Nonlinear preconditioning techniques for unbalanced nonlinear systems

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Outline

Introduction and objectives

Nonlinear preconditioning

- Newton's method
- Domain decomposition: additive vs. multiplicative splitting

Iterative NIEm and block Jacobi/Newton method

- Description, strategy and algorithm
- Global monotone convergence analysis

Some applications

- Richards equation
- Porous medium equation
- Obstacle problem
- Two-phase flow equation

Conclusions

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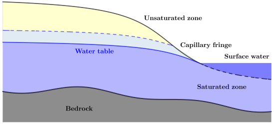
Context:



Physical problem

↓

System of PDEs

↓

Large algebraic nonlinear system: $F(\boldsymbol{u}) = \mathbf{0}, \quad F : \mathbb{R}^N \to \mathbb{R}^N$

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Iterative linearization by **Newton's method** → **Nonlinear preconditioning**

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Resolution of the linear system → Linear preconditioning

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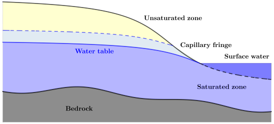

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Objective:

Study of the interaction of the monotone convergence of the semi-smooth Newton method and nonlinear preconditioning techniques and their numerical application

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Nonlinear preconditioning

Newton's method $$F'(\boldsymbol{u}^n)\left(\boldsymbol{u}^{n+1}-\boldsymbol{u}^n\right)+F(\boldsymbol{u}^n)=0$$

Newton-Kantorovich Theorem – semi-local convergence (Kantorovich '48; Ortega '68)

Nonsmooth Monotone Newton Theorem – semi-local convergence (Clarke '90; Qi & Sun '93) – global convergence (Rheinboldt '67)

Assumptions:

- Existence of $\overline{\boldsymbol{u}} \in \mathbb{R}^N$ such that $F(\overline{\boldsymbol{u}}) \geq 0$,
- Existence of $\boldsymbol{J}(\boldsymbol{u}) \in \boldsymbol{\partial F}(\boldsymbol{u})$ such that $\boldsymbol{J}(\boldsymbol{u})^{-1} \geq \mathbf{0}$,
- For all $D \subset \mathbb{R}^N$, there exists Q such that: $Q^{-1} \geq 0$ and $\boldsymbol{J}(\boldsymbol{u}) \leq \boldsymbol{Q}$ for all $\boldsymbol{u} \in D$.

Then:

- $F(\boldsymbol{u}^n) \leq 0$ and $\boldsymbol{u}^n \leq \boldsymbol{u}^{n+1} \leq \boldsymbol{u}^\star$, $\forall\, n \geq 1$,
- $\{\boldsymbol{u}^n\}_n$ converges to the unique solution $\boldsymbol{u}^\star$.

Nonlinear preconditioning

Domain decomposition

Objective: to operate on **smaller subsets of dofs**.

Reasons: treat unbalanced nonlinearities, parallel computation, etc.

Nonlinear preconditioning

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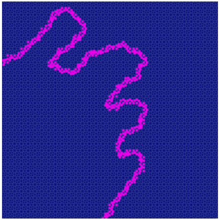
- Partitioning of the unknowns:

$$\boldsymbol{u} = (\underbrace{u_1, \dots, u_{N_1}}_{\boldsymbol{u}_1}, \underbrace{u_{N_1+1}, \dots, u_{N_2}}_{\boldsymbol{u}_2}, \dots, \underbrace{u_{N_{(m-1)+1}}, \dots, u_{N_m}}_{\boldsymbol{u}_m})$$

$m = 2$



$m = 8$

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- Splitting of the system:

$$\begin{cases} F_1(\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_m) = 0, \\ F_2(\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_m) = 0, \\ \vdots \\ F_m(\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_m) = 0. \end{cases}$$

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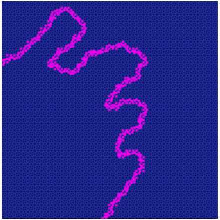

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- Definition of local operators G_i through implicit function theorem:
$$F_i(\boldsymbol{u}_1, \dots, G_i(\boldsymbol{u}_i^c), \dots, \boldsymbol{u}_m) = 0, \quad \forall i = 1, \dots, m.$$

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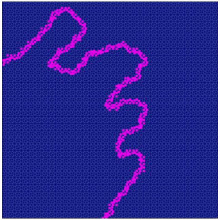

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- Reformulation of the problem:

$$F_i(\boldsymbol{u}) = 0 \iff \boldsymbol{u}_i = G_i(\boldsymbol{u}_1, \ldots, \boldsymbol{u}_{i-1}, \boldsymbol{u}_{i+1}, \ldots, \boldsymbol{u}_m), \quad \forall i = 1, \ldots, m.$$

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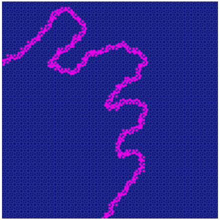

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Nonlinear preconditioning

Additive splitting:

ASPIN (Keyes, Cai, Young 2002)
RASPEN (Bastian, Kamthorncharoen 2021; Gander, Dolean, Masson 2016)

$$\begin{cases} \boldsymbol{u}_1 - G_1(\boldsymbol{u}_2) = 0 \\ \boldsymbol{u}_2 - G_2(\boldsymbol{u}_1) = 0 \end{cases}$$

$$\downarrow$$

- Motivation: high concurrency.
- Symmetric approach of the subdomains.

Newton's method applied to modified systems

Multiplicative splitting:

NEPIN (Liu, Hwang, Cai, Keyes 2022)

$$\begin{cases} \boldsymbol{u}_1 - G_1(\boldsymbol{u}_2) = 0 \\ F_2(\boldsymbol{u}_1, \boldsymbol{u}_2) = 0 \end{cases}$$

INB-NE (Hwang, Lin 2010)
NIEm (Lanzkron, Rose, Wilkes 1996)

$$F_2(G_1(\boldsymbol{u}_2), \boldsymbol{u}_2) = 0$$

MSPIN (Liu, Keyes 2015)

$$\boldsymbol{u}_2 - G_2(G_1(\boldsymbol{u}_2)) = 0$$

$$\downarrow$$

- Motivation: convergence robustness.
- Asymmetric approach of the subdomains $\rightarrow$ field split or bad and good partitioning.

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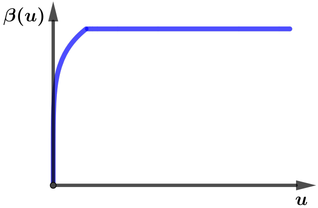
Physical setting:

Richards equation

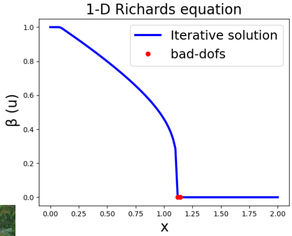
$$\partial_t s - \mathrm{div}\left(\nabla u - k(s)\boldsymbol{g}\right) = 0, \quad s = \beta(u)$$



Closure law.

Discrete nonlinear system

$$F(\boldsymbol{u}) = \beta(\boldsymbol{u}) + A\boldsymbol{u} - \boldsymbol{b} = 0$$



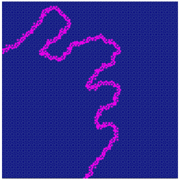
Aquifer zones (Michel et al. '19).

Iterative NIEm

Strategy:

- Identification of **bad dofs** and domain decomposition

$$F(\boldsymbol{u}) = \begin{pmatrix} F_g(\boldsymbol{u}_g, \boldsymbol{u}_b) \\ F_b(\boldsymbol{u}_g, \boldsymbol{u}_b) \end{pmatrix} = 0$$



- **Local implicit nonlinear elimination** of the bad dofs

$$\text{Given } \boldsymbol{u}_g^n, \text{ find } \tilde{\boldsymbol{u}}_b^n = G_b(\boldsymbol{u}_g^n) \text{ such that } F_b(\boldsymbol{u}_g^n, G_b(\boldsymbol{u}_g^n)) = 0$$

- **Global linearization**

$$\text{Given } \tilde{\boldsymbol{u}}^n = (\boldsymbol{u}_g^n, \tilde{\boldsymbol{u}}_b^n), \text{ find } \boldsymbol{u}^{n+1} = \tilde{\boldsymbol{u}}^n - F'(\tilde{\boldsymbol{u}}^n)^{-1} F(\tilde{\boldsymbol{u}}^n)$$

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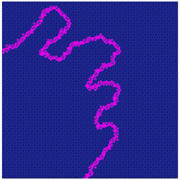

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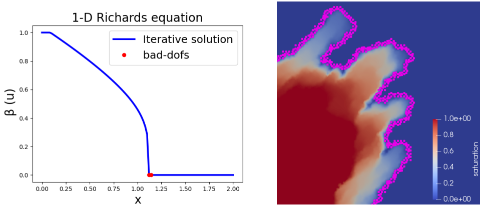
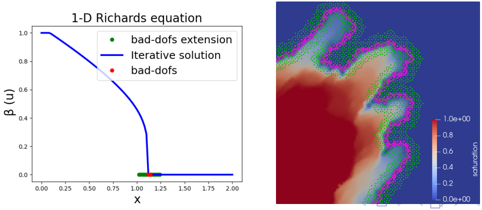
Proposition: the Newton method applied to the reduced system $F_g(\boldsymbol{u}_g, G_b(\boldsymbol{u}_g)) = 0$ is equivalent to the **iterative NIEm algorithm**

Iterative NIEm

- **Identification** criteria for the bad dofs
  - Algebraic criterion:
  $$|F(\boldsymbol{u}^n)_i| > \epsilon.$$
  - Physical criterion: front identification.



- **Extension** of the bad dofs to a fixed number of neighbouring layers of dofs.



Block Jacobi/Newton method

Strategy:

- Splitting of the unknown and of the system (e.g. $N = 8$)

$$F(\boldsymbol{u}) = \begin{pmatrix} F_1(\boldsymbol{u}_1, \ldots, \boldsymbol{u}_8) \\ \vdots \\ F_8(\boldsymbol{u}_1, \ldots, \boldsymbol{u}_8) \end{pmatrix} = 0$$

- **Local implicit nonlinear elimination** of each component

$$\text{Given } \boldsymbol{u}^n = (\boldsymbol{u}_1^n, \ldots, \boldsymbol{u}_8^n), \text{ find } \tilde{\boldsymbol{u}}^n = (\tilde{\boldsymbol{u}}_1^n, \ldots, \tilde{\boldsymbol{u}}_8^n) \text{ satisfying:}$$

$$F_1(\tilde{\boldsymbol{u}}_1^n, \boldsymbol{u}_2^n, \ldots, \boldsymbol{u}_8^n) = 0, \quad F_2(\boldsymbol{u}_1^n, \tilde{\boldsymbol{u}}_2^n, \boldsymbol{u}_3^n, \ldots, \boldsymbol{u}_8^n) = 0, \quad \ldots \quad F_8(\boldsymbol{u}_1^n, \ldots, \boldsymbol{u}_7^n, \tilde{\boldsymbol{u}}_8^n)$$

- **Global linearization**

$$\text{Given } \tilde{\boldsymbol{u}}^n = (\tilde{\boldsymbol{u}}_1^n, \ldots, \tilde{\boldsymbol{u}}_8^n), \text{ find } \boldsymbol{u}^{n+1} = \tilde{\boldsymbol{u}}^n - F'(\tilde{\boldsymbol{u}}^n)^{-1} F(\tilde{\boldsymbol{u}}^n)$$

Convergence analysis

Given $\boldsymbol{u}_g^n$, find $\tilde{\boldsymbol{u}}_b^n$ such that:	$F_b(\boldsymbol{u}_g^n, \tilde{\boldsymbol{u}}_b^n) = 0$
Set $\tilde{\boldsymbol{u}}^n = (\boldsymbol{u}_g^n, \tilde{\boldsymbol{u}}_b^n)$ and solve:	$\boldsymbol{u}^{n+1} = \tilde{\boldsymbol{u}}^n - F'(\tilde{\boldsymbol{u}}^n)^{-1} F(\tilde{\boldsymbol{u}}^n)$

Theorem: Semi-global Monotone Convergence of the Iterative NIEm and block Jacobi/Newton method

- Assumptions:
  - (i) Nonsmooth Monotone Newton Theorem,
  - (ii) $J(\boldsymbol{u})$ and the majorant Q are M-matrices
  - (iii) $F(\boldsymbol{u}^0) \leq 0$
- Proposition:
  - (i) $F(\boldsymbol{u}^n) \leq 0$ and $\boldsymbol{u}^n \leq \boldsymbol{u}^{n+1} \leq \boldsymbol{u}^\star$, $\forall\, n \geq 1$,
  - (ii) $\{\boldsymbol{u}^n\}_n$ converges to the unique solution $\boldsymbol{u}^\star$.
- Remark:
  Convergence is global, since $F(\boldsymbol{u}^0) \leq 0$ is ensured by performing a single Newton's step first.

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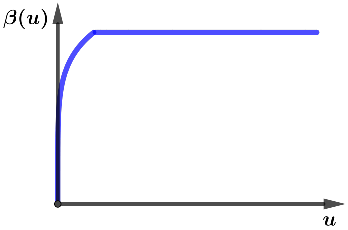
Continuous problem

$$\partial_t \beta(u(\boldsymbol{x}, t)) - \mathrm{div}(\kappa(\boldsymbol{x}) \nabla u(\boldsymbol{x}, t)) = \delta_0(\boldsymbol{x}),$$
$$\beta(u) = \min\left(u^{1/m}, 1\right).$$

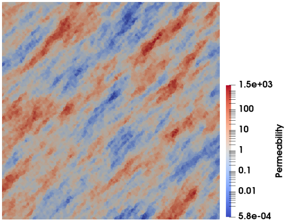
- Top-right edges: homogeneous Dirichlet boundary conditions.
- Bottom-left edges: zero-flux.
- Zero initial condition.



Discrete system

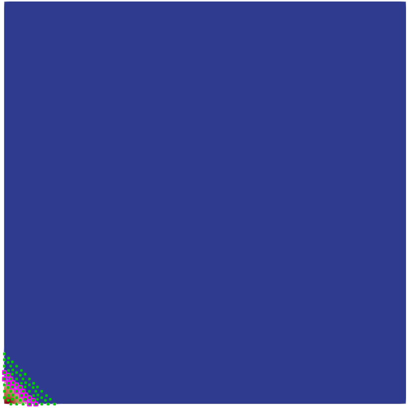
$$\beta_\epsilon(\boldsymbol{u}^{n+1}) - \beta_\epsilon(\boldsymbol{u}^n) + \Delta t \left(A\boldsymbol{u}^{n+1} - \boldsymbol{b}\right) = 0,$$
$$\beta_\epsilon(\boldsymbol{u}) = \min(10^{300}\,\boldsymbol{u}, \boldsymbol{u}^{\frac{1}{m}}, 1).$$

- Mass-lumped $\mathbb{P}_1$ FEM ($\max(\theta) \leq \pi/2$).
  $\beta'_\epsilon(\boldsymbol{u}) + \Delta t\, A$: M-matrix,
  β_ϵ: diagonal and concave.

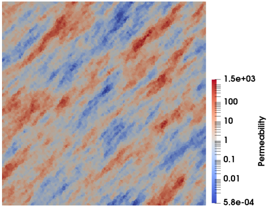


Richards equation

Saturation evolution



Iteration 1



Bad dofs:

- front dofs
- extension

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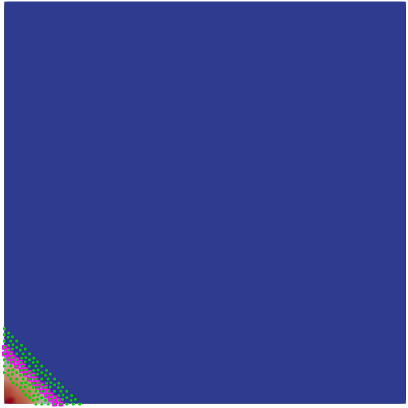
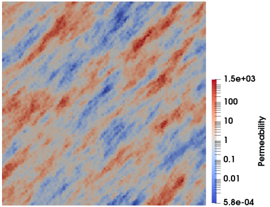


Iteration 2



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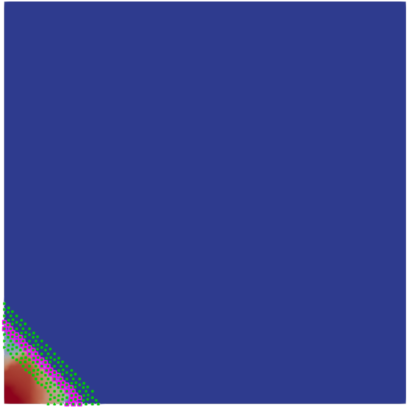
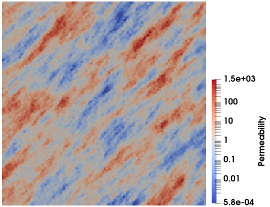


Iteration 3



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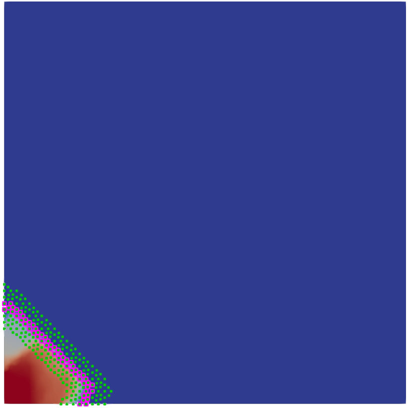
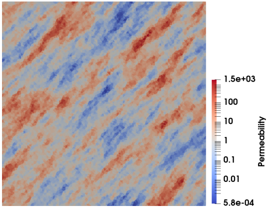


Iteration 4



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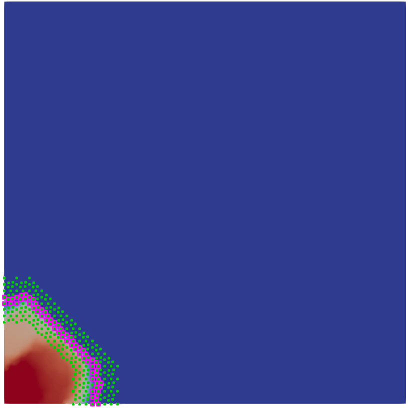
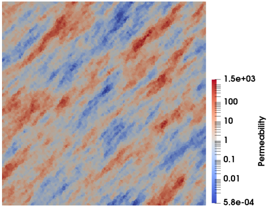


Iteration 5



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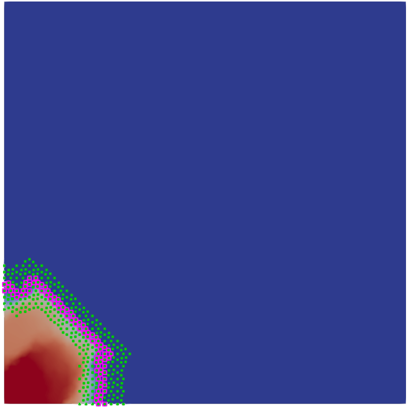
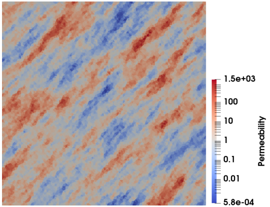


Iteration 6



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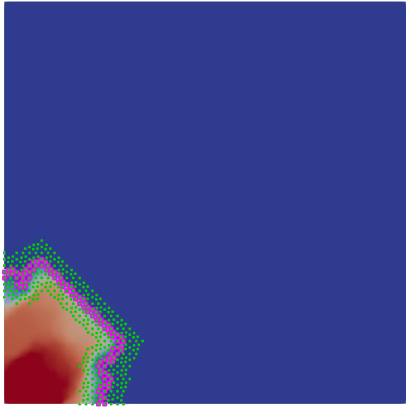
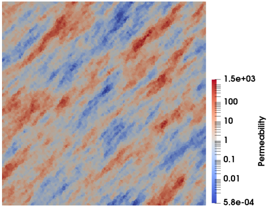


Iteration 7



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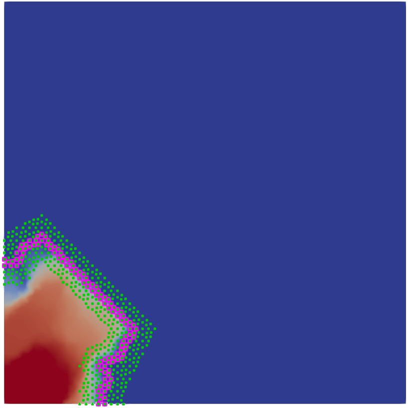
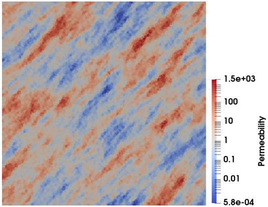


Iteration 8



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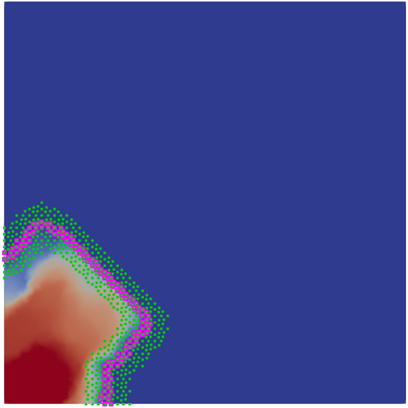
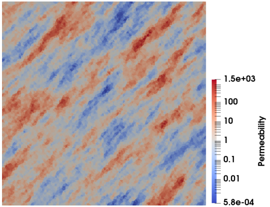


Iteration 9



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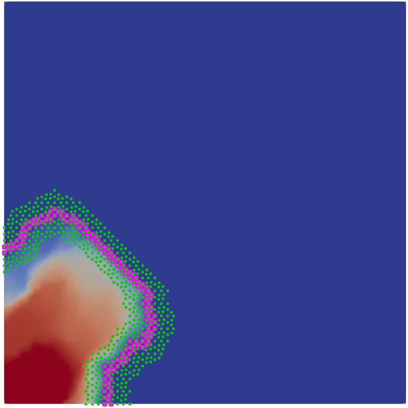
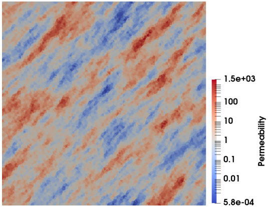
Richards equation

Saturation evolution



Iteration 10

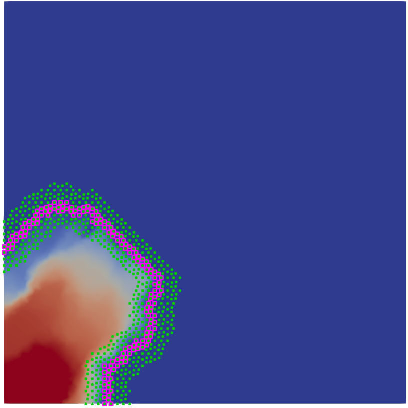


Bad dofs:

- front dofs
- extension

Richards equation

Saturation evolution



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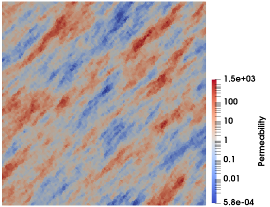

Bad dofs:

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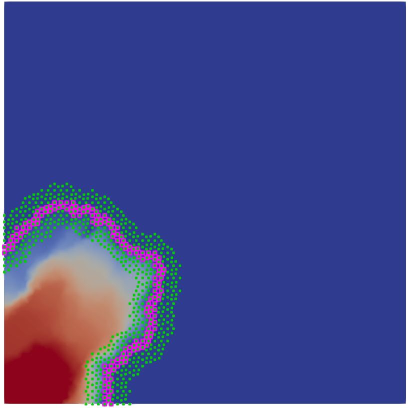
- extension

Richards equation

Saturation evolution



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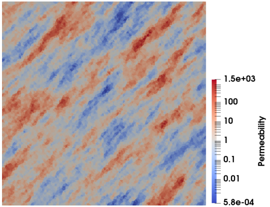

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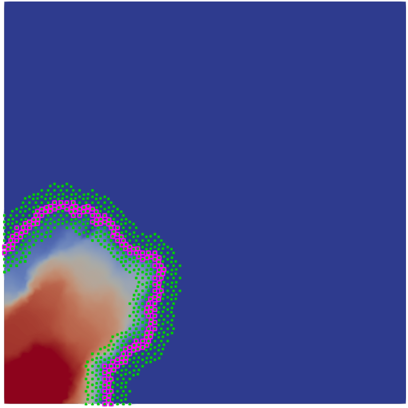
Richards equation

Saturation evolution



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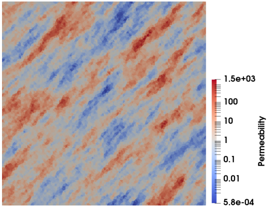

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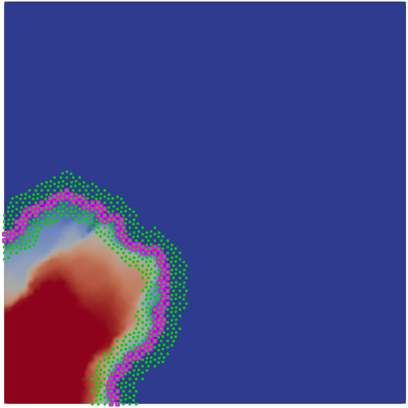
Richards equation

Saturation evolution



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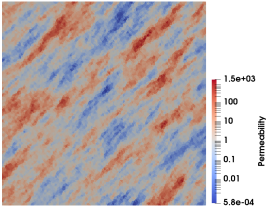

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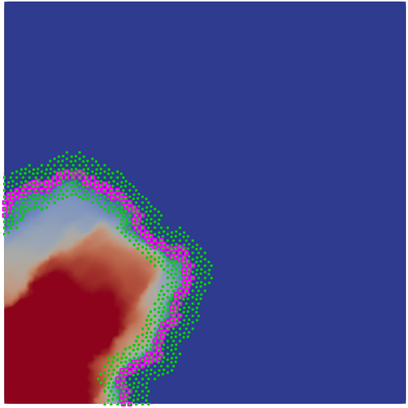
- extension

Richards equation

Saturation evolution



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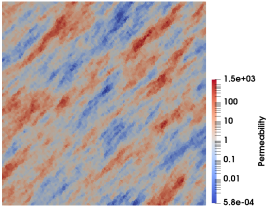

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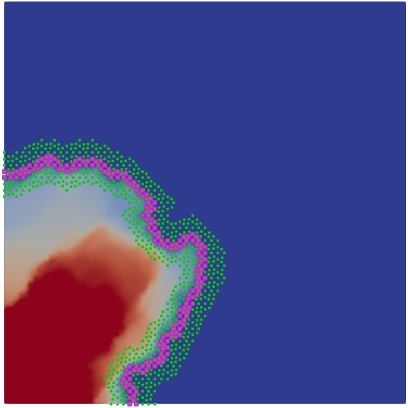
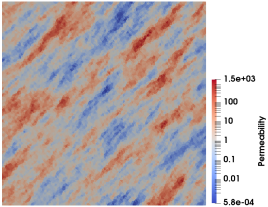
- extension

Richards equation

Saturation evolution



Iteration 16

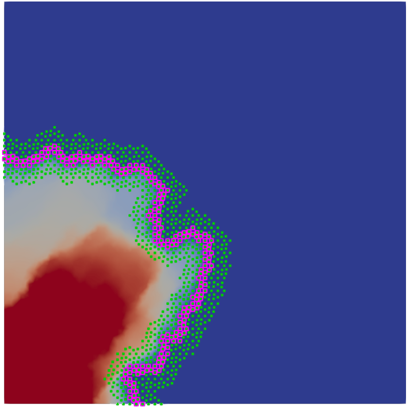


Bad dofs:

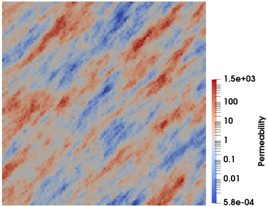
- front dofs
- extension

Richards equation

Saturation evolution



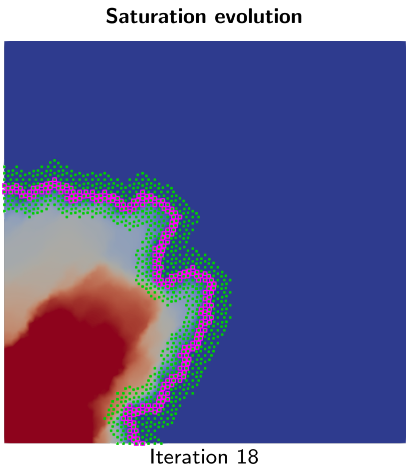
Iteration 17

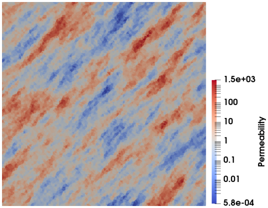


Bad dofs:

- front dofs
- extension

Richards equation





Bad dofs:

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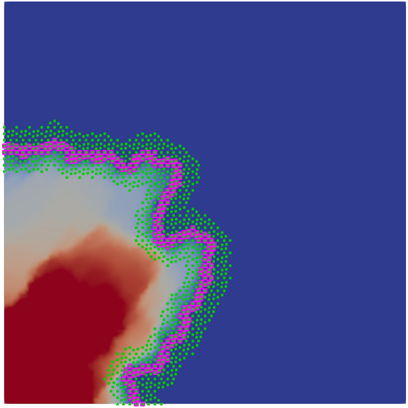
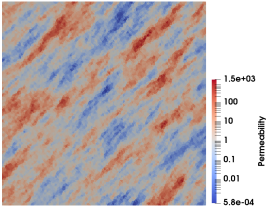
- extension

Richards equation

Saturation evolution



Iteration 19



Bad dofs:

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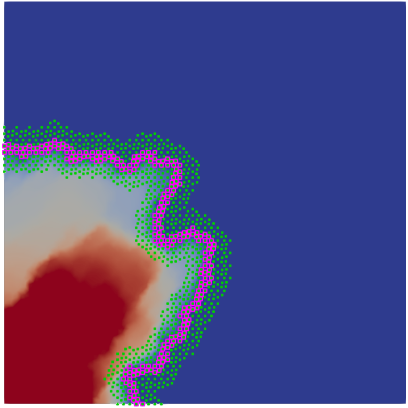
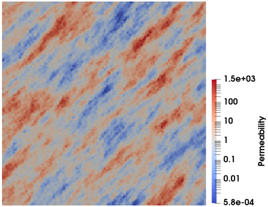
Saturation evolution



Iteration 20



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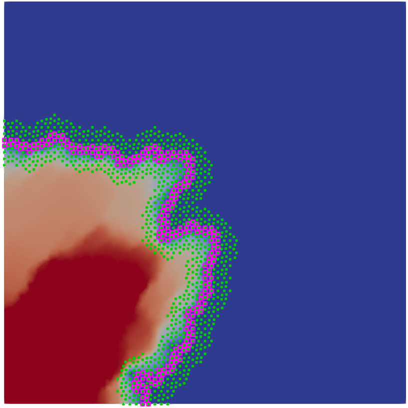
Richards equation

Saturation evolution



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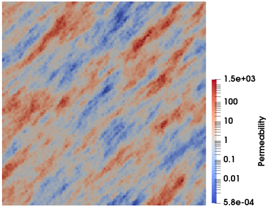

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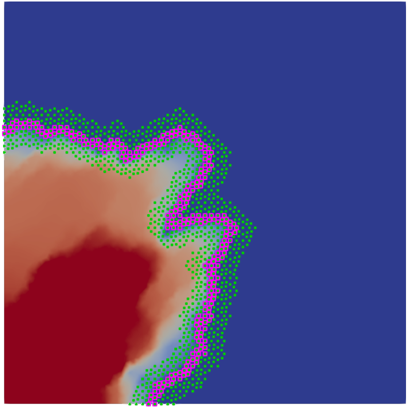
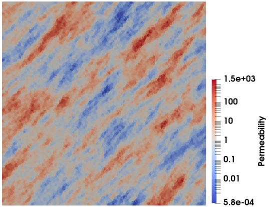
Saturation evolution



Iteration 22



Bad dofs:

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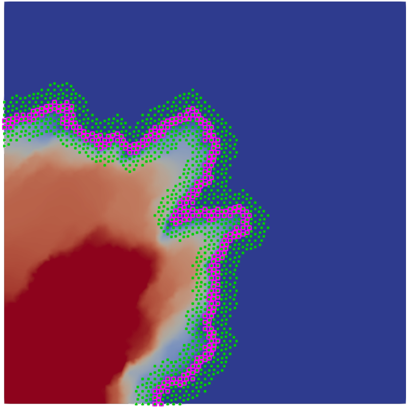
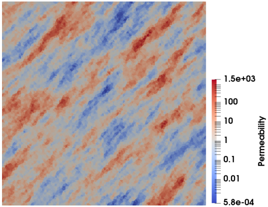
Richards equation

Saturation evolution



Iteration 23



Bad dofs:

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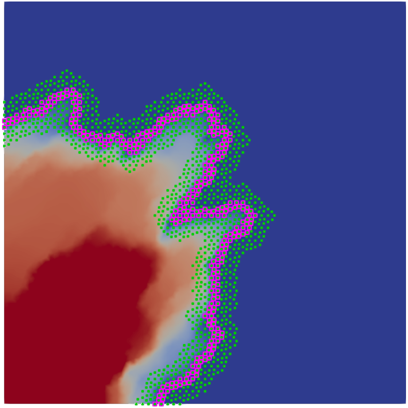
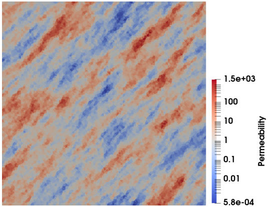
Richards equation

Saturation evolution



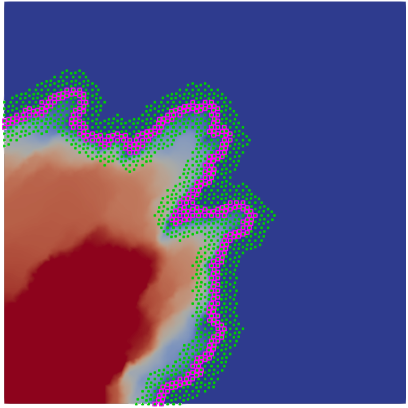
Iteration 24



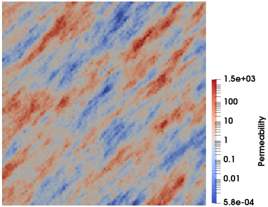
Bad dofs:

- front dofs
- extension

Saturation evolution



Iteration 25



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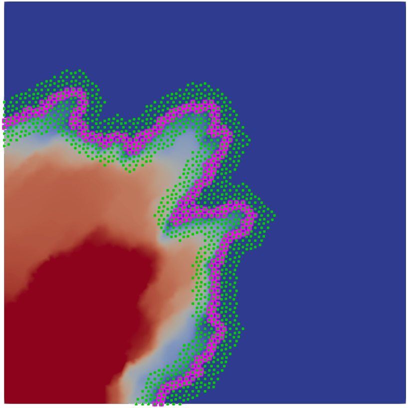
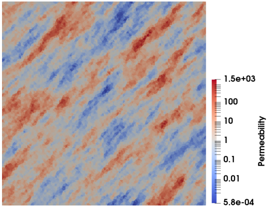
Richards equation

Saturation evolution



Iteration 26

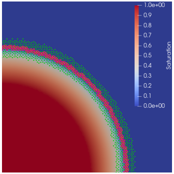


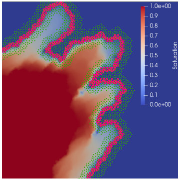
Bad dofs:

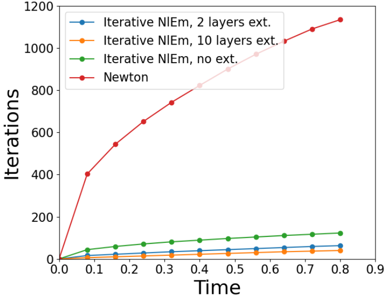
- front dofs
- extension

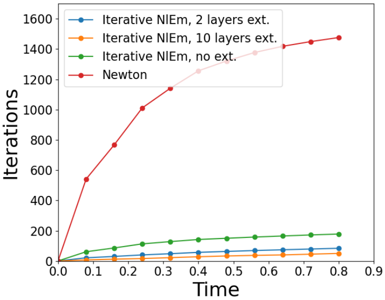
Richards equation

Comparison of the **iterative NIEm** and the **Newton method**: cumulative outer Newton's iterations



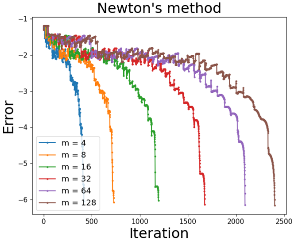


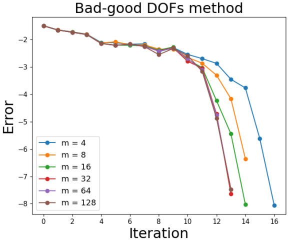




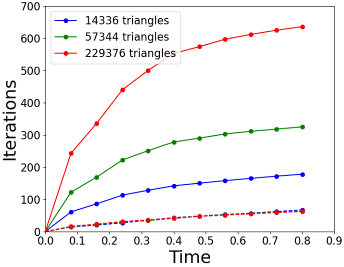
Richards equation

Robustness of the iterative NIEm with respect to the **parameter m**, $\beta(u) = \min\left(u^{1/m}, 1\right)$





Robustness of the iterative NIEm with respect to the **mesh refinements**

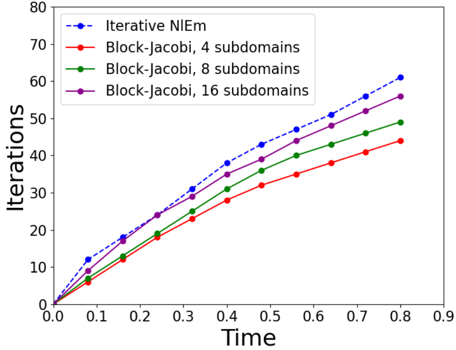


- continuous line: no extension of the bad dofs
- dashed line: bad dofs extended to 4, 8, 16 layers of dofs

Richards equation

Block Jacobi/Newton method

Cumulative outer Newton's iterations.



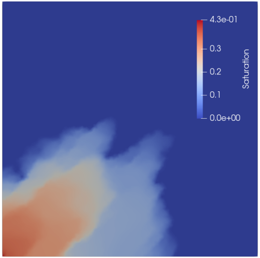
Example of block partitioning of the domain.

Porous medium equation

Continuous problem

$$u(\boldsymbol{x}) - \mathrm{div}(\kappa(\boldsymbol{x})\nabla\varphi(u(\boldsymbol{x}))) = q\,\delta_\varepsilon(\boldsymbol{x}),$$
$$\varphi(v) = \max\left(0, u^m\right), \quad m > 1; \quad q > 0.$$

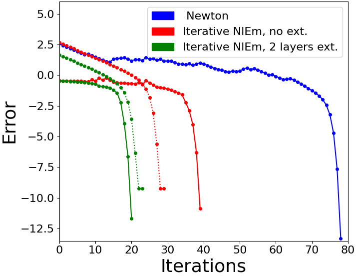
- Top-right edges: homogeneous Dirichlet boundary conditions.
- Bottom-left edges: zero-flux.



Discrete system

$$F_1(\boldsymbol{u}) = \boldsymbol{u} + A\phi(\boldsymbol{u}) - \boldsymbol{b} = 0.$$
$$F_2(\boldsymbol{x}) = \boldsymbol{x} + \phi(A\boldsymbol{x}) - A^{-1}\boldsymbol{b} = 0,$$
$$\boldsymbol{x} = A^{-1}\boldsymbol{u}.$$

- Mass-lumped $\mathbb{P}_1$ FEM, $(\max(\theta) \leq \pi/2)$.



Obstacle problem

Continuous problem

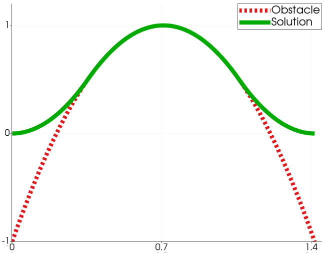
$$-\Delta u(\boldsymbol{x}) \geq 0,\ u(\boldsymbol{x}) \geq \psi,\ \Delta u(\boldsymbol{x})(u(\boldsymbol{x}) - \psi) = 0,$$
$$\psi(\boldsymbol{x}) = \max(1 - 4(\boldsymbol{x} - 0.5)^2, -10).$$

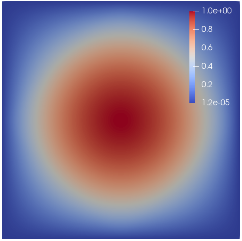
- Homogeneous Dirichlet boundary conditions.

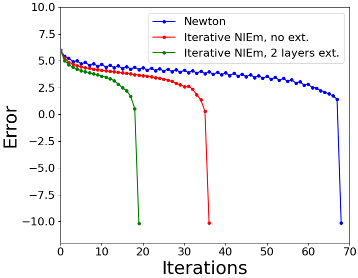
Discrete system

$$F(\boldsymbol{u}) = \min(A\boldsymbol{u}, \boldsymbol{u} - \boldsymbol{\psi}) = 0.$$

- $\mathbb{P}_1$ FEM, $(\max(\theta) \leq \pi/2)$.







Two-phase flow problem

Continuous problem

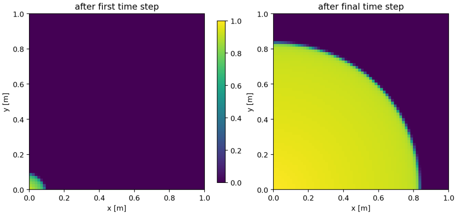
$$\phi\, \partial_t(\rho_\alpha s_\alpha) + \mathrm{div}(\rho_\alpha \boldsymbol{v}_\alpha) = q_\alpha,$$
$$\boldsymbol{v}_\alpha = -\lambda_\alpha\, K\,(\nabla p_\alpha + \rho_\alpha g \nabla z), \quad \alpha \in \{w, nw\}$$
$$s_w + s_{nw} = 1,$$
$$p_c(s_{nw}) = p_{nw} - p_w.$$

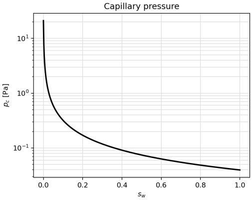
- Brooks-Corey capillary pressure and relative permeability laws.

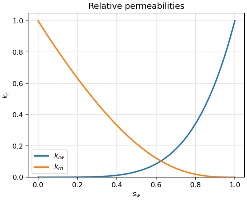
$$p_c(s_w) = p_b\left(10^{-3} + (1-10^{-3})s_w\right)^{-1/\beta},$$
$$k_{rw}(s_w) = s_w^{3+2/\beta},$$
$$k_{rn}(s_w) = (1-s_w)^2\left[1 - s_w^{1+2/\beta}\right].$$

Discrete system

Fully implicit two-point FV scheme.

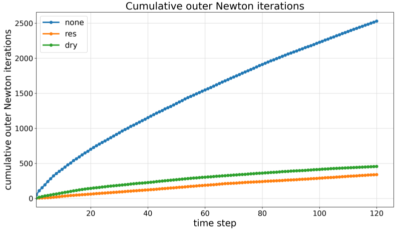


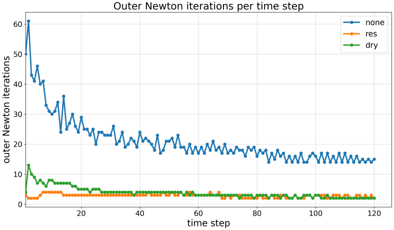


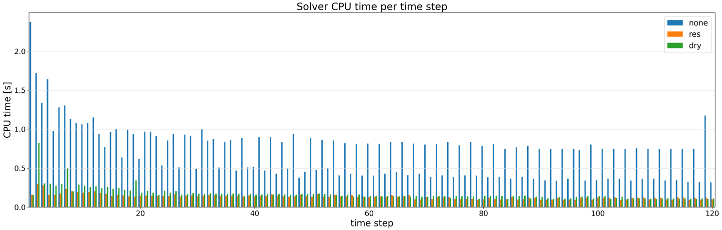


Two-phase flow problem

Comparison **iterative NIEm** and **Newton's method**: outer Newton's iterations and CPU time

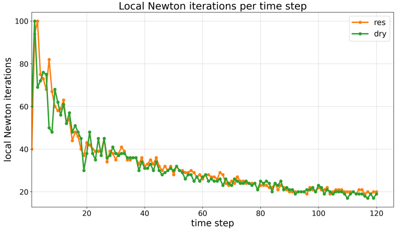


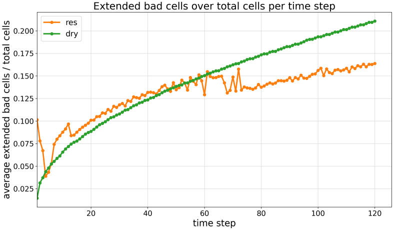


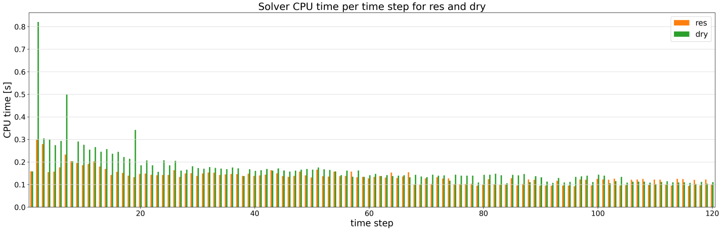


Two-phase flow problem

Comparison of the **residual** and **dry-front** iterative NIEm preconditioners







Outline

Introduction and objectives

Nonlinear preconditioning

- Newton's method
- Domain decomposition: additive vs. multiplicative splitting

Iterative NIEm and block Jacobi/Newton method

- Description, strategy and algorithm
- Global monotone convergence analysis

Some applications

- Richards equation
- Porous medium equation
- Obstacle problem
- Two-phase flow equation

Conclusions

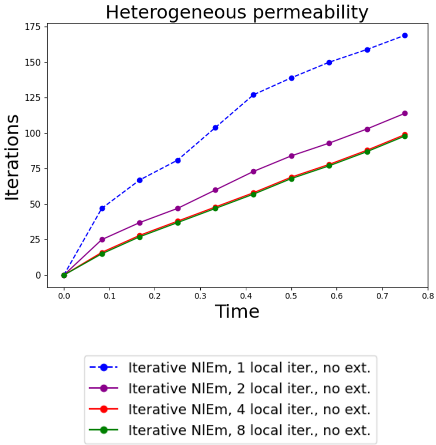
Conclusions

- Nonlinear preconditioning based on a **domain decomposition**: strategy and algorithm of the **iterative NIEm** and the **block Jacobi/Newton method**.
- Study of the interplay between the theory of monotone Newton's method and the nonlinear preconditioning: **global monotone convergence** is preserved under preconditioning.
- **Numerical experiments** on the **Richards equation**, the **porous medium equation**, the **obstacle problem** and the **two-phase flow equation**.
    - Improvement of the performance of Newton's method.
    - Robustness of the iterative NIEm with respect to problem's parameters and mesh refinements.

Thank you for your attention!

Richards equation

Comparison of the **iterative NIEm** with one or **multiple local iterations**: cumulative outer Newton's iterations.



Algorithm:

For $n = 0, 1, ..., N_{Newton}$:

$$\tilde{\boldsymbol{u}}_{b_{k+1}}^{n,k+1} = G_{b_{k+1}}(\boldsymbol{u}_{g_k}^{n,k}), \quad k = 0, 1, ..., m-1$$

$$\tilde{\boldsymbol{u}}^{n,m} = (\boldsymbol{u}_g^{n,m-1}, \tilde{\boldsymbol{u}}_b^{n,m})$$

$$\boldsymbol{u}^{n+1} = \tilde{\boldsymbol{u}}^{n,m} - F'(\tilde{\boldsymbol{u}}^{n,m})^{-1} F(\tilde{\boldsymbol{u}}^{n,m})$$