

Adaptive iterative approximation in nonlinear PDEs II

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in collaboration with

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INSTITUT
POLYTECHNIQUE
DE PARIS

Outline

1 Introduction

- Nonsmooth and degenerate nonlinearities
- Variational inequalities (complementarity problems)
- Setting & achievements

2 Heat equation: robustness wrt final time and space–time error localization

- A posteriori error estimates
- Flux reconstruction

3 The Richards equation: adaptive regularization and linearization

- Discretization, regularization, linearization
- Flux reconstruction
- A posteriori estimates and adaptive iterative approximation

4 Multiphase multicompositional flows (phase appearance and disappearance)

- Adaptive iterative approximation

5 Conclusions

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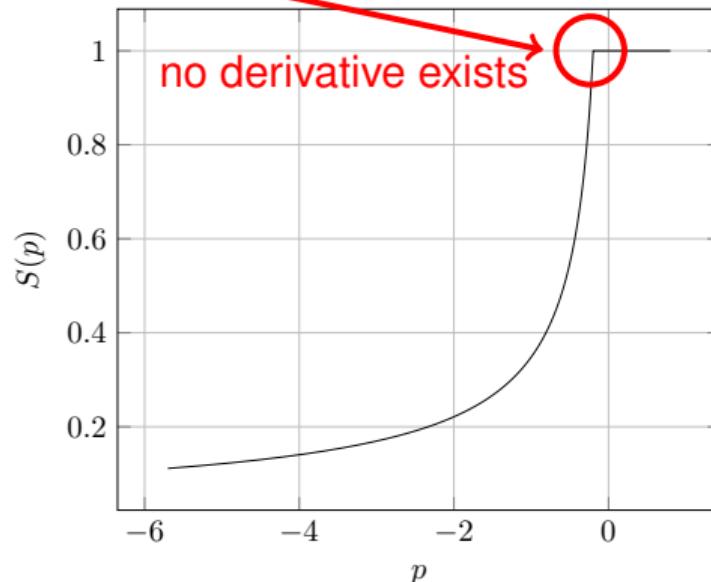
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Nonsmooth and degenerate nonlinearities

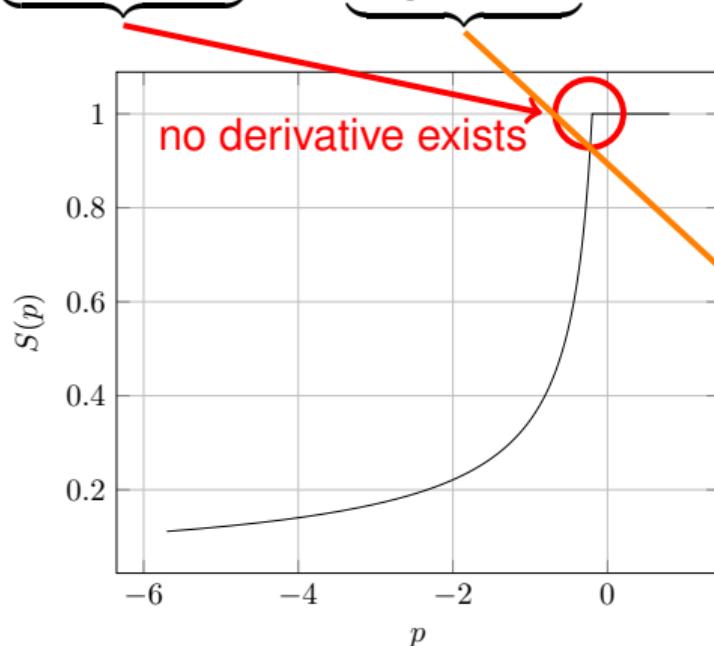
Nonsmooth nonlinearities



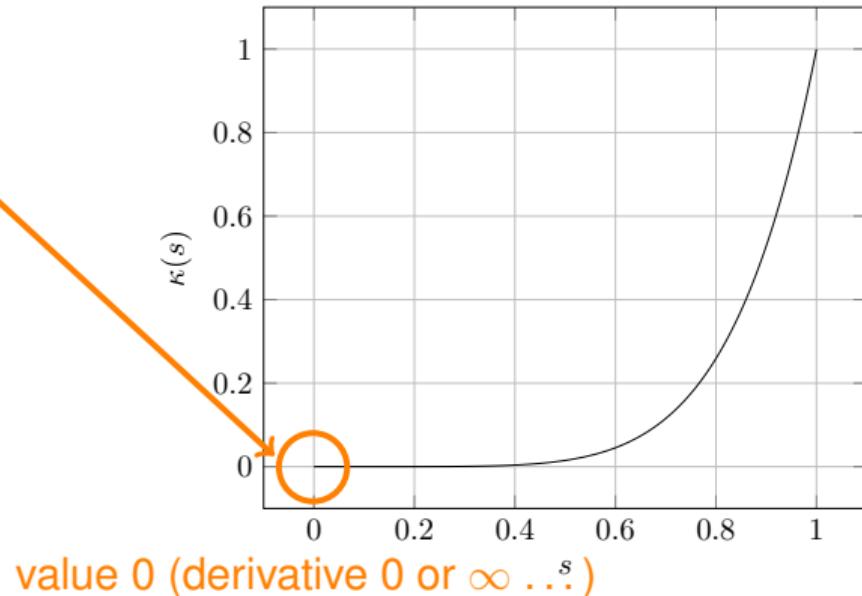
Brooks–Corey pressure–saturation
function

Nonsmooth and degenerate nonlinearities

Nonsmooth and degenerate nonlinearities



Brooks–Corey pressure–saturation
function



value 0 (derivative 0 or $\infty \dots$)
Brooks–Corey saturation–relative
permeability function

Nonsmooth and degenerate nonlinearities

Nonsmooth and degenerate nonlinearities

- omnipresent in applications
- cause **convergence troubles** of **standard iterative linearization methods**

Nonsmooth and degenerate nonlinearities: common recipes

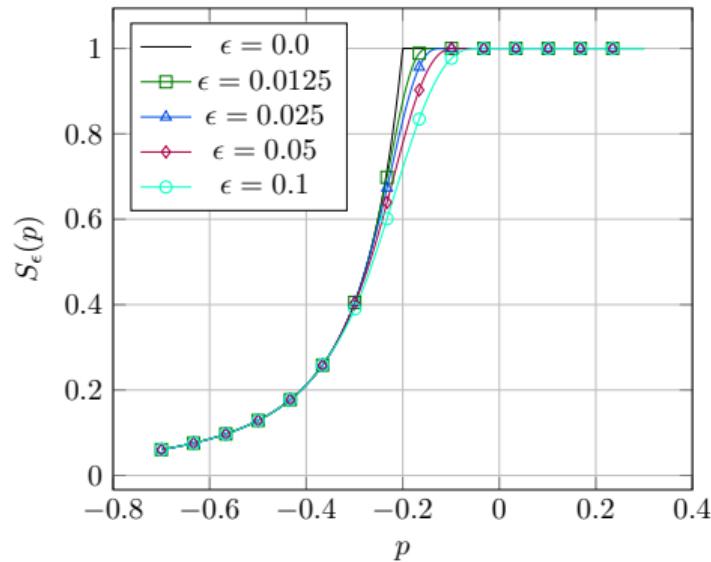
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Common recipes

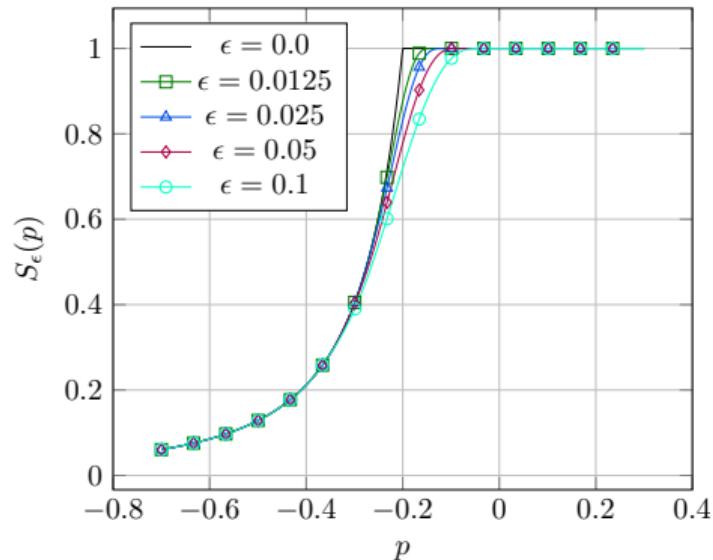
- timestep cutting
- damping
- scheme switching (from Newton to fixed-point ...)
- variable switching
- regularization
- ...

Regularization

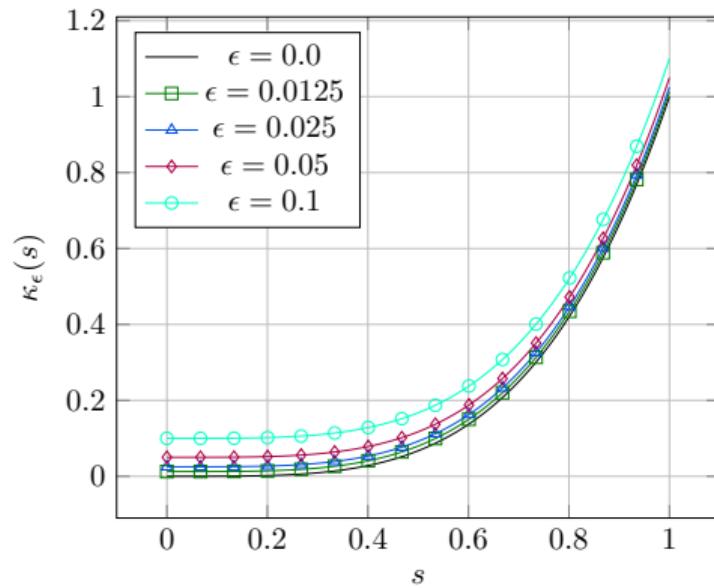


Brooks–Corey **regularized**
pressure–saturation functions

Regularization



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



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

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Variational inequalities (complementarity problems)

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

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

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Common methods

- semismooth Newton methods
- path finding
- interior-point methods
- regularization
- ...

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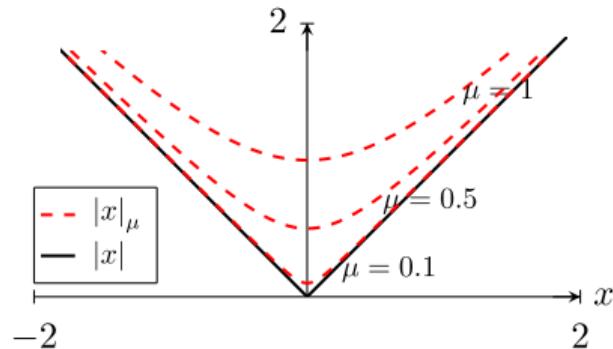
Complementarity functions

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

$$\mathbf{C}(\mathbf{X}) = \mathbf{0}$$

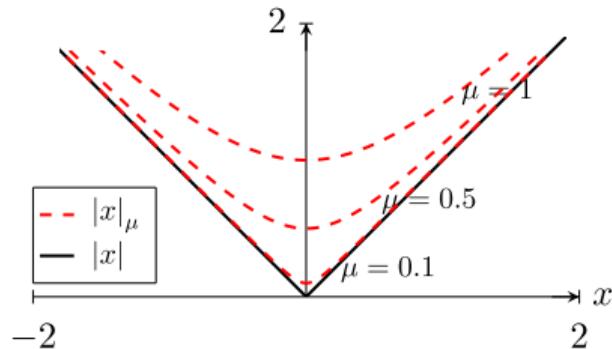
equivalent reformulation as
nonlinear **nonsmooth equalities**

Regularized complementarity functions

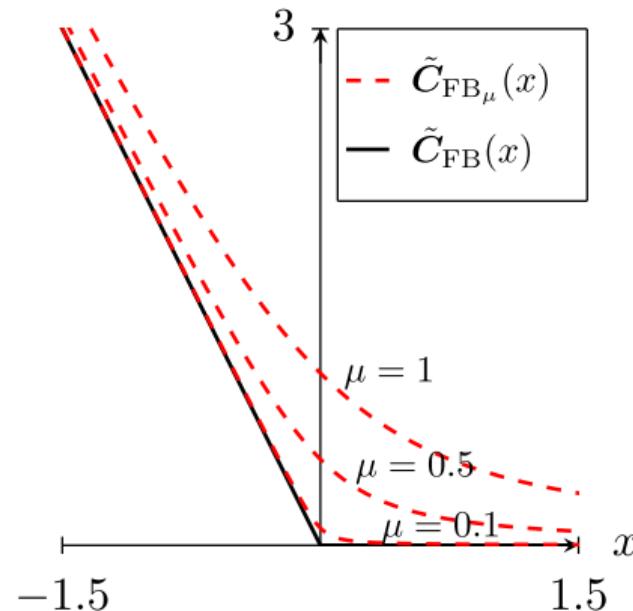


Regularized absolute value
(Newton-min) C -functions

Regularized complementarity functions



Regularized absolute value
(Newton-min) C -functions



Regularized Fischer–Burmeister C -functions

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Numerical approximations of unsteady nonlinear PDEs:

Setting

- u : unknown exact PDE solution
- u_{ℓ}^n : known numerical approximation on space mesh \mathcal{T}_{ℓ} and time t^n

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Numerical approximations of unsteady nonlinear PDEs: 3 crucial questions

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Crucial questions

- ① How **large** is the overall **error** between u and $u_{\ell}^{n,j,k,i}$?

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Suggested answers

- ① Computable **a posteriori** error **estimates**.

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Suggested answers

- ① Computable **a posteriori** error **estimates**.
- ② Identification of **error components**.
- ③ **Balancing** error components, **adaptivity** (working where needed).

Main achievements

A posteriori error estimates

Guaranteed a posteriori error estimates

$$\sum_{n=1}^N \int_{t^{n-1}}^{t^n} \|u - u_\ell^{n,j,k,i}\|^2 \leq \sum_{n=1}^N \sum_{K \in \mathcal{T}_\ell^n} \eta_K(u_\ell^{n,j,k,i})^2$$

Main achievements

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Main achievements

A posteriori error estimates

Guaranteed a posteriori error estimates
with respect to the **final time** **efficient, robust**

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C_{eff} independent of T ,

Main achievements

A posteriori error estimates

Guaranteed a posteriori error estimates **locally space-time efficient, robust** with respect to the **final time**

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Guaranteed a posteriori error estimates **locally space-time efficient, robust** with respect to the **final time**, and identifying **error components**.

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Holistic approach: interplay PDE–numerics–linearization–algebra

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Nonsmooth and degenerate nonlinearities/variational inequalities

Algorithm (adaptive iterative regularization)

- 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**
- **algebraic** error is below linearization: stop algebraic solver
- **linearization** error is below regularization: stop Newton iterations
- **regularization** error is below discretization: stop regularization (ϵ_j is **never brought to zero**)
- **space mesh & time step adaptivity**
- **discretization** is below a specified tolerance: finish

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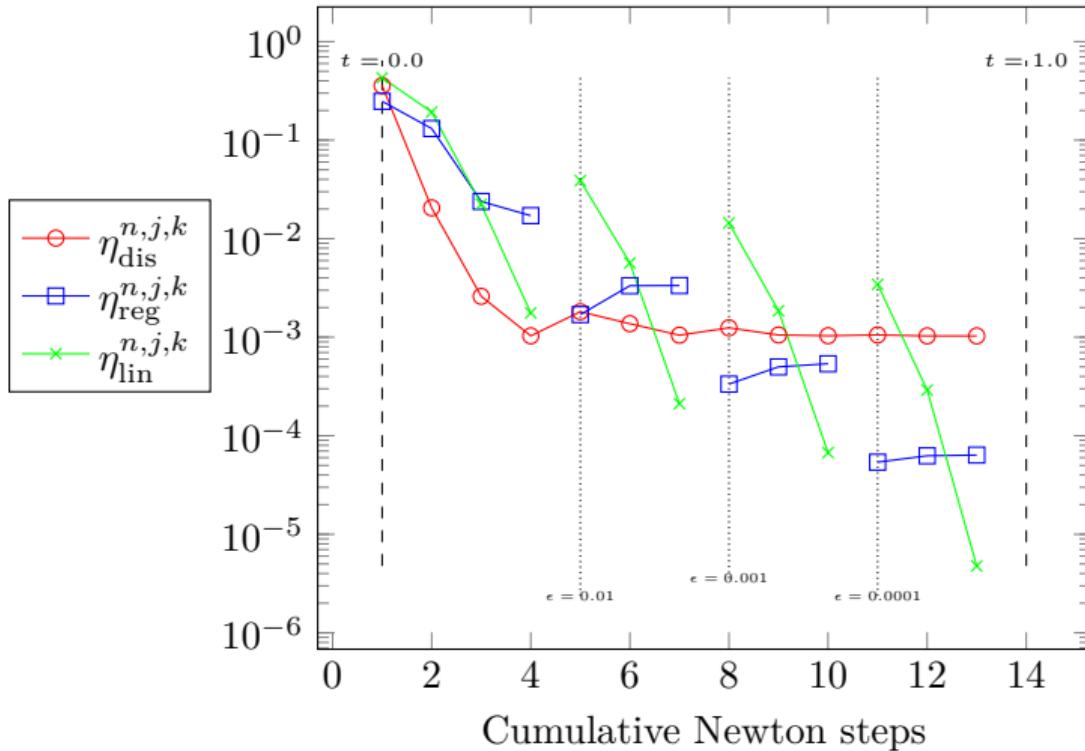
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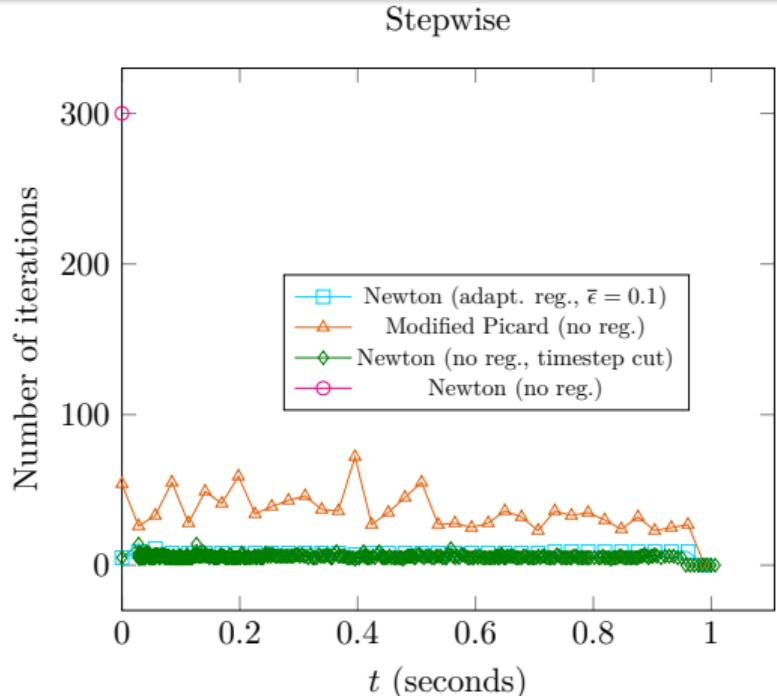
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Example overall behavior (Richards equation, 1 time step)



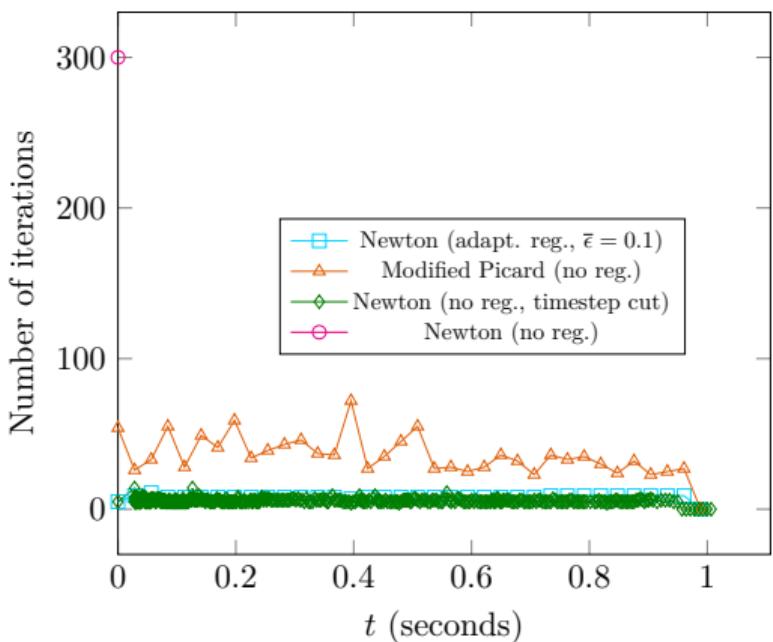
Comparison with existing approaches



Number of linearization iterations on
each time step

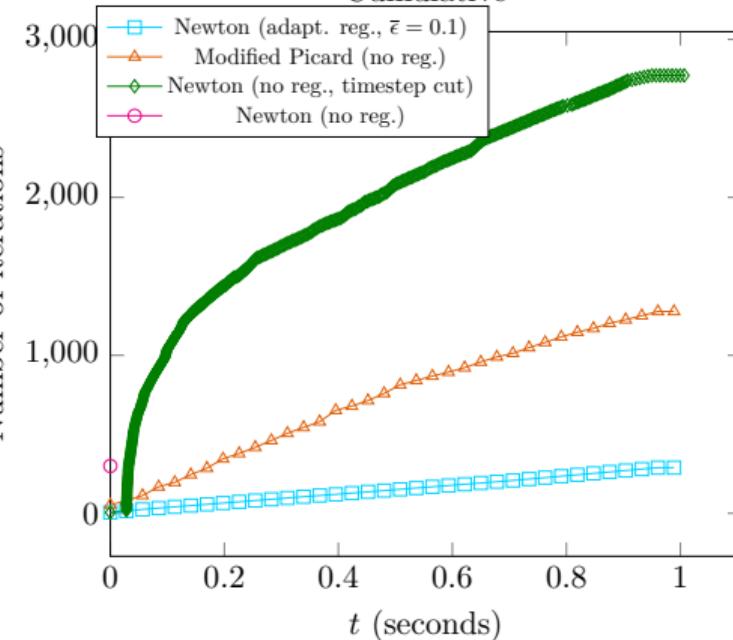
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Stepwise



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Cumulative



Cumulative number of linearization
iterations

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The heat equation ($f \in L^2(0, T; L^2(\Omega))$, $u_0 \in L^2(\Omega)$)

The heat equation

$$\begin{aligned}\partial_t u - \Delta u &= f \quad \text{in } \Omega \times (0, T), \\ u &= 0 \quad \text{on } \partial\Omega \times (0, T), \\ u(0) &= u_0 \quad \text{in } \Omega\end{aligned}$$

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Spaces

$$X := L^2(0, T; H_0^1(\Omega)), \|v\|_X^2 := \int_0^T \|\nabla v\|^2 dt,$$

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Definition (Weak solution)

$u \in Y$ with $u(0) = u_0$ such that

$$\int_0^T \langle \partial_t u, v \rangle + (\nabla u, \nabla v) dt = \int_0^T (f, v) dt \quad \forall v \in X.$$

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Nonsymmetry

Trial space Y , test space X .

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Y norm error is the dual X norm of the residual + initial condition error

$$\|u - u_{h\tau}\|_Y^2 = \sup_{v \in X, \|v\|_X=1} \left[\int_0^T (f, v) - \langle \partial_t u_{h\tau}, v \rangle - (\nabla u_{h\tau}, \nabla v) dt \right]^2 + \|u_0 - u_{h\tau}(0)\|^2$$

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- C_{eff} a generic constant independent of Ω , u , u_h , ℓ , p , τ_h , q ,

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Robust local in space and in time **error lower bound** (efficiency)

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Equilibrated flux reconstruction

Definition (Equilibrated flux reconstruction)

For each time-step interval I_n and for each vertex $\mathbf{a} \in \mathcal{V}^n$, let

$$\sigma_{h\tau}^{\mathbf{a},n} := \arg \min_{\begin{array}{l} \mathbf{v}_\ell \in \mathbf{V}_{h\tau}^{\mathbf{a},n} \\ \nabla \cdot \mathbf{v}_\ell = \psi_{\mathbf{a}}(f - \partial_t \mathcal{I} u_{h\tau}) - \nabla \psi_{\mathbf{a}} \cdot \nabla u_{h\tau} \end{array}} \int_{I_n} \|\mathbf{v}_\ell + \psi_{\mathbf{a}} \nabla u_{h\tau}\|_{\omega_{\mathbf{a}}}^2 dt.$$

Then set

$$\sigma_{h\tau} := \sum_{n=1}^N \sum_{\mathbf{a} \in \mathcal{V}^n} \sigma_{h\tau}^{\mathbf{a},n}.$$

Comments

- satisfies $\sigma_{h\tau} \in L^2(0, T; \mathbf{H}(\text{div}, \Omega))$ with $\nabla \cdot \sigma_{h\tau} = f - \partial_t \mathcal{I} u_{h\tau}$
- a priori a local space-time problem, $\mathbf{V}_{\ell\tau}^{\mathbf{a},n} := \mathcal{Q}_{\mathbf{q}}(I_n; \mathbf{V}_\ell^{\mathbf{a},n})$
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Modelling flow of water and air through soil

The Richards equation

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

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

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Setting

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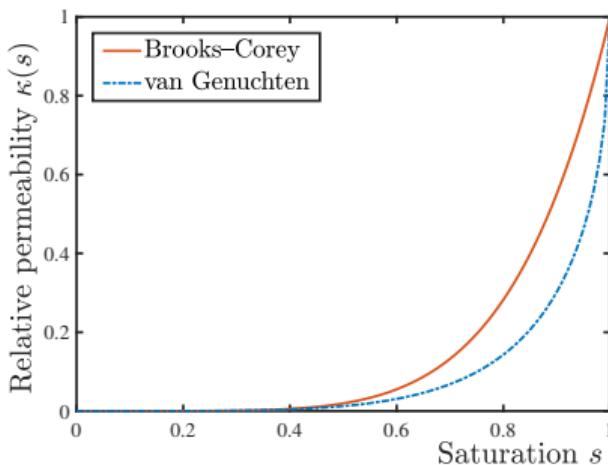
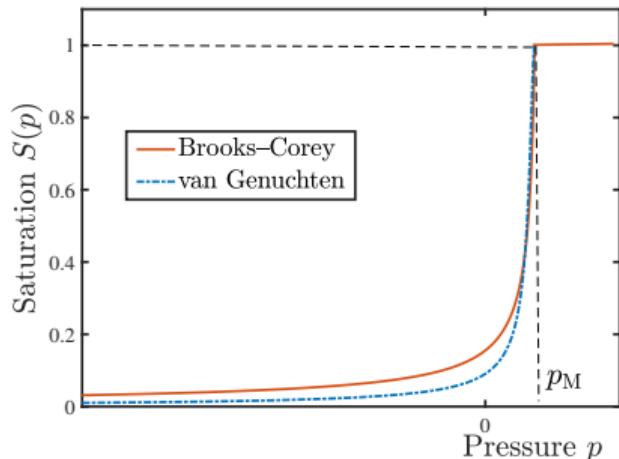
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Nonlinear (nonsmooth and degenerate) functions S and κ



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Backward Euler & finite element discretization

Piecewise polynomial space

$$V_\ell^0 := \mathcal{P}_1(\mathcal{T}_\ell) \cap H_0^1(\Omega)$$

Discretization: finite elements & backward Euler

For each $1 \leq n \leq N$, given $p_\ell^{n-1} \in V_\ell^0$, find the approximate pressure $p_\ell^n \in V_\ell^0$ satisfying

$$\frac{1}{\tau^n} (S(p_\ell^n) - S(p_\ell^{n-1}), v_\ell) + (\mathbf{F}(p_\ell^n), \nabla v_\ell) = (f(\cdot, t_n), v_\ell) \quad \forall v_\ell \in V_\ell^0,$$

where the flux is given by

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

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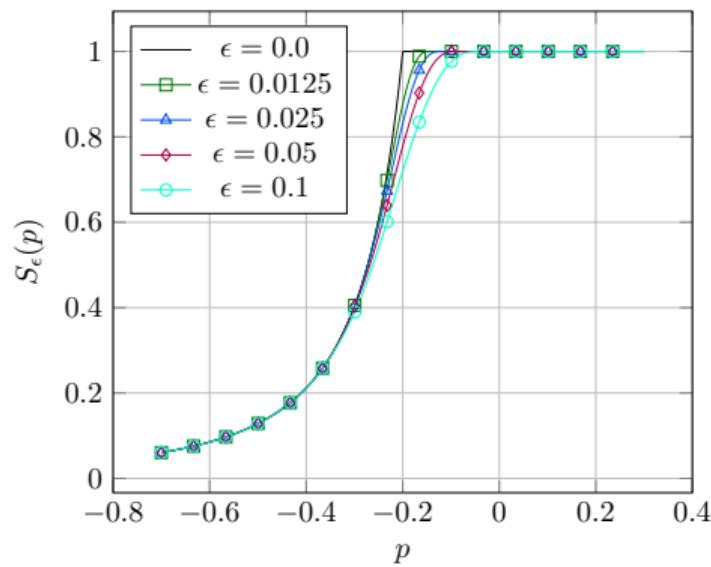
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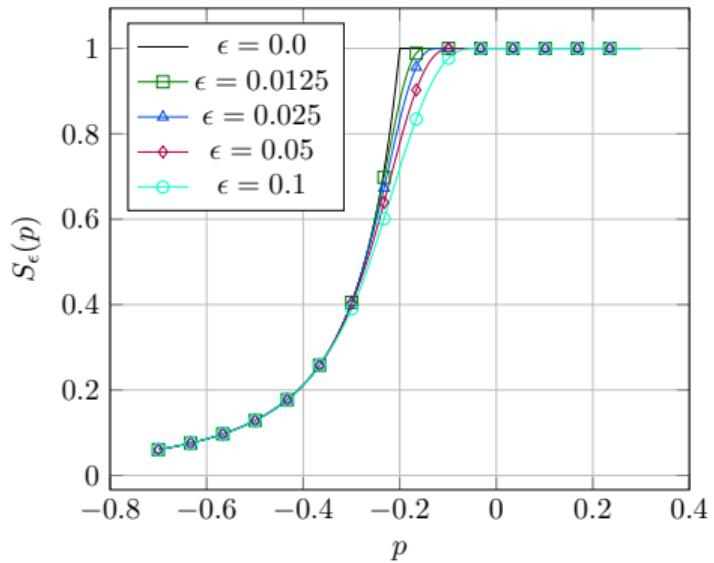
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Example regularizations

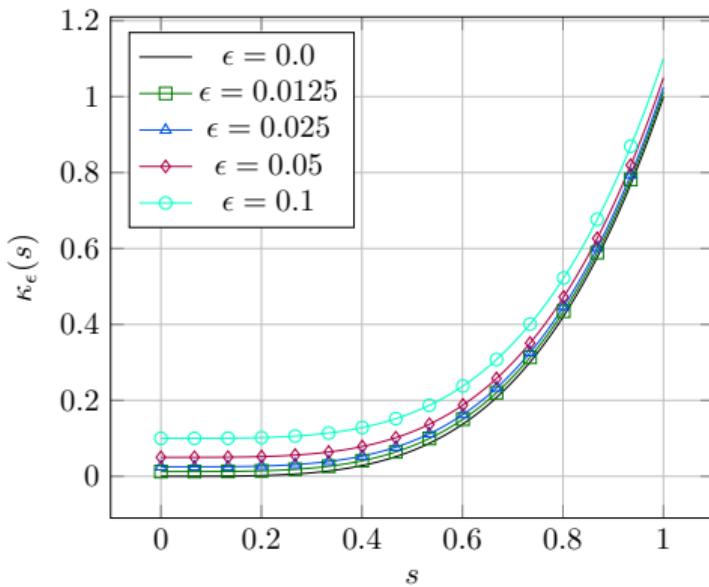


Brooks–Corey **regularized**
pressure–saturation functions

Example regularizations



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



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

Regularization

Regularization

Given $p_\ell^{n-1,\bar{j}} \in V_\ell^0$, find $p_\ell^{n,j} \in V_\ell^0$ satisfying

$$\frac{1}{\tau^n}(S_{\epsilon^j}(p_\ell^{n,j}) - S_{\epsilon^j}(p_\ell^{n-1,\bar{j}}), v_\ell) + (\mathbf{F}_{\epsilon^j}(p_\ell^{n,j}), \nabla v_\ell) = (f(\cdot, t_n), v_\ell) \quad \forall v_\ell \in V_\ell^0,$$

where the **regularized flux** is given by

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

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

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Linearization

Linearization

Given an initial guess $p_\ell^{n,j,k-1}$, find $p_\ell^{n,j,k} \in V_\ell^0$ such that, for all $v_\ell \in V_\ell^0$,

$$\frac{1}{\tau^n}(S_{\epsilon^j}(p_\ell^{n,j,k-1}) - S_{\epsilon^j}(p_\ell^{n-1,\bar{j},\bar{k}}), v_\ell) + \frac{1}{\tau^n}(\mathcal{L}(p_\ell^{n,j,k} - p_\ell^{n,j,k-1}), v_\ell) + (\mathcal{F}_\ell^{n,j,k}, \nabla v_\ell) = (f(\cdot, t_n), v_\ell),$$

where the **linearized flux** is given by

$$\mathcal{F}_\ell^{n,j,k} := \mathbf{K} \kappa_{\epsilon^j}(S_{\epsilon^j}(p_\ell^{n,j,k-1}))[\nabla p_\ell^{n,j,k} + \mathbf{g}] + \boldsymbol{\xi}(p_\ell^{n,j,k} - p_\ell^{n,j,k-1}).$$

- \bar{k} : stopping linearization index

- modified Picard:

$$\mathcal{L} := S'_{\epsilon^j}(p_\ell^{n,j,k-1}), \quad \boldsymbol{\xi} := \mathbf{0}$$

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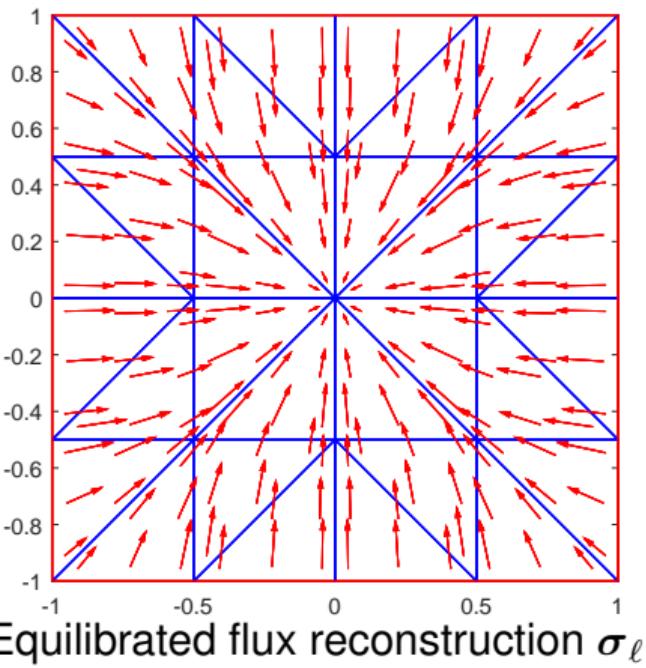
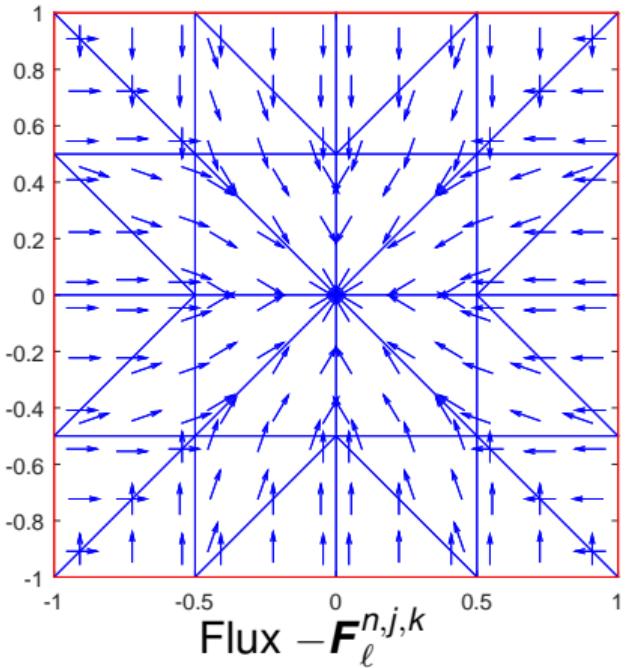
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Flux reconstruction: $-\mathbf{F}_\ell^{n,j,k} \notin \mathbf{H}(\text{div}, \Omega) \rightarrow \sigma_\ell^{n,j,k} \in \mathcal{RT}_0(\mathcal{T}_\ell) \cap \mathbf{H}(\text{div}, \Omega)$



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A posteriori estimates of error components

A posteriori estimates of error components

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

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

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

Adaptive regularization and linearization

Adaptive regularization and linearization ($\gamma_{\text{lin}}, \gamma_{\text{reg}} \approx 0.1$)

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

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

Strictly unsaturated medium

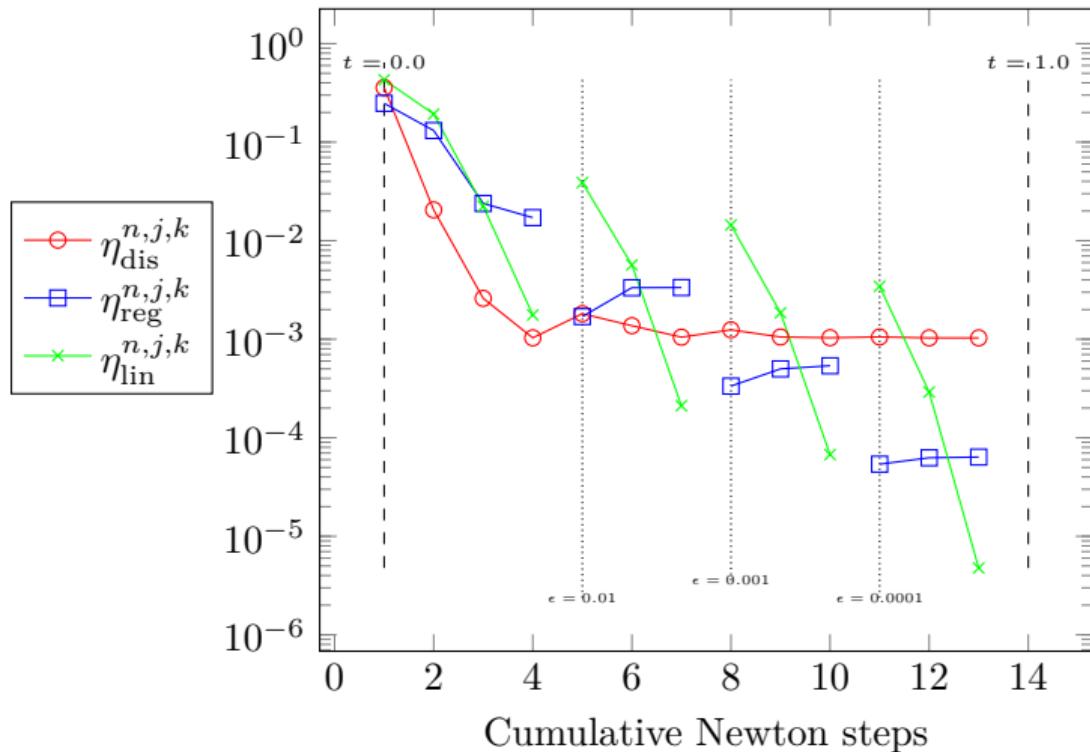
- $\Omega = \Omega_1 \cup \Omega_2$, $\Omega_1 = (0, 1) \times (0, 1/4]$, $\Omega_2 = (0, 1) \times (1/4, 1)$
- $T = 1$, $\mathbf{K} = \mathbf{I}$, $\mathbf{g} = (0, 1)^T$
- effective saturation $\mathcal{S}(s) = \frac{s - S_R}{S_V - S_R}$
- van Genuchten model

$$\kappa(s) = \kappa_c \sqrt{\mathcal{S}(s)} (1 - (1 - \mathcal{S}(s)^{1/\lambda_2})^{\lambda_2})^2,$$

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

- $p_M = 0$, $S_R = 0.026$, $S_V = 0.42$, $\kappa_c = 0.12$, $\alpha = 0.551$, $\lambda_2 = 0.655$
- $f(x, y) = \begin{cases} 0 & (x, y) \in \Omega_1, \\ 0.06 \cos(\frac{4}{3}\pi y) \sin(x) & (x, y) \in \Omega_2 \end{cases}$
- $p_0(x, y) = \begin{cases} -y - 1/4 & (x, y) \in \Omega_1, \\ -4 & (x, y) \in \Omega_2 \end{cases}$
- $s_0 = S(p_0)$
- uniform mesh with $40 \times 40 \times 2$ elements, $\tau^0 = 1$

Adaptive regularization and linearization



Injection case

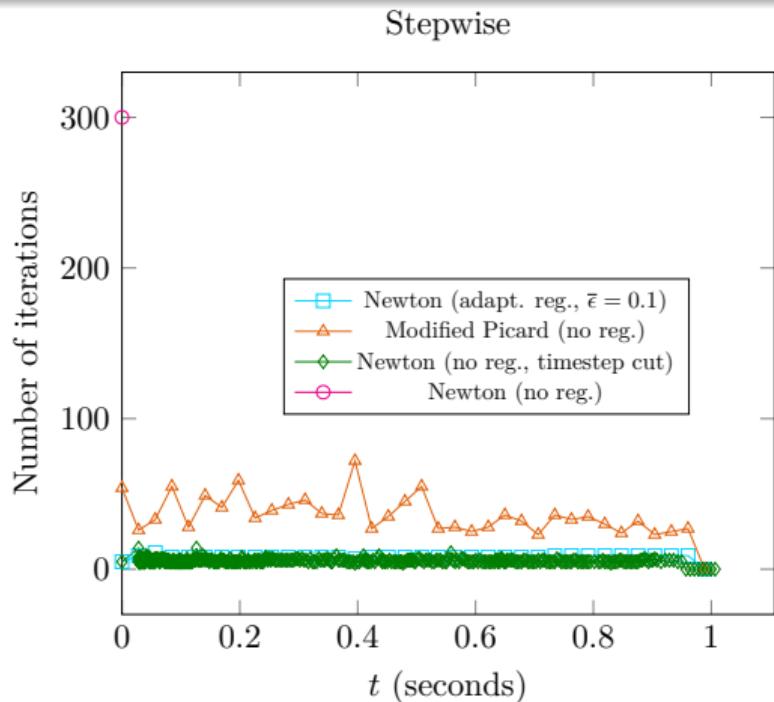
- $\Omega = (0, 1)^2$
- $T = 1, \mathbf{K} = \mathbf{I}, \mathbf{g} = (0, -1)^T$
- effective saturation $\mathcal{S}(s) = \frac{s - S_R}{S_V - S_R}$
- Brooks–Corey model

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

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

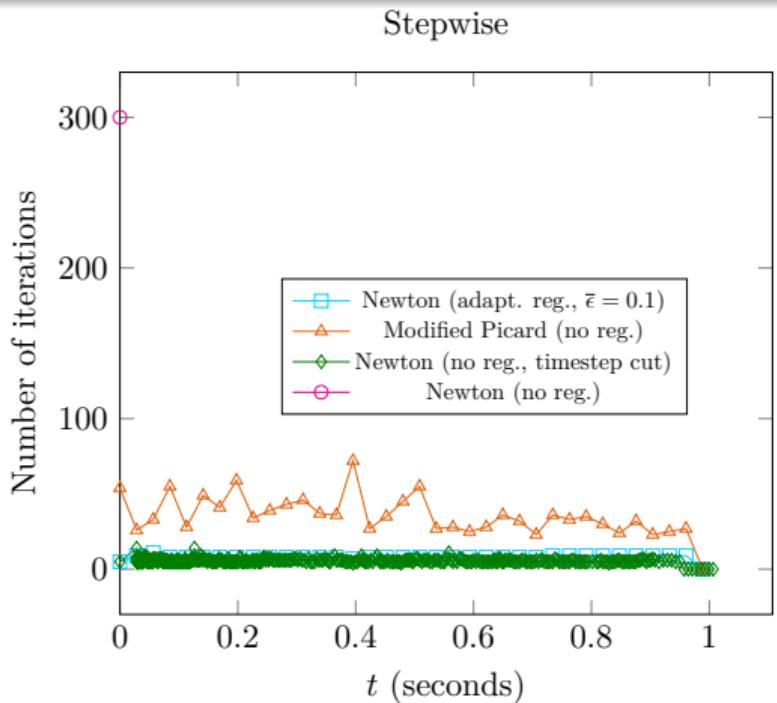
- $p_M = -0.2, \lambda_1 = 2.239$
- $f = 0$
- $p_0 = -1$
- $s_0 = S(p_0)$
- quasi uniform mesh with $\ell = 2.82 \cdot 10^{-2}, \tau^0 = 2.82 \cdot 10^{-2}$

Do we reduce the computational cost?

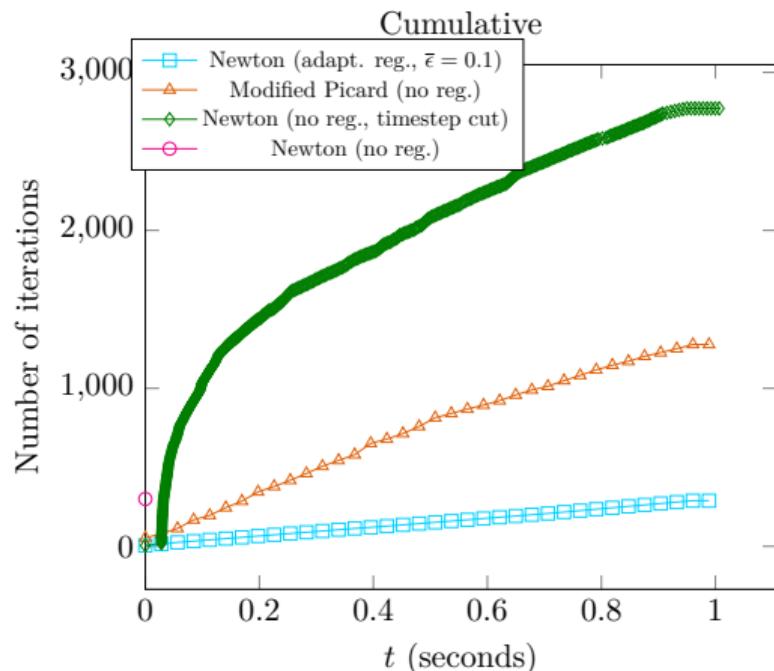


Number of linearization iterations on
each time step

Do we reduce the computational cost?

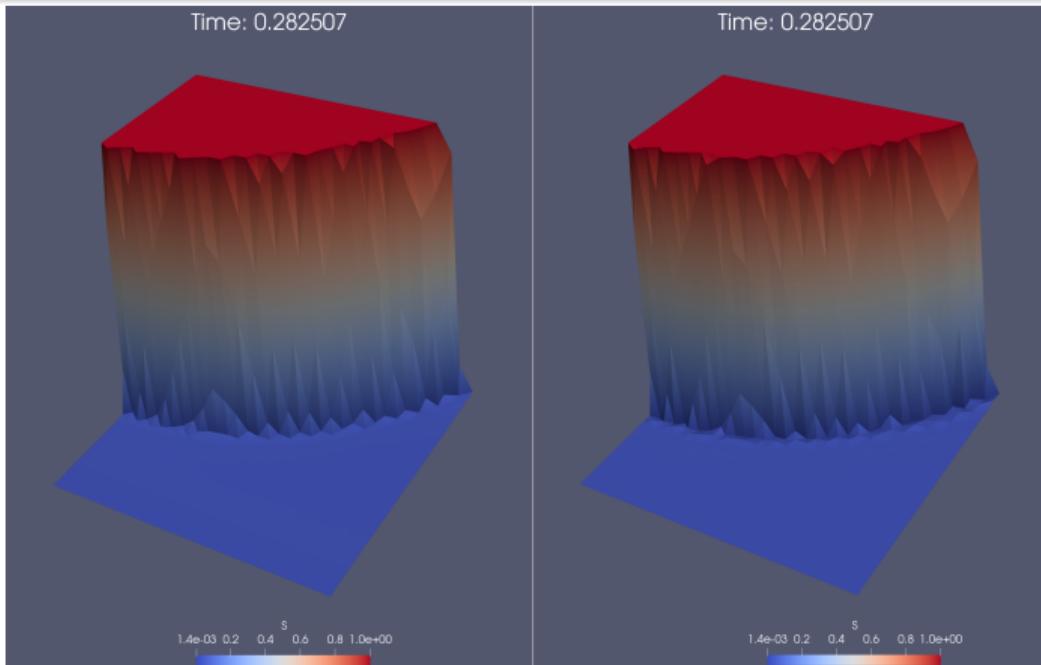


Number of linearization iterations on each time step



Cumulative number of linearization iterations

Do we lose precision?



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

Realistic case

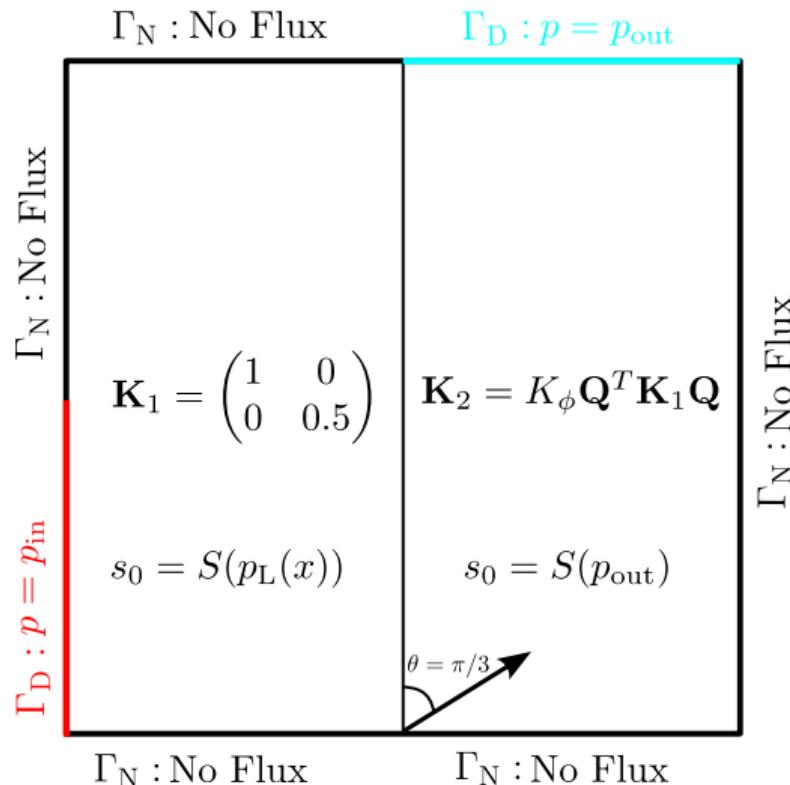
- $\Omega = (0, 1)^2$
- $T = 1$
- $\mathbf{g} = (-1, 0)^T$
- $\mathbf{Q} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$
- $K_\phi = 0.1$
- effective saturation $\mathcal{S}(s) = \frac{s - S_R}{S_V - S_R}$
- Brooks–Corey model

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

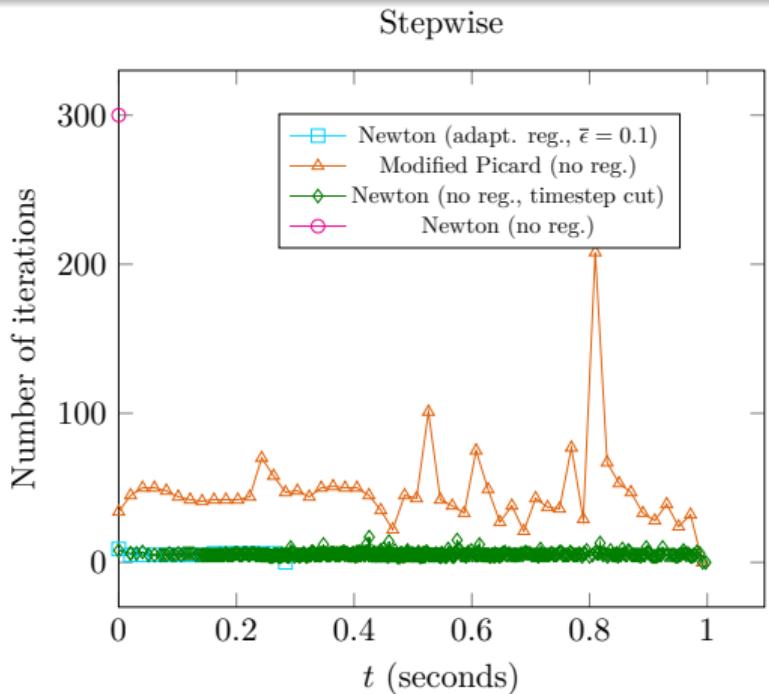
$$S(p) = \begin{cases} (-p/p_M)^{-\lambda_1} & p \leq p_M, \\ 1 & p > p_M \end{cases}$$

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

Realistic case setting

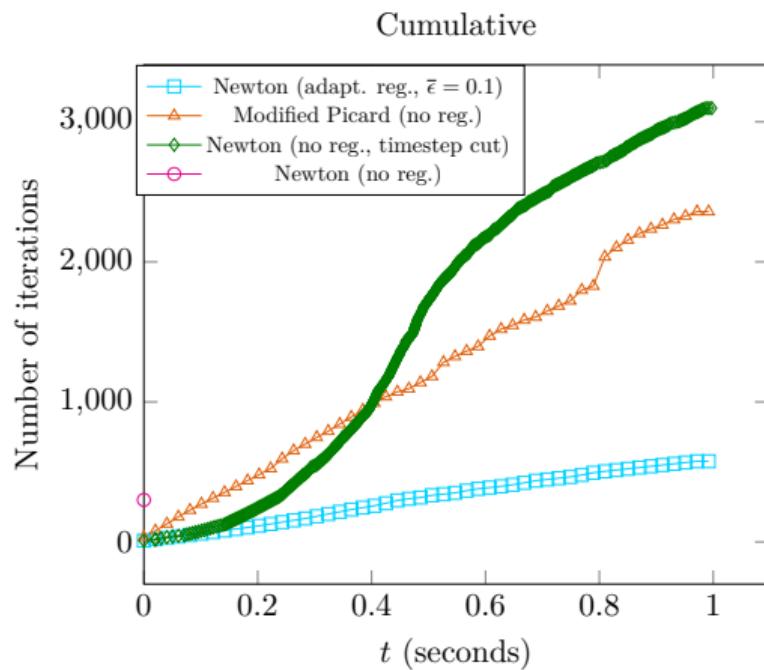
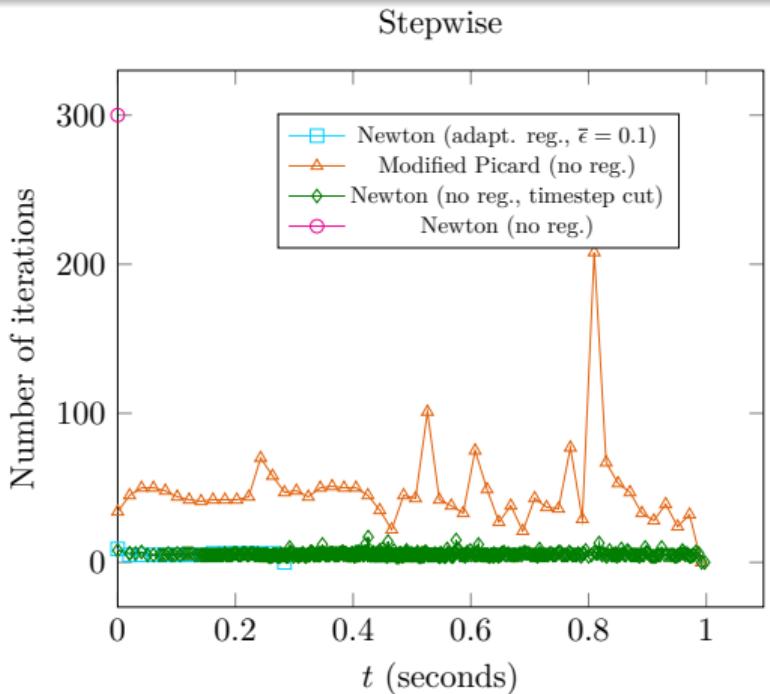


Do we reduce the computational cost?



Number of linearization iterations on
each time step

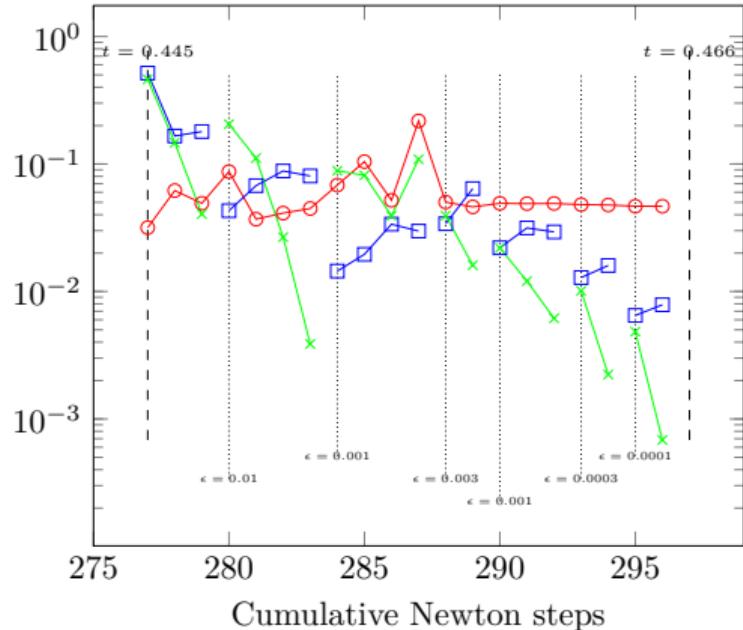
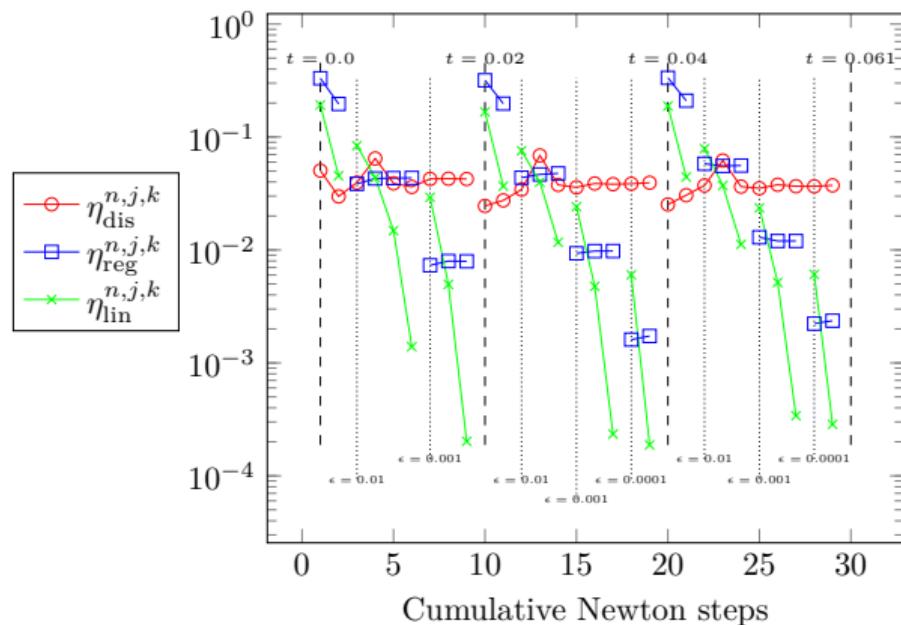
Do we reduce the computational cost?



Number of linearization iterations on each time step

Cumulative number of linearization iterations

Adaptive regularization and linearization



Perched water table case

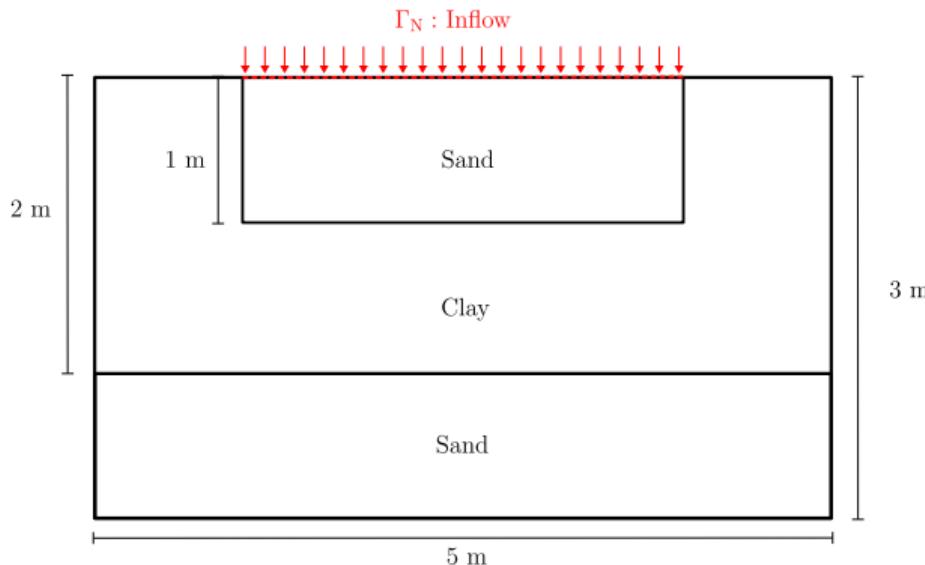
- $\Omega = (-2.5 \text{ m}, 2.5 \text{ m}) \times (-3 \text{ m}, 0 \text{ m})$
- $T = 86400 \text{ s}$ (one day)
- $\mathbf{K} = \mathbf{I}$
- $\mathbf{g} = (-1, 0)^T$
- effective saturation $\mathcal{S}(s) = \frac{s - S_R}{S_V - S_R}$
- van Genuchten model

$$\kappa(s) = \kappa_c \sqrt{\mathcal{S}(s)} (1 - (1 - \mathcal{S}(s)^{1/\lambda_2})^{\lambda_2})^2,$$

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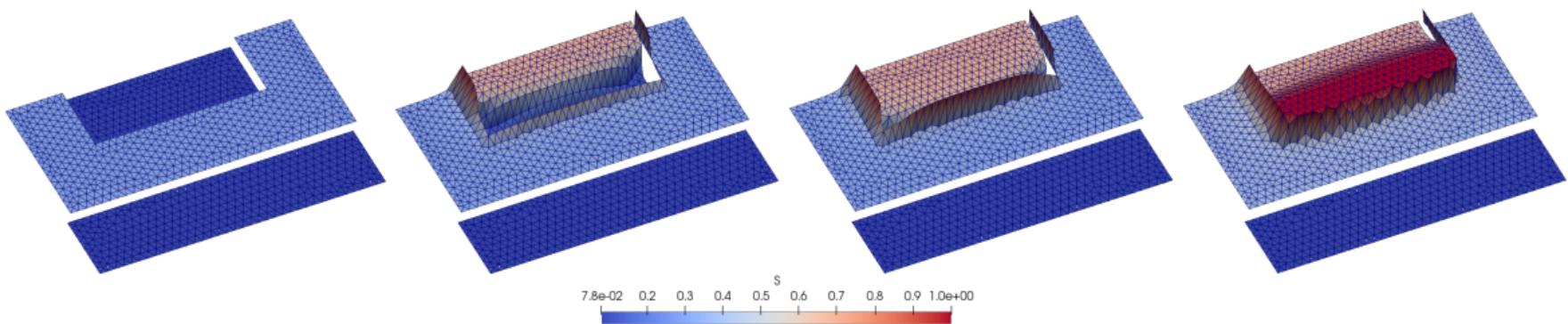
- $f = 0$
- quasi uniform mesh with $h = 8.2 \cdot 10^{-2}$
- $\tau^0 = 60 \text{ s}$, (increase $\tau^n := 1.2\tau^{n-1}$ for $n \geq 1$)
- initial condition $s_0 = S(p_0)$ with $p_0 = -300 \text{ m}$

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

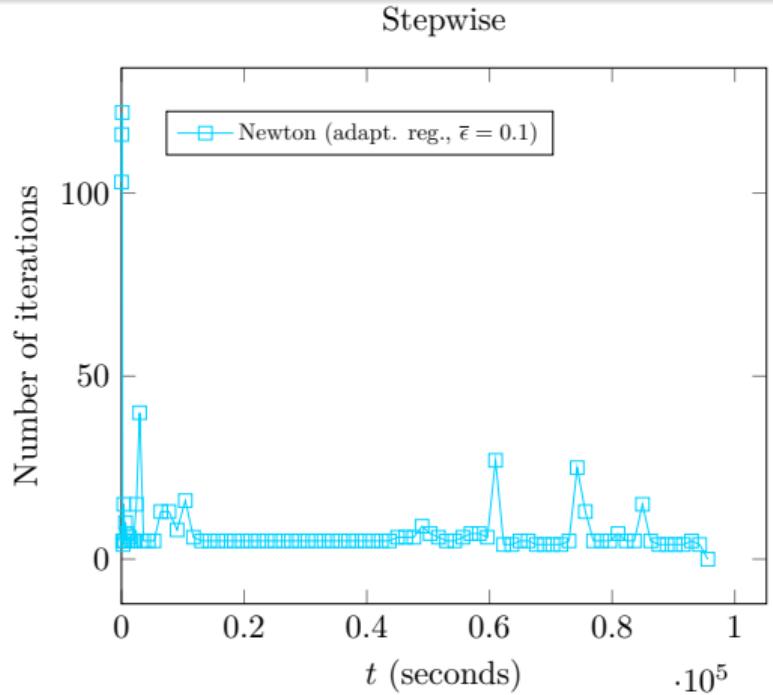
Perched water table case saturation evolution



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

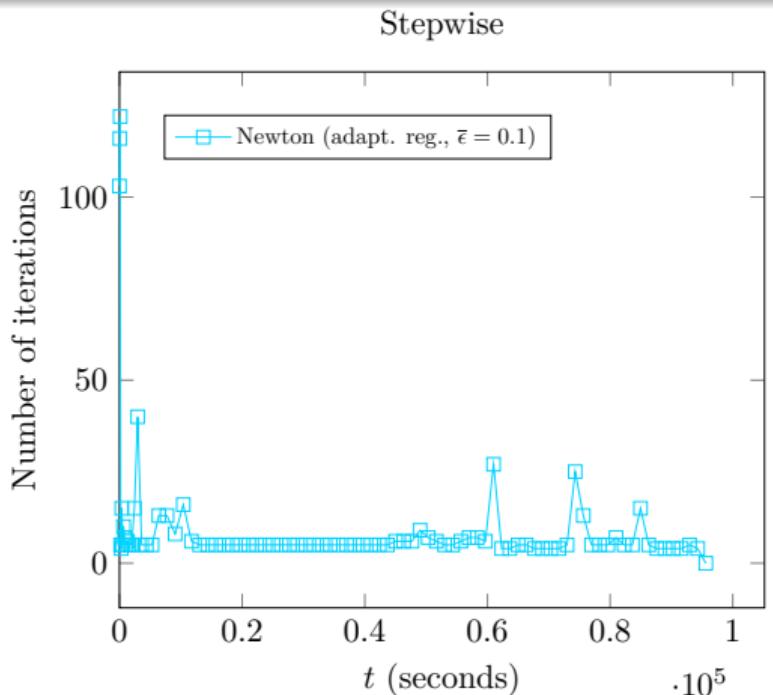
F. Févotte, A. Rappaport, M. Vohralík, Computational Geosciences (2024)

Performance: only adaptive regularization and linearization works

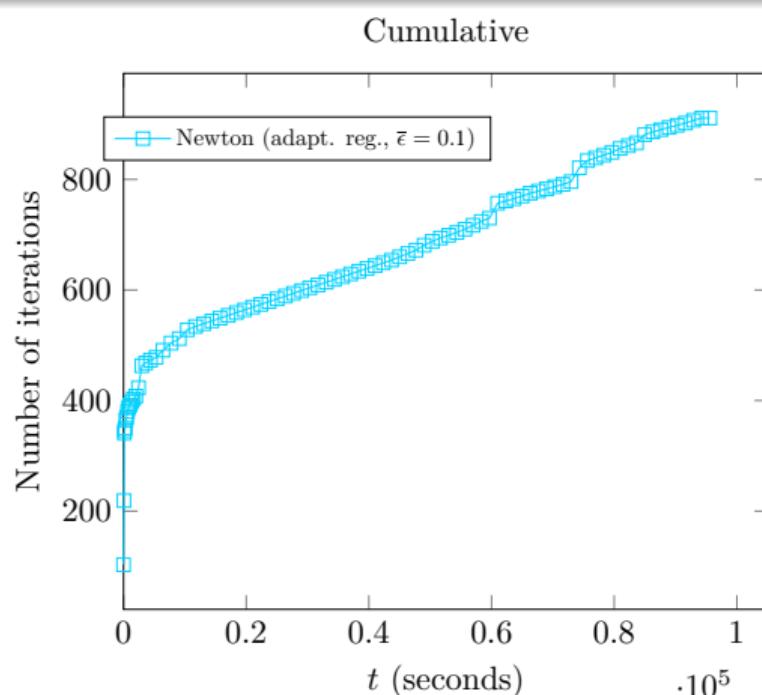


Number of linearization iterations on
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Performance: only adaptive regularization and linearization works



Number of linearization iterations on each time step



Cumulative number of linearization iterations

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- Variational inequalities (complementarity problems)
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Two-phase flow

Incompressible two-phase flow in porous media

Find *saturations* s_α and *pressures* p_α , $\alpha \in \{g, w\}$, such that

$$\begin{aligned} \partial_t(\phi s_\alpha) - \nabla \cdot \left(\frac{k_{r,\alpha}(s_w)}{\mu_\alpha} \mathbf{K} (\nabla p_\alpha + \rho_\alpha g \nabla z) \right) &= q_\alpha, \quad \alpha \in \{g, w\}, \\ s_g + s_w &= 1, \\ p_g - p_w &= p_c(s_w) \end{aligned}$$

- unsteady, nonlinear, and degenerate problem
- coupled system of PDEs & algebraic constraints

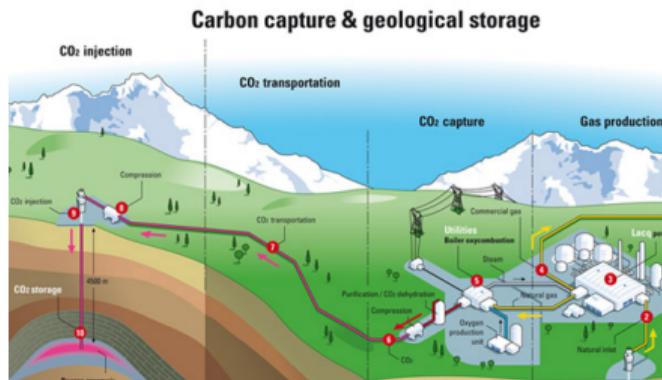
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Theorem (Multi-phase multi-compositional Darcy flow with phase (dis)appearance)

There holds

$$\text{error on time interval } I_n \leq \left\{ \sum_{c \in \mathcal{C}} (\eta_{\text{sp},c}^{n,j,k,i} + \eta_{\text{tm},c}^{n,j,k,i} + \eta_{\text{reg},c}^{n,j,k,i} + \eta_{\text{lin},c}^{n,j,k,i} + \eta_{\text{alg},c}^{n,j,k,i})^2 \right\}^{1/2}.$$

Error components

- $\eta_{\text{sp},c}^{n,j,k,i}$: spatial discretization
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Error control

- at **any moment** during the simulation
- price: sparse **matrix-vector** multiplication

Full adaptivity

- **same physical units** of all component estimators
- **balance** all component estimators
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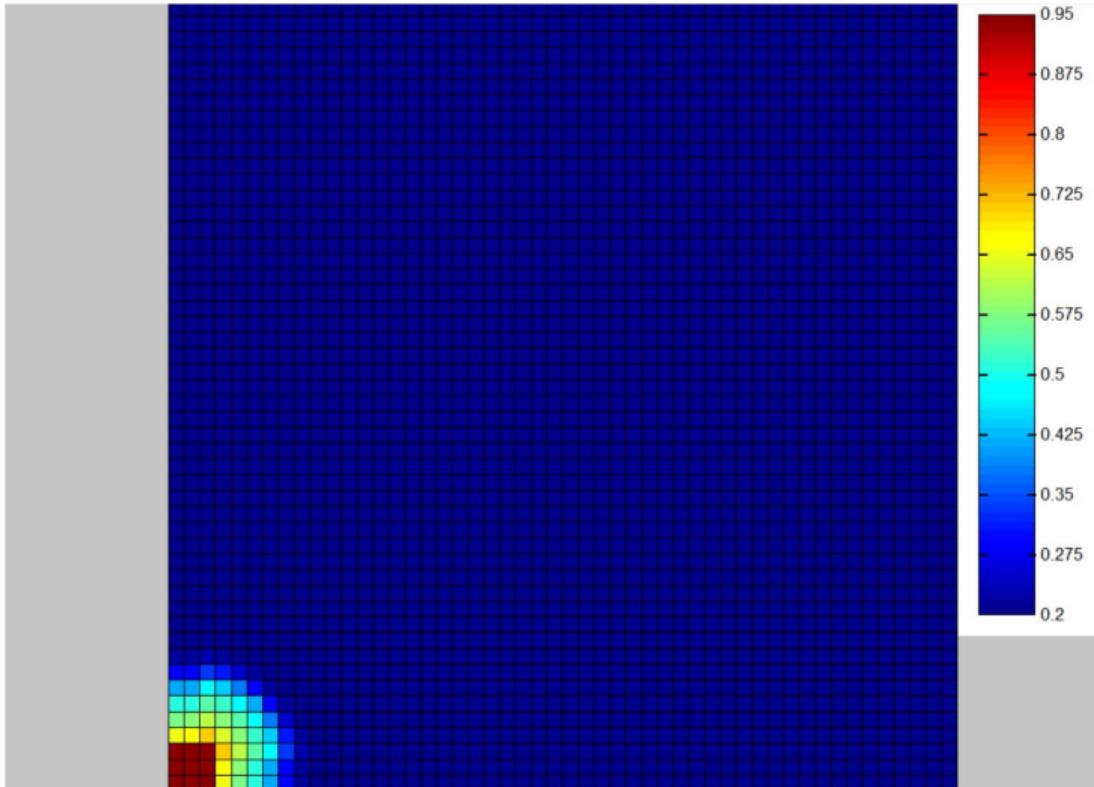
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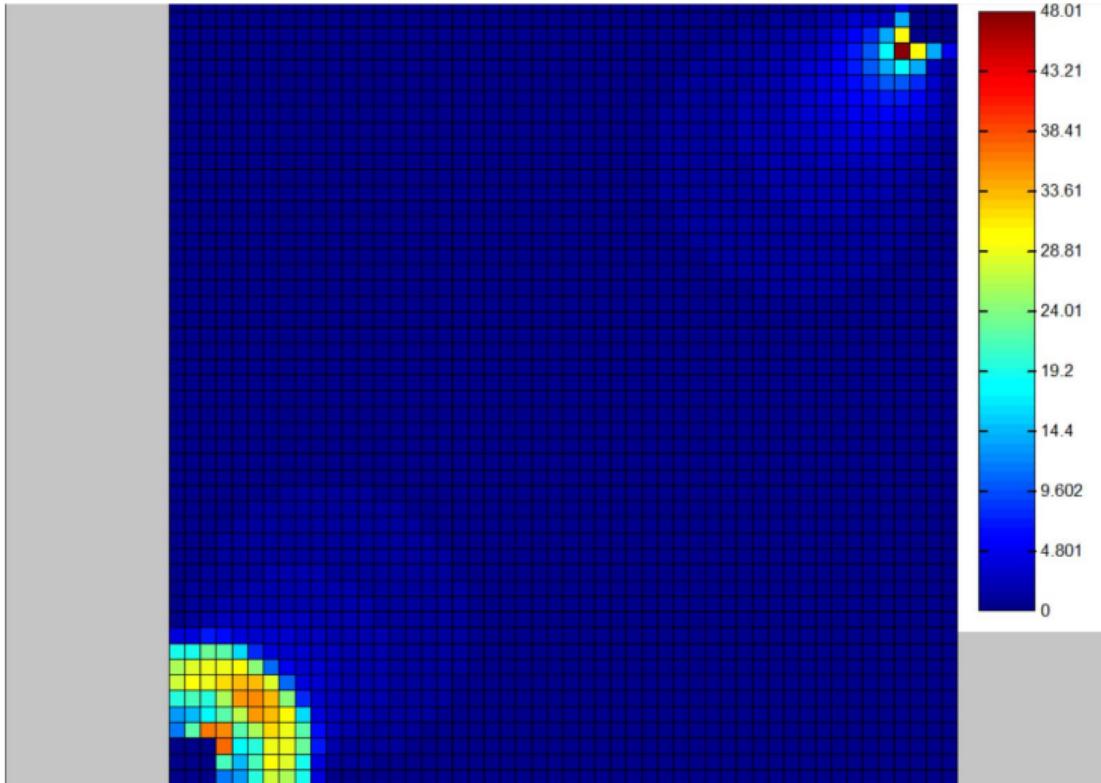
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Geological sequestration of CO₂, CO₂ saturation



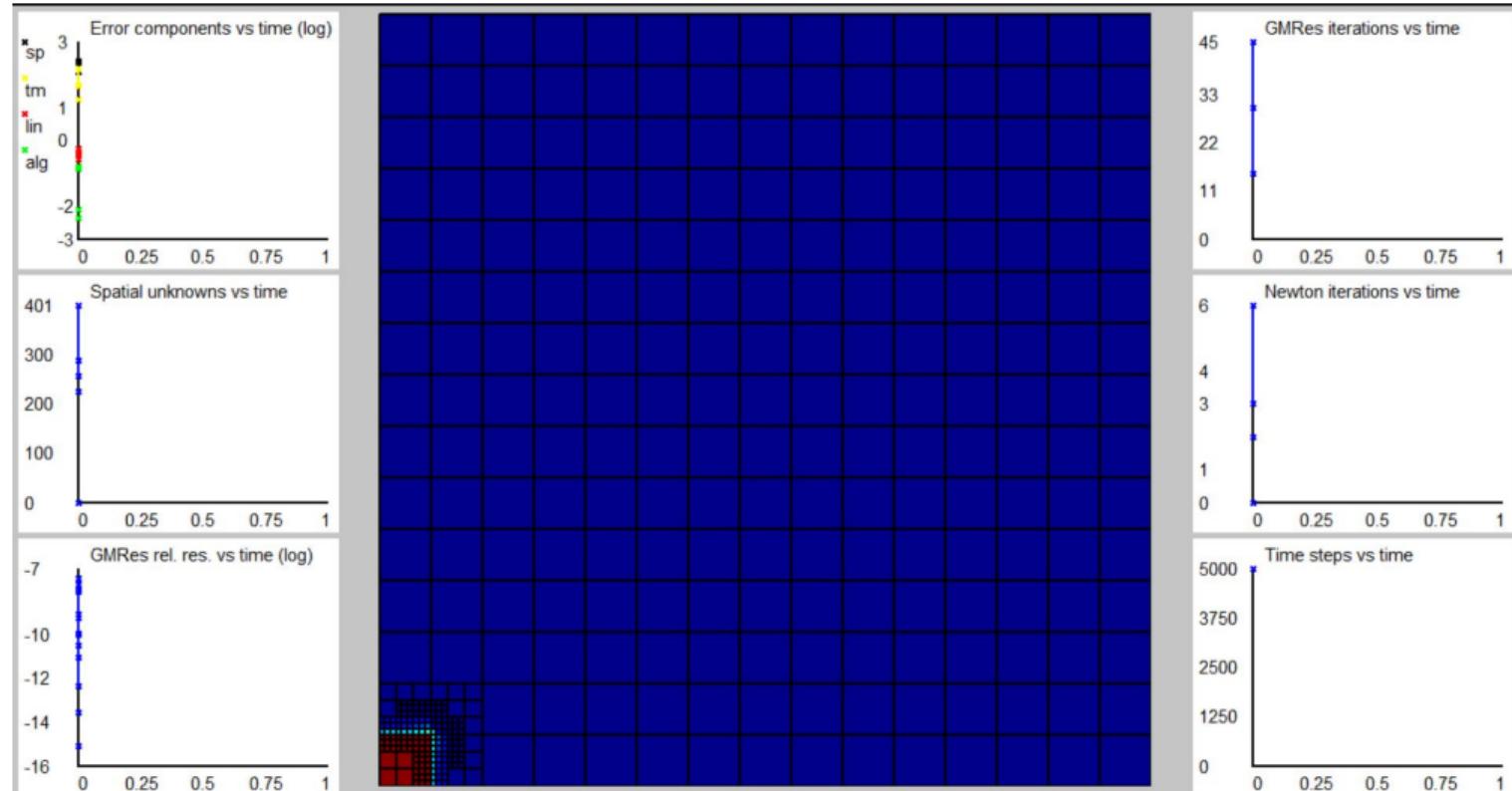
M. Vohralík, M. Wheeler, Computational Geosciences (2013)

Geological sequestration of CO₂, overall a posteriori estimate

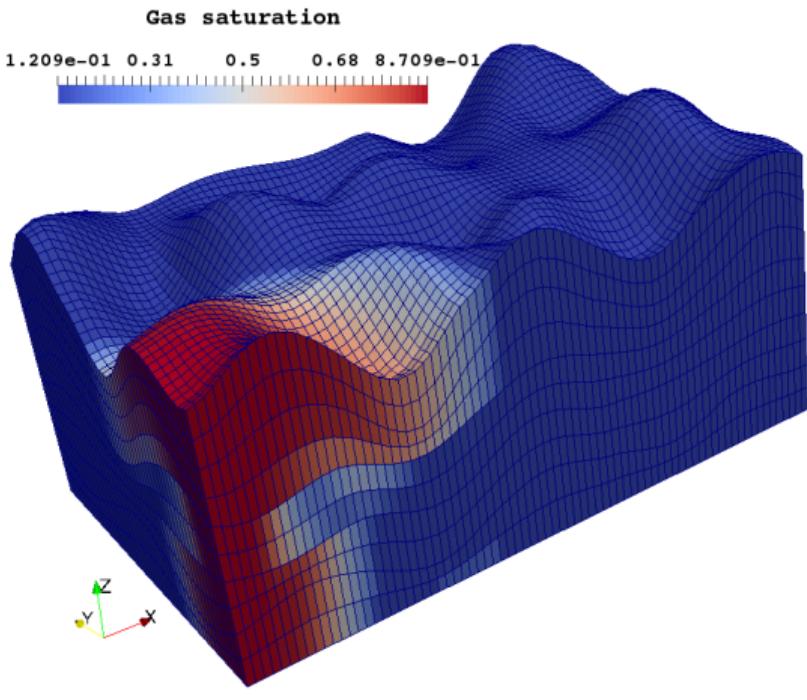


M. Vohralík, M. Wheeler, Computational Geosciences (2013)

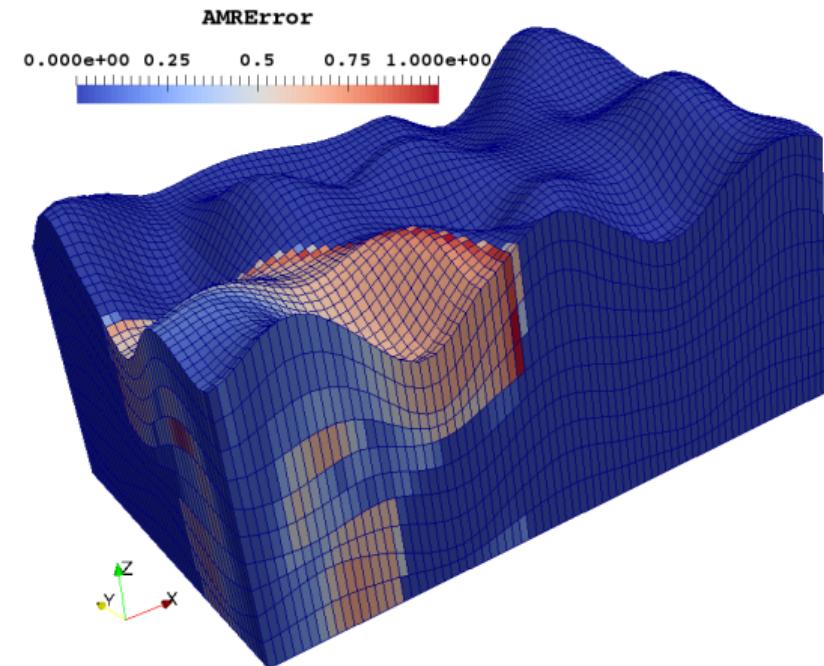
Geological sequestration of CO₂, adaptive iterative approximation



Adaptivity: 3 phases, 3 components (black-oil) problem



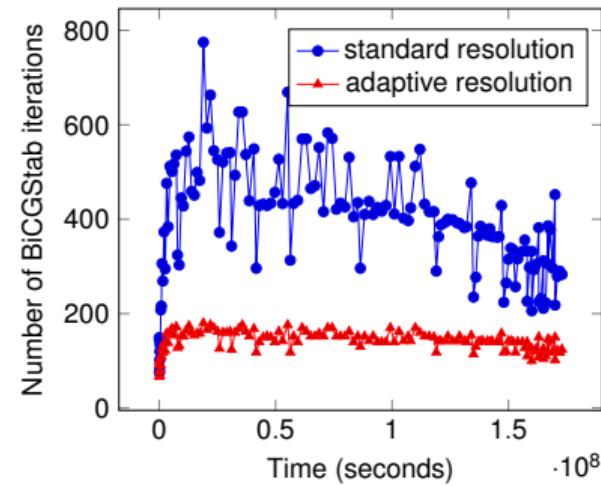
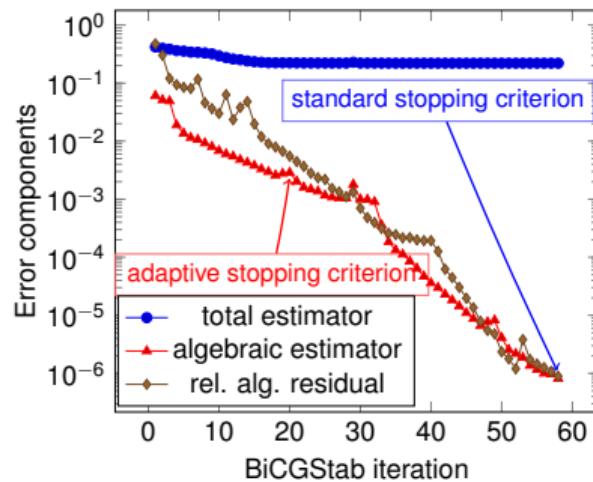
Gas saturation



A posteriori error estimate

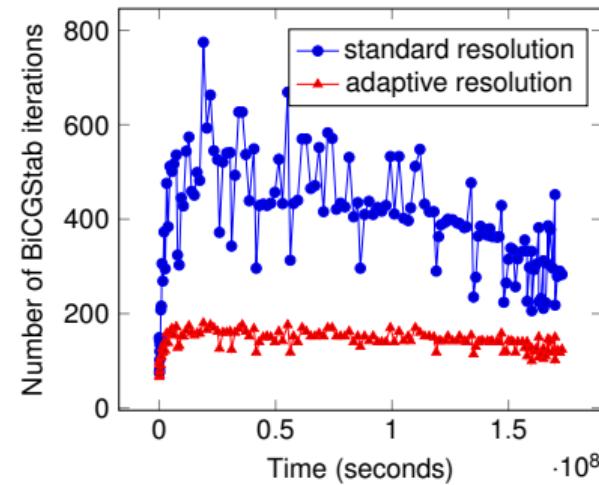
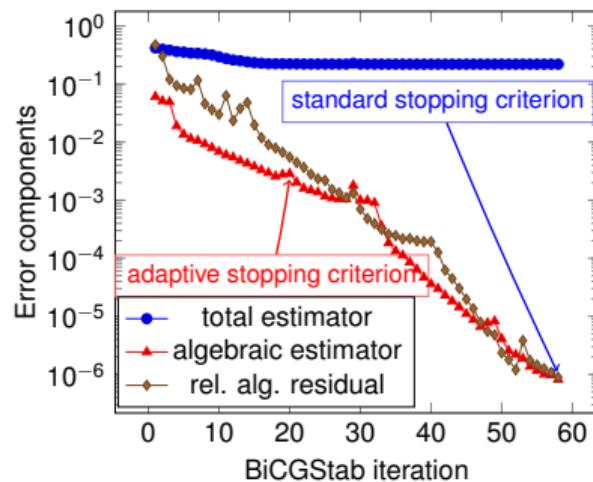
M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2018)

Three-phases, three-components (black-oil) problem: algebraic solver & spatial mesh adaptivity



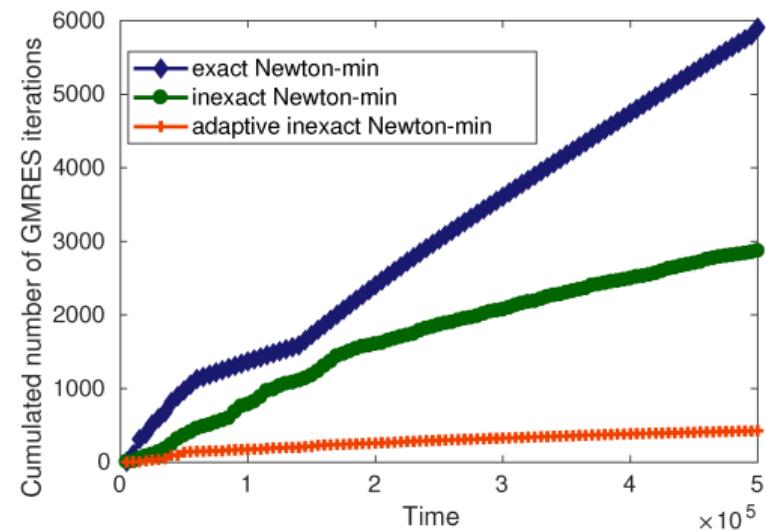
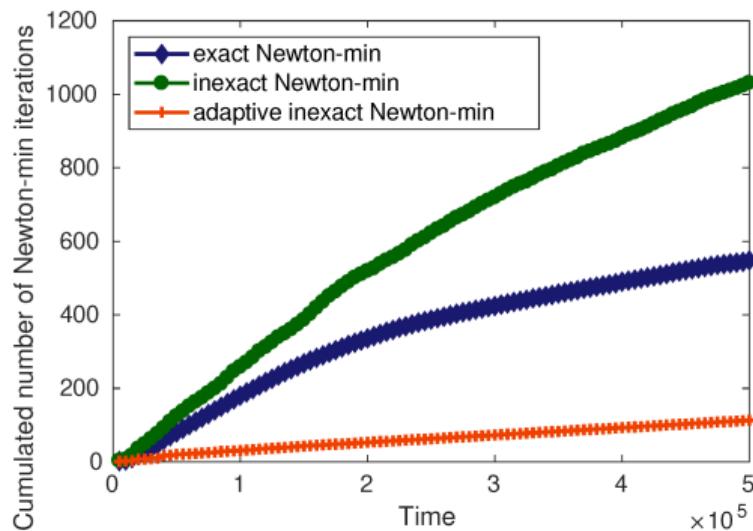
	Linear solver steps	Resolution time	AMR time	Estimators evaluation	Gain factor
Standard resolution	66386	1023s	-	-	-
Adaptive resolution	20184	201s	42s	26s	3.8

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Phase (dis)appearance: Couplex-gas benchmark



Adaptive linear and nonlinear solvers

I. Ben Ghabria, J. Dabaghi, V. Martin, M. Vohralík, Computational Geosciences (2020)

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References

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-  BEN GHARBIA I., FERZLY J., VOHRALÍK M., YOUSEF S., Semismooth and smoothing Newton methods for nonlinear systems with complementarity constraints: Adaptivity and inexact resolution, *J. Comput. Appl. Math.* **420** (2023), 114765.
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Thank you for your attention!