Quasi-Newton iterative methods for nonlinear elliptic PDEs

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Outline

- Introduction, motivation
- Theoretical background
- Applications to PDE types
  - A summary of some earlier and recent examples
  - Recent joint work with Stansislav Sysala and Michal Béreš

Other collaborators: I. Faragó, B. Borsos, B. Hingyi, S. Castillo

Nonlinear elliptic PDEs

The studied class: PDEs with divergence structure

Linear case:

$-\operatorname{div}\mathbf{B} = \rho$ ↘ ↙ $\mathbf{B} = k\nabla u$

$$-\operatorname{div}\left(k\nabla u\right) = \rho$$

Nonlinear elliptic PDEs

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$$-\mathrm{div}\,\mathbf{B} = \rho \qquad\qquad \mathbf{B} = k(|\nabla u|)\,\nabla u$$

$$\searrow \qquad\qquad \swarrow$$

$$-\mathrm{div}\,\big(k(|\nabla u|)\,\nabla u\big) = \rho$$

Nonlinear elliptic PDEs

The studied class: PDEs with divergence structure

Nonlinear case more generally: + extra terms; higher order ...

Nonlinear elliptic PDEs

Some typical stationary models:

- Elasto-plastic torsion in 2D
- Electromagnetic potentials (nonlinear stationary Maxwell equation)
- Subsonic flow
- Electrorheology
- Minimal surfaces
- Glaciologic flow
- Deformation of plates
- Gao beam model

The steps of modelling

Physical, chemical etc. model of a real process

↓

Mathematical model (e.g. PDE)

↓

Numerical model (e.g. algebraic system)

↓

Computer model

The steps of modelling

Physical, chemical etc. model of a real process

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Numerical model (e.g. algebraic system)

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Computer model

Approach: abstract spaces

Background for the numerical solution:

- Hilbert or Banach space
- operator theory

Why does this help?

- Well-posedness, weak solution
  $\Rightarrow$ natural base space (Sobolev space)
- Finite element method (FEM)
- principle of J. Neuberger (Sobolev gradients):
  numerical difficulties $\leftrightarrow$ analytic difficulties

Approach: abstract spaces

↓

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Newton type iterative methods

Numerical solution of elliptic problems:

discretization (we use FEM)

$\rightarrow$ a nonlinear algebraic system $F_h(u_h) = 0$

$\rightarrow$ needs iterative solution

Our starting point: we study the underlying PDE $F(u) = 0$

$\rightarrow$ define an iterative method in function space

$\rightarrow$ project it into the FEM subspace

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Newton type iterative methods

Two typical approaches:

Newton's method (fast but costly):	Sobolev gradients /simple preconditioning (slow but cheap):
$u_{n+1} := u_n - F'(u_n)^{-1} F(u_n)$	$u_{n+1} := u_n - B^{-1} F(u_n)$

Newton type iterative methods

Newton's method
(fast but costly):

$$u_{n+1} := u_n - \underbrace{F'(u_n)^{-1}}_{\text{to be approximated:}} F(u_n)$$

Sobolev gradients
/simple preconditioning
(slow but cheap):

$$u_{n+1} := u_n - \underbrace{B^{-1}}_{\text{to be varied:}} F(u_n)$$

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$$u_{n+1} := u_n - B_n^{-1} F(u_n)$$

quasi-Newton method = variable preconditioning

Choice of B_n? A balance between cost and speed.

Algebraic choices (Davidon-Fletcher-Powell, Broyden...):
they use matrix properties and not the PDE

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The general iteration scheme (quasi-Newton)

Consider an operator equation

$$F(u) = 0\,.$$

Construction of the iteration:

- Let B_n be linear operators such that, for some $M_n \geq m_n > 0$,

$$m_n\langle B_n h, h\rangle \leq \langle F'(u_n)h, h\rangle \leq M_n\langle B_n h, h\rangle \qquad (\forall h).$$

- Choose u_0 and then define the sequence

$$u_{n+1} = u_n - \frac{2}{M_n + m_n}\, B_n^{-1} F(u_n) \qquad (n \in \mathbf{N}).$$

The general iteration scheme (quasi-Newton)

"Main convergence theorems": under proper conditions on F,

$$\limsup \frac{\|F(u_{n+1})\|}{\|F(u_n)\|} \leq \limsup \frac{M_n - m_n}{M_n + m_n} =: Q < 1\,.$$

Special (extreme) cases:

- Simple preconditioning (Sobolev gradient method):
  $B_n \equiv B \quad \Rightarrow \quad M_n \equiv M, \quad m_n \equiv m, \quad Q = \frac{M-m}{M+m}.$
- Newton iteration:
  $B_n = F'(u_n) \quad \Rightarrow \quad M_n = 1, \quad m_n = 1, \quad Q = 0$ (superlinear).
- Intermediate choice? Problem-dependent.

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Some conditions

1. Uniformly elliptic problems in Hilbert space

(i) $F : H \to H$ has a bihemicontinuous Gâteaux derivative.

(ii) For any $u \in H$ the operator $F'(u)$ is self-adjoint.

(iii) $\exists$ constants $\mu_1 \geq \mu_2 > 0$:

$$\mu_2 \|h\|^2 \leq \langle F'(u)h, h \rangle \leq \mu_1 \|h\|^2 \qquad (\forall u, h \in H).$$

(iv) F' is Lipschitz continuous.

[with I. Faragó]

Some conditions – extensions

2. Non-uniformly elliptic problems in Banach space

(i) $F : X \to X'$ has a bihemicontinuous Gâteaux derivative.

(ii) For any $u \in X$ the operator $F'(u)$ is symmetric.

(iii) $\exists$ functions $\lambda : \mathbb{R}^+ \to \mathbb{R}^+$, $\searrow$, and $\Lambda : \mathbb{R}^+ \to \mathbb{R}^+$, $\nearrow$:

$$\lambda(\|u\|)\,\|h\|^2 \le \langle F'(u)h, h\rangle \le \Lambda(\|u\|)\,\|h\|^2 \qquad (\forall u, h \in X)$$

$$\text{and} \qquad \int_0^{+\infty} \lambda(t)\,dt \;=\; +\infty.$$

(iv) F' is locally Lipschitz continuous.

[with B. Borsos]

Some conditions – extensions

3. Nonsmooth problems in Hilbert space

(i) $F : H \to H$ is Lipschitz continuous and uniformly monotone.

For all $u \in H \quad \exists$ a bounded self-adjoint linear operator $F^o(u) : H \to H$ with the conditions below:

(ii) $\exists$ constants $\mu_1 \geq \mu_2 > 0$:

$$\mu_2 \|h\|^2 \leq \langle F^o(u)h, h\rangle \leq \mu_1 \|h\|^2 \qquad (\forall u, h \in H).$$

(iii) $\forall u \in H \;\; \exists\, \delta_u > 0$ and $L_u > 0$ such that

$$\|F(v) - F(u) - F^o(v)(v-u)\| \leq L_u \|u-v\|^2 \qquad (\text{if } \|u-v\| \leq \delta_u).$$

Restrictions on m_n, M_n: see later.

[with S. Sysala, M. Béres]

Some conditions – extensions

4. Non-selfadjoint problems in Hilbert space

- $F'(u)$ need not be self-adjoint (non-potential problems).

  Non-spectral conditions:

- For the operators:

  $\langle F'(u)h, h\rangle \leq \mu_1 \|h\|^2$ replaced by $\langle F'(u)h, v\rangle \leq \mu_1 \|h\|\|v\|$

- For the preconditioning:

  $\langle F'(u_n)h, h\rangle \leq M_n \langle B_n h, h\rangle$ repl. by $\langle F'(u_n)h, v\rangle \leq M_n \|h\|_{B_n} \|v\|_{B_n}$

[with S. Castillo, in progress]

Uniformly elliptic nonlinear PDEs

(i) Elasto-plastic torsion in 2D cross-sections:

$$-\mathrm{div}\big(\overline{g}(|\nabla u|)\nabla u\big) = 2\omega \quad \text{in } \Omega \quad (+b.c.)$$

Uniform ellipticity:

$$0 < \mu_1 \leq \overline{g}(T) \leq (\overline{g}(T)T)' \leq \mu_2$$

(ii) Electromagnetic potential (nonlinear stationary 2D Maxwell eqn)

$$-\mathrm{div}\left(a(|\nabla u|^2)\nabla u\right) = \rho \quad \text{in } \Omega \quad (+b.c.)$$

Uniform ellipticity:

$$0 < \mu_1 \leq a(r^2) \leq (a(r^2)r)' \leq \mu_2$$

$\Rightarrow$ These problems are well-posed in the real Hilbert space $H_0^1(\Omega)$

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Uniformly elliptic nonlinear PDEs

Abstract formulation.

Weak form: find $u \in H_0^1(\Omega)$ such that

$$\int_\Omega a(|\nabla u|^2)\nabla u \cdot \nabla v - \int_\Omega gv = 0 \qquad (\forall v \in H_0^1(\Omega))$$

$\sim$ operator equation $F(u) = 0$ in $H := H_0^1(\Omega)$

Uniform ellipticity:

$$\mu_1 \|h\|^2 \leq \langle F'(u)h, h\rangle \leq \mu_2 \|h\|^2 \qquad (\forall h \in H)$$

$+$ local Lipschitz: $\rightarrow$ conditions that ensure the "main theorem".

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Uniformly elliptic nonlinear PDEs

Further models with the same operator properties.

(iii) Deformation of elastic plates (4th order problem):

$$\begin{cases} \operatorname{div}^2\Big(\overline{g}(E(D^2u))\ \tilde{D}^2u\Big) = \alpha \\ u_{|\partial\Omega} = \frac{\partial^2 u}{\partial \nu^2}\Big|_{\partial\Omega} = 0\,, \end{cases}$$

where:

modified Hessian: $$\tilde{D}^2u = \begin{pmatrix} \frac{\partial^2 u}{\partial x^2} + \frac{1}{2}\frac{\partial^2 u}{\partial y^2} & \frac{1}{2}\frac{\partial^2 u}{\partial x \partial y} \\ \frac{1}{2}\frac{\partial^2 u}{\partial x \partial y} & \frac{\partial^2 u}{\partial y^2} + \frac{1}{2}\frac{\partial^2 u}{\partial x^2} \end{pmatrix};$$

matrix divergence: $$\operatorname{div}^2\begin{pmatrix} a & b \\ b & d \end{pmatrix} = \frac{\partial^2 a}{\partial x^2} + 2\frac{\partial^2 b}{\partial x \partial y} + \frac{\partial^2 d}{\partial y^2}\,.$$

Uniform ellipticity:

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Uniformly elliptic nonlinear PDEs

(iv) Nonlinear elasticity systems.

$$\left\{ \begin{aligned} -\operatorname{div}\, T_i(x,\varepsilon(\mathbf{u})) &= \varphi_i(x) && \text{in } \Omega \\ T_i(x,\varepsilon(\mathbf{u}))\cdot\nu &= \gamma_i(x) && \text{on } \Gamma_N \\ u_i &= 0 && \text{on } \Gamma_D \end{aligned} \right\} \qquad (i=1,2,3).$$

Stress-strain tensor: $T:\Omega\times\mathbf{R}^{3\times 3}\to\mathbf{R}^{3\times 3}$,

$$T(x,A) = 3k(x,|\mathrm{vol}\,A|^2)\,\mathrm{vol}\,A + 2\mu(x,|\mathrm{dev}\,A|^2)\,\mathrm{dev}\,A,$$

where $k =$ bulk modulus, $\mu =$ Lamé's coefficient.

Uniform ellipticity:

$$\mu_1|B|^2 \le \underline{\mathbb{C}}(x,A)B:B \le T'_A(x,A)B:B \le \overline{\mathbb{C}}(x,A)B:B \le \mu_2|B|^2.$$

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Nonsmooth PDEs

Nonlinear elasto-plasticity systems: similar form as before,

$$\left\{ \begin{aligned} -\operatorname{div} \, T_i(x, \varepsilon(\mathbf{u})) &= \varphi_i(x) \quad \text{in } \Omega \\ T_i(x, \varepsilon(\mathbf{u})) \cdot \nu &= \gamma_i(x) \quad \text{on } \Gamma_N \\ u_i &= 0 \quad \text{on } \Gamma_D \end{aligned} \right\} \qquad (i = 1, 2, 3)$$

with

$$T(x, A) = 3k(x) \operatorname{vol} A + 2\mu(x, |\operatorname{dev} A|^2) \operatorname{dev} A,$$

but now μ is Lipschitz continuous and only piecewise C^1.

(Details later)

Non-uniformly elliptic nonlinear PDEs

(v) An electrorheologic model: electric potential in a stationary fluid

$$-\mathrm{div}\Big(\big(\chi_1 + \chi_2 |\nabla u|^2\big)\ \nabla u\Big) = g\,.$$

(vi) A parallel sided slab in glaciology:

$$-\mathrm{div}\Big(\frac{2}{T_0 + \sqrt{T_0^2 + |\nabla u|}}\ \nabla u\Big) = P,$$

(vii) Subsonic flow:

$$-\mathrm{div}\left(\left(1 + \frac{1}{5}(M_\infty^2 - |\nabla u|^2\right)^{5/2}\ \nabla u\right) \ = \ 0\,.$$

(viii) Minimal surface:

$$-\mathrm{div}\Big(\frac{\nabla u}{\sqrt{1 + |\nabla u|^2}}\Big) = 0\,.$$

Non-uniformly elliptic nonlinear PDEs

Function space: $X := W^{1,p}(\Omega)$

Non-uniform ellipticity:

$$\lambda(\|u\|)\|h\|^2 \leq \langle F'(u)h, h\rangle \leq \Lambda(\|u\|)\|h\|^2 \qquad (\forall h \in X)$$

where λ and Λ are decreasing resp. increasing functions;

+ lower restriction: $\int_0^{+\infty} \lambda(t)\, dt = +\infty$

+ local Lipschitz

$\rightarrow$ these conditions also ensure the "main theorem".

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The choice of B_n

(i) Consider the example class (2nd order PDE)

$$\begin{cases} -\mathrm{div}\big(a(|\nabla u|^2)\,\nabla u\big) = g \\ u_{|\partial\Omega} = 0\,. \end{cases}$$

FEM stiffness matrices:

(a) Newton linearization:

$\langle F'(u_n)\varphi_i, \varphi_j\rangle =$

$$= \int_\Omega a(|\nabla u_n|^2)\,\nabla\varphi_i\cdot\nabla\varphi_j + 2\,a'(|\nabla u_n|^2)(\nabla u_n\cdot\nabla\varphi_i)\,(\nabla u_n\cdot\nabla\varphi_j)$$

(b) The operators B_n (quasi-Newton/var. prec.):

$$\langle B_n\varphi_i, \varphi_j\rangle = \int_\Omega b(|\nabla u_n|^2)\,\nabla\varphi_i\cdot\nabla\varphi_j \qquad \text{(where } b\approx a,\ a'\text{)}$$

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The choice of B_n

The operators B_n:

$$\langle B_n \varphi_i, \varphi_j \rangle = \int_\Omega b(|\nabla u_n|^2) \nabla \varphi_i \cdot \nabla \varphi_j \qquad \text{(where } b \approx a,\ a'\text{)}$$

i.e. $b(|\nabla u_n|^2)$ is a scalar coefficient

Some possibilities:

- Sobolev gradient: $b \equiv const.$
- frozen coefficient: $b = a$
- improved approximation: $a(r^2) \le b(r^2) \le \big(a(r^2)r\big)'$

The choice of B_n

(ii) 4th order PDE (like elastic plates):

$$\langle B_n \varphi_i, \varphi_j \rangle = \int_\Omega w(E(D^2 u_n))\, \tilde{D}^2 \varphi_i : \tilde{D}^2 \varphi_j$$

i.e. $w(E(D^2 u_n))$ is a scalar coefficient.

The choice of B_n

(iii) Reaction-convection-diffusion systems (ongoing work).

Time-discretized parabolic transport system on a time layer:

$$-K\Delta u_i + \mathbf{b}_i \cdot \nabla u_i + \left(R_i(x, u_1, \dots, u_\ell) + \frac{1}{\tau} u_i \right) = \frac{1}{\tau} u_i^{\text{prev}}$$

$+$ b.c.

(for $i = 1, \dots, \ell$, where ℓ can be large)

The choice of B_n

FEM stiffness matrices:

$$F'(u_n) \sim \begin{pmatrix} \mathbf{L}_n^{11} & \mathbf{L}_n^{12} & \dots & \dots & \mathbf{L}_n^{1\ell} \\ \mathbf{L}_n^{21} & \mathbf{L}_n^{22} & \dots & \dots & \mathbf{L}_n^{2\ell} \\ \dots & \dots & \dots & \dots & \dots \\ \mathbf{L}_n^{\ell 1} & \mathbf{L}_n^{\ell 2} & \dots & \dots & \mathbf{L}_n^{\ell\ell} \end{pmatrix}$$

The choice of B_n

FEM stiffness matrices:

$$B_n \sim \begin{pmatrix} \mathbf{S}_h^1 & 0 & \dots & \dots & 0 \\ 0 & \mathbf{S}_h^2 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & 0 & \mathbf{S}_h^\ell \end{pmatrix}$$

Numerical applications – Model 1: Gao beam

Gao's model for a nonlinear Euler–Bernoulli type beam:

$$EI\, u^{IV} - E\alpha (u')^2 u'' + k_F u = f \qquad \text{in } J := [0, b].$$

[papers of Gao, Machalova, ...]

Constants:

- $E > 0$: elastic modulus
- $I > 0$: moment of inertia for the cross-section
- $h > 0$: thickness; $\nu > 0$: Poisson ratio
- $\alpha = 3h(1-\nu^2)$
- $k_F > 0$: foundation stiffness coefficient
- q: transverse distributed load; $f = (1-\nu^2)q$

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Model 1: Gao beam

Reformulation of the eqn: here $(u')^2 u'' = \frac{1}{3}\big((u')^3\big)'$ $\Rightarrow$

$$u^{IV} - \beta\big((u')^3\big)' + ku = g$$

Clamped boundary conditions: $u(0) = u'(0) = u(b) = u'(b) = 0$

Weak form: find $u \in H_0^2(J)$ satisfying

$$\int_0^b \left(u''v'' + \beta(u')^3 v' + kuv\right) = \int_0^b gv \qquad (\forall v \in H_0^2(J)).$$

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Model 1: Gao beam

Properties of the linearized operator:

- Ellipticity (upper non-uniform):

$$\|h\|^2_{H_0^2} \leq \langle F'(u)h, h\rangle_{H_0^2} \leq \Lambda(\|u\|_{H_0^2})\,\|h\|^2_{H_0^2} \qquad (\forall u, h \in V_h),$$

  where $\Lambda(t) = 1 + kC_2^4 + 3\beta C_4^4 t^2$;

- Local Lipschitz continuity:

$$\|F'(u)-F'(v)\| \leq L(\max\{\|u\|_{H_0^2},\ \|v\|_{H_0^2}\})\,\|u-v\|_{H_0^2} \quad (\forall u,\ h \in V_h),$$

  where $L(t) = 6C_4^4\beta t$.

Model 1: Gao beam

Quasi-Newton iteration:

$$u_{n+1} := u_n - \sigma_n z_n ,$$

where $\sigma_n > 0$ const.,
and z_n solves the linear problem:

$$\underbrace{z_n^{IV} - w_n z_n'' + k z_n}_{\text{preconditioning operator on } z_n} = r_n \text{ (residual)} \quad + \text{b.c.}$$

where $w_n > 0$ is a constant, e.g. $w_n := \frac{3\beta}{2} \max(u_n')^2$.

Stiffness matrix:

$$\mathbf{K} + w_n \mathbf{M} \qquad (\text{where } \mathbf{K} \sim z^{IV} + kz, \quad \mathbf{M} \sim z'')$$

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Model 1: Gao beam

Numerical experiments for some parameters

	$E = E_1,\, \nu = \nu_1$			$E = E_2,\, \nu = \nu_2$		
DOF	$q = q_1$	$q = q_2$	$q = q_3$	$q = q_4$	$q = q_5$	$q = q_6$
8	3	4	5	3	4	5
80	3	4	5	3	4	5
800	3	4	5	3	4	5
8000	4	4	5	3	4	5

Table: Number of iterations for the quasi-Newton method: mesh independence

Tolerance: 10^{-4}. Materials: steel and concrete beam

Model 1: Gao beam

Numerical experiments for some parameters

	$E = E_1,\ \nu = \nu_1$			$E = E_2,\ \nu = \nu_2$		
DOF	$q = q_1$	$q = q_2$	$q = q_3$	$q = q_4$	$q = q_5$	$q = q_6$
8	0.656	0.814	0.739	0.733	0.831	0.757
80	0.570	0.679	0.603	0.654	0.722	0.648
800	0.508	0.586	0.500	0.571	0.611	0.527
8000	0.458	0.454	0.370	0.451	0.362	0.372

Table: Ratios of quasi-Newton / full Newton runtimes.

Tolerance: 10^{-4}. Materials: steel and concrete beam

Model 2: shallow ice in glaciology

A shallow ice model for the motion of a glacier in a valley:

$$-\mathrm{div}\left(|\nabla u|^{-2/3}\,\nabla u\right) = \alpha\,, \qquad u = 0 \quad \text{on } \Gamma_D, \quad \frac{\partial u}{\partial \mathbf{n}} = 0 \quad \text{on } \Gamma_N$$

Here:

- Ω: planar profile of the glacier
- u = sliding velocity
- $\alpha = A^{1/3}$, where $A = 0.2\ \mathrm{bar}^{-3}\mathrm{y}^{-1}$ (rate factor)
- $-2/3 = -(n-1)/n$ for $n = 3$ (Glen's law)

[Fowler, Glowinski, Rappaz...]

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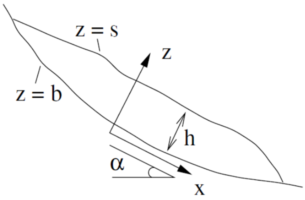

Figure: A compressed profile scheme of the glacier [Fowler 2011]

Model 2: shallow ice in glaciology

The preconditioning operators B_n:

$$\langle B_n h, v\rangle = \int_\Omega |\nabla u_n|^{-2/3} \, \nabla h \cdot \nabla v \qquad (\forall h, v \in V_h).$$

$\rightarrow$ FEM stiffness matrix:

$$\langle B_n \varphi_i, \varphi_j\rangle = \int_\Omega |\nabla u_n|^{-2/3} \, \nabla \varphi_i \cdot \nabla \varphi_j$$

Difficulty: a singular problem. Theory only works for

$$\langle B_n \varphi_i, \varphi_j\rangle = \int_\Omega \left(\varepsilon + |\nabla u_n|^2\right)^{-1/3} \, \nabla \varphi_i \cdot \nabla \varphi_j$$

but then the convergence is independent of ε!

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Unsymmetric domain/mesh: $\surd$

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Numerical results:

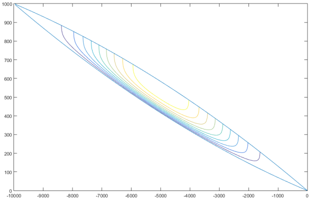

Figure: Contours of the velocity u

Model 2: shallow ice in glaciology

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Unsymmetric domain/mesh: $\surd$

Numerical results:

DOF	# iter	time ratio
3394	21	0.365
12845	21	0.382
52040	21	0.426

Table: Number of iterations; ratio of quasi-Newton and full Newton runtimes. (Tolerance: 10^{-4}. Meshes generated by ANSYS.)

Model 3: nonlinear heat radiation in 3D

Stationary heat conduction with nonlinear Stefan-Boltzmann radiation boundary conditions.

The problem:

$$-\operatorname{div}\big(A\nabla u\big) = f \quad \text{in } \Omega$$

$$u_{|\partial\Omega} = \overline{u} \quad \text{on } \Gamma_D,$$

$$\alpha u + \nu^{\mathrm{T}} A\nabla u + \beta u^4 = g \quad \text{on } \Gamma_N,$$

Here:

- $\Omega \subset \mathbb{R}^3$ bounded; $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$;
- $u \geq 0$: absolute temperature;
- A : an s.p.d. 3×3 matrix of heat conductivities;
- $f, g \geq 0$: density of body/boundary heat sources;
- $\alpha, \beta > 0$: physical constants.

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The preconditioning operators B_n:

$$\langle B_n h,\ v\rangle := \int_\Omega G(x)\ \nabla h \cdot \nabla v + (\alpha_0 + w_n) \int_{\Gamma_N} hv \qquad (\forall v, h \in V_h),$$

$\rightarrow$ FEM stiffness matrix:

$$\mathbf{B}_n = \mathbf{G} + (\alpha_0 + w_n)\mathbf{M},$$

where:

- $\mathbf{G}$ = weighted elliptic stiffness matrix
- $\mathbf{M}$ = boundary mass matrix on Γ_N

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Model 3: nonlinear heat radiation in 3D

Numerical tests for some parameters; $A = \mathit{tridiag}(\mu, 1, \mu)$.

	$\mu = 0.2$			$\mu = 0.4$		
DOF	$\bar{u} = 300$	600	1500	$\bar{u} = 300$	600	1500
2940	3	4	4	3	4	4
8400	3	3	4	3	3	4
27900	3	3	4	3	3	4
65600	3	3	4	3	3	4

Table: Number of quasi-Newton iterations.

Model 3: nonlinear heat radiation in 3D

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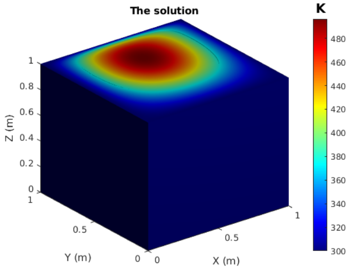
	$\mu = 0.2$			$\mu = 0.4$		
DOF	$\bar{u} = 300$	600	1500	$\bar{u} = 300$	600	1500
2940	0.9009	1.1895	0.8843	0.8884	1.1850	0.8881
8400	0.8863	0.8819	0.8855	0.8923	0.8728	0.8830
27900	0.9095	0.9082	0.9056	0.9048	0.9199	0.9029
65600	0.9086	0.9083	0.9103	0.9068	0.9126	0.9108

Table: Ratio of runtimes of quasi-Newton and full Newton for tolerance $\varepsilon = 10^{-6}$.

Model 3: nonlinear heat radiation in 3D

Numerical tests: heat colourmaps.
$(\mathrm{DoF} = 65600,\ \bar{u} = 300,\ \mu = 0.4)$



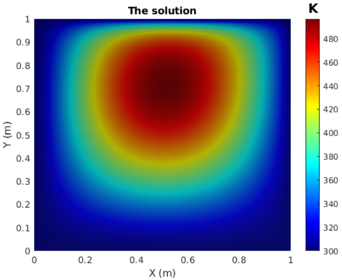


Figure: The numerical solution on the whole cube and on Γ_N, respectively.

Model 3: nonlinear heat radiation in 3D

Numerical tests: heat colourmaps.
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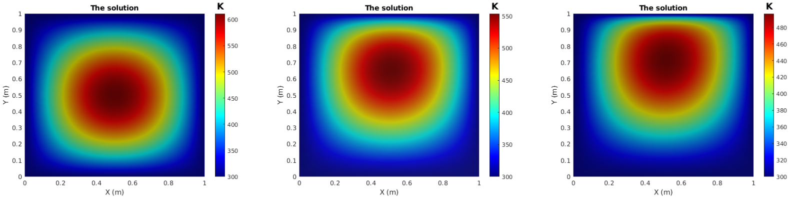

Figure: The effect of anisotropy: $\mu = 0$, $\mu = 0.2$, $\mu = 0.4$.

Model 4: excursion – reaction-diffusion equations

A stationary reaction-diffusion problem with isothermal reaction:

$$\begin{aligned} -\Delta u + ku^\gamma &= 0, \\ u|_{\partial\Omega} &= u_0 > 0, \end{aligned}$$

where $0 < \gamma < 1$. [Diaz, Gomez, Castro,...]

Singularity: $f(u) := ku^\gamma$ is

- not differentiable
- not Lipschitz

$\Rightarrow$ "dead core" phenomenon: u may be $\equiv 0$ in parts of Ω
(altogether $u \geq 0$)

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Iteration: Sobolev gradient method (Newton not applicable)

Some test results ($\gamma = \frac{1}{2}$, $k = 80$) – shape of the dead core:

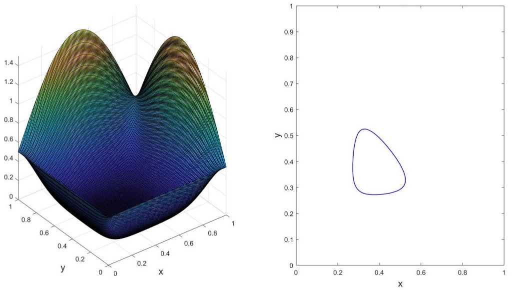

Figure: Square domain, $u_0(x, y) = \frac{1}{2} + \sin(\pi xy)$.

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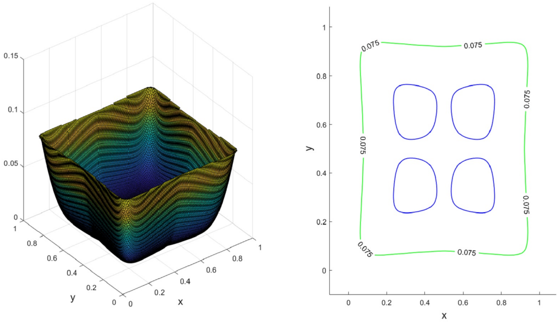

Figure: Concave domain, $u_0 = 0.075$.

Model 5: nonlinear elasticity systems

Recent joint work with Stanislav Sysala and Michal Béreš [Numer. Linear Alg. Appl., 2024]. The BVP:

$$\left\{ \begin{aligned} -\operatorname{div}\, T_i(x,\varepsilon(\mathbf{u})) &= \varphi_i(x) \quad \text{in } \Omega \\ T_i(x,\varepsilon(\mathbf{u}))\cdot\nu &= \gamma_i(x) \quad \text{on } \Gamma_N \\ u_i &= 0 \quad \text{on } \Gamma_D \end{aligned} \right\} \qquad (i=1,2,3).$$

Stress-strain tensor: $T:\Omega\times\mathbf{R}^{3\times3}\to\mathbf{R}^{3\times3}$,

$$T(x,A) = 3k\ \mathrm{vol}\, A + 2\mu(|\mathrm{dev}\, A|^2)\ \mathrm{dev}\, A,$$

where k = bulk modulus, μ = Lamé's coefficient, and

$$0<\mu_0\le\mu(x,s^2)\le\tilde\mu_0\,, \qquad 0<\mu_0\le\left(\mu(x,s^2)s\right)'_s\le\tilde\mu_0\,.$$

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Model 5: nonlinear elasticity systems

Some models for the Lamé coefficient $z \mapsto \mu(z)$ $(z \in \mathbf{R}^+)$:

Model 1: $$\mu(z) := \mu_0 + \frac{\tilde{\mu}_0 - \mu_0}{1 + \varepsilon\sqrt{z}}$$

Model 2: $$\mu(z) := \tilde{\mu}_0 - \frac{\tilde{\mu}_0 - \mu_0}{1 + \varepsilon\sqrt{z}}$$

where $\tilde{\mu}_0 > \mu_0 > 0$ are constant.

[R. Blaheta – P. Byczanski, 2001]

Model 5: nonlinear elasticity systems

Some models for the Lamé coefficient $z \mapsto \mu(z)$ $(z \in \mathbf{R}^+)$:

Model 3:

$$\mu(z) := \begin{cases} \mu_0, & 2\mu_0\sqrt{z} \in I_1 \\ (1-\alpha)\mu_0 + \frac{\alpha}{2\sqrt{z}}[Y - \frac{1}{4\varepsilon}(2\mu_0\sqrt{z} - Y - \varepsilon)^2], & 2\mu_0\sqrt{z} \in I_2 \\ (1-\alpha)\mu_0 + \frac{\alpha}{2\sqrt{z}} Y, & 2\mu_0\sqrt{z} \in I_3 \end{cases}$$

where $I_1 = [0,\ Y - \varepsilon]$, $I_2 = [Y - \varepsilon, Y + \varepsilon]$, $I_3 = [Y + \varepsilon, +\infty)$, and:

$\alpha \in (0,1)$: isotropic hardening parameter,
$Y > 0$: initial yield stress,
$\mu_0 > 0$: Lamé constant
$\varepsilon > 0$: regularization parameter.

[O. Axelsson – S. Sysala, 2015]

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Model 5: choices of B_n

Preconditioner 1:
elastic stiffness matrix with variable parameters.

$$\langle B_n^{(1)}\mathbf{h},\mathbf{v}\rangle = \int_\Omega \Big(3k\ \mathrm{vol}\,\varepsilon(\mathbf{h}) : \mathrm{vol}\,\varepsilon(\mathbf{v}) + 2\mu_n\ \mathrm{dev}\,\varepsilon(\mathbf{h}) : \mathrm{dev}\,\varepsilon(\mathbf{v})\Big)$$

where $k > 0$ is constant and

$$\underline{\mu}(|\mathrm{dev}\,\varepsilon(\mathbf{u}_n)(x)|^2) \le \mu_n(x) \le \overline{\mu}(|\mathrm{dev}\,\varepsilon(\mathbf{u}_n)(x)|^2) \qquad (x \in \Omega),$$

e.g., for some $0 < \delta < 1$,

$$\mu_n := \delta\underline{\mu} + (1-\delta)\overline{\mu}.$$

Model 5: choices of B_n

Preconditioner 2:
elastic stiffness matrix with fixed parameters.

$$\langle B_n^{(2)}\mathbf{h},\mathbf{v}\rangle = \int_\Omega \Big(3k\ \mathrm{vol}\,\varepsilon(\mathbf{h}) : \mathrm{vol}\,\varepsilon(\mathbf{v}) + 2\mu_0\ \mathrm{dev}\,\varepsilon(\mathbf{h}) : \mathrm{dev}\,\varepsilon(\mathbf{v})\Big)$$

where $k,\mu_0 > 0$ are constant.

Preconditioner 3:
motivated by separate displacements.

$$\langle B_n^{(3)}\mathbf{h},\mathbf{v}\rangle = \int_\Omega \Big(\lambda_n\ (\mathrm{div}\mathbf{h})\,(\mathrm{div}\mathbf{v}) + 2\mu_n\,\nabla\mathbf{h} : \nabla\mathbf{v}\Big)\,.$$

where μ_n is from Prec 1 and $\lambda_n(x) := k_n(x) - \frac{2}{3}\,\mu_n(x) > 0$.

The convergence theory applies to all 3 preconditioners.

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Preconditioner 3:

motivated by separate displacements.

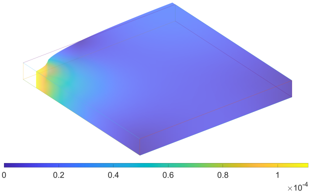
$$\langle B_n^{(3)}\mathbf{h}, \mathbf{v}\rangle = \int_\Omega \Big(\lambda_n \ (\mathrm{div}\mathbf{h})\,(\mathrm{div}\mathbf{v}) + 2\mu_n \nabla\mathbf{h} : \nabla\mathbf{v}\Big) .$$

where μ_n is from Prec 1 and $\lambda_n(x) := k_n(x) - \frac{2}{3}\,\mu_n(x) > 0$.

The convergence theory applies to all 3 preconditioners.

Model 5: numerical tests

Strip-footing problem



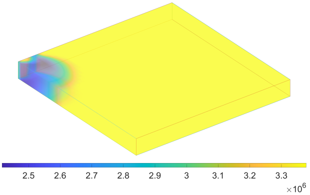


Figure: Left – displacement field u, right – shear moduli field μ.

Meshes with P1 elements:

- coarse: 38,400 elements
- finer: 307,200 elements.
- finest: 1,036,800 elements.

Model 5: numerical tests

Comparison of iteration numbers and computational times with tolerance 10^{-12}. Best: elastic preconditioners.

	Newton it / time [s]	q-Newton 1 it / time [s]	q-Newton 2 it / time [s]	q-Newton 3 it / time [s]
M1 - coarse	6 / 1.5	14 / 1.1	21 / **1.0**	42 / 1.7
M2 - coarse	7 / 1.6	17 / **1.2**	40 / 1.4	68 / 2.4
M3 - coarse	6 / 1.3	18 / 1.4	26 / **1.0**	48 / 2.4
M1 - fine	6 / 20.5	15 / 13.9	22 / **12.4**	45 / 20.9
M2 - fine	7 / 19.9	17 / **13.9**	40 / 17.5	59 / 23.4
M3 - fine	7 / 20.2	19 / 17.1	26 / **13.1**	52 / 26.4
M1 - finest	6 / 101.7	16 / 67.9	23 / **64.3**	47 / 91.9
M2 - finest	7 / 98.3	17 / **64.9**	40 / 80.1	68 / 112.9
M3 - finest	7 / 95.1	19 / 76.4	27 / **70.9**	54 / 118.9

Model 6: nonsmooth elasto-plasticity systems

More recent joint work with Stansislav Sysala and Michal Béreš [Comput. Math. Appl., 2025].

Structure of the BVP: similar to the previous one,

$$\left\{ \begin{array}{rcll} -\mathrm{div}\ T_i(x,\varepsilon(\mathbf{u})) & = & \varphi_i(x) & \text{in } \Omega \\ T_i(x,\varepsilon(\mathbf{u}))\cdot\nu & = & \gamma_i(x) & \text{on } \Gamma_N \\ u_i & = & 0 & \text{on } \Gamma_D \end{array} \right\} \qquad (i=1,2,3).$$

Stress-strain tensor: $T : \Omega \times \mathbf{R}^{3\times 3} \to \mathbf{R}^{3\times 3}$,

$$T(x,A) = 3k\ \mathrm{vol}\, A + 2\mu(|\mathrm{dev}\, A|^2)\ \mathrm{dev}\, A.$$

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Model 6: nonsmooth elasto-plasticity systems

Nonsmooth nonlinear Lamé coefficient:

$$\mu(z) := \begin{cases} \mu_0, & \text{if } 2\mu_0\sqrt{z} \leq Y, \\ (1-\alpha)\mu_0 + \frac{\alpha}{2\sqrt{z}} Y & \text{if } 2\mu_0\sqrt{z} \geq Y. \end{cases}$$

New theory: convergence

- with regularization;
- without regularization.

Model 6: nonsmooth elasto-plasticity systems

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Model 6: nonsmooth elasto-plasticity systems

1. Theory with regularization.

- Using smooth operators F_ε such that

$$\|F(u) - F_\varepsilon(u)\| \leq K\varepsilon\|u\| \qquad (\forall u \in H),$$

where we allow $\lim_{\varepsilon\to 0} L(F'_\varepsilon) = +\infty$.

- Preconditioners:

$$m_n^{(\varepsilon)}\langle B_n^{(\varepsilon)}h, h\rangle \leq \langle F'_\varepsilon(u_n)h, h\rangle \leq M_n^{(\varepsilon)}\langle B_n^{(\varepsilon)}h, h\rangle$$

where $\underline{m} \leq m_n^{(\varepsilon)} \leq M_n^{(\varepsilon)} \leq \overline{M} \quad (\forall n \in \mathbf{N})$.

- Convergence:

$$\limsup \frac{\|F_\varepsilon(u_{n+1})\|_*}{\|F_\varepsilon(u_n)\|_*} \leq Q < 1\,.$$

Model 6: nonsmooth elasto-plasticity systems

2. Theory without regularization (directly).

Use generalized derivatives $F^\circ(u)$ instead of $F'(u)$ as in extension 3 previously.

Convergence under some restrictions:

- $\sup \frac{\mu_1}{\mu_2} \frac{M_n - m_n}{M_n + m_n} \leq \overline{Q} < 1$, or
- $\exists$ locally Lipschitz F' near u^*.

Implementation for the BVP

Solution of the linear problems:

- deflated CG method;
- separate displacement + AGMG preconditioners.

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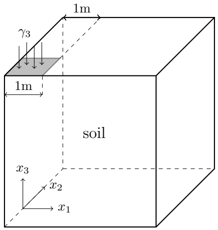
Model 6: numerical tests

Test 1. Homogeneous material: strip-footing problem.



Preconditioners (QNVP:= Quasi-Newton/variable prec.):

- QNVP1a = Prec1 from before (variable elastic stiffness mtx)
- QNVP1b = freeze B_n as $B_n := B_{n-1}$ if $\frac{|\mu_n - \mu_{n-1}|}{|\mu_n|} \leq 0.1$
- QNVP2 = Prec2 from before (fixed elastic stiffness mtx)

Model 6: numerical tests

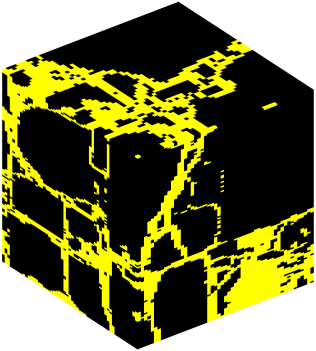
Test 1. Comparison of results with tolerance 10^{-10}:

Newton iterations/cumulative CG iterations/runtime[s].

Setup	α	**Newton**	**QNVP1a**	**QNVP1b**	**QNVP2**
$\varepsilon = 0$	**0.3**	6/305/194.3	12/195/195.9	12/195/**141.0**	16/192/146.6
	0.5	6/313/192.5	15/222/238.7	15/222/**174.1**	22/221/175.3
	0.9	7/460/**257.8**	49/385/774.2	49/385/442.9	115/531/511.3
$\varepsilon = 0.1$	**0.3**	5/249/155.4	12/196/197.2	12/196/**114.8**	16/192/148.2
	0.5	6/313/193.3	15/224/238.2	15/225/**140.0**	22/221/176.4
	0.9	7/469/**256.5**	47/393/731.4	47/394/388.0	115/521/521.9

Model 6: numerical tests

Test 2. Heterogeneous material: coal–polyurethane composite



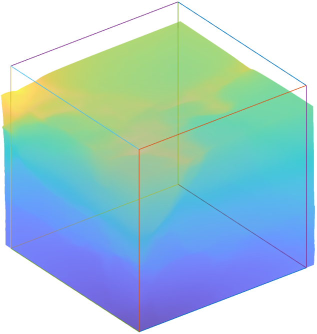


Figure: Left – the composite material, right – the displacement field

Model 6: numerical tests

Test 2. Comparison of results with tolerance 10^{-10}:

Newton iterations/cumulative CG iterations/runtime[s].

Mesh 1: DOF=1.094.364, Mesh 2: DOF=4.404.888 M.

Setup	ε	Newton	q-Newton 1a	q-Newton 1b	q-Newton 2
Mesh 1	**0**	6/124/31.4	16/83/42.3	16/83/28.0	22/80/**14.9**
	0.001	6/115/32.7	16/83/44.1	16/83/24.2	22/80/**15.6**
	0.01	6/117/31.9	16/83/44.4	16/83/22.2	22/80/**15.4**
	0.1	6/120/32.4	15/81/40.8	15/81/19.0	22/80/**15.6**
	0.5	6/120/43.9	13/79/38.0	13/80/18.8	21/82/**17.1**
Mesh 2	**0**	6/113/126.6	16/79/181.3	16/79/117.1	22/69/**59.3**
	0.001	6/113/128.7	16/79/180.3	16/79/103.9	22/69/**58.4**
	0.01	6/115/126.5	16/79/179.6	16/79/95.6	22/69/**58.0**
	0.1	6/118/129.9	15/77/169.0	15/78/77.7	22/71/**59.3**
	0.5	6/117/182.0	14/77/168.2	14/76/81.9	21/70/**70.1**

Closing remarks

Future work:

- Experiments for further scalar problems: electromagnetic potentials, non-Newtonian fluids
- More general elasto-plastic operators
- Survey of the QNVP approach

Closing remarks

Some references:

Faragó I., Karátson J., Numerical Solution of Nonlinear Elliptic Problems via Preconditioning Operators: Theory and Application, NOVA Science Publishers, New York, 2002.

Borsos, B., Karátson, J., Quasi-Newton variable preconditioning for nonlinear nonuniformly monotone elliptic problems posed in Banach spaces, IMA J. Numer. Anal. 42, no. 2, 1806–1830 (2022).

Karátson, J.; Sysala, S.; Béreš, M., Quasi-Newton variable preconditioning for nonlinear elasticity systems in 3D, Numer. Lin. Alg. Appl. 31:3, pp. 1-20 (2024)

Karátson, J.; Sysala, S.; Béreš, M., Quasi-Newton iterative solution approaches for nonsmooth elliptic operators with applications to elasto-plasticity, Comput. Math. Appl. 178, pp. 61-80 (2025)

Closing remarks

Thank you for your attention!