Multilevel Optimization

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SIAM Conference on Optimization, Boston, May 2008

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$$\min_{x\in \mathbf{R}^n} f(x)$$

▶ $f : \mathbb{R}^n \to \mathbb{R}$ nonlinear, $\in C^2$ and bounded below

- No convexity assumption
- Results from the discretization of some infinite-dimensional problem on a relatively fine grid for instance (*n* large)

 \longrightarrow Iterative search of a first-order critical point x_* (s.t. $\nabla f(x_*) = 0$)

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Newton's method

$$x_{k+1} = x_k + s_k^N$$
 with $\nabla^2 f(x_k) s_k^N = -\nabla f(x_k)$

- ► Fast convergence (quadratic) to a local minimizer x_{*} of f
- ▶ If *x*⁰ sufficiently close to *x*[∗]
- → Requires a globalization technique in order to:
 - Ensure convergence of the iterates from every starting point
 - Take account of the nonconvexity when far from a local min.

Line search — Trust region — Adaptive regularization

Hierarchy of problem descriptions

Assume now that a hierarchy of problem descriptions is available, linked by known operators

Finest problem description					
Restriction $\downarrow R$	$P \uparrow Prolongation$				
Fine problem description					
Restriction $\downarrow R$ $P \uparrow$ Prolongation					
•••					
Restriction $\downarrow R$	$P \uparrow Prolongation$				
Coarse proble	m description				
Restriction $\downarrow R$ $P \uparrow$ Prolongation					
Coarsest probl	em description				

Grid transfer operators

Restriction

$$\mathbf{R}_i: \mathbb{R}^{n_i} \to \mathbb{R}^{n_{i-1}}$$



$$P_i: \mathbb{R}^{n_{i-1}} \to \mathbb{R}^{n_i}$$





$$R_i = \sigma P_i^T$$

Sources for such problems

- Parameter estimation in
 - discretized ODEs
 - discretized PDEs
- Optimal control problems
- Variational problems (minimum surface problem)
- Optimal surface design (shape optimization)
- Data assimilation in weather forecast (different levels of physics in the models)

The minimum surface problem

$$\min_{v} \int_{0}^{1} \int_{0}^{1} \left(1 + (\partial_{x}v)^{2} + (\partial_{y}v)^{2} \right)^{\frac{1}{2}} dx dy$$

with the boundary conditions:

$$\begin{cases} f(x), & y = 0, & 0 \le x \le 1\\ 0, & x = 0, & 0 \le y \le 1\\ f(x), & y = 1, & 0 \le x \le 1\\ 0, & x = 1, & 0 \le y \le 1 \end{cases}$$

where

$$f(x) = x * (1 - x)$$

→ Discretization using a finite element basis



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The solution at different levels















 $n = 31^2 = 961$ $n = 63^2 = 3969$ $n = 127^2 = 16129$

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(Unconstrained case)

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Past and recent developments

Line-search

- Fisher (1998), Frese-Bouman-Sauer (1999), Nash (2000)
- Lewis-Nash (2000, 2002, to appear)
- Oh-Milstein-Bouman-Webb (2003)
- Wen-Goldfarb (2007, report 2008)
- Gratton-Toint (report 2007)

Trust-region

- Gratton-Sartenaer-Toint (to appear in SIOPT)
- Gratton-Mouffe-Toint-Weber Mendonça (to appear in IMAJNA)

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- Mouffe-Gratton-Sartenaer-Toint-Tomanos (in preparation)
- Toint-Tomanos-Weber Mendonça (report 2007)

Adaptive regularization

Toint-Tomanos (in preparation)

A very active field

- Large Scale Optimization and PDE-Based Problems (MS2, MS12, MS42, MS52)
- Multigrid/Multilevel Optimization Methods and Their Applications (MS62)
- Numerical Treatment of PDE Constrained Optimization Problems:
 - A: Numerical Analysis (MS3, MS13)
 - B: Algorithms (MS23, MS33)
 - C: Applications (MS53, MS63, MS73)
- Optimization with PDE Constraints (CP3)





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- 1. Trust-region methods for beginners
- 2. Multigrid for beginners
- 3. **RMTR** (a Recursive Multilevel Trust-Region Method)

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- Theoretical aspects
- Practical aspects
- 4. Some numerical flavor

Trust-region philosophy

<u>At iteration k</u> (until convergence):

- Choose a local model m_k of f around x_k (Taylor's model)
- Compute a trial step s_k that suff. reduces m_k in a trust region:

{	(approx.) minimize $s \in \mathbb{R}^n$	$m_k(x_k+s)$
t	SUDJECT TO	$\ s\ \leq \Delta_k$

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- Evaluate $f(x_k + s_k)$
- ▶ If achieved decrease (Δf) \approx predicted decrease (Δm_k), then
 - accept the trial point $(x_{k+1} = x_k + s_k)$
 - possibly enlarge the trust region $(\Delta_k \nearrow)$

else

- keep the current point $(x_{k+1} = x_k)$
- shrink the trust region $(\Delta_k \searrow)$

minimize : $f(\alpha, \beta) = -10\alpha^2 + 10\beta^2 + 4\sin(\alpha\beta) - 2\alpha + \alpha^4$



Two local minima: (-2.20, 0.32) and (2.30, -0.34)

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 $x_0 = (0.71, -3.27)$ and $f(x_0) = 97.630$

Contours of f

Contours of m_0 around x_0 (quadratic model)





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$k \parallel \Delta_k$	Sk	$f(x_k+s_k)$	$\Delta f/\Delta m_k$	x_{k+1}
0 1	(0.05, 0.93)	43.742	0.998	$x_0 + s_0$



k	Δ_k	Sk	$f(x_k+s_k)$	$\Delta f/\Delta m_k$	x_{k+1}
0	1	(0.05, 0.93)	43.742	0.998	$x_0 + s_0$
1	2	(-0.62, 1.78)	2.306	1.354	$x_1 + s_1$





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0	1	(0.05, 0.93)	43.742	0.998	$x_0 + s_0$
1	2	(-0.62, 1.78)	2.306	1.354	$x_1 + s_1$
2	4	(3.21, 0.00)	6.295	-0.004	<i>x</i> ₂





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1	2	(-0.62, 1.78)	2.306	1.354	$x_1 + s_1$
2	4	(3.21, 0.00)	6.295	-0.004	<i>x</i> ₂
3	2	(1.90, 0.08)	-29.392	0.649	$x_2 + s_2$





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2	4	(3.21, 0.00)	6.295	-0.004	<i>x</i> ₂
3	2	(1.90, 0.08)	-29.392	0.649	$x_2 + s_2$
4	2	(0.32, 0.15)	-31.131	0.857	$x_3 + s_3$





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2	4	(3.21, 0.00)	6.295	-0.004	<i>x</i> ₂
3	2	(1.90, 0.08)	-29.392	0.649	$x_2 + s_2$
4	2	(0.32, 0.15)	-31.131	0.857	$x_3 + s_3$
5	4	(-0.03, -0.02)	-31.176	1.009	$x_4 + s_4$





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k	Δ_k	Sk	$f(x_k+s_k)$	$\Delta f/\Delta m_k$	x_{k+1}
0	1	(0.05, 0.93)	43.742	0.998	$x_0 + s_0$
1	2	(-0.62, 1.78)	2.306	1.354	$x_1 + s_1$
2	4	(3.21, 0.00)	6.295	-0.004	<i>x</i> ₂
3	2	(1.90, 0.08)	-29.392	0.649	$x_2 + s_2$
4	2	(0.32, 0.15)	-31.131	0.857	$x_3 + s_3$
5	4	(-0.03, -0.02)	-31.176	1.009	$x_4 + s_4$
6	8	(-0.02, 0.00)	-31.179	1.013	$x_5 + s_5$





Path of iterates:

From another x_0 :





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What makes it work ?

 $\begin{cases} \text{ (approx.) minimize}_{s \in \mathbb{R}^n} & m_k(x_k + s) \\ \text{subject to} & \|s\| \leq \Delta_k \end{cases}$

$$(g_k =
abla m_k(x_k) =
abla f(x_k))$$



(Best decrease of the model within the trust region along the steepest descent direction $-g_k$)

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$$m_k(x_k) - m_k(x_k^C) \ge \frac{1}{2} ||g_k|| \min\left[\frac{||g_k||}{\beta_k}, \Delta_k\right]$$

Illustration from [Conn, Gould, Toint, 2000]

positive curvature and minimum inside	$m_k(x_k) - m_k(x_k^C) \ge \frac{1}{2} \frac{\ g_k\ ^2}{\beta_k}$
positive curvature and minimum outside	$m_k(x_k) - m_k(x_k^C) \ge \frac{1}{2} \ g_k\ \Delta_k$
negative curvature	$m_k(x_k) - m_k(x_k^C) \ge \ g_k\ \Delta_k$

 β_k = upper bound on the curvature of m_k

First-order convergence

Sufficient decrease condition:

$$m_k(x_k) - m_k(x_k + s_k) \ge \kappa (m_k(x_k) - m_k(x_k^C))$$

$$\lim_{k\to\infty}\|\nabla f(x_k)\|=0$$

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What makes it fast ?

$$m_k(x_k+s) = f(x_k) + g_k^T s + \frac{1}{2} s^T H_k s$$

where $g_k = \nabla f(x_k)$ and $H_k \approx \nabla^2 f(x_k)$ (possibly indefinite)

Any global minimizer *s*^{*} of

$$\begin{cases} \text{minimize}_{s \in \mathbf{R}^n} & m_k(x_k + s) \\ \text{subject to} & \|s\|_2 \le \Delta_k \end{cases}$$

satisfies:

$$(H_k + \lambda^* I) s^* = -g_k$$

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where $H_k + \lambda^* I$ is pos. (semi)def., $\lambda^* \ge 0$ and $\lambda^* (||s^*||_2 - \Delta_k) = 0$

Exact solution: search for λ^* (Moré-Sorensen)

For Δ_k fixed, find $\lambda \geq \max\{0, -\lambda_{\min}(H_k)\}$ such that:

• $H_k + \lambda I$ is positive semidefinite

$$\blacktriangleright \quad s(\lambda) = -(H_k + \lambda I)^{-1} g_k \text{ satisfies } \begin{cases} \|s(\lambda)\|_2 \le \Delta_k \text{ for } \lambda = 0\\ \|s(\lambda)\|_2 - \Delta_k = 0 \end{cases}$$

by applying a safeguarded Newton's method to the secular equation:

$$\phi(\lambda) \stackrel{\text{def}}{=} \frac{1}{\|s(\lambda)\|_2} - \frac{1}{\Delta_k} = 0$$

Dominating cost: $s(\lambda)$ (a small number of Cholesky factorizations)

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Inexact solution: Krylov method (Steihaug-Toint)

- Adapt the (preconditioned) conjugate gradient method:
 - iterative method (*n* iterations) that generates a sequence {*p_j*} of mutually conjugate directions with respect to *H_k*:

$$p_j^T H_k p_i = 0 \quad i \neq j$$

- along which $m_k(x_k + s)$ is exactly minimized
- ► for the solution of the trust-region subproblem:

$$\begin{cases} \text{ (approx) } \min_{s \in \mathbb{R}^n} & m_k(x_k + s) \\ \text{ subject to } & \|s\|_2 \le \Delta_k \end{cases}$$

Start from the Cauchy point x_k^C (that is, with $p_0 = -g_k$)

• in order to ensure a further reduction in the model m_k

Terminate

- when an approximate minimizer is found (Stop)
- when the trust-region boundary is passed (Stop at the boundary)
- when a direction of negative curvature is encountered (move to the boundary and Stop)

For instance:
• The Steihaug-Toint algorithm

• The Generalized Lanczos Trust-Region algorithm (GLTR)

Book on trust-region methods



Trust-region methods [Conn, Gould, Toint, 2000]

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On the side of multigrid methods

where

Consider the linear system (discrete Poisson equation, for instance):

$$Ax = b \quad \rightsquigarrow \quad Ae = r \quad \text{(residual equation)}$$

here
$$\bullet \ e = x_* - \tilde{x} \quad \text{(error)} \quad \bullet \ x_* \quad \text{(exact solution)}$$

 $\blacktriangleright r = b - A\tilde{x}$ (residual) $\blacktriangleright \tilde{x}$ (approximation)

Expansion of e in Fourier modes shows high (oscillatory) and low (smooth) frequency components:



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Relaxation methods

Basic iterative methods:

- correct the i^{th} component of x_k in the order $1, 2, \ldots, n$
- to annihilate the i^{th} component of r_k

Jacobi

$$[x_{k+1}]_i = \frac{1}{a_{ii}} \left(-\sum_{j=1, \ j \neq i}^n a_{ij} [x_k]_i + [b]_i \right)$$

Gauss-Seidel

$$[x_{k+1}]_i = \frac{1}{a_{ii}} \left(-\sum_{j=1}^{i-1} a_{ij} [x_{k+1}]_i - \sum_{j=i+1}^n a_{ij} [x_k]_i + [b]_i \right)$$

 \longrightarrow Solve the equations of the linear system one by one

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Smoothing effect

Very effective methods at "smoothing", i.e., eliminating the high-frequency (oscillatory) components of the error:



error oferror after 10error after 100initial guessGS iterationsGS iterations

But they leave the low-frequency (smooth) components relatively unchanged

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Assume now (two levels):

• A fine grid (f) description
$$Ae = r \rightarrow A^f e^f = r^f$$

• A coarse grid (c) description
$$A^c e^c = r^c$$

Linked by transfer operators
$$A^c = RA^f P$$
, $e^c = Re^f$, $r^c = Rr^f$

Smooth error modes on a fine grid "look less smooth" on a coarse grid

- \longrightarrow When relaxation begins to stall at the finer level:
 - Move to the coarser grid where the smooth error modes appear more oscillatory

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- Apply a relaxation at the coarser level:
 - more efficient
 - substantially less expensive

Two-grid correction scheme



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Smoothing on fine grid only:



Two-grid correction scheme:



 $k = 0 \qquad \qquad k = 10 \qquad \qquad k = 100$

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Multigrid scheme



Recursive use to annihilate oscillatory error level by level $(\mathcal{O}(n))$

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Smoothing

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Smoothing

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Mesh Refinement

Solve the problem on the coarsest level

 \Rightarrow Good starting point for the next fine level

Do the same on each level

 \Rightarrow Good starting point for the finest level

Finally solve the problem on the finest level



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Combination of Mesh Refinement and V-cycles



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Books on multigrid



A Multigrid Tutorial [Briggs, Henson, McCormick, 2000]



Multigrid [Trottenberg, Oosterlee, Schüller, 2001]

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Back to our main issue Trust-region technique Hierarchy of problem descriptions Efficiency – Robustness Multilevel optimization method

<u>Note</u>: Multilevel Moré-Sorensen algorithm: $(H_k + \lambda I) s = -g_k$ [Toint, Tomanos, Weber Mendonça, report 2007]



Assume that we have:

► A hierarchy of problem descriptions of *f*:

$${f_i}_{i=0}^r$$
 with $f_r(x) = f(x)$

• Transfer operators, for
$$i = 1, ..., r$$
:

Terminology: a particular *i* is referred to as a level



$$\min_{x \in \mathbb{R}^n} f_r(x) = f(x) \longrightarrow \underline{\text{at } x_k}: \quad \text{minimize Taylor's model of } f_r \text{ around } x_k \text{ in the trust region of radius } \Delta_k$$

\downarrow or (whenever suitable and desirable)



 \rightarrow If more than two levels are available (r > 1), do this recursively

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Example of recursion with 5 levels (r = 4)



i: level index
$$(0 \le i \le r)$$

Notation:

k: index of the current iteration within level *i*

Construction of the coarse local models

If $f_i \neq 0$ for $i = 0, \ldots, r-1$

Impose first-order coherence via a correction term:

$$g_{\mathsf{low}} = Rg_{\mathsf{up}}$$

Impose second-order coherence^(*) via two correction terms:

$$g_{\text{low}} = Rg_{\text{up}}$$
 and $H_{\text{low}} = RH_{\text{up}}P$

(*) Not needed to derive first-order global convergence

If
$$f_i = 0$$
 for $i = 0, ..., r - 1$

 <u>Galerkin model</u>: Restricted version of the quadratic model at the upper level

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Preserving the trust-region constraint



<u>Note</u>: Motivation to switch to ∞ -norm [Gratton, Mouffe, Toint, Weber Mendonça, to appear] Use the coarse model whenever suitable

• When
$$||g_{\text{low}}|| \stackrel{\text{def}}{=} ||Rg_{\text{up}}|| \ge \kappa ||g_{\text{up}}||$$
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("Coarsening condition")

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<u>and</u>

• When
$$||g_{low}|| \stackrel{\text{def}}{=} ||Rg_{up}|| > \epsilon_{low}$$

<u>and</u>



Use the coarse model whenever desirable



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Recursive multilevel trust-region algorithm (RMTR)

<u>At iteration k</u> (until convergence):

- Choose either a Taylor or (if suitable) a coarse local model (first-order coherent):
 - Taylor model: compute a Taylor step (sufficient decrease condition OK)
 - Coarse local model: apply the algorithm recursively

(sufficient decrease condition KO)

- Evaluate the change in the objective function
- If achieved decrease \approx predicted decrease, then
 - accept the trial point
 - possibly enlarge the trust region

else

- keep the current point
- shrink the trust region
- Impose current trust region \subseteq upper level trust region

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Global convergence

Based on the trust-region technology

- Uses the sufficient decrease argument (imposed in Taylor's iterations)
- ▶ Plus the coarsening condition $(||Rg_{up}|| \ge \kappa ||g_{up}||)$

Main result

$$\lim_{k\to\infty}\|g_{r,k}\|=0$$

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[Gratton, Sartenaer, Toint, to appear]

Intermediate results

At iteration (i, k) we associate the set:

 $\mathcal{R}(i,k) \stackrel{\text{def}}{=} \{(j,\ell) \mid \text{iteration } (j,\ell) \text{ occurs within iteration } (i,k)\}$



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Let

$$\mathcal{V}(i,k) \stackrel{\text{def}}{=} \{ (j,\ell) \in \mathcal{R}(i,k) \mid \underbrace{\Delta m_{j,\ell} \ge \kappa \|g_{i,k}\|\Delta_{j,\ell}}_{\text{``sufficient decrease''}} \}$$

Then, at a non critical point and if the trust region is small enough:

$$\mathcal{V}(i,k) = \mathcal{R}(i,k)$$

→ Back to "classical" trust-region arguments

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Premature termination

For a recursive iteration (i, k):

A minimization sequence at level i - 1 initiated at iteration (i, k)denotes all successive iterations at level i - 1until a return is made to level i



Properties of RMTR

 Each minimization sequence contains at least one successful iteration

Premature termination in that case does not affect the convergence results at the upper level

Which allows

- Stop a minimization sequence after a preset number of successful iterations
- Use fixed lower-iterations patterns like the V or W cycles in multigrid methods

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A practical RMTR algorithm: Taylor iterations

At the coarsest level

 Solve using the exact Moré-Sorensen method (small dimension)

At finer levels

 Smooth using a smoothing technique from multigrid (to reduce the high frequency residual/gradient components)

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Adaptation of the Gauss-Seidel smoothing technique to optimization:

Sequential Coordinate Minimization (SCM smoothing)

Successive one-dimensional minimizations of the model along the coordinate axes when positive curvature

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▶ Cost: 1 SCM smoothing cycle ≈ 1 matrix-vector product



How to impose sufficient decrease in the model ?

How to impose the trust-region constraint ?

What to do if a negative curvature is encountered ?

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Start the first SCM smoothing cycle

 by minimizing along the largest gradient component (enough to ensure sufficient decrease)

Perform (at most) *p* SCM smoothing cycles

while inside the trust region (reasonable cost)

Terminate

- when an approximate minimizer is found (Stop)
- when the trust-region boundary is passed (Stop at the boundary)
- when a direction of negative curvature is encountered (move to the boundary and Stop)

SCM smoothing limits its exploration of the model's curvature to the coordinate axes \rightarrow only guarantees asymptotic positive curvature:

- along the coordinate axes at the finest level (i = r)
- ► along the the prolongation of the coordinate axes at levels i = 1,...,r-1
- along the prolongation of the coarsest subspace (i = 0)

"Weak" minimizers

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Some numerical flavor

[Gratton, Mouffe, Sartenaer, Toint, Tomanos, in preparation]

All on Finest (**AF**)

Standard Newton trust-region algorithm (TCG) Applied at the finest level

Multilevel on Finest (MF)

Algorithm RMTR Applied at the finest level

Mesh Refinement (**MR**)

Standard Newton trust-region algorithm (TCG) Applied successively from coarsest to finest level^(*)

Full Multilevel (FM)

Algorithm RMTR Applied successively from coarsest to finest level^(*)

(*) Starting point at level i + 1 obtained by prolongating the solution at level i

Test problem characteristics

Problem name	n _r	r	Туре	Bounds	Description
P2D	1.046.529	9	2-D, quadratic		Poisson model problem
P3D	250.047	5	3-D, quadratic		Poisson model problem
DEPT	1.046.529	9	2-D, quadratic		Elastic-plastic torsion problem
DPJB	1.046.529	9	2-D, quadratic	x	Journal bearing problem
DODC	1.046.529	9	2-D, convex		Optimal design problem
MINS-SB	1.046.529	9	2-D, convex		Minimium surface problem
MINS-OB	1.046.529	9	2-D, convex		Minimium surface problem
MINS-DMSA	1.046.529	9	2-D, convex		Minimium surface problem
IGNISC	3.969	5	2-D, convex		Combustion problem
DSSC	1.046.529	9	2-D, convex		Combustion problem
BRATU	1.046.529	9	2-D, convex		Combustion problem
MINS-BC	1.046.529	9	2-D, convex	X	Minimium surface problem
MEMBR	16.383	6	2-D, convex	X	Membrane problem
NCCS	7.938	6	2-D, nonconvex		Optimal control problem
NCCO	7.938	6	2-D, nonconvex		Optimal control problem
MOREBV	1.046.529	9	2-D, nonconvex		Boundary value problem

Performance profiles

CPU time



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Problem name	AF	MF	MR	FM
P2D	1061.2	70.3	532.1	25.9
P3D	626.1	60.9	18.3	71.7
DEPT	1350.5	70.1	97.1	8.7
DPJB	3600.0	506.6	249.8	63.2
DODC	868.1	57.4	171.6	29.2
MINS-SB	3600.0	3600.0	3600.0	153.6
MINS-OB	1433.6	54.0	114.0	21.9
MINS-DMSA	1155.7	89.8	281.0	19.2
IGNISC	8.5	4.7	2.0	1.7
DSSC	3183.8	3600.0	116.1	12.1
BRATU	2020.7	1227.3	80.1	9.9
MINS-BC	2706.4	97.0	524.6	57.9
MEMBR	18.2	10.0	5.9	3.9
NCCS	146.1	2212.6	6.7	7.0
NCCO	145.6	3600.0	0.0	0.0
MOREBV	3600.0	1572.7	3600.0	34.0

Best

Second best





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