Accélération de la méthode de Newton par le préconditionnement de Jacobi non linéaire

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Journées scientifiques du GdR MaNu

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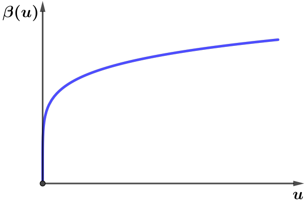
Nonlinear algebraic system

Model problem: Find $\mathbf{u} \in \mathbb{R}^N$

$$\beta(\mathbf{u}) + A\mathbf{u} = \mathbf{b}, \qquad \mathbf{b} \geqslant 0$$



Assumptions:

- $\beta_i : \mathbb{R}^+ \to \mathbb{R}^+$ increasing and concave, $\beta_i'(0) \leqslant +\infty$
- $J(\mathbf{u}) = \beta'(\mathbf{u}) + A$ is M-matrix:
  $J(\mathbf{u})^{-1} \geqslant 0$ and $(J(\mathbf{u}))_{ij} \leqslant 0, i \neq j$

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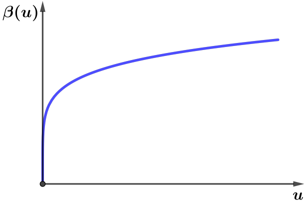

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Objective: Efficient Newton-like method

Outline

Motivation

Monotone Newton Theorem versus numerical experiment

Variable switching by parametrization

Nonlinear Jacobi preconditioning

Motivation

Nonlinear PDE

$$\partial_t \beta(u) + L(u) = 0$$

L is a linear elliptic operator.

Nonlinear discrete problem

$$\frac{\beta(u^{n+1}) - \beta(u^n)}{\Delta t_n} + Au^{n+1} = 0$$

Discretization

- Implicit in time
- Monotone discretization of L:
  - TPFA finite volumes
  - $\mathbf{P_1}$ finite elements with mass-lumping (on an appropriate mesh)
  - Upstream weighting for convection

Nonlinear PDE

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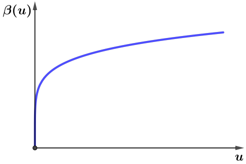
Applications in Geosciences:

- Porous media equation
- Contaminant transport with adsorption
- Richards' equation
- ...

Porous media equation

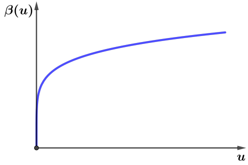
$$\partial_t u^{1/m} - \Delta u = 0, \qquad m > 1$$



Applications: porous media-like equations

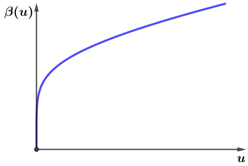
Porous media equation

$$\partial_t u^{1/m} - \Delta u = 0, \qquad m > 1$$



Contaminant transport with adsorption

$$\partial_t \underbrace{(u + a(u))}_{\text{dissolved + adsorbed conc.}} - \text{div}\,(\nabla u + u\mathbf{V}) = 0$$



Freundlich isotherm

$$a(u) = cu^{1/m}, \quad c > 0, \quad m > 1$$

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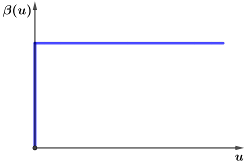

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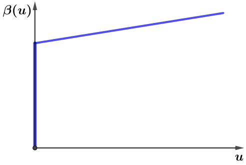

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Limit case $m \to +\infty$

$$\partial_t v + L(u) = 0, \qquad v \in \beta(u)$$

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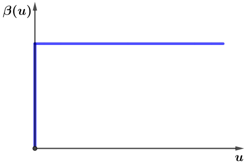

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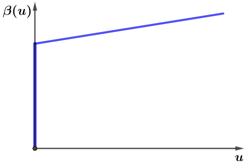

Limit case $m \to +\infty$

$$\partial_t v + L(u) = 0, \qquad v \in \beta(u)$$

- β is maximal monotone
- Connections with obstacle problems (Brugnano & Sestini '09)

Porous media equation

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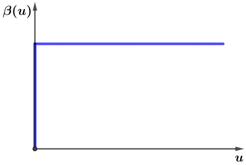

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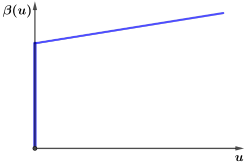


Limit case $m \to +\infty$

$$\partial_t v + L(u) = 0, \qquad v \in \beta(u)$$

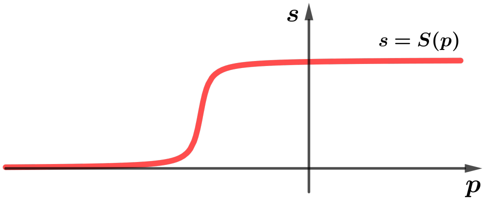
Nonlinear solver must be robust w.r.t. to the shape of β

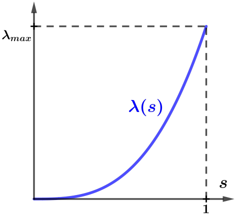
Richards' equation

$$\partial_t s - \operatorname{div}\left(\lambda(s)\left(\nabla p - \mathbf{g}\right)\right) = 0, \qquad s = S(p)$$

Natural variables

- pressure p
- saturation s





Curve $s = S(p)$ reflects the macroscopic capillary effects

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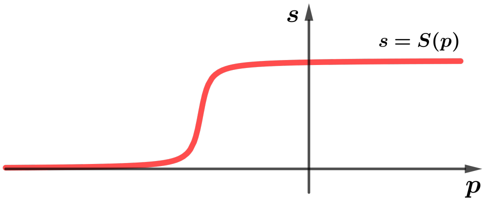
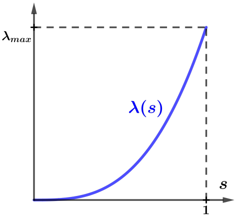




Introducing Kirchhoff transform

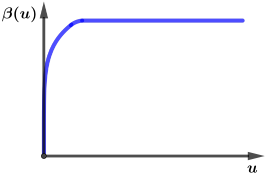
$$U(p) = \int_0^p \lambda(S(a))\mathrm{d}a$$

Richards' equation

We obtain Richards' equation using generalized pressure

$$\partial_t s - \Delta u = -\mathrm{div}\,(\lambda(s)\mathbf{g})\,, \qquad s = \beta(u)$$

with $\beta(u) := S(U^{-1}(u))$



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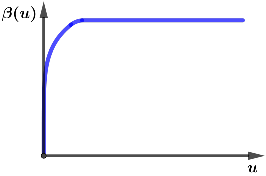

- Using semi-implicit discretization we find

$$\beta(\mathbf{u}) + A\mathbf{u} = \mathbf{b}$$

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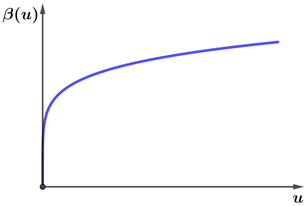

Assumptions:

- $\beta_i : \mathbb{R}^+ \to \mathbb{R}^+$ increasing and concave, $\beta_i'(0) \leqslant +\infty$
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Objective: Newton-like iterative method

- efficient and robust w.r.t. to the shape of β
- with guarantied (semi-)global convergence

Objectives

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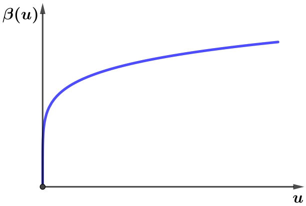

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Monotone Newton Theorem versus numerical experiment

Monotone Newton's method

Let

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

Newton's method:

$$\mathbf{u}_{k+1} = \mathbf{u}_k - F'(\mathbf{u}_k)^{-1} F(\mathbf{u}_k), \qquad k \geqslant 0$$

Theorem (Monotone Newton Theorem (Baluev '52; Ortega & Rheinboldt '70))

Let $\mathbf{u}_0$ *satisfy* $F(\mathbf{u}_0) \leqslant 0$, *then*

- $\mathbf{u}_k$ *converges to the unique solution* $\mathbf{u}_\star$
- $\mathbf{u}_k \leqslant \mathbf{u}_{k+1} \leqslant \mathbf{u}_\star$ *for all* $k \geqslant 0$

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Main ingredients:

- F is concave (or convex)
- $F'(\mathbf{u})$ is an M-matrix

Illustration (N = 1)

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Using nested iterations concavity (convexity) assumption can be removed

- Piece-wise linear systems: Brugnano & Casulli '09
- Systems with diagonal nonlinearities: Casulli & Zanolli '12

Monotone Newton's method

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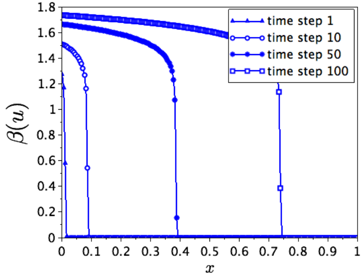
The method is semi-globally convergent. Is it efficient?

Porous media equation on $(0,1) \times (0,T)$

$$\partial_t \beta(u) - \partial_{xx}^2 u = 0, \qquad \beta(u) = u^{1/m}$$

with Neumann boundary conditions

- Inflow at $x = 0$: $-\partial_x u(0,t) = q > 0$
- No-flow at $x = 1$
- Almost "dry" initial condition: $\beta(u(x,0)) = 10^{-10}$



Solution profile at different time steps

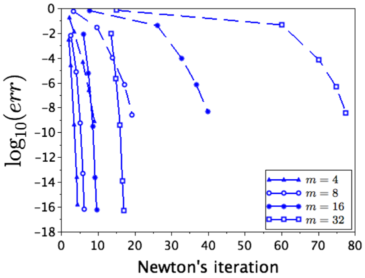
Original u-formulation:

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

Alternative v-formulation:

$$\mathbf{v} + A\beta^{-1}(\mathbf{v}) - \mathbf{b} = 0$$

Different values of $m > 1$ in $\beta(u) = u^{1/m}$



- Dashed: Original formulation is inefficient, manly because $\beta'(0) = +\infty$.
- Solid: Alternative formulation is more efficient, but concavity is lost: note that $(A)_{ii}(A)_{ij} \leqslant 0, i \neq j$

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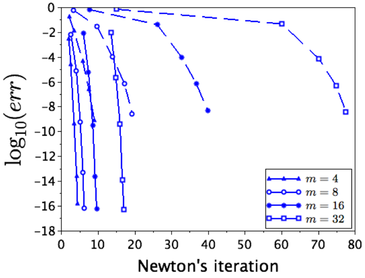
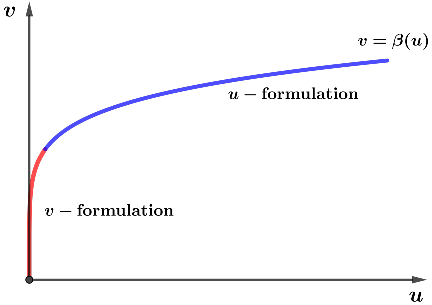


- Performance of both formulations depends on m
- Can we find some even more efficient primary variable?

Variable switching by parametrization

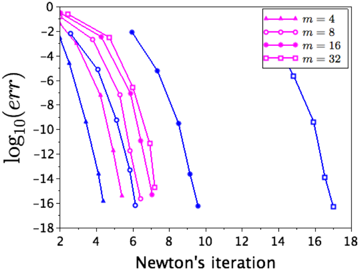
Adaptive choice of the variable



- Switching between v and u may be a good idea
- Well known for Richards' equation

Efficiency of variable switching

- v-formulation: $\partial_t v - \triangle\beta^{-1}(v) = 0$
- variable switching: PDE?

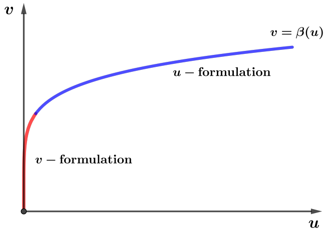


- Variable switching: is more **efficient** and is **robust** w.r.t. m
- Drawback: implementation using **if/else** conditions

Parametrization of the graph $v = \beta(u)$:

Let $\overline{u}, \overline{v} : \mathbb{R}^+ \to \mathbb{R}^+$ such that

$$\overline{v}(\tau) = \beta(\overline{u}(\tau)) \qquad \forall \tau \in \mathbb{R}^+$$

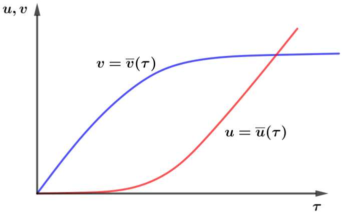


PDE in terms of the new variable τ

$$\partial_t \overline{v}(\tau) - \Delta \overline{u}(\tau) = 0$$

Variable switching:

$$\max(\overline{v}'(\tau), \overline{u}'(\tau)) = 1$$



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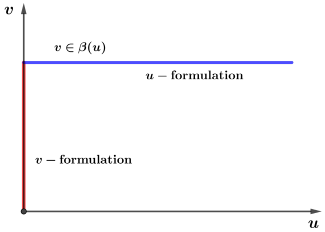
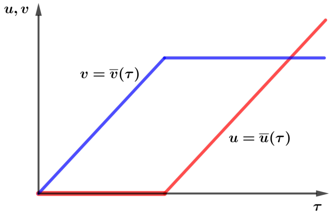
- Multi-valued closure $v \in \beta(u)$ is Ok



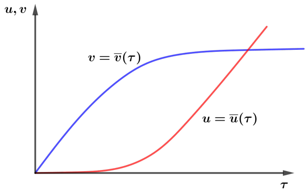


Define $F_\tau(\boldsymbol{\tau}) = \overline{v}(\boldsymbol{\tau}) + A\overline{u}(\boldsymbol{\tau}) - b$

Estimates on $F'_\tau(\boldsymbol{\tau})$

$$\|F'_\tau(\boldsymbol{\tau})\|, \|F'_\tau(\boldsymbol{\tau})\|^{-1} < C$$

uniformly w.r.t. $\boldsymbol{\tau}$ and the shape of β.



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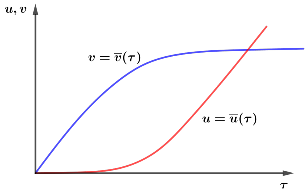
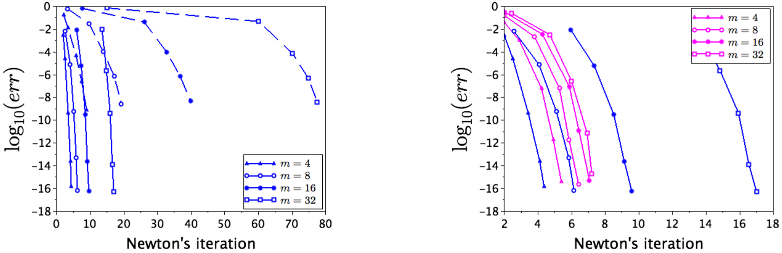


Corollaries:

- Control of $\mathrm{cond}(F'_\tau)$
- Justified stopping criterion:

$$\|F_\tau(\boldsymbol{\tau})\| < \epsilon \Rightarrow \|\boldsymbol{\tau} - \boldsymbol{\tau}_\star\| < C\epsilon \Rightarrow \begin{cases} \|\overline{v}(\boldsymbol{\tau}) - v_\star\| < C\epsilon, \\ \|\overline{u}(\boldsymbol{\tau}) - u_\star\| < C\epsilon \end{cases}$$

Nonlinear Jacobi preconditioning



$$
\begin{aligned}
u - \text{formulation}: \quad & \beta(\mathbf{u}) + A\mathbf{u} - \mathbf{b} && = 0 \\
v - \text{formulation}: \quad & \mathbf{v} + A\beta^{-1}(\mathbf{v}) - \mathbf{b} && = 0 \\
\tau - \text{formulation}: \quad & \overline{v}(\boldsymbol{\tau}) + A\overline{u}(\boldsymbol{\tau}) - \mathbf{b} && = 0
\end{aligned}
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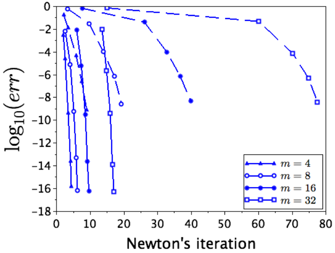
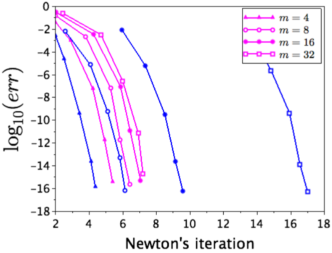
- $u-$formulations: catastrophic performance, but convergence theorem
- $\tau-$formulations: excellent performance, but no convergence theorem





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Can we have both performance and convergence result?

Nonlinear Jacobi preconditioner

Nonlinear Jacobi method:

- Separate diagonal and off-diagonal terms

$$\underbrace{\beta(\mathbf{u}) + \mathrm{diag}(A)\mathbf{u}}_{f(\mathbf{u})} + \underbrace{(A - \mathrm{diag}(A))\mathbf{u}}_{B\mathbf{u}} = \mathbf{b}$$

- Use fixed-point iterations

$$\mathbf{u}_{k+1} = g(\mathbf{b} - B\mathbf{u}_k), \qquad g = f^{-1}$$

Nonlinear Jacobi method:

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- Use fixed-point iterations

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Our idea: Use Jacobi method as preconditioner not as a solver

- Left preconditioned method: apply Newton to

$$\mathbf{u} - g(\mathbf{b} - B\mathbf{u}) = 0$$

Nonlinear Jacobi method:

- Separate diagonal and off-diagonal terms

$$\underbrace{\beta(\mathbf{u}) + \mathrm{diag}(A)\mathbf{u}}_{f(\mathbf{u})} + \underbrace{(A - \mathrm{diag}(A))\mathbf{u}}_{B\mathbf{u}} = \mathbf{b}$$

- Use fixed-point iterations

$$\mathbf{u}_{k+1} = g(\mathbf{b} - B\mathbf{u}_k), \qquad g = f^{-1}$$

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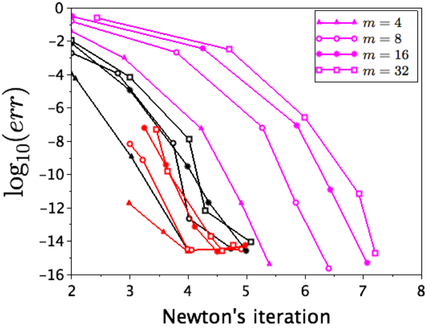
Preconditioned methods satisfy MNT: note that $B \leqslant 0$.

Left-preconditioned:

$$\mathbf{u} - g(\mathbf{b} - A\mathbf{u}) = 0$$

Right-preconditioned:

$$\boldsymbol{\xi} + Ag(\boldsymbol{\xi}) - \mathbf{b} = 0$$

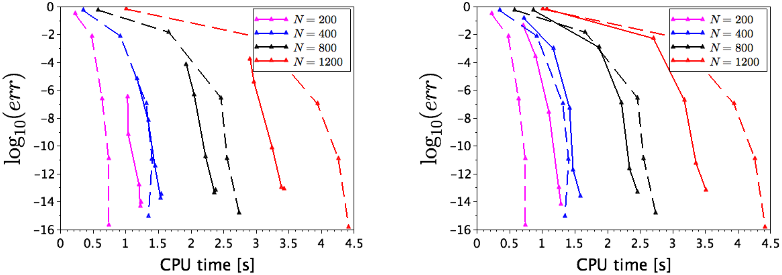


- **Left** and **right** preconditioned methods beat $\tau-$ formulation!

Preconditioned methods have to evaluate $g = f^{-1}$:

- At each Newton's iteration one solves N uncoupled equations

  How expensive is that?

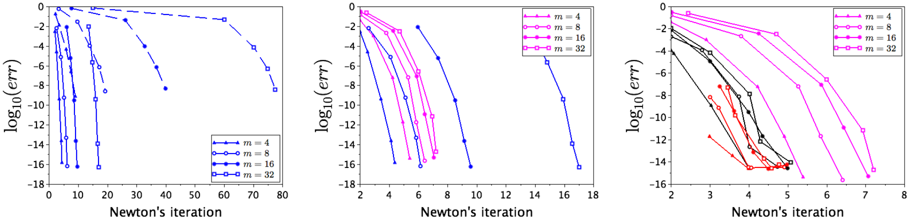


Relative error versus CPU time for different grid sizes:
$\tau-$formulation = dashed lines
preconditioned method = solid lines

- Efficient for all except very small problems ($N \gtrsim 400$) because less linear solves

Nonlinear Jacobi preconditioning

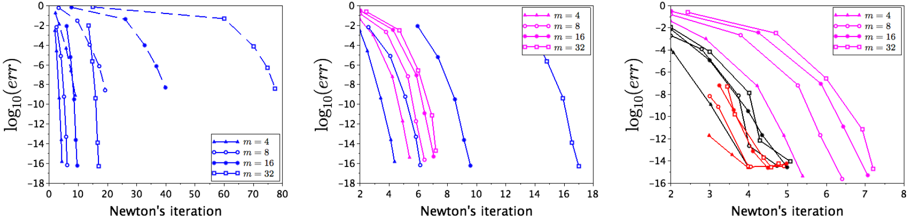
- accelerates convergence of Newton's method,
- while preserving monotone convergence



Conclusion

Nonlinear Jacobi preconditioning

- accelerates convergence of Newton's method,
- while preserving monotone convergence



$$
\begin{aligned}
u-\text{formulation}: &\quad \beta(\mathbf{u}) + A\mathbf{u} - \mathbf{b} &= 0\\
v-\text{formulation}: &\quad \mathbf{v} + A\beta^{-1}(\mathbf{v}) - \mathbf{b} &= 0\\
\tau-\text{formulation}: &\quad \overline{v}(\boldsymbol{\tau}) + A\overline{u}(\boldsymbol{\tau}) - \mathbf{b} &= 0\\
\text{Left-preconditioned}: &\quad \mathbf{u} - g(\mathbf{b} - A\mathbf{u}) &= 0\\
\text{Right-preconditioned}: &\quad \boldsymbol{\xi} + Ag(\boldsymbol{\xi}) - \mathbf{b} &= 0
\end{aligned}
$$

Inexact preconditioning (B. '20 $+ \epsilon$)

Non diagonal nonlinearities and non monotone discretizations (with R. Masson): two-phase flow, heterogeneous media, etc, ...

- Works well with parametrization
- Ongoing work on Jacobi

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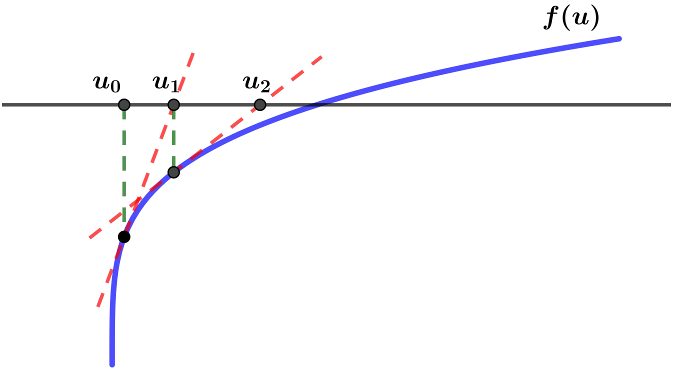
Newton's method for

$$f(u) = 0, \qquad u \in \mathbb{R}$$

- f concave and increasing



Go back

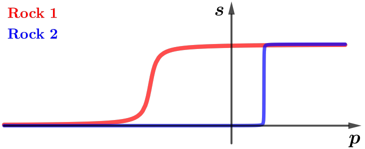
Heterogeneous toy problem

Heterogeneous model PDE

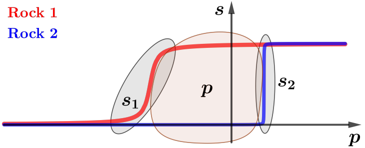
$$\partial_t \beta(u, \mathbf{x}) - \triangle u = 0$$

Piece-wise constant $\beta(\cdot, \mathbf{x})$

- $\beta(p, x)|_{\Omega_i} = \beta_i(p), \quad i = 1, 2$



Multiple variable switching



via simultaneous parametrization of $\beta_1(u)$ and $\beta_2(u)$