Adaptive regularization and linearization for nonsmooth and degenerate problems

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in collaboration with

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Inria Paris & Ecole des Ponts

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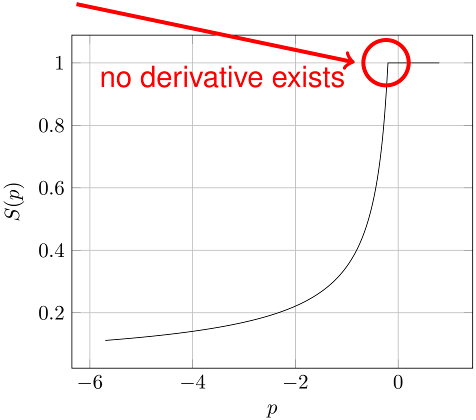
École des Ponts ParisTech

Outline

1. Introduction
2. The Richards equation: adaptive regularization and linearization
   - Discretization
   - Regularization
   - Linearization
   - Flux reconstruction
   - A posteriori estimates of error components
   - Adaptive regularization and linearization
   - Numerical experiments
3. Multi-phase flow with phase transition
4. The Richards equation: overall error certification
   - A posteriori error estimates
   - Numerical experiments
5. Conclusions

Nonsmooth and degenerate nonlinearities

Nonsmooth **nonlinearities**



Brooks–Corey pressure–saturation function

Nonsmooth and degenerate nonlinearities

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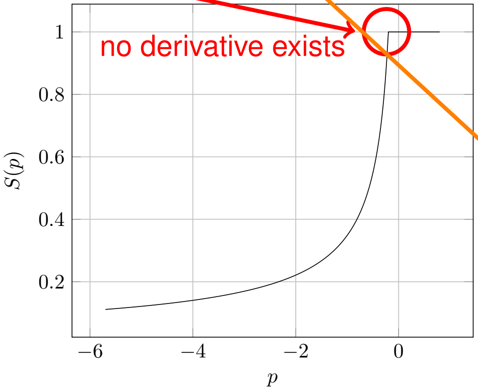

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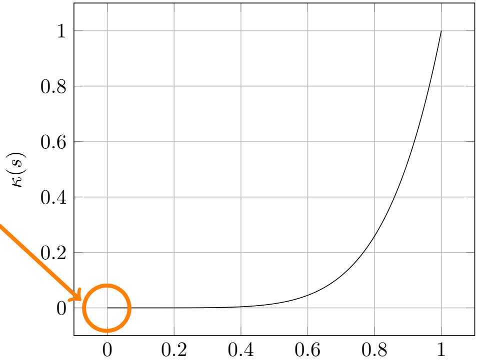

value 0 (derivative 0 or ∞ . . .)

Brooks–Corey saturation–relative permeability function

Nonsmooth and degenerate nonlinearities

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- omnipresent in flows and transport in porous media
- cause **convergence troubles** of **standard iterative linearization schemes**

Nonsmooth and degenerate nonlinearities: common recipes

Nonsmooth and degenerate nonlinearities

- omnipresent in flows and transport in porous media
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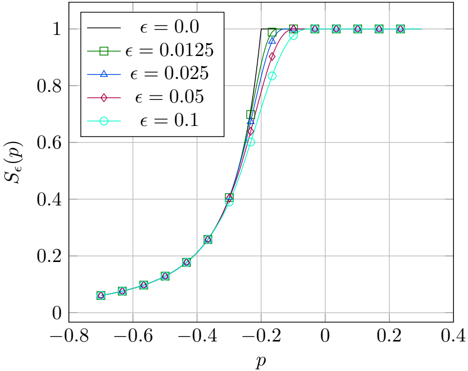
Common recipes

- timestep cutting
- damping
- scheme switching (from Newton to fixed-point . . .)
- semismooth methods
- path finding
- variable switching
- . . .

Example regularizations



Brooks–Corey **regularized** pressure–saturation functions

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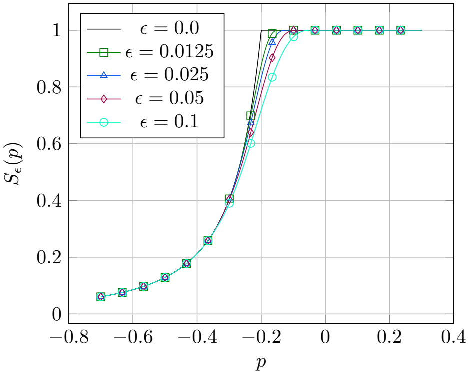

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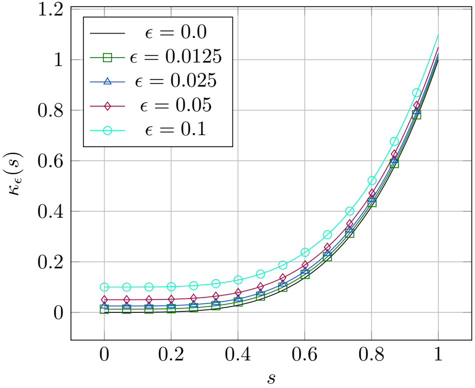

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Nonsmooth and degenerate nonlinearities: our approach

Algorithm

1. regularization parameter $\epsilon_j > 0$
2. replace the nonsmooth and degenerate functions by smooth and nondegenerate ϵ_j-approximations
3. a few steps of Newton linearization (gentle nonlinearity, good initial guess)
4. decrease ϵ_j and go back to step 2

Steering

- a posteriori estimates of error components
- linearization is below regularization: stop Newton iterations
- regularization is below discretization: stop regularization (ϵ_j is never brought to zero)
- discretization is below a specified tolerance: finish

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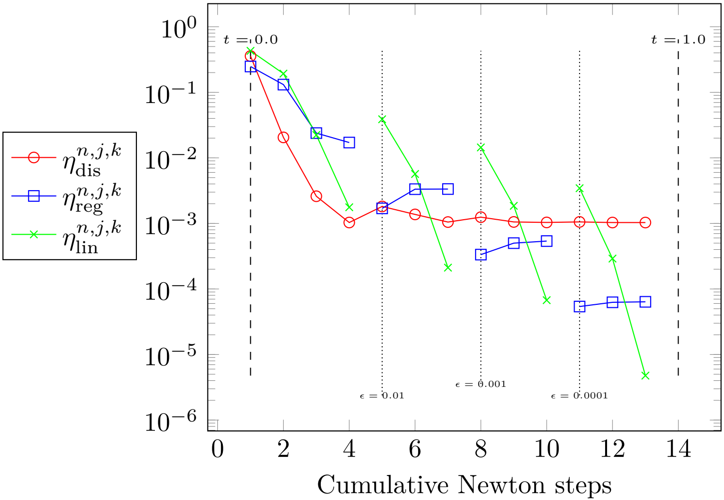
Example overall behavior



Richards equation, unsaturated medium, 1 time step

Outline

Outline

Modelling flow of water and air through soil

The Richards equation

Find $p : \Omega \times (0, T) \to \mathbb{R}$ such that

$$\begin{aligned} \partial_t S(p) - \nabla\cdot[\boldsymbol{K}\kappa(S(p))(\nabla p + \boldsymbol{g})] &= f && \text{in } \Omega \times (0, T), \\ p &= 0 && \text{on } \partial\Omega \times (0, T), \\ (S(p))(\cdot, 0) &= s_0 && \text{in } \Omega. \end{aligned}$$

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Setting

- p: pressure
- $S(p)$: saturation
- $\Omega \subset \mathbb{R}^d$, $1 \le d \le 3$, open polytope with Lipschitz boundary $\partial\Omega$
- T: final time
- diffusion tensor $\boldsymbol{K}$, source term $f \in C^1([0, 1])$, gravity $\boldsymbol{g}$, initial saturation $s_0 \in L^\infty(\Omega)$, $0 \le s_0 \le 1$
- **nonlinear (nonsmooth and degenerate) functions** S and κ

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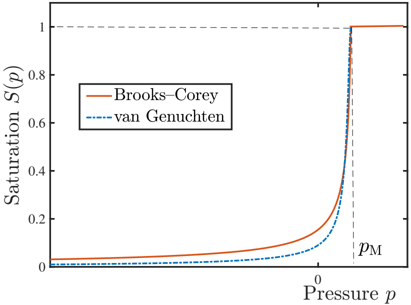

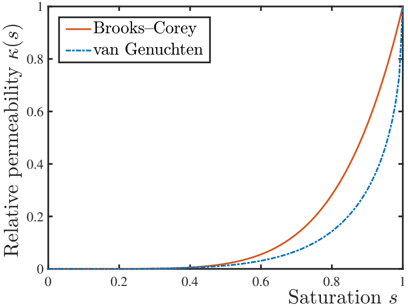

Outline

Backward Euler & finite element discretization

Lowest-order continuous finite element space

$$V_h^0 := \{v_h \in H_0^1(\Omega),\ v_h|_K \in \mathcal{P}_1(K) \quad \forall K \in \mathcal{T}_h\}$$

Discretization

For each $n \in \{1, \ldots, N\}$, given $p_{n-1,h} \in V_h^0$, find the approximate pressure $p_{n,h} \in V_h^0$ satisfying

$$\frac{1}{\tau}(S(p_{n,h}) - S(p_{n-1,h}), \varphi_h) + (\boldsymbol{F}(p_{n,h}), \nabla \varphi_h) = (f(\cdot, t_n), \varphi_h) \qquad \forall \varphi_h \in V_h^0,$$

where

$$\boldsymbol{F}(q) := \boldsymbol{K}\kappa(S(q))[\nabla q + \boldsymbol{g}].$$

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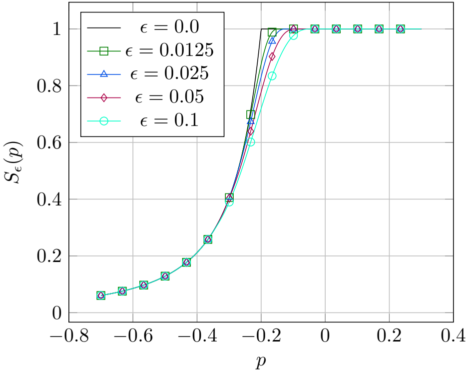
Example regularizations



Brooks–Corey **regularized** pressure–saturation functions

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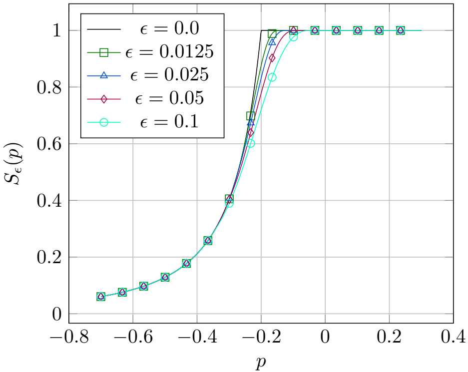

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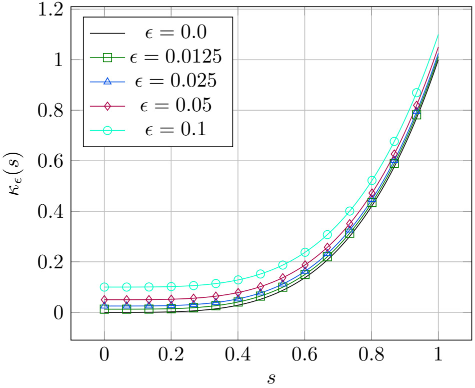

Brooks–Corey **regularized** saturation–relative permeability functions

Regularization

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Given $p^{\bar{j}}_{n-1,h} \in V^0_h$, find $p^j_{n,h} \in V^0_h$ satisfying

$$\frac{1}{\tau}(S_{\epsilon^j}(p^j_{n,h}) - S_{\epsilon^j}(p^{\bar{j}}_{n-1,h}), \varphi_h) + (\boldsymbol{F}_{\epsilon^j}(p^j_{n,h}), \nabla \varphi_h) = (f(\cdot, t_n), \varphi_h) \quad \forall \varphi_h \in V^0_h,$$

where the **regularized flux** is given by

$$\boldsymbol{F}_{\epsilon^j}(q) := \boldsymbol{K} \kappa_{\epsilon^j}(S_{\epsilon^j}(q))[\nabla q + \boldsymbol{g}].$$

- ϵ^j: sequence of regularization parameters
- $\bar{j}$: stopping regularization index

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Given an initial guess $p_{n,h}^{j,k-1}$, find $p_{n,h}^{j,k} \in V_h^0$ such that, for all $\varphi_h \in V_h^0$,

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- modified Picard:

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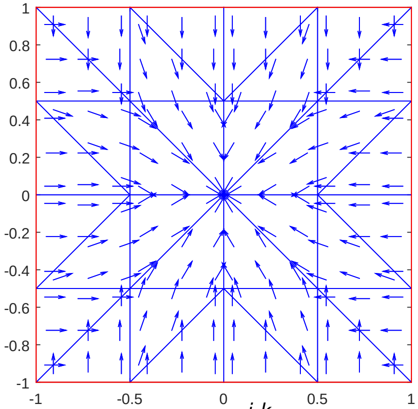
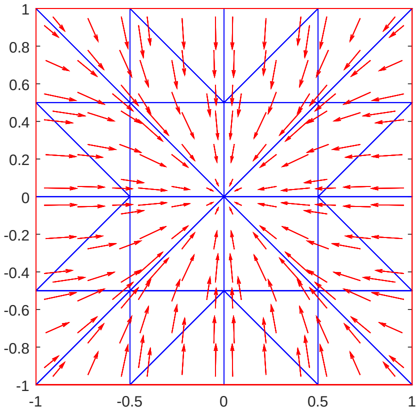
Outline

Flux reconstruction: $-\boldsymbol{F}_{n,h}^{j,k} \notin \boldsymbol{H}(\mathrm{div},\Omega) \to \boldsymbol{\sigma}_{n,h}^{j,k} \in \mathcal{RT}_0(\mathcal{T}_\ell) \cap \boldsymbol{H}(\mathrm{div},\Omega)$



Flux $-\boldsymbol{F}_{n,h}^{j,k}$



(Equilibrated) flux reconstruction $\boldsymbol{\sigma}_\ell$

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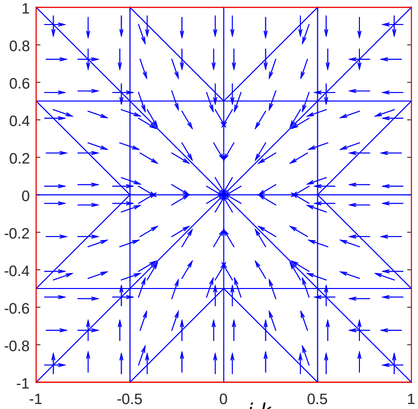

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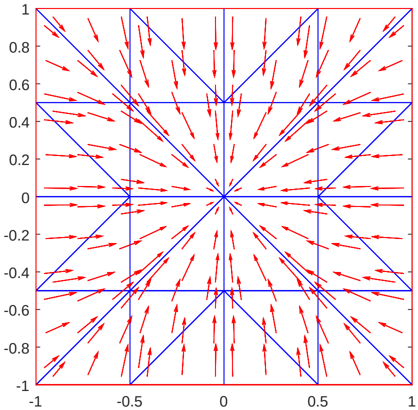


(Equilibrated) flux reconstruction $\boldsymbol{\sigma}_\ell$

normal trace averaging: $$\frac{1}{|F|}\int_F \boldsymbol{\sigma}_{n,h}^{j,k}\cdot \boldsymbol{n}_F = \frac{1}{|\mathcal{T}_F||F|}\sum_{K\in\mathcal{T}_F}\int_F -\boldsymbol{F}_{n,h}^{j,k}\cdot\boldsymbol{n}_F \quad \forall F\in\mathcal{F}$$

Outline

A posteriori estimates of error components

A posteriori estimates of error components

$$\eta_{\mathrm{dis}}^{n,j,k} := \|\mathbf{F}_{n,h}^{j,k} + \boldsymbol{\sigma}_{n,h}^{j,k}\| \qquad \text{(discretization)}$$

$$\eta_{\mathrm{lin}}^{n,j,k} := \|\mathbf{F}_{\epsilon^j}(p_{n,h}^{j,k}) - \mathbf{F}_{n,h}^{j,k}\| \qquad \text{(linearization)}$$

$$\eta_{\mathrm{reg}}^{n,j,k} := \|\mathbf{F}(p_{n,h}^{j,k}) - \mathbf{F}_{\epsilon^j}(p_{n,h}^{j,k})\| \qquad \text{(regularization)}$$

Outline

Adaptive regularization and linearization

Adaptive regularization and linearization ($\gamma_{\text{lin}}, \gamma_{\text{reg}} \approx 0.3$)

$$\eta_{\text{lin}}^{n,j,\bar{k}} < \gamma_{\text{lin}} \eta_{\text{reg}}^{n,j,\bar{k}}$$
$$\eta_{\text{reg}}^{n,\bar{j},\bar{k}} < \gamma_{\text{reg}} \eta_{\text{dis}}^{n,\bar{j},\bar{k}}$$

Outline

Strictly unsaturated medium

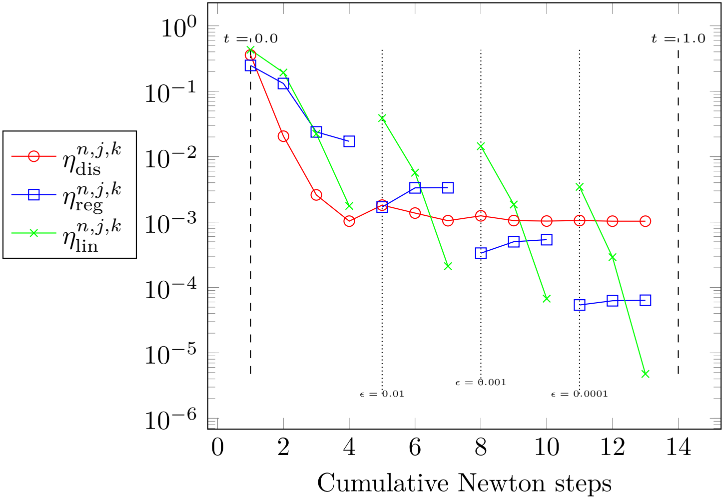
- $\Omega = \Omega_1 \cup \Omega_2$, $\Omega_1 = (0,1) \times (0,1/4]$, $\Omega_2 = (0,1) \times (1/4,1)$
- $T = 1$, $\boldsymbol{K} = \boldsymbol{I}$, $\boldsymbol{g} = (0,1)^T$
- effective saturation $\mathscr{S}(s) = \frac{s - S_{\mathrm{R}}}{S_{\mathrm{V}} - S_{\mathrm{R}}}$
- van Genuchten model

$$\kappa(s) = \kappa_{\mathrm{c}} \sqrt{\mathscr{S}(s)} (1 - (1 - \mathscr{S}(s)^{1/\lambda_2})^{\lambda_2})^2,$$

$$S(p) = \begin{cases} \left[(1 + (-\alpha p)^{\frac{1}{1-\lambda_2}} \right]^{-\lambda_2} & p \leq p_{\mathrm{M}}, \\ 1 & p > p_{\mathrm{M}} \end{cases}$$

- $p_{\mathrm{M}} = 0$, $S_{\mathrm{R}} = 0.026$, $S_{\mathrm{V}} = 0.42$, $\kappa_{\mathrm{c}} = 0.12$, $\alpha = 0.551$, $\lambda_2 = 0.655$
- $f(x,y) = \begin{cases} 0 & (x,y) \in \Omega_1, \\ 0.06 \cos(\frac{4}{3}\pi y) \sin(x) & (x,y) \in \Omega_2 \end{cases}$
- $p_0(x,y) = \begin{cases} -y - 1/4 & (x,y) \in \Omega_1, \\ -4 & (x,y) \in \Omega_2 \end{cases}$
- $s_0 = S(p_0)$
- uniform mesh with $40 \times 40 \times 2$ elements, $\tau_0 = 1$

Adaptive regularization and linearization



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Injection case

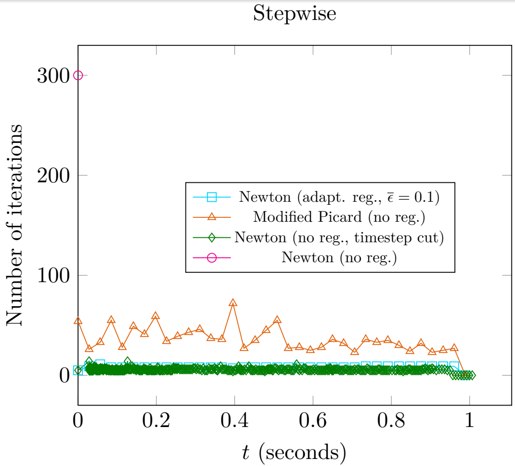
- $\Omega = (0,1)^2$
- $T = 1, \boldsymbol{K} = \boldsymbol{I}, \boldsymbol{g} = (0,-1)^T$
- effective saturation $\mathscr{S}(s) = \frac{s - S_R}{S_V - S_R}$
- Brooks–Corey model

$$\kappa(s) = \mathscr{S}(s)^{\frac{2+3\lambda_1}{\lambda_1}},$$

$$S(p) = \begin{cases} (-p/p_M)^{-\lambda_1} & p \le p_M, \\ 1 & p > p_M \end{cases}$$

- $p_M = -0.2$, $\lambda_1 = 2.239$
- $f = 0$
- $p_0 = -1$
- $s_0 = S(p_0)$
- quasi uniform mesh with $h = 2.82 \cdot 10^{-2}$, $\tau_0 = 2.82 \cdot 10^{-2}$

Do we reduce the **computational cost**?



Number of linearization iterations on each time step

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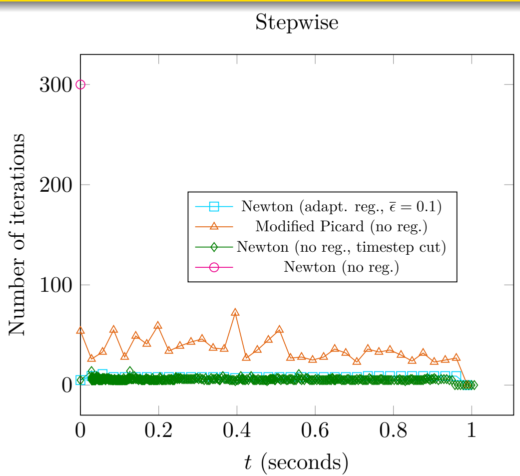

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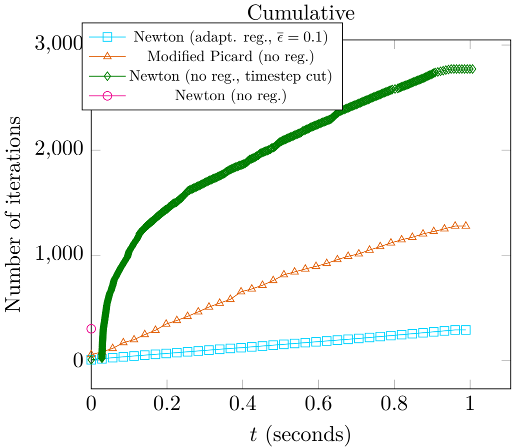

Cumulative number of linearization iterations

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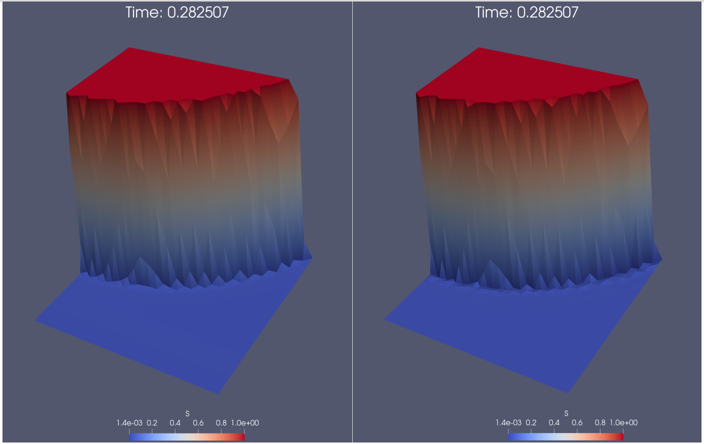
Do we **lose precision**?



Saturation field $s = S(p_{n,h}^{\bar{j},\bar{k}})$ using Newton's method and adaptive regularization $\epsilon^1 = 0.1$ (left) and modified Picard with no regularization (right)

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Realistic case

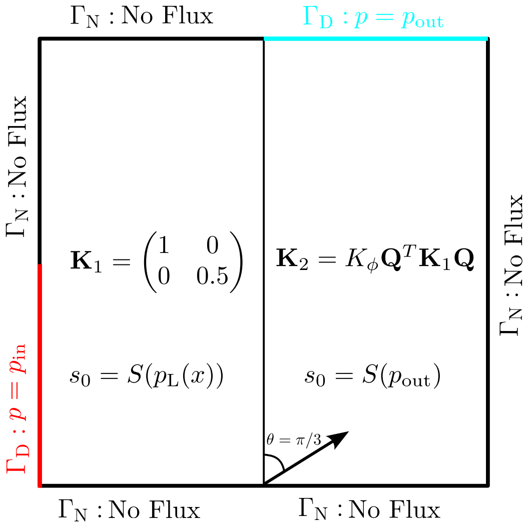
- $\Omega = (0,1)^2$
- $T = 1$
- $\boldsymbol{g} = (-1, 0)^T$
- $\mathbf{Q} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$
- $K_\phi = 0.1$
- effective saturation $\mathscr{S}(s) = \frac{s - S_R}{S_V - S_R}$
- Brooks–Corey model

$$\kappa(s) = \mathscr{S}(s)^{\frac{2+3\lambda_1}{\lambda_1}},$$

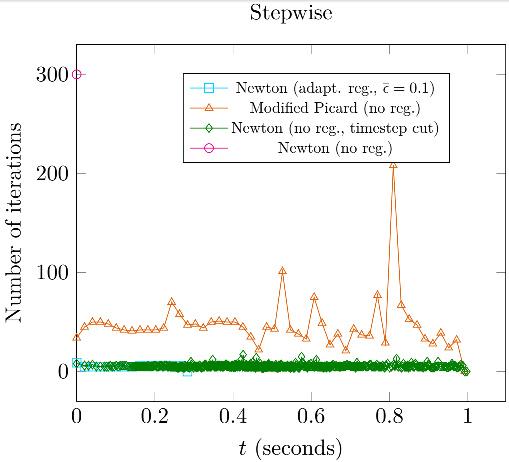
$$S(p) = \begin{cases} (-p/p_M)^{-\lambda_1} & p \le p_M, \\ 1 & p > p_M \end{cases}$$

- $p_M = -0.2$, $\lambda_1 = 2$
- $f = 0$
- quasi uniform mesh with $h = 2.02 \cdot 10^{-2}$, $\tau_0 = 2.02 \cdot 10^{-2}$
- $p_L(\boldsymbol{x}) = \left(\frac{p_{out} - p_{in}}{0.5}\right) \boldsymbol{x}$, $p_{out} = -2.0$, $p_{in} = -0.2$, $p_D = p_0|_{\Gamma_D}$

Realistic case setting



Do we reduce the **computational cost**?



Number of linearization iterations on each time step

F. Févotte, A. Rappaport, M. Vohralík, Computational Geosciences (2024)

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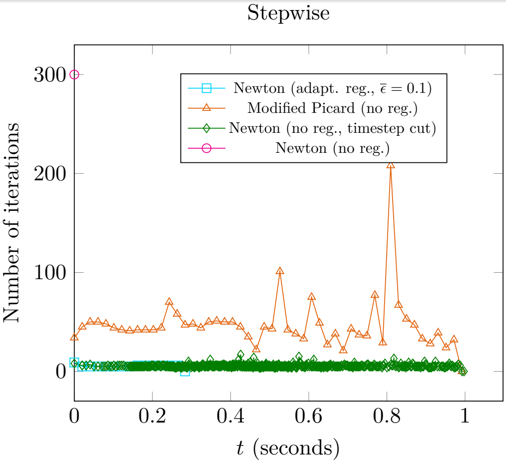

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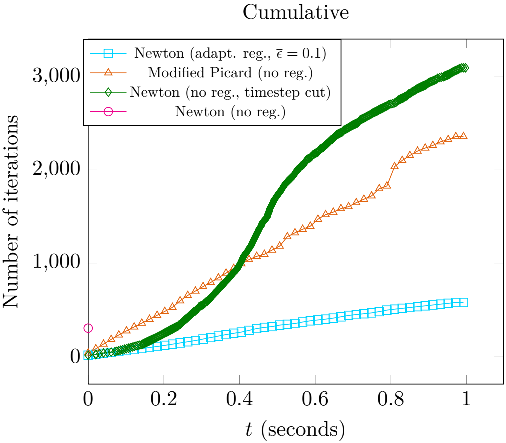
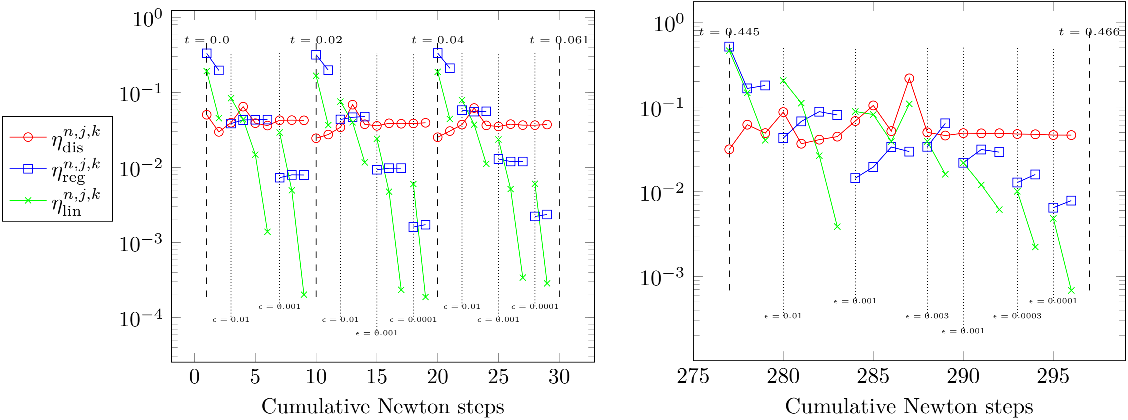


Cumulative number of linearization iterations

F. Févotte, A. Rappaport, M. Vohralík, Computational Geosciences (2024)

Adaptive regularization and linearization



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Perched water table case

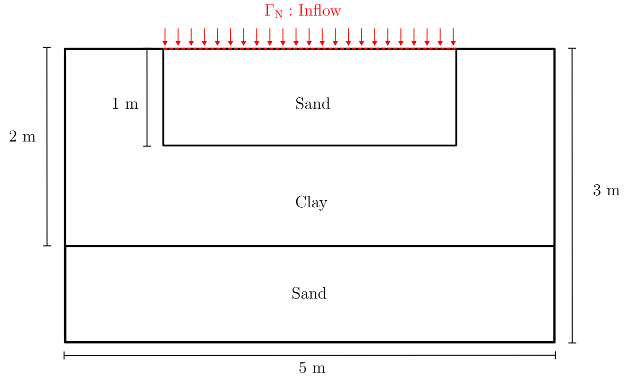
- $\Omega = (-2.5\text{ m}, 2.5\text{ m}) \times (-3\text{ m}, 0\text{ m})$
- $T = 86400$ s (one day)
- $\mathbf{K} = \boldsymbol{I}$
- $\boldsymbol{g} = (-1, 0)^T$
- effective saturation $\mathscr{S}(s) = \frac{s - S_\mathrm{R}}{S_\mathrm{V} - S_\mathrm{R}}$
- van Genuchten model

$$\kappa(s) = \kappa_\mathrm{c} \sqrt{\mathscr{S}(s)} (1 - (1 - \mathscr{S}(s)^{1/\lambda_2})^{\lambda_2})^2,$$

$$S(p) = \begin{cases} \left[(1 + (-\alpha p)^{\frac{1}{1-\lambda_2}} \right]^{-\lambda_2} & p \le p_\mathrm{M}, \\ 1 & p > p_\mathrm{M} \end{cases}$$

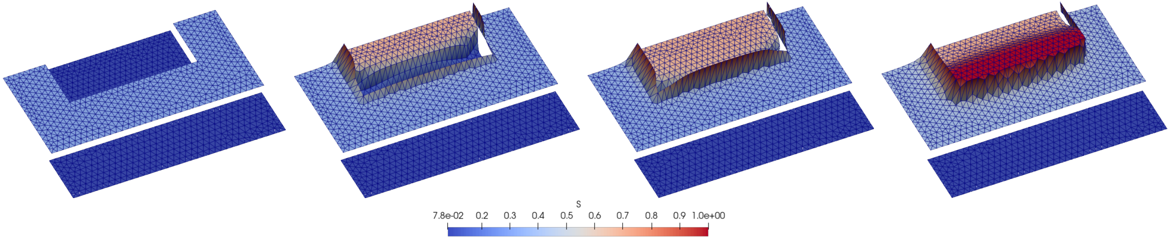
- $f = 0$
- quasi uniform mesh with $h = 8.2 \cdot 10^{-2}$
- $\tau_0 = 60$ s, (increase $\tau_n := 1.2\tau_{n-1}$ for $n \ge 1$)
- initial condition $s_0 = S(p_0)$ with $p_0 = -300$ m

Perched water table case setting



Material	κ_c	ϕ	S_R	S_V	λ_2	α
Sand	6.262×10^{-5}	0.368	0.07818	1	0.553	2.8
Clay	1.516×10^{-6}	0.4686	0.2262	1	0.2835	1.04

Perched water table case saturation evolution



Saturation at $t = 0$ s, $21 \cdot 10^3$ s, $41 \cdot 10^3$ s, $86.1 \cdot 10^3$ s

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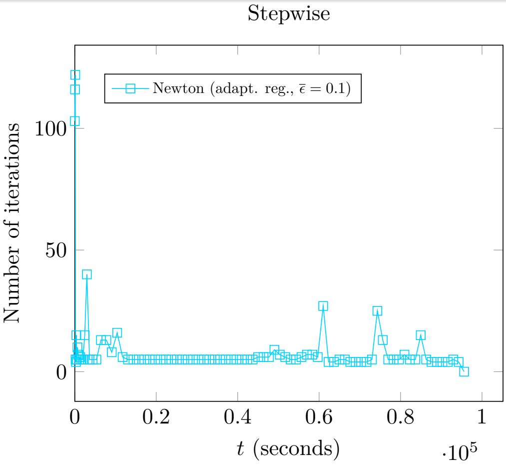
Performance: only adaptive regularization and linearization works



Number of linearization iterations on each time step

F. Févotte, A. Rappaport, M. Vohralík, Computational Geosciences (2024)

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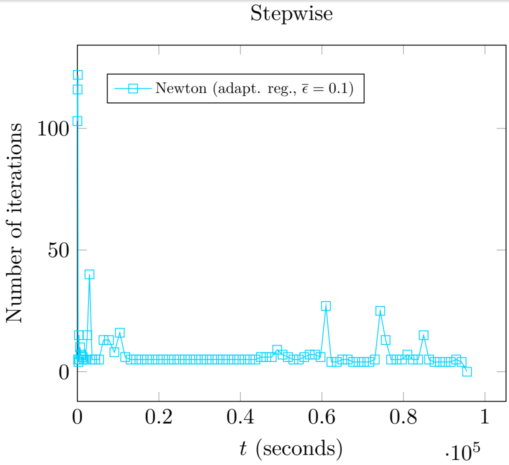

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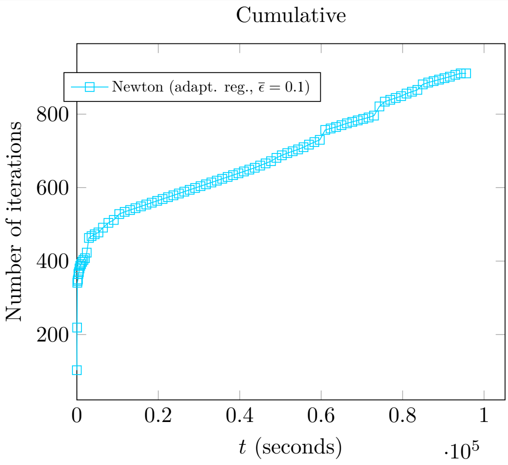

Cumulative number of linearization iterations

F. Févotte, A. Rappaport, M. Vohralík, Computational Geosciences (2024)

Outline

Complementarity problems

System of (nonlinear) algebraic equations with complementarity constraints

$$\boldsymbol{F}(\boldsymbol{X}) = \boldsymbol{0},$$
$$\boldsymbol{K}(\boldsymbol{X}) \geq \boldsymbol{0},\ \boldsymbol{G}(\boldsymbol{X}) \geq \boldsymbol{0},\ \ \boldsymbol{K}(\boldsymbol{X}) \cdot \boldsymbol{G}(\boldsymbol{X}) = 0$$

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Nonlinear algebraic **inequalities** $\overset{?}{\rightarrow}$ nonlinear algebraic **equalities**

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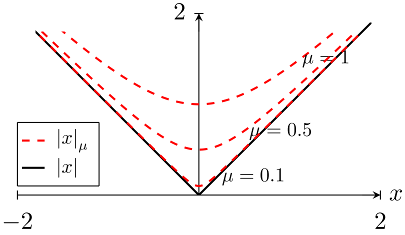
Nonlinear algebraic **inequalities** $\overset{?}{\to}$ nonlinear algebraic **equalities**

Complementarity functions: equivalent reformulation as algebraic equalities

$$\boldsymbol{F}(\boldsymbol{X}) = \mathbf{0},$$
$$\boldsymbol{C}(\boldsymbol{X}) = \mathbf{0}$$

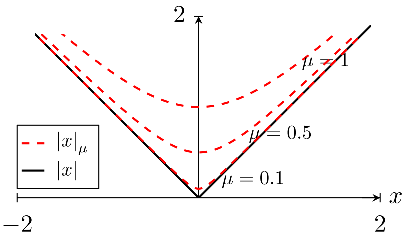
nonlinear **nonsmooth** system

Regularized complementary functions



Regularized absolute value
(Newton-min) functions

Regularized complementary functions



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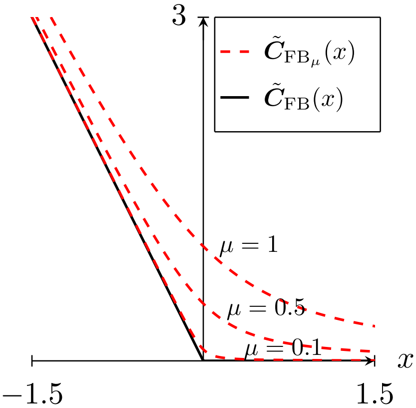
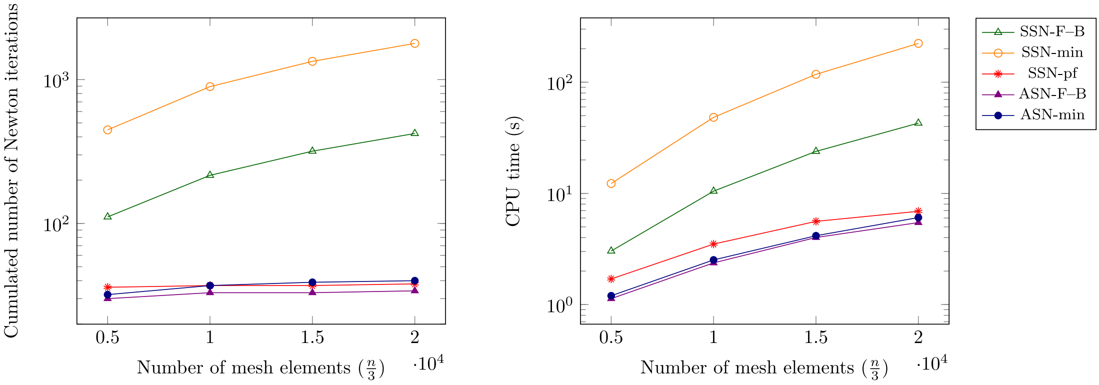


Regularized Fischer–Burmeister functions

Numerical performances



I. Ben Gharbia, J. Ferzly, M. Vohralík, S. Yousef, Journal of Computational and Applied Mathematics (2023)

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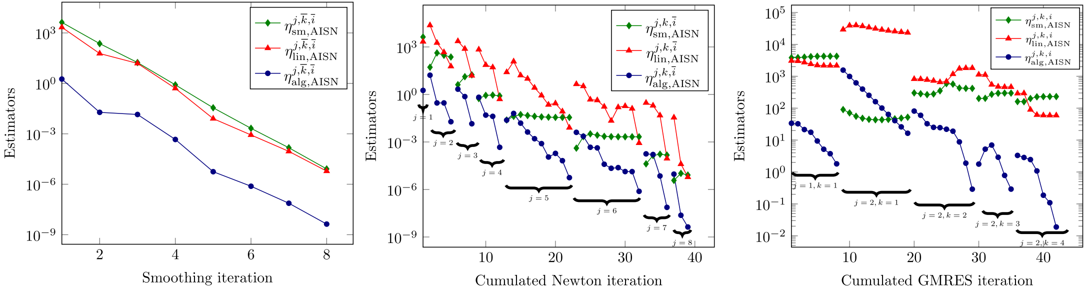

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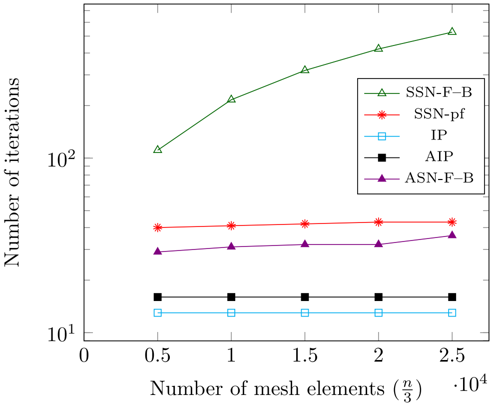

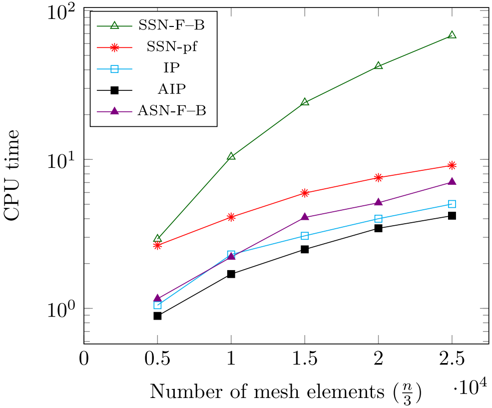

I. Ben Gharbia, J. Ferzly, M. Vohralík, S. Yousef, Journal of Computational and Applied Mathematics (2023)

Outline

Modelling flow of water and air through soil

The Richards equation

Find $p : \Omega \times (0, T) \to \mathbb{R}$ such that

$$\begin{aligned} \partial_t S(p) - \nabla\cdot[\boldsymbol{K}\kappa(S(p))(\nabla p + \boldsymbol{g})] &= f(S(p)) && \text{in } \Omega \times (0, T), \\ p &= 0 && \text{on } \partial\Omega \times (0, T), \\ (S(p))(\cdot, 0) &= s_0 && \text{in } \Omega. \end{aligned}$$

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Setting

- p: pressure
- $S(p)$: saturation
- $\Omega \subset \mathbb{R}^d$, $1 \leq d \leq 3$, open polytope with Lipschitz boundary $\partial\Omega$
- T: final time
- diffusion tensor $\boldsymbol{K}$, source term $f \in C^1([0, 1])$, gravity $\boldsymbol{g}$, initial saturation $s_0 \in L^\infty(\Omega)$, $0 \leq s_0 \leq 1$
- **nonlinear (nonsmooth and degenerate) functions** S and κ

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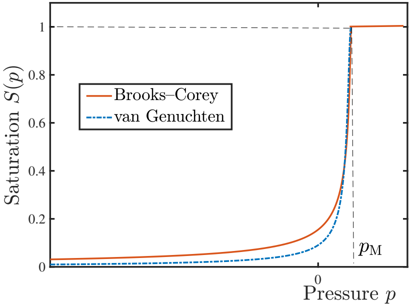

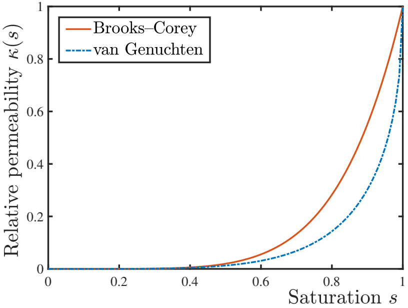

Outline

Weak formulation

Spaces

$$X := L^2(0, T; H_0^1(\Omega)), \qquad Z := H^1(0, T; H^{-1}(\Omega))$$

Total pressure (Kirchhoff transform)

$$\mathcal{K}(p) := \begin{cases} \int_0^p \kappa(S(\varrho))\,\mathrm{d}\varrho & \text{for } p \le p_{\mathrm{M}}, \\ P_{\mathrm{M}} + \kappa(1)(p - p_{\mathrm{M}}) & \text{for } p > p_{\mathrm{M}}, \end{cases} \qquad \theta \circ \mathcal{K} = S$$

Weak formulation

$$\Psi \in X \qquad \text{with } s := \theta(\Psi) \in Z, \qquad s(0) = s_0 \quad \text{in } \Omega,$$

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Residual $\mathcal{R}(\Psi_{h\tau}) \in X'$**, for** $\Psi_{h\tau} \in X$ **such that** $s_{h\tau} := \theta(\Psi_{h\tau}) \in Z$

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Time-integration functionals based on the **sharp Grönwall** lemma

Time-integration functionals, $\alpha : [0, T] \to [0, \infty)$

$$\mathcal{J}_\alpha : L^2([0,T]) \to [0,\infty),$$

$$\mathcal{J}_\alpha(\varrho) := \left[\exp\left(-\int_0^T \alpha\right) \int_0^T \left(\varrho^2(t) + \alpha(t) \exp\left(\int_t^T \alpha\right) \int_0^t \varrho^2\right) \mathrm{d}t\right]^{\frac{1}{2}}$$

- define norm on $L^2([0,T])$
- actually equivalent to the $L^2([0,T])$ norm

$$\exp\left(-\frac{1}{2}\int_0^T \alpha\right) \|\varrho\|_{L^2([0,T])} \le \mathcal{J}_\alpha(\varrho) \le \|\varrho\|_{L^2([0,T])}$$

- yield an almost constant value of error independent of $T \geq 1$ in applications

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Time-integration functionals, $\alpha : [0, T] \to [0, \infty)$

$$\mathcal{J}_\alpha : L^2([0,T]) \to [0,\infty),$$

$$\mathcal{J}_\alpha(\varrho) := \left[\exp\left(-\int_0^T \alpha\right) \int_0^T \left(\varrho^2(t) + \alpha(t) \exp\left(\int_t^T \alpha\right) \int_0^t \varrho^2\right) \mathrm{d}t\right]^{\frac{1}{2}}$$

- define norm on $L^2([0, T])$
- actually equivalent to the $L^2([0, T])$ norm

$$\exp\left(-\frac{1}{2}\int_0^T \alpha\right) \|\varrho\|_{L^2([0,T])} \leq \mathcal{J}_\alpha(\varrho) \leq \|\varrho\|_{L^2([0,T])}$$

- yield an almost constant value of error independent of $T \geq 1$ in applications

Relation error – residual **without e^T** by the **sharp Grönwall** lemma

Theorem (Relation error – residual without e^T)

Let $\Psi_{h\tau} \in X$ such that $s_{h\tau} := \theta(\Psi_{h\tau}) \in Z$. Then

$$e^{-\int_0^T(\lambda+\mathfrak{C}_1)}\|(s-s_{h\tau})(T)\|^2_{H^{-1}(\Omega)} + \mathcal{J}_{\lambda+\mathfrak{C}_1}\left(\theta_{\partial,\mathrm{M}}^{-\frac{1}{2}}\|s-s_{h\tau}\|\right)^2$$

$$\leq \|s_0 - s_{h\tau}(0)\|^2_{H^{-1}(\Omega)} + \mathcal{J}_{\lambda+\mathfrak{C}_1}(\lambda^{-\frac{1}{2}}\|\mathcal{R}(\Psi_{h\tau})\|_{H^{-1}(\Omega)})^2,$$

$$e^{-\int_0^T\mathfrak{C}_2}\|(s-s_{h\tau})(T)\|^2 + \frac{1}{2}\mathcal{J}_{\mathfrak{C}_2}\left(\left\|D(s)^{-\frac{1}{2}}\mathcal{K}^{\frac{1}{2}}\nabla(\Psi-\Psi_{h\tau})\right\|\right)^2$$

$$\leq \|s_0 - s_{h\tau}(0)\|^2 + \mathcal{J}_{\mathfrak{C}_2}\left(\eta^{\mathrm{deg}}\right)^2 + 4\,\mathcal{J}_{\mathfrak{C}_2}\left(D_{\mathrm{m}}^{-\frac{1}{2}}\|\mathcal{R}(\Psi_{h\tau})\|_{H^{-1}(\Omega)}\right)^2,$$

$$\mathcal{J}_\lambda(\|\partial_t(s-s_{h\tau})\|_{H^{-1}(\Omega)})^2$$

$$\leq 3\left[\mathcal{J}_\lambda(\|\Psi-\Psi_{h\tau}\|_{H^{-1}(\Omega)})^2 + \mathfrak{C}_3(T)\,\mathcal{J}_\lambda(\|s-s_{h\tau}\|)^2 + \mathcal{J}_\lambda(\|\mathcal{R}(\Psi_{h\tau})\|_{H^{-1}(\Omega)})^2\right].$$

Guaranteed a posteriori error estimate

Theorem (Guaranteed a posteriori error estimate)

Let $\Psi_{h\tau} \in X$ such that $s_{h\tau} := \theta(\Psi_{h\tau}) \in Z$. Then

$$\|\mathcal{R}(\Psi_{h\tau}(t))\|_{H^{-1}(\Omega)} \leq \eta_{\mathcal{R}}(t).$$

Consequently,

$$\begin{aligned}
\mathcal{E}_{L^2}^2 &:= e^{-\int_0^T(\lambda+\mathfrak{C}_1)}\|(s - s_{h\tau})(T)\|_{H^{-1}(\Omega)}^2 + \mathcal{J}_{\lambda+\mathfrak{C}_1}(\theta_{\partial,\mathrm{M}}^{-\frac{1}{2}}\|s - s_{h\tau}\|)^2 \\
&\leq [\eta^{\mathrm{ini},H^{-1}}]^2 + \mathcal{J}_{\lambda+\mathfrak{C}_1}(\lambda^{-\frac{1}{2}}\eta_{\mathcal{R}})^2 =: \eta_{L^2}^2, \\
\mathcal{E}_{H^1}^2 &:= e^{-\int_0^T \mathfrak{C}_2}\|(s - s_{h\tau})(T)\|^2 + \frac{1}{2}\mathcal{J}_{\mathfrak{C}_2}(\|D(s)^{-\frac{1}{2}}\mathcal{K}^{\frac{1}{2}}\nabla(\Psi - \Psi_{h\tau})\|)^2 \\
&\leq [\eta^{\mathrm{ini},L^2}]^2 + \mathcal{J}_{\mathfrak{C}_2}\left(\eta^{\mathrm{deg}}\right)^2 + 4\,\mathcal{J}_{\mathfrak{C}_2}\left(D_{\mathrm{m}}^{-\frac{1}{2}}\eta_{\mathcal{R}}\right)^2 =: \eta_{H^1}^2.
\end{aligned}$$

Outline

Degenerate case with known solution

- unit square $\Omega = (0, 1)^2$
- $T = 1$
- $\boldsymbol{K} = \boldsymbol{I}$
- nonlinearities

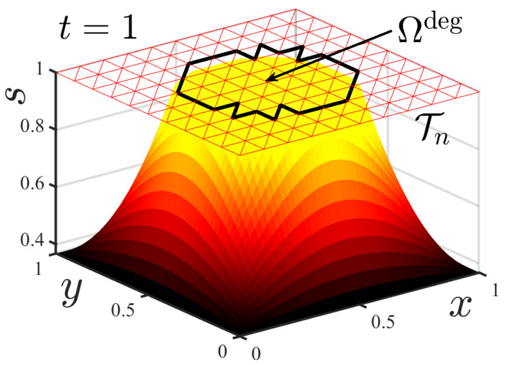
$$\kappa(s) = 1, \quad S(p) = \begin{cases} \exp(p-1) & \text{if } p < 1, \\ 1 & \text{if } p \geq 1 \end{cases}$$

- exact solution

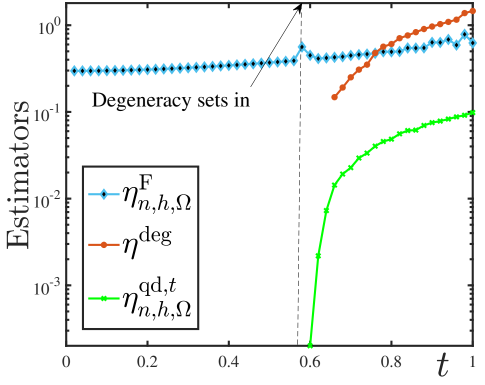
$$p_{\text{exact}}(x, y, t) = 12\,(1 + t^2)\,x\,y\,(1 - x)\,(1 - y)$$

- f and s_0 chosen accordingly
- $(h, \tau) = (h_0, \tau_0)/\ell$ with $\ell \in \{1, 2, 4\}$, $h_0 = 0.2$, $\tau_0 = 0.04$

Evolution of the solution and of the estimators



Saturation of the exact solution p_{exact} and the domain $\Omega^{\text{deg}}(t)$ at $t = 1$



Principal estimators $\eta^{\text{F}}_{n,h,\Omega}(t)$, $\eta^{\text{deg}}(t)$, and $\eta^{\text{qd},t}_{n,h,\Omega}(t)$ for $\ell = 2$

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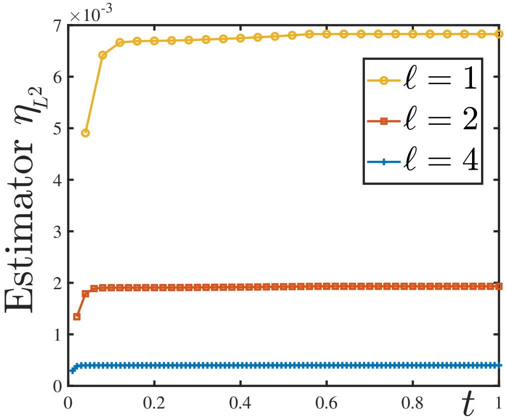
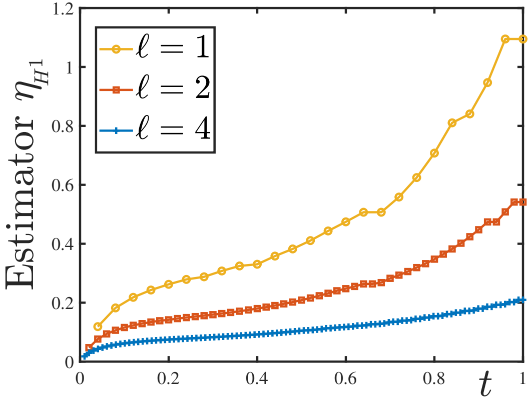
How **large** is the error?



Overall η_{L^2} a posteriori error estimator



Overall η_{H^1} a posteriori error estimator

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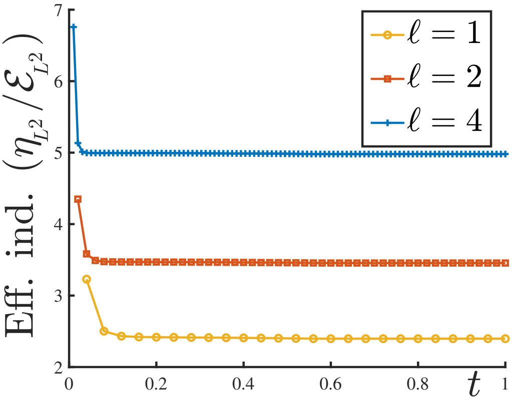
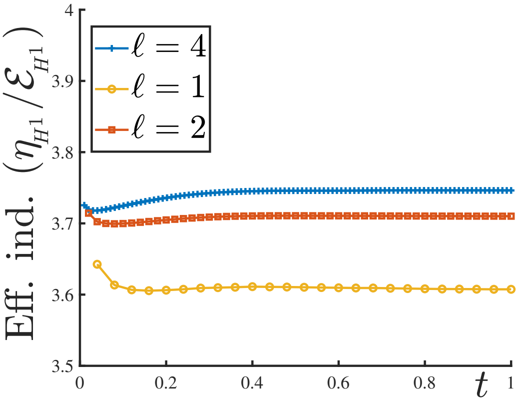
Is our prediction **efficient** and **robust** wrt the final time?



$\mathcal{E}_{L^2}$ effectivity indices



$\mathcal{E}_{H^1}$ effectivity indices

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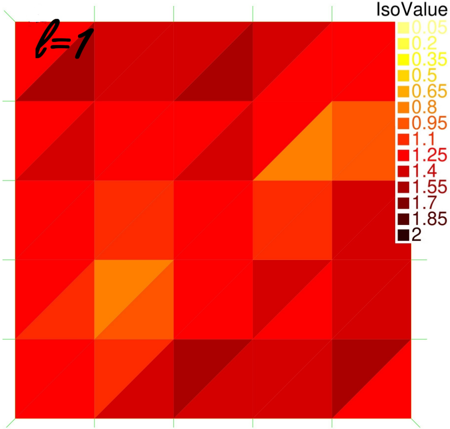
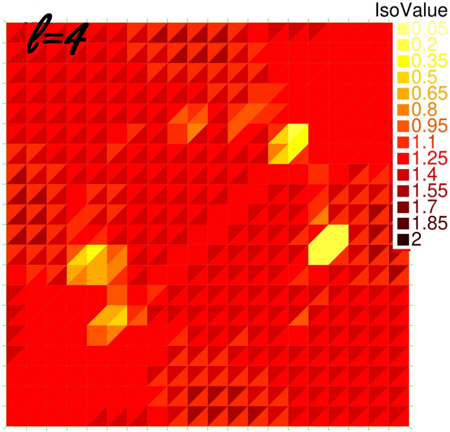
Where (in space and time) is the error **localized**?



Elementwise effectivity indices ($t = 1$, $\ell = 1$)



Elementwise effectivity indices ($t = 1$, $\ell = 4$)

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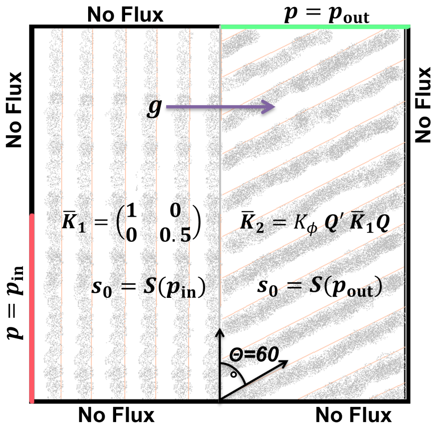
Realistic case

- unit square $\Omega = (0,1)^2$
- $T = 1$
- $f = 0$, heterogeneous and anisotropic $\boldsymbol{K}$, $\boldsymbol{g} = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$
- **Brooks–Corey**-type **saturation** and **permeability** laws

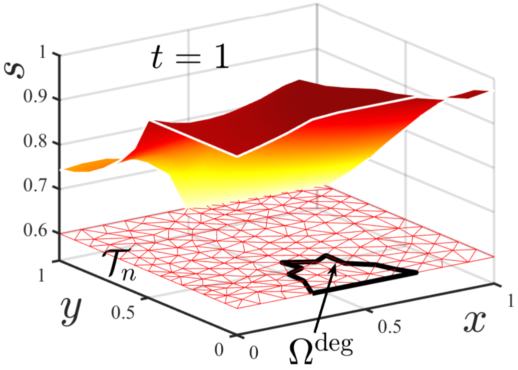
$$S(p) = \begin{cases} \frac{1}{(2-p)^{\frac{1}{3}}} & \text{if } p < 1, \\ 1 & \text{if } p \geq 1 \end{cases}, \quad \kappa(s) = s^3$$

- unknown exact solution
- $(h, \tau) = (h_0, \tau_0)/\ell$ with $\ell \in \{1, 2, 4\}$, $h_0 = 0.2$, $\tau_0 = 0.04$

Realistic case

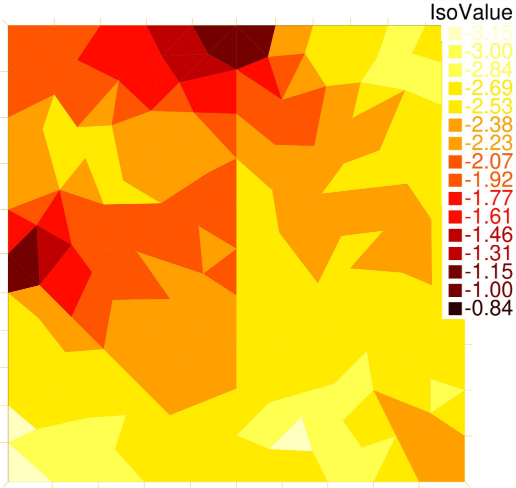


Setting

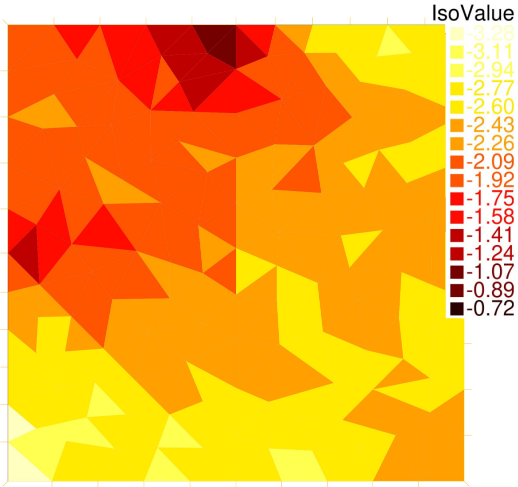


Numerical saturation for $\ell = 2$ at $t = 1$

Where (in space and time) is the error **localized**?



Estimated local error ($t = 1$, $\ell = 2$)



Exact local error ($t = 1$, $\ell = 2$)

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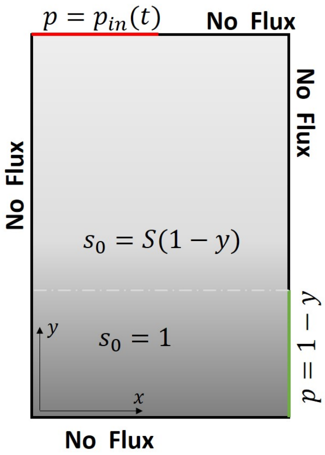
Benchmark case (infiltration in a vadose zone from a water body)

- $\Omega = (0,2) \times (0,3)$
- $T = 1$
- $f = 0$, $\boldsymbol{K} = 4.96 \times 10^{-2} \boldsymbol{I}$, $\boldsymbol{g} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
- **van Genuchten saturation** and **permeability** laws

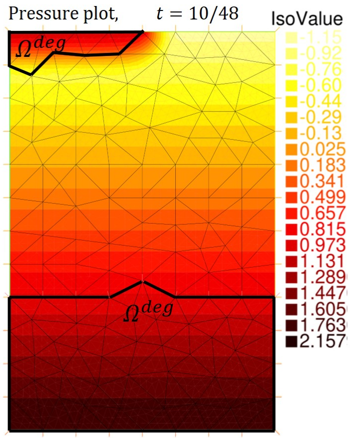
$$S(p) = \begin{cases} 1/(1 + (p_{\mathrm{M}} - p)^{\frac{1}{1-\lambda_2}})^{\lambda_2} & \text{if } p < p_{\mathrm{M}}, \\ 1 & \text{if } p \geq p_{\mathrm{M}} \end{cases}, \qquad \kappa(s) = \sqrt{s}\,(1 - (1 - s^{1/\lambda_2})^{\lambda_2})^2$$

- $\lambda_2 = 1 - 1/2.06$, $p_{\mathrm{M}} = 1$
- unknown exact solution
- $h = 1/4$, $\tau = 10/48$

Benchmark case

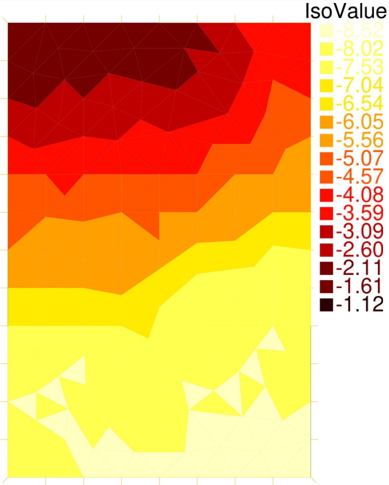


Setting

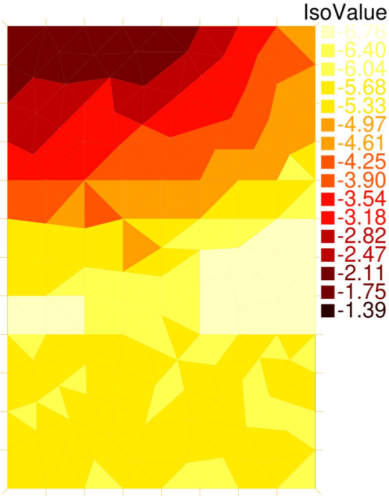


Numerical pressure at $t = 10/48$

Where (in space and time) is the error **localized**?



Estimated local error ($t = 10/48$)



Exact local error ($t = 10/48$)

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Outline

Conclusions

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- **adaptive regularization**: keep Newton linearization and avoid timestep cutting, damping, scheme switching, or variable switching
- steered by **a posteriori estimates**
- **certification** of the overall **error** committed in the numerical simulation
- **sound numerical performance** (Richards equation, multiphase flows, multicompositional flows, complementarity problems)

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Thank you for your attention!