Numerical Solution II

Instationary Flow and Transport

R. Kornhuber (FU Berlin),

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

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

heat equation

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

boundary conditions:

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

initial conditions: $u(x,0) = u_0(x)$ in Ω

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

choice of 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:

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

Diagonalization

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

matrix T of eigenvectors:

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

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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discretization:

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

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

truncation error:

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

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):

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

- 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:

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

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:

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

stability:

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

convergence:

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

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

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

Implicit Euler Scheme

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

matrix form: $BU_{j+1} = U_j, \quad B = (I + \frac{\Delta t}{h^2} A),$

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

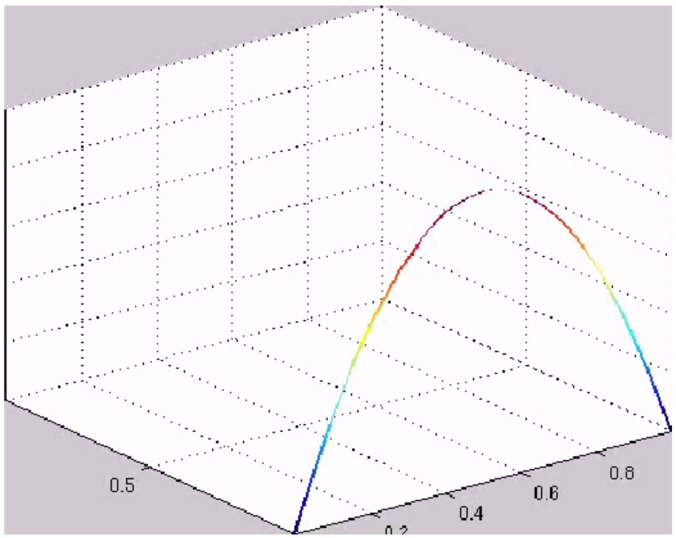
Theorem (cf., e.g., Hackbusch 1994, p.154)
B satisfies: sign pattern, strongly diagonally dominant
$\Longrightarrow$ B is an "M-Matrix" (B regular, $B^{-1} > 0$), $\|B^{-1}\|_\infty \leq 1$

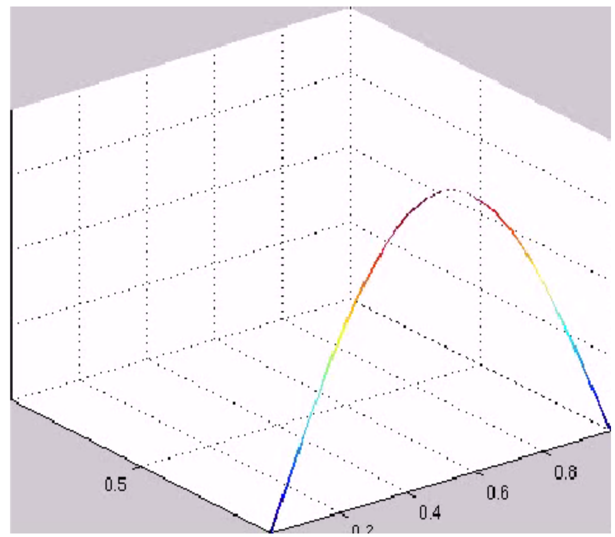
consequence: convergence with order $\mathcal{O}(\Delta t + h^2)$

Numerical Experiments

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

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





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

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

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:

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

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

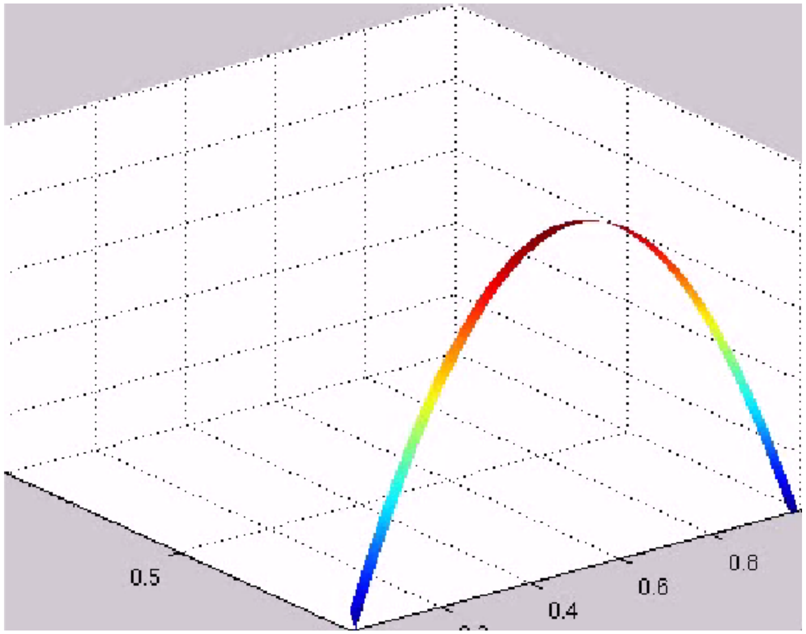
$$u(x,0) = u_0(x) \qquad x \in (0,1) \qquad \text{initial condition}$$

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



Implicit Euler Scheme

initial-boundary-value problem:

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

$$u(0,t) = u(1,t) = 0 \qquad t \in (0,T]$$ initial condition

$$u(x,0) = u_0(x) \qquad x \in (0,1)$$ boundary condition

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

unstable!

Stability Condition

matrix form: $BU_{j+1} = U_j, \quad B = I + \frac{\varepsilon \Delta t}{h^2}(A - C)$

$$C = \begin{pmatrix} 0 & -P & & \\ P & \ddots & \ddots & \\ & \ddots & \ddots & -P \\ & & P & 0 \end{pmatrix} \qquad P = \frac{h}{2\varepsilon} \text{ "Peclet number"}$$

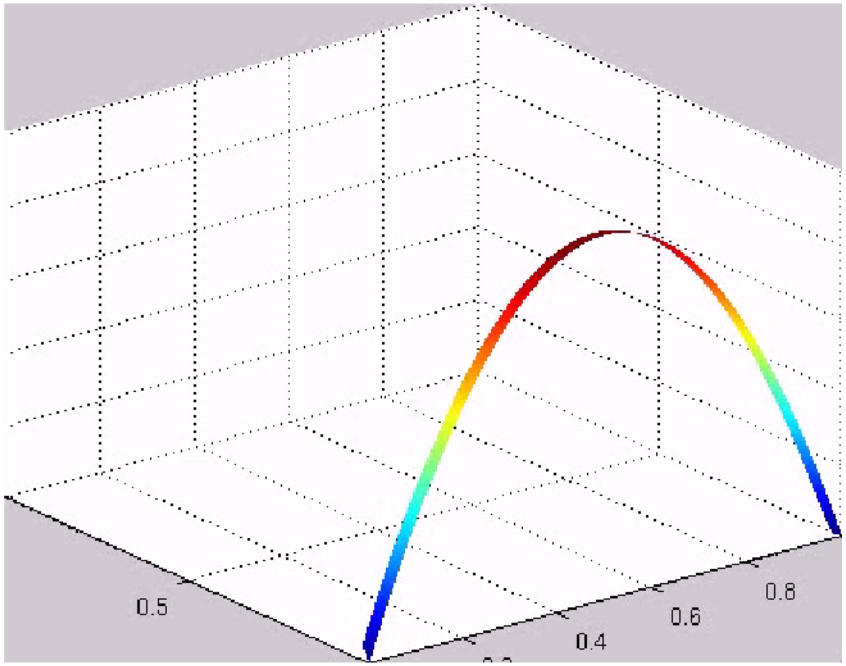
M-Matrix criterion:

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

sign pattern: $P \leq 1 \quad \Longleftrightarrow \quad h \leq 2\varepsilon$

Numerical Experiment

parameter: $\varepsilon = 0.001, \quad h = 2\varepsilon = 0.002, \quad \Delta t = 0.01$



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: $BU_{j+1} = U_j, \quad B = I + \frac{\varepsilon \Delta t}{h^2}((1+P)A - C)$

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

sign pattern $\quad \Longrightarrow \quad \|B^{-1}\|_\infty \leq 1 \quad$ for all $h > 0$

discretization error estimate:

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

Outlook

another perspective: upwind schemes

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

extensions to two and three space dimensions:

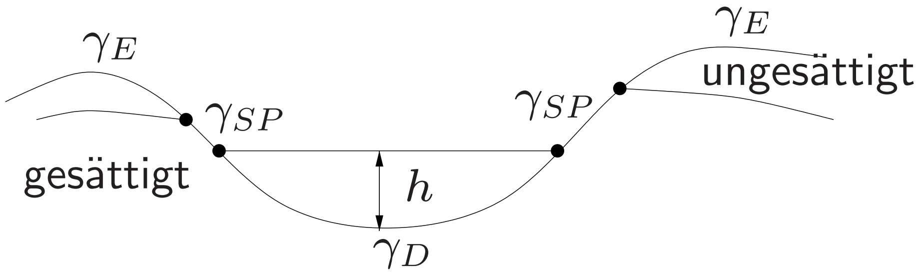
streamline diffusion, finite volumes, discontinuous Galerkin methods, ...

even more complicated: the hyperbolic limit $\varepsilon = 0$

linear and nonlinear conservation laws

Unsaturated Groundwater Flow

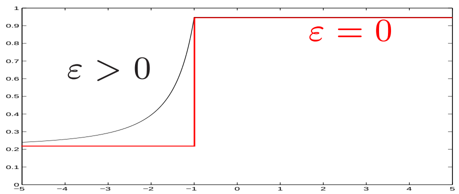
given water table h: dam problem



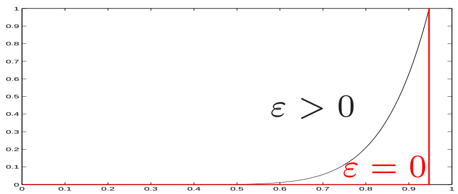
Richards Equation with Solution-Dependent BC

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

state equations: (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:

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

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

Implicit Time Discretization

nonlinear algebraic system

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

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

Monotone Multigrid Methods Berninger, Kornhuber, Sander 09

exploit convexity rather than smoothness:

homogeneous state equation:

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

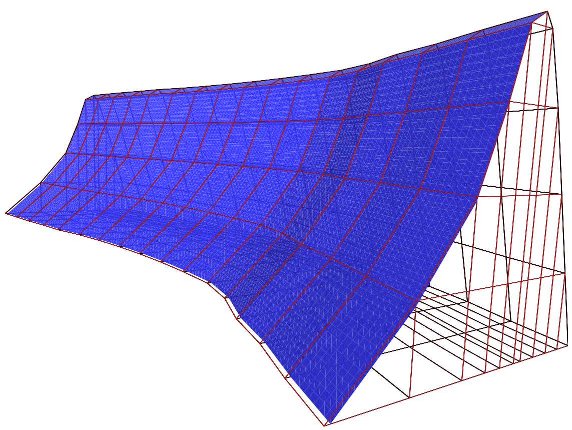
piece-wise constant parameters in state equation:

- nonlinear domain decomposition

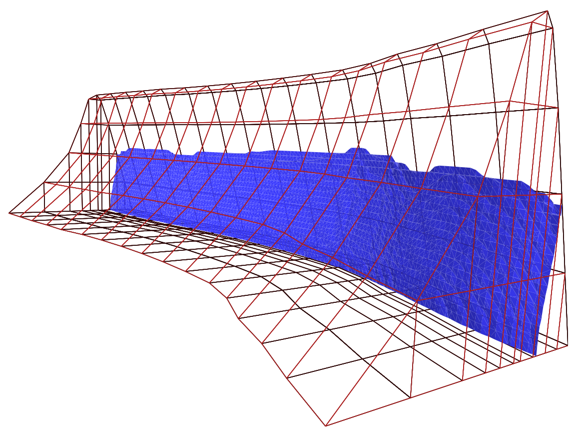
Evolution of a Wetting Front in a Porous Dam

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

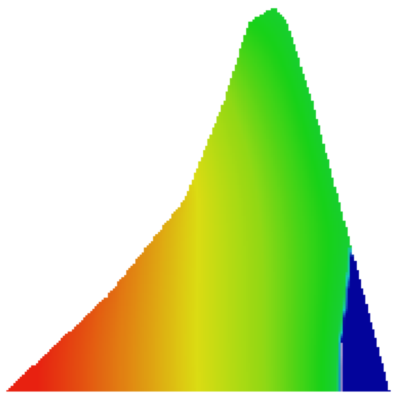
triangulation; uniformly refined triangulation $\mathcal{T}_4$ (216 849 nodes)



initial wetting front



wetting front for $t = 100s$

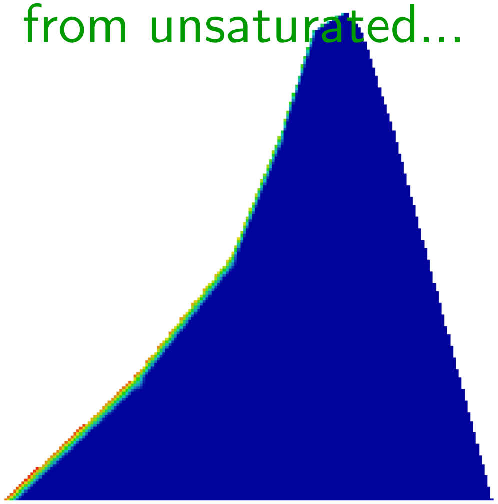


pressure p_j

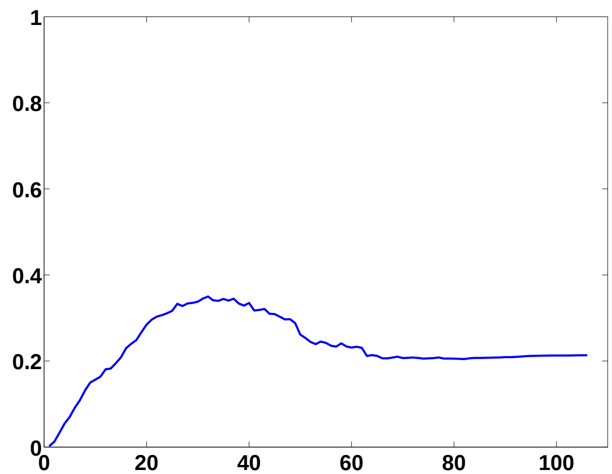
Efficiency and Robustness of the Multigrid Solver

pre- and postsmoothing steps: V(3,3) cycle

from unsaturated...

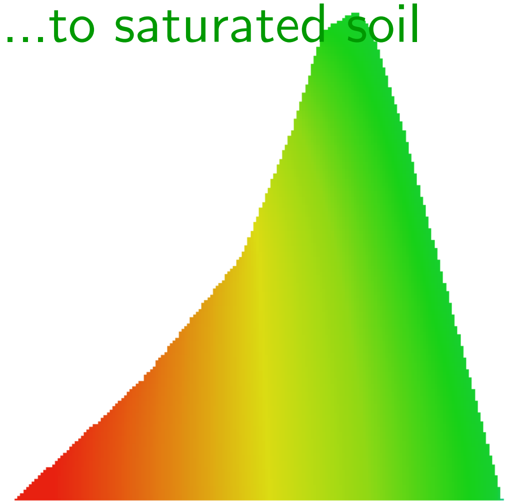


$t = 0$



convergence rates ρ over time t

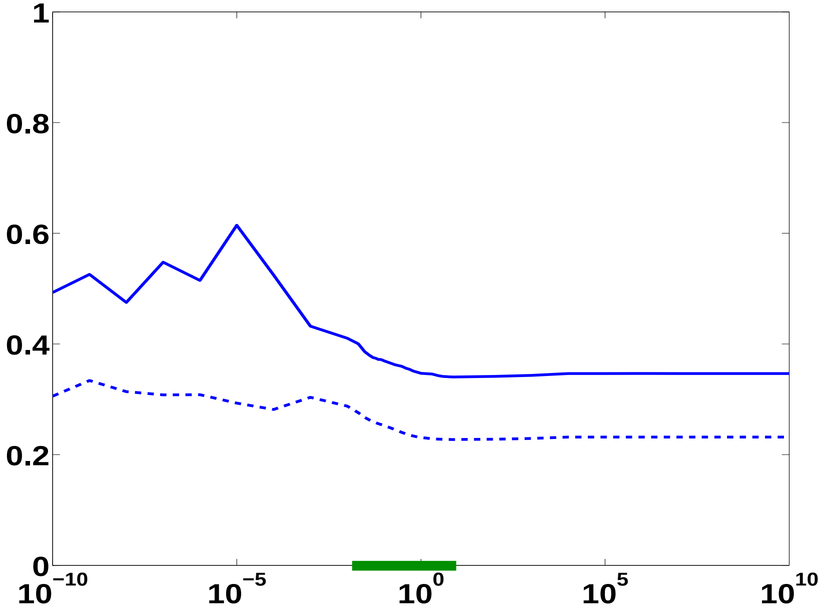
...to saturated soil



$t = 250s$

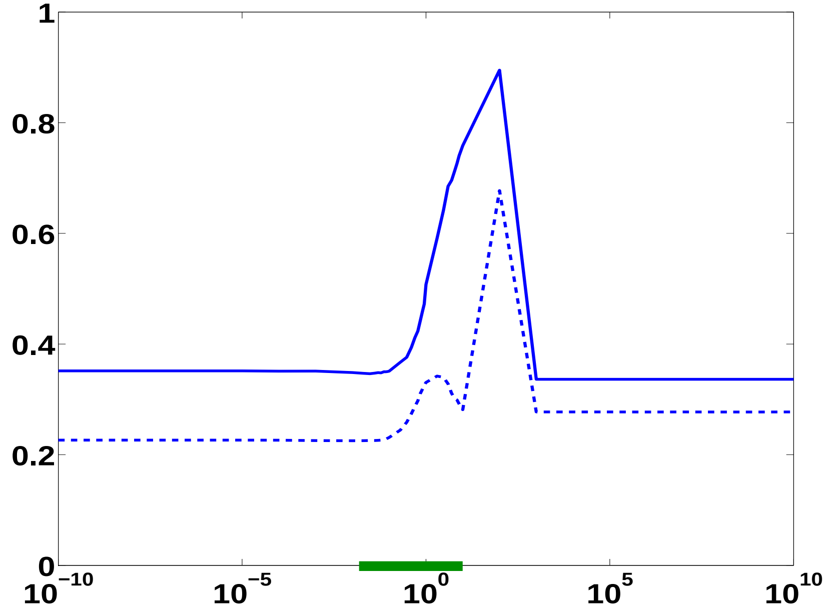
Robustness with respect to Soil Parameters

variation of ε:



$\rho_{\max}$ and ρ_{ave} over ε

variation of $-p_b$:



$\rho_{\max}$ and ρ_{ave} over $-p_b$

Coupling of Ground and Surface Water

supercritical surface flow over dry Soil: clogging interface condition