max}(B) \leq \mathcal{O}(h^{-2})$$

- explicit Euler: time step restriction $\Delta t \leq \mathcal{O}(h^2)$
- Crank-Nicolson: bounded oscillations
- implicit Euler: no time step restriction, no oscillations

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Upshot: implicit time discretization + fast spatial solvers

Example: Finite Differences in 1D

Initial-boundary-value problem

$$
\begin{aligned}
u_t &= u_{xx} & (x,t) &\in (0,1)\times(0,T) & &\text{heat equation}\\
u(0,t) &= u(1,t) = 0 & t &\in (0,T] & &\text{boundary condition}\\
u(x,0) &= u_0(x) & x &\in (0,1) & &\text{initial condition}
\end{aligned}
$$

Finite differences

$$u_{xx}(x_i) \approx D_{xx}u(x_i) = \frac{1}{h^2}\left(u(x_{i-1}) - 2u(x_i) + u(x_{i+1})\right)$$

Explicit Euler scheme

$$U_{ij+1} - U_{ij} = \Delta t D_{xx} U_{ij}, \quad U_{0j} = U_{nj} = 0$$

Matrix form

$$U_{j+1} = U_j - \frac{\Delta t}{h^2} A U_j, \qquad A = \begin{pmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix}$$

Convergence

Consistency

$$\|\tau_j\|_\infty = \mathcal{O}(\Delta t + h^2), \quad \tau_{ij} = \frac{1}{\Delta t}(u(x_i, t_{j+1}) - u(x_i, t_j)) - D_{xx}u(x_i, t_j)$$

Stability

$$\Delta t \leq \frac{1}{2}h^2 \quad \Longrightarrow \quad (I - \frac{\Delta t}{h^2}A) \geq 0 \quad \Longrightarrow \quad \|(I - \frac{\Delta t}{h^2}A)\|_\infty = 1$$

Convergence

$$e_{j+1} = \left(I - \frac{\Delta t}{h^2}A\right)e_j + \Delta t \tau_j, \qquad e_j = u(t_j) - U_j$$

$$e_j = \Delta t \sum_{k=1}^{j} \left(I - \frac{\Delta t}{h^2}A\right)^{j-k} \tau_k$$

$$\max_{j=1,\ldots,m} \|e_j\|_\infty \leq \Delta t \sum_{k=1}^{j} \left\|I - \tfrac{\Delta t}{h^2}A\right\|_\infty^{j-k} \|\tau_k\|_\infty \leq \mathcal{O}(\Delta t + h^2)$$

Implicit Euler Scheme

$$U_{ij+1} - U_{ij} = \Delta t D_{xx} U_{ij+1}$$

Matrix form $BU_{j+1} = U_j$

$$B = (I + \frac{\Delta t}{h^2} A) = \begin{pmatrix} \ddots & \ddots & \\ -\frac{\Delta t}{h^2} & +(1 + 2\frac{\Delta t}{h^2}) & -\frac{\Delta t}{h^2} \\ & \ddots & \ddots \end{pmatrix}$$

Theorem (cf., e.g., Hackbusch 1994, p.154)

B satisfies: sign pattern, strongly diagonally dominant
$\Longrightarrow$ *B is an "M-Matrix" (B regular, $B^{-1} > 0$), $\|B^{-1}\|_\infty \leq 1$*

Consequence
Convergence with order $\mathcal{O}(\Delta t + h^2)$

Parameter

$u_t = \varepsilon u_{xx}, \quad u_0 = 4x(1-x), \quad \varepsilon = 0.1,\ h = 1/50$

Time step

explicit Euler: $\Delta t \leq h^2/2\varepsilon = 1/500$, implicit Euler: $\Delta t = h$

unstable unstable

Computing time

explicit Euler: 1.83e-02 sec $>$ implicit Euler: 1.22e-03 sec

Rothe's-Method

Disadvantage of the method of lines

fixed spatial mesh for all times

Change of perspective

ordinary differential equation in Hilbert space

$$u' = -Lu + f, \qquad L : \mathcal{D} \in H_0^1(\Omega) \to H_0^1(\Omega)$$

$$Lu \in H_0^1(\Omega) : \quad (Lu, v) = a(u, v) \quad \forall v \in H_0^1(\Omega)$$

Discretization

- first discretize in time (e.g. by the implicit Euler scheme)
- then (approximate) spatial solution (e.g. by adaptive finite elements)

Transport of mass

$$\rho u_t = \mathrm{div}(D\nabla u) + \beta \cdot \nabla u + \sigma u + f$$

ρ: density

$D \in \mathbb{R}^{d,d}$: diffusion and dispersion

$\beta = \nabla p \in \mathbb{R}^d$: flow field (convection)

σ: adsorption

Convection-diffusion equation

$$u_t = \varepsilon \Delta u + \beta \cdot \nabla u + f$$

Implicit Euler Scheme

Initial-boundary-value problem

$$
\begin{aligned}
u_t &= \varepsilon u_{xx} + u_x \quad && (x,t) \in (0,1) \times (0,T), && \\
u(0,t) &= u(1,t) = 0 && t \in (0,T] && \text{boundary condition} \\
u(x,0) &= u_0(x) && x \in (0,1) && \text{initial condition}
\end{aligned}
$$

Finite differences

$$u_x(x_i) \approx D_x u(x_i) = \frac{1}{2h}\left(u(x_{i+1}) - u(x_{i-1})\right)$$

Implicit Euler scheme

$$U_{ij+1} - U_{ij} = \varepsilon \Delta t D_{xx} U_{ij+1} + \Delta t D_x U_{ij+1}$$

Numerical Experiment

Parameter

$\varepsilon = 0.001, \quad h = 0.01, \quad \Delta t = 0.01$

True solution

Numerical solution

unstable

unstable

Numerical Experiment

Parameter

$\varepsilon = 0.001, \quad h = 0.01, \quad \Delta t = 0.01$

True solution | Numerical solution

unstable

unstable

Unstable!

Implicit Euler Scheme

Initial-boundary-value problem

$$u_t = \varepsilon u_{xx} + u_x \quad (x,t) \in (0,1) \times (0,T),$$

$$u(0,t) = u(1,t) = 0 \qquad t \in (0,T] \qquad \text{boundary condition}$$

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$$u_x(x_i) \approx D_x u(x_i) = \frac{1}{2h}\left(u(x_{i+1}) - u(x_{i-1})\right)$$

Implicit Euler scheme

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Unstable!

Stability Condition

Matrix form $BU_{j+1} = U_j$

$$B = I + \frac{\varepsilon \Delta t}{h^2}(A - C), \qquad C = \begin{pmatrix} 0 & -P & & \\ P & \ddots & \ddots & \\ & \ddots & \ddots & -P \\ & & P & 0 \end{pmatrix}$$

"Peclet number": $P = \frac{h}{2\varepsilon}$

M-Matrix criterion

$$B = \begin{pmatrix} & \ddots & & \ddots & \\ & -\frac{\varepsilon \Delta t}{h^2}(1 - P) & & +(1 + 2\frac{\varepsilon \Delta t}{h^2}) & & -\frac{\varepsilon \Delta t}{h^2}(1 + P) \\ & & & \ddots & & \ddots \end{pmatrix}$$

Sign pattern $P \leq 1 \quad \Longleftrightarrow \quad h \leq 2\varepsilon$

Numerical Experiment

Parameter

$\varepsilon = 0.001, \quad h = 2\varepsilon = 0.002, \quad \Delta t = 0.01 \qquad \Rightarrow P = 1$

unstable

Numerical Experiment

Parameter

$\varepsilon = 0.001, \quad h = 2\varepsilon = 0.002, \quad \Delta t = 0.01 \qquad \Rightarrow P = 1$

unstable

Stable!

Stabilization by Artificial Viscosity

$$U_{ij+1} = U_{ij} + \varepsilon\Delta t(1+P)D_{xx}U_{ij+1} + \Delta t D_x U_{ij+1}, \qquad \text{if } P > 1$$

Matrix form $BU_{j+1} = U_j$

$$B = I + \frac{\varepsilon\Delta t}{h^2}((1+P)A - C), \qquad B = \begin{pmatrix} \ddots & \ddots & \\ -\frac{\varepsilon\Delta t}{h^2} & 1 + 2\frac{\varepsilon\Delta t}{h^2}(1+P) & -\frac{\varepsilon\Delta t}{h^2}(1+2P) \\ & \ddots & \ddots \end{pmatrix}$$

Sign pattern $\implies$ $\|B^{-1}\|_\infty \le 1$ for all $h > 0$

Discretization error estimate

$$\max_{j=1,\dots,m} \|u(t_j) - U_j\|_\infty = \mathcal{O}(\Delta t + h)$$

Outlook

Another perspective

upwind schemes

domain of dependence, **C**ourant-**F**riedrichs-**L**evy (CFL) condition

Extensions to two and three space dimensions

streamline diffusion

finite volumes, discontinuous Galerkin methods, ...

Even more complicated

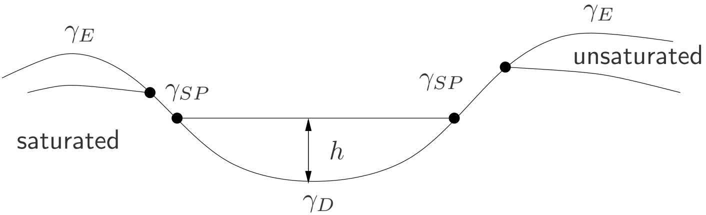
the hyperbolic limit $\varepsilon = 0$

linear and nonlinear conservation laws

Unsaturated Groundwater Flow

Given water table h

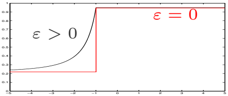
Dam problem



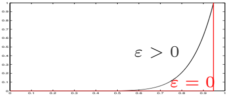
Richards Equation with Solution-Dependent BC

$$\frac{\partial}{\partial t}\theta(p) + \operatorname{div} \mathbf{v}(x,p) = 0, \quad \mathbf{v}(x,p) = -K(x)\kappa\big(\theta(p)\big)\nabla(p - \rho g z)$$

State equation
(Brooks-Corey, van Genuchten)



saturation/capillary pressure: $\theta = \theta_\varepsilon(p)$



relative permeability/saturation $\kappa = \kappa_\varepsilon(\theta)$

Quasilinear degenerate pde
$p > p_b$: elliptic
$p < p_b$: parabolic
$\theta = 0$: hyperbolic

$\varepsilon = 0$: jump discontinuity

Signorini-type boundary conditions

$$p \leq 0, \quad \mathbf{v}\cdot\mathbf{n} \geq 0, \quad \langle \mathbf{v}\cdot\mathbf{n}, p\rangle = 0$$

on $\gamma_S := \gamma_E \cup \gamma_{SP}$

Implicit Time Discretization

Nonlinear algebraic system

$$\theta_h(p_{j+1}) - \theta_h(p_j) + \mathrm{div}\,\big(-K\kappa\big(\theta(p_{j+1})\big)\nabla(p_{j+1} - \rho g z)\big) = 0$$

Solution techniques

- ‘freezing’ of the nonlinearities (Picard-Iteration)
- damped Newton linearization

Lack of robustness coupling of

- smoothness of $\theta(p)$, $\kappa(\theta)$
- time step size
- algebraic convergence speed

Exploit convexity rather than smoothness

Homogeneous state equation

- Kirchhoff transformation
- discretization $\rightarrow$ convex minimization
- multilevel descent method
- discrete inverse Kirchhoff transformation

Piece-wise constant parameters in state equation

- nonlinear domain decomposition

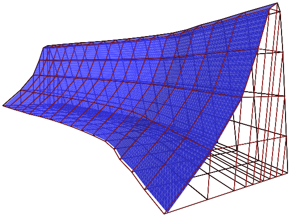
Evolution of a Wetting Front in a Porous Dam

Physical parameters

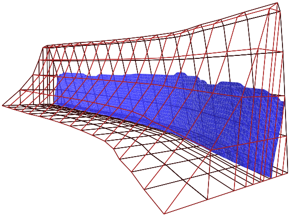
$\Omega = (0,2) \times (0,1)$, sand $\rightarrow \varepsilon,\ \theta_m,\ \theta_M,\ p_b,\ n$

Triangulation

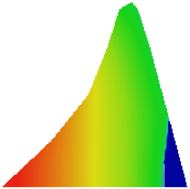
uniformly refined triangulation $\mathcal{T}_4$ (216 849 nodes)



initial wetting front



wetting front for $t = 100s$



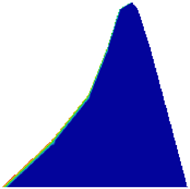
pressure p_j

Efficiency and Robustness of the Multigrid Solver

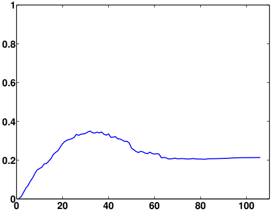
Pre- and postsmoothing steps

V(3,3) cycle

From unsaturated ... ... to saturated



$t = 0$

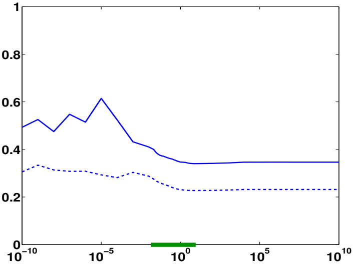


convergence rates ρ over time t

$t = 250s$

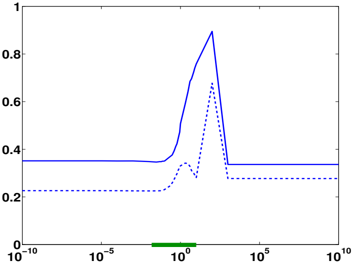
Robustness with Respect to Soil Parameters

variation of ε



$\rho_{\max}$ and ρ_{ave} over ε

variation of $-p_b$



$\rho_{\max}$ and ρ_{ave} over $-p_b$