



An Inexact Trust-Region Algorithm for Nonsmooth Nonconvex Optimization



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2 Problem Formulation



Goal: Develop an efficient algorithm to solve the **nonsmooth optimization problem**,

$$\min_{x \in H} f(x) + \phi(x).$$

- H is a **Hilbert space** with inner product (\cdot, \cdot) and associated norm $\|\cdot\|$;
- $f : H \rightarrow \mathbb{R}$ has **Lipschitz continuous gradients** on an open set containing $\text{dom } \phi$;
- $\phi : H \rightarrow [-\infty, +\infty]$ is proper, **closed** and **convex**, but may be **nonsmooth**;
- $F := f + \phi$ is **bounded below** on $\text{dom } \phi$.

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- $F := f + \phi$ is **bounded below** on $\text{dom } \phi$.

Key Requirements of Algorithm

- 1. Large-Scale Problems:** Rapid convergence, mesh independence, and matrix free.
- 2. Leverage Inexactness:** Converges even when f and ∇f are computed inexactly via adaptive discretization, reduced-order modelling, compression, etc.

3 Inexact Computations

Motivation



In infinite-dimensional optimization, the objective function and its gradient are often **impossible** to compute without discretization, iteration, etc., leading to **inexactness**.

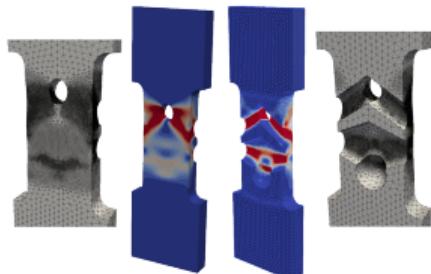
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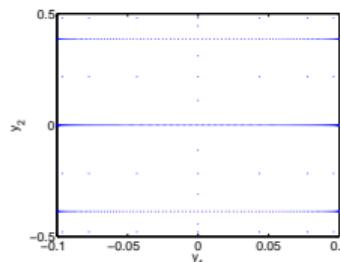
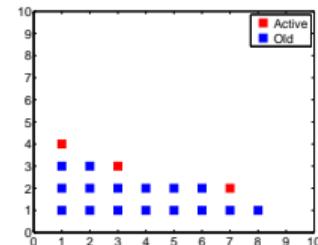


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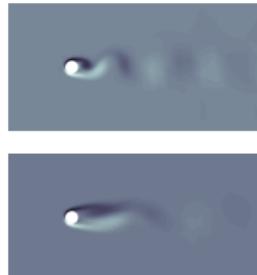
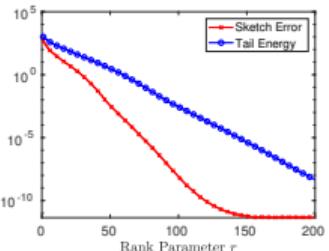
Adaptive Finite Elements



Adaptive Quadrature



Adaptive Compression



Goal: Determine a control z that produces a state close to w and that has **small support**.

Given a domain $\Omega \subset \mathbb{R}^d$, a target state $w \in L^2(\Omega)$, bounds $a \leq 0 \leq b$ a.e., and penalty parameters $\alpha, \beta \geq 0$,

$$\min_{z \in L^2(\Omega)} \int_{\Omega} |S(z) - w|^2(x) \, dx + \frac{\alpha}{2} \int_{\Omega} |z|^2(x) \, dx + \beta \int_{\Omega} |z|(x) \, dx$$

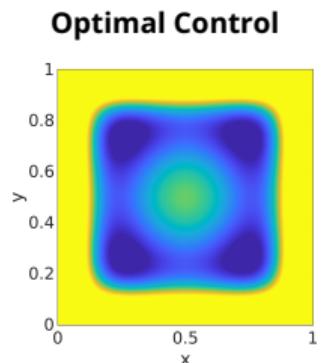
subject to $a \leq z \leq b$ a.e.,

where $S(z) = u \in H_0^1(\Omega)$ solves

$$-\Delta u + u^3 = z \quad \text{in } \Omega$$

$$u = 0 \quad \text{in } \partial\Omega$$

Challenges: Objective function is **nonsmooth**, **nonconvex**, and **expensive**.



5 | Sparse Control

Existing Methods



1. Subgradient and Bundle Methods: Iterates x_{k+1} solve the optimization problem

$$\min_{x \in H} \frac{t_k}{2} \|x - x_k\|_H^2 + \sup_{j \in I_k} \{f(y_j) + \phi(y_j) + (\nabla f(y_j) + \eta_j, x - y_j)_H\},$$

where $t_k \geq 0$ and $\eta_j \in \partial\phi(y_j)$. Typically, **convergence is slow** (e.g., sublinear).

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2. **Proximal Gradient Methods:** Iterates x_{k+1} solve the optimization problem

$$\min_{x \in H} (\nabla f(x_k), x - x_k)_H + \frac{1}{2\gamma_k} \|x - x_k\|_H^2 + \phi(x) \iff x_{k+1} = \text{prox}_{\gamma_k \phi}(x_k - \gamma_k \nabla f(x_k)).$$

PG methods are robust, but **slow**. Can use acceleration (Nesterov) or momentum (heavy balls).

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3. **Proximal Newton-Type Methods:** Iterates x_{k+1} solve the optimization problem

$$\min_{x \in H} (\nabla f(x_k), x - x_k)_H + \frac{1}{2} (B_k(x - x_k), x - x_k)_H + \phi(x),$$

where $B_k \in L(X)$ approximates the Hessian of f . PN methods require **positive definite** B_k (e.g., convexity) and **nonstandard/nontrivial prox computations**.

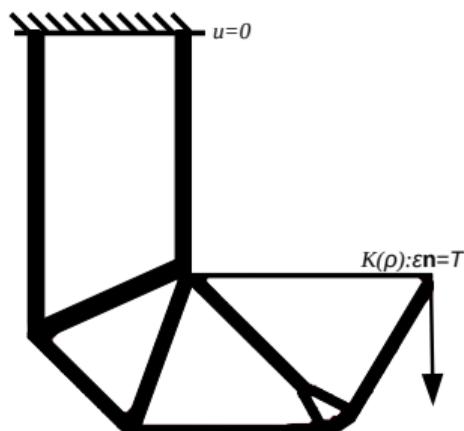
6 Motivating Application

Elastic Topology Optimization



Goal: Determine a *binary* ρ that is maximally stiff and that satisfies the volume constraint.

Given a domain $\Omega \subset \mathbb{R}^d$ and a volume fraction $v \in (0, 1)$,



$$\begin{aligned} & \min_{\rho \in L^2(\Omega)} \int_{\Gamma_t} T(x) \cdot [S(\rho)](x) \, dx \\ & \text{subject to} \quad \int_{\Omega} \rho(x) \, dx \leq v|\Omega|, \quad 0 \leq \rho \leq 1 \text{ a.e.}, \end{aligned}$$

where $S(\rho) = u \in (H^1(\Omega))^d$ solves

$$\begin{aligned} -\nabla \cdot (K(\rho) : \varepsilon) &= 0, & \varepsilon = \frac{1}{2}(\nabla u + \nabla u^\top) & \text{in } \Omega \\ K(\rho) : \varepsilon \mathbf{n} &= T & & \text{on } \Gamma_t \\ u &= 0 & & \text{on } \Gamma_d \end{aligned}$$

Challenges: Objective function is **expensive** and highly **nonconvex** due to material models like the **Solid Isotropic Material with Penalization (SIMP)**.



1. **Optimality Criterion Method:** A **heuristic** fixed-point iteration that is related to a projected gradient method.

Bendsøe & Kikuchi, [Generating optimal topologies in structural design using a homogenization method](#), CMAME, 1988.



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It is extremely difficult to handle *inexact* objective values and gradients in these methods!

8 Nonsmooth Trust Regions

Basic Algorithm



Require: An initial guess x_1 , initial trust-region radius $\Delta_1 > 0$, $0 < \eta_1 < \eta_2 < 1$ and $0 < \gamma_1 \leq \gamma_2 < 1$

1: **for** $k = 1, 2, \dots$ **do**

2: **Model Selection:** Choose a subproblem model f_k of f near x_k

3: **Step Computation:** Compute x_k^+ that *approximately* solves

$$\min_{x \in H} \{m_k(x) := f_k(x) + \phi(x)\} \quad \text{subject to} \quad \|x - x_k\| \leq \Delta_k$$

4: **Evaluate Objective:** Compute the actual reduction $\text{ared}_k := F(x_k) - F(x_k^+)$

5: **if** $\rho_k := \frac{\text{ared}_k}{m_k(x_k) - m_k(x_k^+)} < \eta_1$ **then**

6: $x_{k+1} \leftarrow x_k$ and $\Delta_{k+1} \in [\gamma_1 \Delta_k, \gamma_2 \Delta_k]$

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Trust-Region Subproblem: At each iteration, we approximately solve

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Recall: TR methods do **not** solve the subproblem, but rather use a **Cauchy point** to ensure **sufficient decrease** of the trial iterate x_k^+ .

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Subproblem



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Recall: TR methods do **not** solve the subproblem, but rather use a **Cauchy point** to ensure **sufficient decrease** of the trial iterate x_k^+ .

We generalize the **Cauchy point** to nonsmooth problems using the **proximal gradient path**

$$x_k^{\text{cp}} = p_k(t_k) \quad \text{with} \quad p_k(t) := \text{prox}_{t\phi}(x_k - tg_k),$$

where $g_k \approx \nabla f(x_k)$ and the **proximity operator** is given by

$$\text{prox}_{t\phi}(x) := \arg \min_{y \in H} \left\{ \frac{1}{2t} \|y - x\|^2 + \phi(y) \right\}.$$



We set $x_k^{cp} = p_k(t_k)$, where the step length t_k satisfies both

1. Trust-Region Feasibility:

$$\|x_k^{cp} - x_k\| \leq \nu_1 \Delta_k$$

2. Sufficient Decrease:

$$m_k(x_k^{cp}) - m_k(x_k) \leq \mu_1 [(g_k, x_k^{cp} - x_k) + \phi(x_k^{cp}) - \phi(x_k)]$$

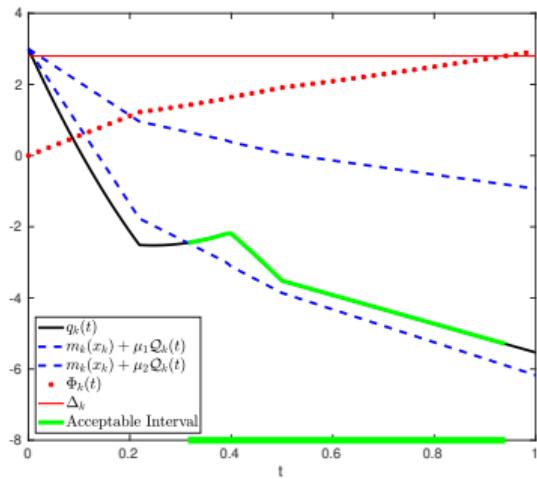
and at least one of the following conditions:

$$t_k \geq \nu_2 t'_k \quad \text{or} \quad t_k \geq \nu_3,$$

where t'_k either satisfies

$$m_k(p_k(t'_k)) - m_k(x_k) \geq \mu_2 [(g_k, p_k(t'_k) - x_k) + \phi(p_k(t'_k)) - \phi(x_k)]$$

$$\text{or} \quad \|p_k(t'_k) - x_k\| \geq \nu_4 \Delta_k.$$



The interval of **acceptable** t_k is depicted by the **green** line on the horizontal axis.



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$$\|x_k^+ - x_k\| \leq \nu_{\text{rad}} \Delta_k, \quad \nu_{\text{rad}} \geq \nu_1$$

$$m_k(x_k) - m_k(x_k^+) \geq \mu_3 [m_k(x_k) - m_k(x_k^{\text{cp}})], \quad 0 < \mu_3 \leq 1.$$



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- ▶ **Trial Iterate Requirements:** Avoid CP computation by ensuring that x_k^+ satisfies

$$\|x_k^+ - x_k\| \leq \nu_{\text{rad}} \Delta_k$$

$$m_k(x_k) - m_k(x_k^+) \geq \kappa_{\text{fcd}} h_k \min \left\{ \frac{h_k}{1 + \omega_k}, \Delta_k \right\}, \quad (\text{FCD})$$

where $h_k := \|p_k(r_0) - x_k\|/r_0$ for fixed $r_0 > 0$ and $\omega_k \geq 0$ measures the curvature of f_k .



Model: For the SPG subproblem solver, we employ the models

$$f_k(x) = \frac{1}{2}(B_k(x - x_k), x - x_k) + (g_k, x - x_k) \quad \text{and} \quad \phi_k(x) = \begin{cases} \phi(x) & \text{if } \|x - x_k\| \leq \Delta_k \\ +\infty & \text{otherwise} \end{cases}$$

Algorithm: Set $x_{k,0} = x_k^{\text{cp}}$, $s_{k,0} = x_{k,0} - x_k$ to ensure (FCD) is satisfied and compute

$$x_{k,\ell+1} = x_{k,\ell} + \alpha_{k,\ell} s_{k,\ell} \quad \text{with} \quad s_{k,\ell} = \text{prox}_{\lambda_{k,\ell}\phi_k}(x_{k,\ell} - \lambda_{k,\ell} \nabla f_k(x_{k,\ell})) - x_{k,\ell},$$

where $\alpha_{k,\ell} \in [0, 1]$ minimizes the quadratic upper bound

$$\begin{aligned} q_{k,\ell}(t) &:= f_k(x_{k,\ell} + ts_{k,\ell}) + t[\phi_k(x_{k,\ell} + s_{k,\ell}) - \phi_k(x_{k,\ell})] + \phi_k(x_{k,\ell}) \\ &\geq f_k(x_{k,\ell} + ts_{k,\ell}) + \phi_k(x_{k,\ell} + ts_{k,\ell}) = m_k(x_{k,\ell} + ts_{k,\ell}) \end{aligned}$$

and $\lambda_{k,\ell}$ is the the safeguarded spectral step length given by

$$\lambda_{k,\ell} = \max \left\{ \lambda_{\min}, \min \left\{ \lambda_{\max}, \frac{(s_{k,\ell-1}, s_{k,\ell-1})}{(B_k s_{k,\ell-1}, s_{k,\ell-1})} \right\} \right\}.$$

Birgin, et al., Nonmonotone spectral projected gradient methods on convex sets, SIOPT, 2000.

Kouri, A matrix-free trust-region Newton algorithm for convex-constrained optimization, Opt. Letters, 2022.

Baraldi & Kouri, A proximal trust-region method for nonsmooth optimization with inexact function and gradient evaluations, Math. Prog., 2022.



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3:   Step Computation: Compute a trial step  $x_k^+$  that satisfies (FCD)
4:   Evaluate Objective: Evaluate the computed reduction  $\text{cred}_k \approx \text{ared}_k$  Inexact!
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When evaluating the of reduction of the objective function, we approximate

$$\text{cred}_k \approx \text{ared}_k := (f(x_k) + \phi(x_k)) - (f(x_{k+1}) - \phi(x_{k+1})),$$

where cred_k satsfies:

$$\begin{aligned} & \exists \kappa_{\text{obj}} > 0, \quad \zeta > 1, \quad \eta < \min\{\eta_1, 1 - \eta_2\}, \quad \text{and} \quad \theta_k \searrow 0 \quad \text{such that} \\ & |\text{ared}_k - \text{cred}_k| \leq \kappa_{\text{obj}} [\eta \min\{m_k(x_k) - m_k(x_{k+1}), \theta_k\}]^\zeta \quad \forall k. \end{aligned}$$



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We also require that the model gradient g_k must satisfy:

$$\exists \kappa_{\text{grad}} > 0 \quad \text{such that} \quad \|\nabla f(x_k) - g_k\| \leq \kappa_{\text{grad}} \min\{h_k, \Delta_k\} \quad \forall k.$$



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$$\exists \kappa_{\text{grad}} > 0 \quad \text{such that} \quad \|\nabla f(x_k) - g_k\| \leq \kappa_{\text{grad}} \min\{h_k, \Delta_k\} \quad \forall k.$$

Can compute model gradient g_k in *finitely* many iterations!



Under the stated assumptions, the iterates produced by the TR algorithm satisfy

$$\liminf_{k \rightarrow \infty} h_k = 0 \implies \liminf_{k \rightarrow \infty} h(x_k, t) = 0 \quad \forall t > 0,$$

where $h_k := \frac{1}{r_0} \|\text{prox}_{r_0 \phi}(x_k - r_0 g_k) - x_k\|$ and $h(x, t) := \frac{1}{t} \|\text{prox}_{t \phi}(x - t \nabla f(x)) - x\|$.

Finite Termination: $\forall \tau > 0 \quad \exists K_\tau \in \mathbb{N} \quad \text{such that} \quad h_{K_\tau} \leq \tau h_1$.

Tikhonov Regularization: If $f(x) = f_0(x) + \frac{\alpha}{2} \|x - x_0\|^2$, where $\alpha > 0$, $x_0 \in H$, ∇f_0 is **completely continuous** and $r_0 \geq \alpha^{-1}$, then any **weak accumulation point** of $\{x_k\}$ is a **critical point** of $f + \phi$. See, e.g., **sparse control**.



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Finite Termination: $\forall \tau > 0 \quad \exists K_\tau \in \mathbb{N} \quad \text{such that} \quad h_{K_\tau} \leq \tau h_1$.

Strong Local Convergence: Suppose f is **strongly convex** on a convex set $U \subseteq H$ with $U \cap \text{dom} \phi \neq \emptyset$ and $\exists K_0 \in \mathbb{N}$ such that $x_k \in U$ for $k \geq K_0$. If $\exists \bar{x} \in U$ satisfying $h(\bar{x}, t) = 0 \quad \forall t > 0$, then $x_k \rightarrow \bar{x}$. That is, $\{x_k\}$ **converges strongly to a critical point**.



Under the stated assumptions, the iterates produced by the TR algorithm satisfy

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where $h_k := \frac{1}{r_0} \|\text{prox}_{r_0\phi}(x_k - r_0 g_k) - x_k\|$ and $h(x, t) := \frac{1}{t} \|\text{prox}_{t\phi}(x - t \nabla f(x)) - x\|$.

Finite Termination: $\forall \tau > 0 \quad \exists K_\tau \in \mathbb{N} \quad \text{such that} \quad h_{K_\tau} \leq \tau h_1$.

Convergence Rates: Further, suppose f_k is the quadratic model and $\nabla^2 f$ is Lipschitz.*

1. If $\frac{1}{r_0} \|\text{prox}_{r_0\phi}(x_k^+ - r_0 \nabla f_k(x_k^+)) - x_k^+\| \leq \tau_k h_k$ and $\tau_k \rightarrow 0$, then x_k converges **superlinearly**.
2. If $\tau_k \leq \tau h_k^{1+\alpha}$ for $\tau > 0$ and $\alpha \geq 0$, then x_k converges **quadratically**.

*Also requires **modest** assumptions on the iterates generated by the subproblem solver.

Baraldi & Kouri, [A proximal trust-region method for nonsmooth optimization with inexact function and gradient evaluations](#), Math. Prog., 2022.
 Kouri, [A matrix-free trust-region Newton algorithm for convex-constrained optimization](#), Opt. Letters, 2022.



Goals:

1. Comparison of TR method with modern nonsmooth methods.
2. Demonstration of mesh independence for TR method.

Let $\Omega = (0, 1)^2$, $w \equiv -1$, $a \equiv -25$, $b \equiv 25$, $\alpha = 10^{-4}$ and $\beta = 10^{-2}$, and consider

$$\min_{z \in L^2(\Omega)} \int_{\Omega} |S(z) - w|^2(x) \, dx + \frac{\alpha}{2} \int_{\Omega} |z|^2(x) \, dx + \beta \int_{\Omega} |z|(x) \, dx$$

subject to $a \leq z \leq b$ a.e.,

where $S(z) = u \in H_0^1(\Omega)$ solves

$$\begin{aligned} -\Delta u + u^3 &= z && \text{in } \Omega \\ u &= 0 && \text{in } \partial\Omega \end{aligned}$$

Discretization: P1 FEM for state variables and piecewise constant for controls.

Problem Size: 131,072 control degrees of freedom.



method	iter	fval	grad	hess	phi	prox	time (s)	TR	speedup*
TR	4	5	5	39	57	142	22.88	1.0000	
PG	59	149	60	0	149	209	498.56		21.79
SPG	30	46	31	0	46	62	168.26		7.35
R2	106	107	46	0	107	153	368.27		16.10
nmAPG	93	194	186	0	194	196	1018.66		44.52
iPiano	103	240	104	0	104	344	816.96		35.71
FISTA	141	430	283	0	430	290	1532.58		66.98
PANOC	83	285	108	0	272	287	948.04		41.44
ZeroFPR	21	70	43	0	45	93	247.39		10.81

Proximal Gradient Methods

Accelerated Methods

Proximal Quasi-Newton Methods

*TR speedup is the ratio of the wallclock time for TR divided by the times for the other methods.



τ_{op}	1e-4				1e-6				1e-8			
mesh	iter	npde	lpde	prox	iter	npde	lpde	prox	iter	npde	lpde	prox
64x64	3	4	56	80	5	6	108	129	7	8	186	181
128x128	3	4	54	79	4	5	79	102	6	7	129	151
256x256	3	4	56	80	5	6	108	129	6	7	133	153
512x512	3	4	54	78	5	6	102	123	6	7	127	147

Trust-region algorithm demonstrates **mesh independence** with respect to the number of iterations and the number of PDE solves!

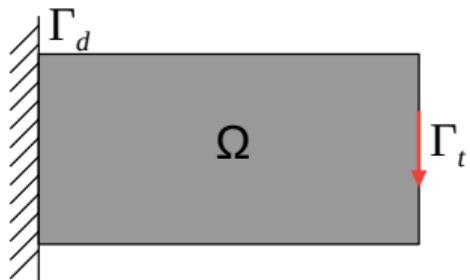
Requires only modest additional computational work to achieve tight tolerances!



Goals:

1. Comparison of TR method with modern projected and AL methods.
2. Demonstration of TR inexactness control for 3D problems.

Let $\Omega = (0, 2) \times (0, 1)^d$, $d = 1, 2$, and $\nu = 0.4$, and consider



$$\begin{aligned} & \min_{\rho \in L^2(\Omega)} \int_{\Gamma_t} T(x) \cdot [S(\rho)](x) \, dx \\ & \text{subject to} \quad \int_{\Omega} \rho(x) \, dx = \nu |\Omega|, \quad 0 \leq \rho \leq 1 \text{ a.e.}, \end{aligned}$$

where $S(\rho) = u \in (H^1(\Omega))^{d+1}$ solves

$$-\nabla \cdot (K(\rho) : \varepsilon) = 0 \quad \text{in } \Omega$$

$$\varepsilon = \frac{1}{2}(\nabla u + \nabla u^\top) \quad \text{in } \Omega$$

$$K(\rho) : \varepsilon \mathbf{n} = T \quad \text{on } \Gamma_t$$

$$u = 0 \quad \text{on } \Gamma_d$$





Formulation: SIMP power $p = 3$ with Helmholtz filtering (radius= 0.1).

Discretization: Q1 FEM for displacement variables and piecewise constant for density.

Problem Size: 26,880 density degrees of freedom.

method	iter	fval	grad	hess	proj	time(s)	TR	speedup*
TR	9	10	10	236	1200	16.49	1.0000	
LMTR	33	34	31	418	391	32.42	1.9660	
PQN	126	235	127	0	4972	164.49	9.9751	
SPG	84	90	85	0	170	52.36	3.1753	
AL-TR	9	52	51	1153	0	61.98	3.7586	
AL-LMTR	11	276	263	4368	0	280.77	17.0267	

Projected Newton-Type Methods

Spectral Projected Gradient

AL Methods

*TR speedup is the ratio of the wallclock time for TR divided by the times for the other methods.

Numerical Results

3D Elastic Topology Optimization



Formulation: SIMP power $p = 3$ with Helmholtz filtering (radius = 0.1).

Discretization: Q1 FEM for displacement variables and piecewise constant for density.

Problem Size: 221,184 density degrees of freedom.

Inexact Solves: Solve using CG with AMG preconditioning.

- **Helmholtz Filter:** Requires ~ 8 iterations to achieve the relative error of $\sim 10^{-12}$
 \Rightarrow Considered to be **exact**.

- **Elasticity Equations:** Trust-region algorithm controls accuracy of linear solver.

k	$F(x_k)$	h_k	$\ x_k - x_{k-1}\ $	Δ_k	fval	grad	hess	proj	obj tol	grad tol
0	1.0000	4.017e-2	---	1e1	1	1	0	3	1.000e-2	1.000e-2
1	0.8157	1.927e-2	1.000e1	1e2	2	2	12	44	1.000e-2	1.000e-2
2	0.4716	1.279e-2	5.420e1	1e3	3	3	25	75	1.000e-2	1.000e-2
3	0.4144	6.280e-3	1.260e1	1e4	4	4	39	103	4.632e-3	1.000e-2
4	0.1600	3.101e-3	1.990e2	1e4	5	5	52	132	1.000e-2	1.000e-2
5	0.1300	1.226e-3	1.085e2	1e5	6	6	65	161	2.970e-3	1.000e-2
6	0.1262	1.242e-5	6.044e1	1e6	7	7	78	190	3.539e-4	1.000e-2
7	0.1254	6.590e-6	5.821e1	1e7	8	8	91	220	6.971e-5	6.590e-3
8	0.1251	3.221e-6	3.599e1	1e8	9	9	104	249	1.942e-5	3.221e-3

Conclusions:

- **Numerical solution** of infinite-dimensional problems requires **expensive approximations**
- Often, the objective function and its gradient can only be computed **inexactly**
- Nonsmooth trust region is **provably convergent** even with **inexact computations**
- **We can efficiently compute a trial step using the spectral proximal gradient method**
- SPG trust-region subproblem solver is **matrix free**, but may **require** many prox computations
Future: Can we incorporate inexact prox computations? Can we handle nonconvex ϕ ?
- Nonsmooth trust-region method **outperforms** existing nonsmooth methods!

References:

- R. J. Baraldi & D. P. Kouri, **Local Convergence Analysis of an Inexact Trust-Region Method for Nonsmooth Optimization**, Submitted, 2023.
- R. J. Baraldi & D. P. Kouri, **A proximal trust-region method for nonsmooth optimization with inexact function and gradient evaluations**, Math Programming, 2022.
- D. P. Kouri, **A matrix-free trust-region Newton algorithm for convex-constrained optimization**, Optimization Letters, 2022.
- D. P. Kouri & D. Ridzal, **Inexact trust-region methods for PDE-constrained optimization**, Frontiers in PDE-Constrained Optimization, 2018.



Trilinos package for **large-scale optimization**. Uses: optimal design, optimal control and inverse problems in engineering applications; mesh optimization; image processing.



- ▶ **Modern optimization algorithms.**
- ▶ **Maximum HPC hardware utilization.**
- ▶ **Special programming interfaces for simulation-based optimization.**
- ▶ **Optimization under uncertainty.**

- ▶ Hardened, production-ready algorithms for **unconstrained, equality-constrained, inequality-constrained and nonsmooth optimization**.
- ▶ Novel algorithms for **optimization under uncertainty** and **risk-averse optimization**.
- ▶ Unique capabilities for optimization-guided **inexact and adaptive computations**.
- ▶ Geared toward **maximizing HPC hardware utilization** through direct use of application data structures, memory spaces, linear solvers and nonlinear solvers.
- ▶ Special interfaces for **engineering applications**, for streamlined and efficient use.
- ▶ Rigorous **implementation verification**: finite difference and linear algebra checks.
- ▶ **Hierarchical and custom** (user-defined) algorithms and stopping criteria.