Recursive trust-region methods for multilevel nonlinear optimization

Philippe Toint[1] Annick Sartenaer[1] Serge Gratton[2]

[1]Department of Mathematics,University of Namur, Belgium

(philippe.toint@fundp.ac.be)

[2]CERFACS, Toulouse, France

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Outline for Annick's talk and mine

Outline

The problem

$$\min_{x \in \mathbf{R}^n} f(x) \qquad (1)$$

- $f : \mathbf{R}^n \to \mathbf{R}$ nonlinear, twice-continuously differentiable and bounded below
- No convexity assumption
- (1) 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. $\nabla f(x_*) = 0$)

Basic trust-region algorithm

At iteration k (at x_k):

1. Define a local model $m_k(x_k + s)$ of f around x_k (Taylor's model)
2. Compute a candidate step s_k that (approximately) solves

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

3. Compute $f(x_k + s_k)$ and $\rho_k = \dfrac{f(x_k) - f(x_k + s_k)}{m_k(x_k) - m_k(x_k + s_k)}$
4. Update the iterate x_k and the trust-region radius Δ_k

$$x_{k+1} = \begin{cases} x_k + s_k & \text{if } \rho_k \ge \eta_1 \\ x_k & \text{if } \rho_k < \eta_1 \end{cases} \qquad \Delta_{k+1} = \begin{cases} \max(\alpha_2 \|s_k\|, \ \Delta_k) & \text{if } \rho_k \ge \eta_2 \\ \Delta_k & \text{if } \rho_k \in [\eta_1, \eta_2) \\ \alpha_1 \|s_k\| & \text{if } \rho_k < \eta_1 \end{cases}$$

where $0 < \eta_1 \le \eta_2 < 1$ and $0 < \alpha_1 < 1 < \alpha_2$

Dominating cost per iteration

- Computation of $f(x_k + s_k)$ and its derivatives
- Numerical solution of the subproblem $\left\{ \begin{array}{ll} \text{minimize}_{s \in \mathbf{R}^n} & m_k(x_k + s) \\ \text{subject to} & \|s\| \leq \Delta_k \end{array} \right.$

Assume now that

A set of alternative simplified models of f is known

$\longrightarrow$ how can we exploit this knowledge to reduce the cost

of solving the trust-region subproblem?

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Example: hierarchy of problem descriptions

Finest problem description	
Restriction ↓ R	P ↑ Prolongation
Fine problem description	
Restriction ↓ R	P ↑ Prolongation
...	
Restriction ↓ R	P ↑ Prolongation
Coarse problem description	
Restriction ↓ R	P ↑ Prolongation
Coarsest problem description	

Sources for such problems

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

The minimum surface problem

$$\min_v \int_0^1 \int_0^1 \left(1 + (\partial_x v)^2 + (\partial_y v)^2\right)^{\frac{1}{2}} \, dx\, dy$$

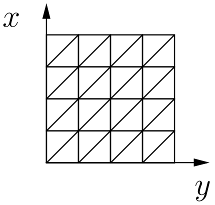
with the boundary conditions:

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

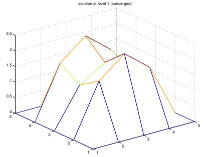
where

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

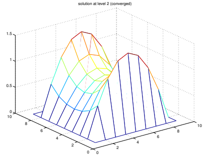
$\longrightarrow$ Discretization using a finite element basis



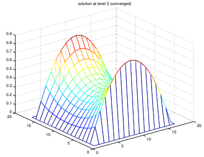
The solution at different levels



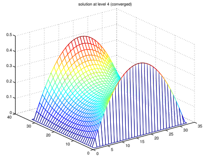
$n = 3^2 = 9$



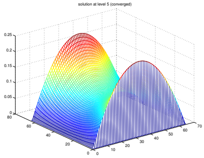
$n = 7^2 = 49$



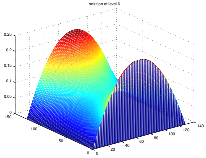
$n = 15^2 = 225$



$n = 31^2 = 961$



$n = 63^2 = 3969$



$n = 127^2 = 16129$

The framework

Assume that

- we know a collection of functions $\{f_i\}_{i=0}^r$ s.t. $f_i : \mathbf{R}^{n_i} \to \mathbf{R} \in \mathcal{C}^2$ and $n_i \geq n_{i-1}$
- $n_r = n$ and $f_r(x) = f(x)$ for all $x \in \mathbf{R}^n$

such that, for each $i = 1, \ldots, r$

- f_i is "more costly" to minimize than f_{i-1}
- there exist full-rank linear operators:

$$\left.\begin{array}{ll} R_i : \mathbf{R}^{n_i} \to \mathbf{R}^{n_{i-1}} & \text{(the restriction)} \\ P_i : \mathbf{R}^{n_{i-1}} \to \mathbf{R}^{n_i} & \text{(the prolongation)} \end{array}\right\} \text{ such that } \sigma_i P_i = R_i^T \qquad (\sigma_i = \|P_i\|^{-1})$$

Terminology

- a particular i is referred to as a level
- a subscript i is used to denote a quantity corresponding to the i-th level

The idea

$\min_{x \in \mathbb{R}^n} f_r(x) = f(x)$ $\longrightarrow$ at x_k: $\begin{cases} \min_{s \in \mathbb{R}^n} & m_k(x_k + s) = f_r(x_k) + \nabla f_r(x_k)^T s + \frac{1}{2} s^T H_k s \\ \text{s.t.} & \|s\| \leq \Delta_k \end{cases}$

$\downarrow$ or (whenever suitable)

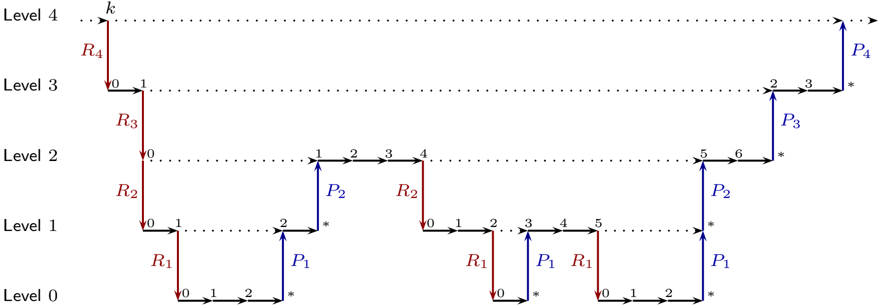
at x_k: Compute $\nabla f_r(x_k)$ (possibly H_k) | Candidate step s_k

Restriction $\downarrow$ R | P $\uparrow$ Prolongation

use f_{r-1} to construct a **coarse** local model of f_r
and minimize it within the **fine** trust region (Δ_k)

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

Example of recursion with 5 levels $(r = 4)$



Notation: double subscript $\begin{cases} i : \text{level index } (0 \le i \le r) \\ k : \text{index of the current iteration within level } i \end{cases}$

Additional ingredients

- Construction of the coarse local models: first-order coherence
- Use of the coarse local models: coarsening condition
- Trust-region constraint preservation

Construction of the coarse models

At a given iteration (i,k) with current iterate $x_{i,k}$

- Restrict $x_{i,k}$ to create the starting iterate $x_{i-1,0}$ at level $i-1$

$$x_{i-1,0} = R_i x_{i,k}$$

- Define the lower level model h_{i-1} around $x_{i-1,0}$

$$h_{i-1}(x_{i-1,0}+s_{i-1}) \stackrel{\text{def}}{=} f_{i-1}(x_{i-1,0}+s_{i-1}) + \boxed{v_{i-1}^T s_{i-1}}$$

where

$$v_{i-1} = R_i \nabla h_i(x_{i,k}) - \nabla f_{i-1}(x_{i-1,0})$$

so that

$$\nabla h_{i-1}(x_{i-1,0}) = R_i \nabla h_i(x_{i,k})$$

$\longrightarrow$ **Coherence of first-order information**

Use of the coarse models

- When $\|R_i \nabla h_i(x_{i,k})\| \geq \kappa \; \|\nabla h_i(x_{i,k})\|$ where $\kappa \in (0, \min[1, \min_i \|R_i\|])$ (0.01)

and

- When $\|R_i \nabla h_i(x_{i,k})\| > \epsilon_{i-1}$ where $\epsilon_{i-1} \in (0,1)$ is a measure of the first-order criticality for h_{i-1} judged sufficient at level $i-1$

and

- When $i > 0$

Choosing a model

Assume that we enter level i and want to (locally) minimize h_i starting from $x_{i,0}$

At iteration k of this minimization

- Choose a local model of h_i at $x_{i,k}$: { Taylor's model / the coarse model }
- Compute a candidate step $s_{i,k}$ that generates a decrease on this model within

$$\mathcal{B}_{i,k} = \{s_i \mid \|s_i\|_i \leq \Delta_{i,k}\}$$

where $\Delta_{i,k} > 0$ and $\|\cdot\|_i$ is a level-dependent norm

Using Taylor's model

The step $s_{i,k}$ is computed such that it approximately solves

$$\begin{cases} \text{minimize}_{s_i \in \mathbb{R}^{n_i}} & m_{i,k}(x_{i,k}+s_i) = h_i(x_{i,k}) + g_{i,k}^T s_i + \frac{1}{2}\ s_i^T H_{i,k} s_i \\ \text{subject to} & \|s_i\|_i \le \Delta_{i,k} \end{cases}$$

where $g_{i,k} \stackrel{\text{def}}{=} \nabla h_i(x_{i,k})$ and $H_{i,k} \approx \nabla^2 h_i(x_{i,k})$

The decrease of $m_{i,k}$ is understood in its usual meaning for trust-region methods, i.e., $s_{i,k}$ must satisfy the "sufficient decrease" condition:

$$m_{i,k}(x_{i,k}) - m_{i,k}(x_{i,k}+s_{i,k}) \ge \kappa_{\text{red}} \|g_{i,k}\| \min\left[\frac{\|g_{i,k}\|}{1+\|H_{i,k}\|}, \Delta_{i,k}\right]$$

for some $\kappa_{\text{red}} \in (0,1)$

Using the coarse model

Defining the level-dependent norm $\| \cdot \|_{i-1}$ by

$$\| \cdot \|_r = \| \cdot \|_2 \quad \text{and} \quad \|s_{i-1}\|_{i-1} = \|P_i s_{i-1}\|_i \quad \text{for} \quad i = 1, \ldots, r$$

then the lower level subproblem consists in approximately solving

$$\begin{cases} \text{minimize}_{s_{i-1} \in \mathbb{R}^{n_{i-1}}} & h_{i-1}(x_{i-1,0} + s_{i-1}) \\ \text{subject to} & \|s_{i-1}\|_{i-1} \leq \boxed{\Delta_{i,k}} \end{cases}$$

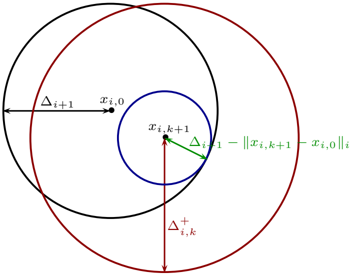
yielding a point $x_{i-1,*}$ such that

$$h_{i-1}(x_{i-1,*}) < h_{i-1}(x_{i-1,0})$$

and a corresponding step $x_{i-1,*} - x_{i-1,0}$ which is brought back to level i

$$s_{i,k} = P_i(x_{i-1,*} - x_{i-1,0})$$

Preserving the trust-region constraint



Trust-region radius update:

$$\Delta_{i,k+1} = \min\left[\Delta^+_{i,k},\ \Delta_{i+1} - \|x_{i,k+1} - x_{i,0}\|_i\right]$$

where

$$\Delta^+_{i,k} = \begin{cases} \max[\ \alpha_2\|s_{i,k}\|, \Delta_{i,k}] & \text{if } \rho_{i,k} \geq \eta_2 \\ \Delta_{i,k} & \text{if } \rho_{i,k} \in [\eta_1, \eta_2) \\ \alpha_1\|s_{i,k}\| & \text{if } \rho_{i,k} < \eta_1 \end{cases}$$

Algorithm RMTR(i, $x_{i,0}$,$g_{i,0}$, Δ_{i+1})

(First call with arguments r, $x_{r,0}$, $\nabla f_r(x_{r,0})$ and ∞)

Step 0: Initialization

- Compute v_i and $h_i(x_{i,0})$
- Set $\Delta_{i,0} = \Delta_{i+1}$ (or some Δ_r^{s} if $i = r$) and $k = 0$

Step 1: Model choice

- If $i = 0$ or if $\|R_i g_{i,k}\| < 0.01\|g_{i,k}\|$ or if $\|R_i g_{i,k}\| \leq \epsilon_{i-1}$, go to Step 3
- Otherwise, choose to go to Step 2 (recursive step) or to Step 3 (Taylor step)

Step 2: Recursive step computation

- Call Algorithm RMTR($i-1$, $R_i x_{i,k}$, $R_i g_{i,k}$, $\Delta_{i,k}$), yielding an approximate solution

  $x_{i-1,*}$ of

$$\begin{cases} \text{minimize}_{s_{i-1} \in \mathbf{R}^{n_{i-1}}} & h_{i-1}(R_i x_{i,k} + s_{i-1}) \\ \text{subject to} & \|s_{i-1}\|_{i-1} \le \boxed{\Delta_{i,k}} \end{cases}$$

- Define $s_{i,k} = P_i(x_{i-1,*} - R_i x_{i,k})$
- Set $\delta_{i,k} = h_{i-1}(R_i x_{i,k}) - h_{i-1}(x_{i-1,*})$ and go to Step 4

Step 3: Taylor step computation

- Choose $H_{i,k}$ and compute $s_{i,k} \in \mathbf{R}^{n_i}$ that approximately solves

$$\begin{cases} \text{minimize}_{s_i \in \mathbf{R}^{n_i}} & m_{i,k}(x_{i,k} + s_i) = h_i(x_{i,k}) + g_{i,k}^T s_i + \frac{1}{2}\, s_i^T H_{i,k} s_i \\ \text{subject to} & \|s_i\|_i \le \boxed{\Delta_{i,k}} \end{cases}$$

- Set $\delta_{i,k} = m_{i,k}(x_{i,k}) - m_{i,k}(x_{i,k} + s_{i,k})$ and go to Step 4

Step 4: Acceptance of the trial point

- Compute $h_i(x_{i,k}+s_{i,k})$ and $\rho_{i,k} = \frac{h_i(x_{i,k})-h_i(x_{i,k}+s_{i,k})}{\delta_{i,k}}$
- Define $x_{i,k+1} = \begin{cases} x_{i,k}+s_{i,k} & \text{if } \rho_{i,k} \geq \eta_1 \\ x_{i,k} & \text{if } \rho_{i,k} < \eta_1 \end{cases}$ (successful iteration)

Step 5: Termination

- Compute $g_{i,k+1}$
- If $\|g_{i,k+1}\|_\infty \leq \boxed{\epsilon_i}$ or $\|x_{i,k+1}-x_{i,0}\|_i > (1-\varepsilon)\Delta_{i+1}$

  return with $x_{i,*} = x_{i,k+1}$

Step 6: Trust-region radius update

- Set

$$\Delta^+_{i,k} = \begin{cases} \max[\,\alpha_2\|s_{i,k}\|, \Delta_{i,k}] & \text{if } \rho_{i,k} \geq \eta_2 \quad \text{(very successful iteration)} \\ \Delta_{i,k} & \text{if } \rho_{i,k} \in [\eta_1, \eta_2) \\ \alpha_1\|s_{i,k}\| & \text{if } \rho_{i,k} < \eta_1 \end{cases}$$

- Set $\boxed{\Delta_{i,k+1}} = \min\left[\Delta^+_{i,k},\; \Delta_{i+1} - \|x_{i,k+1}-x_{i,0}\|_i\right]$
- Increment k by one and go to Step 1

Outline

Global convergence and complexity

Based on the trust-region technology:

- Uses the sufficient decrease argument (imposed in Taylor's iterations)
- Plus the coarsening condition $(\|R_i g_{i,k}\| \geq 0.01 \; \|g_{i,k}\|)$

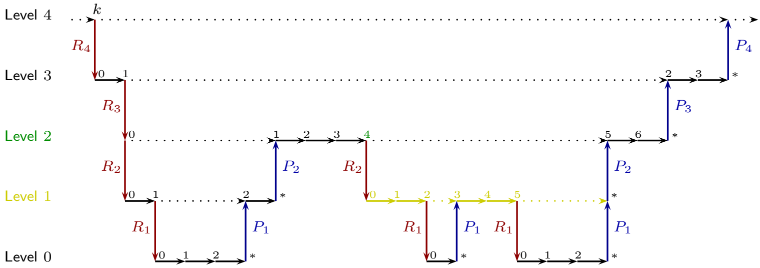
Main results:

- Convergence to first-order critical points at all levels
- Weak upper bound $(\mathcal{O}(1/\epsilon_r^2))$ on the number of iterations to achieve a given accuracy

Minimization sequence

If iteration (i,k) is a recursive iteration:

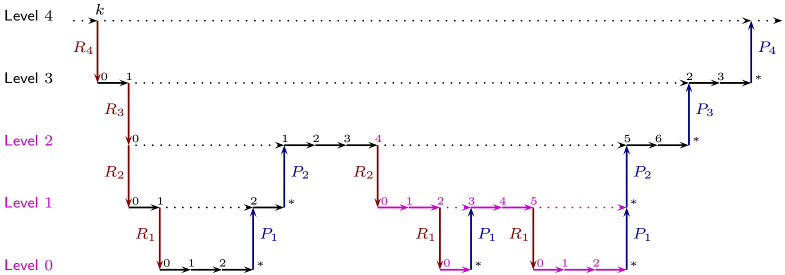
a minimization sequence at level $i-1$ initiated at iteration (i,k)
denotes all successive iterations at level $i-1$ until a return is made to level i



The set $\mathcal{R}(i,k)$

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

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



Key results

Consider the set

$$\mathcal{V}(i,k) \stackrel{\text{def}}{=} \{ (j,\ell) \in \mathcal{R}(i,k) \mid \underbrace{\delta_{j,\ell} \geq c\|g_{i,k}\|\Delta_{j,\ell}}_{\text{"sufficient decrease"}} \} \quad c \in (0,1)$$

If $x_{i,k}$ is non-critical and $\Delta_{i,k}$ is small enough

then:
- $\mathcal{V}(i,k) = \mathcal{R}(i,k)$
- The total number of iterations in $\mathcal{R}(i,k)$ is finite
- All iterations $(j,\ell) \in \mathcal{R}(i,k)$ are very successful
- $\Delta^+_{i,k} \geq \Delta_{i,k}$

Because we impose nonzero tolerances ϵ_i on the gradient norms

then:
- Each minimization sequence contains at least one successful iteration
- All the trust-region radii are bounded away from zero

Complexity result

Furthemore:

- The number of iterations at each level is finite
- Algorithm RMTR needs at most

$$\left\lceil \frac{f(x_{r,0}) - f_{\text{low}}}{\theta(\epsilon_{min})} \right\rceil$$

successful Taylor iterations at any level to obtain an iterate $x_{r,k}$ such that

$$\|g_{r,k}\| \leq \epsilon_r$$

where

- $\epsilon_{min} = \min_{i=0,\dots,r} \epsilon_i$
- f_{low} is a known lower bound on f
- $\theta(\epsilon) = \mathcal{O}(\epsilon^2)$ for small values of ϵ (can be estimated)

This complexity bound in $1/\epsilon^2$ for small ϵ:

- is in terms of iteration numbers, thus only implicitly accounts for the cost of computing a Taylor step
- is only modified by a constant factor if all iterations (successful and unsucessful) are considered
- thus gives a worst case upper bound on the number of function and gradient evaluations
- is of the same order as the corresponding bound for the pure gradient method (not surprising since based on the "sufficient decrease" condition)
- involves the number of successful Taylor iterations summed up on all levels, meaning that successful such iterations at cheap low levels decrease the number of necessary expensive ones at higher levels
- does not depend on the problem dimension but on the properties of the problem and of the algorithm

Global convergence result

If Algorithm RMTR is called at the uppermost level with $\epsilon_r = 0$, then:

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

If the trust region becomes asymptotically inactive at all levels and all ϵ_i are driven to zero, then each minimization sequence becomes infinite and:

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

for every level $i = 0, \ldots, r$

Two comments

"Premature" termination does not affect the convergence results at the upper level provided each minimization sequence contains at least one successful iteration

One can:

- 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

We did not use the form of the lower levels functions $\{f_i\}_{i=0}^{r-1}$

One can:

- Choose $f_i = 0$ for $i = 0, \ldots, r-1$, which implies that the lower level model $h_{i-1}(x_{i-1,0} + s_{i-1})$ reduces to the linear model $(R_i g_{i,k})^T s_{i-1}$

Outline

A practical RMTR algorithm

- How to efficiently compute appropriate steps at Taylor iterations?
- How to improve the coarse models to ensure second-order coherence?
- Which structure consider for the recursions?
- How to compute the starting point at the finest level?
- Which choice for the prolongation and restriction operators (P_i and R_i)?

Taylor iterations: solving and smoothing

$$\begin{cases} \text{minimize}_{s_i \in \mathbf{R}^{n_i}} & m_{i,k}(x_{i,k} + s_i) = h_i(x_{i,k}) + g_{i,k}^T s_i + \frac{1}{2}\; s_i^T H_{i,k} s_i \\ \text{subject to} & \|s_i\|_i \le \Delta_{i,k} \end{cases}$$

- At the coarsest level:
  - Solve using the exact Moré-Sorensen method (small dimension)
- At finer levels:
  - Solve using a Truncated Conjugate-Gradient (TCG) algorithm

or

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

SCM Smoothing

⟶ 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)

  From $s_i^0 = 0$ and for $j = 1, \ldots, n_i$:

  $$s_i^j \Longleftarrow \min_{\alpha} m_{i,k}(x_{i,k} + s_i^{j-1} + \alpha e_{i,j})$$

  where $e_{i,j}$ is the jth vector of the canonical basis of $\mathbb{R}^{n_i}$

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

Three issues

- How to impose sufficient decrease in the model?
- How to impose the trust-region constraint?
- What to do if a negative curvature is encountered?

- Start the first SCM smoothing cycle by minimizing along the largest gradient component (enough to ensure sufficient decrease)
- While inside the trust region, perform (at most p) SCM smoothing cycles (reasonable cost)
- If the step lies outside the trust region, apply a variant of the dogleg strategy (very rare in practice)
- If negative curvature is encountered during a cycle:
  - Remember the step to the trust-region boundary which produces the largest model reduction during the cycle (stop the SCM smoothing)
  - Select the final step as that giving the maximum reduction

Second-order and Galerkin models

At level $i-1$ (model for level i):

- First-order coherence

$$h_{i-1}(x_{i-1,0}+s_{i-1}) = f_{i-1}(x_{i-1,0}+s_{i-1}) + v_{i-1}^T s_{i-1}$$

with $x_{i-1,0} = R_i x_{i,k}$ and $v_{i-1} = R_i g_{i,k} - \nabla f_{i-1}(x_{i-1,0})$

$$\Rightarrow \quad g_{i-1,0} = \nabla h_{i-1}(x_{i-1,0}) = R_i g_{i,k}$$

- Second-order coherence (more costly)

$$h_{i-1}(x_{i-1,0}+s_{i-1}) = f_{i-1}(x_{i-1,0}+s_{i-1}) + v_{i-1}^T s_{i-1} + \tfrac{1}{2} s_{i-1}^T W_{i-1} s_{i-1}$$

with $W_{i-1} = R_i H_{i,k} P_i - \nabla^2 f_{i-1}(x_{i-1,0})$

$$\Rightarrow \quad \nabla^2 h_{i-1}(x_{i-1,0}) = R_i H_{i,k} P_i$$

- Galerkin model (second-order coherent)

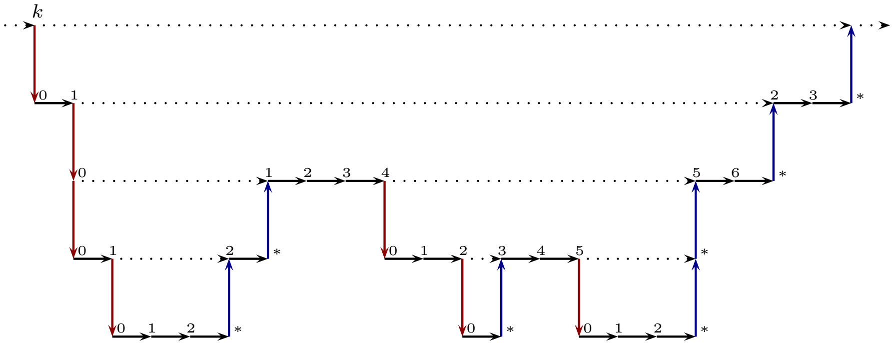
$$h_{i-1}(x_{i-1,0} + s_{i-1}) = v_{i-1}^T s_{i-1} + \frac{1}{2} s_{i-1}^T W_{i-1} s_{i-1}$$

with

- $v_{i-1} = R_i g_{i,k}$
- $W_{i-1} = R_i H_{i,k} P_i$

$\Rightarrow$ "Restricted" version of the quadratic model at the upper level

Recursion forms



Example of recursion with 5 levels $(r = 4)$

Free and fixed form recursions

Because:

- The convergence properties of Algorithm RMTR still hold if the minimization at lower levels ($i = 0, \dots, r-1$) is stopped after the first successful iteration

$\Rightarrow$ Flexibility that allows different recursion patterns

- Alternance of successful SCM smoothing iterations with recursive or TCG successful iterations (at all levels but the coarsest) is very fruitful

$\Rightarrow$ This alternance is imposed for each recursion form

- TCG iterations are much more expensive than recursive iterations

$\Rightarrow$ A recursive iteration is always attempted whenever allowed
(i.e., when $i > 0$ and $\|R_i g_{i,k}\| \geq 0.01 \|g_{i,k}\|$ and $\|R_i g_{i,k}\| > \epsilon_{i-1}$)

Free form recursion

- The minimization at each level is stopped when the termination condition on the gradient norm or on the step size is satisfied (Step 5 of Algorithm RMTR)
- Alternance of successful SCM smoothing iterations with recursive (or TCG) iterations is imposed

Fixed form recursion (possibly truncated)

- A maximum number of successful iterations at each level is specified

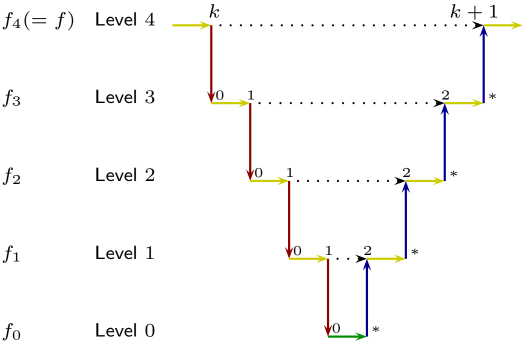
V-form recursion:

One succ. SCM smoothing
followed by
One succ. recursive (or TCG) iteration
followed by
One succ. SCM smoothing

W-form recursion:

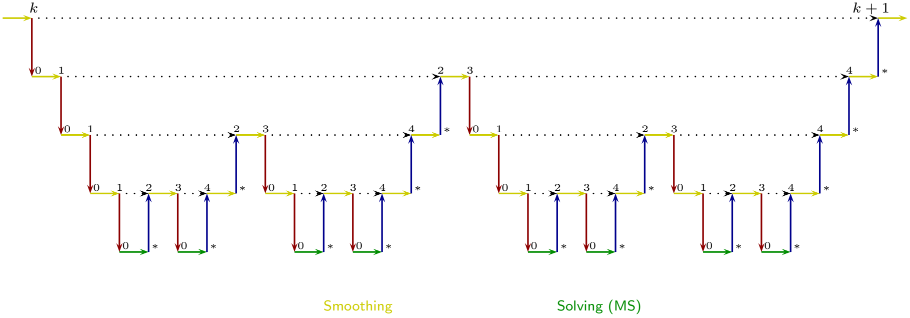
One succ. SCM smoothing
followed by
One succ. recursive (or TCG) iteration
followed by
One succ. SCM smoothing
followed by
One succ. recursive (or TCG) iteration
followed by
One succ. SCM smoothing

V-form recursion



Smoothing Solving (MS)

W-form recursion



Computing the starting point at the finest level

Use a mesh refinement technique to compute $x_{r,0}$:

- Select a random starting point $x_{0,0}$ at level 0

For $i = 0, \ldots, r-1$

- Apply Algorithm RMTR to solve

$$\min_x f_i(x)$$

(with increasing accuracy)

- Prolongate the solution to level $i+1$ using cubic interpolation

Prolongations and restrictions

- The prolongation P_i is the linear interpolation operator
- The restriction R_i is P_i^T normalized to ensure that $\|R_i\| = 1$
- P_i and R_i are never assembled

Outline

Convergence to weak minimizers

- Convergence to second-order critical points requires the eigen-point condition

If $\tau_{i,k}$ (the smallest eigenvalue of $H_{i,k}$) is negative, then

$$m_{i,k}(x_{i,k}) - m_{i,k}(x_{i,k} + s_{i,k}) \geq \kappa_{\text{eip}} |\tau_{i,k}| \min[\tau_{i,k}^2, \Delta_{i,k}^2]$$

where $\kappa_{\text{eip}} \in (0, \frac{1}{2})$

$\longrightarrow$ Too costly to impose a posteriori on recursive iterations

- The SCM smoothing technique limits its exploration of the model's curvature to the coordinate axes and thus only guarantees

If $\mu_{i,k}$ (the most negative diagonal element of $H_{i,k}$) is negative, then

$$m_{i,k}(x_{i,k}) - m_{i,k}(x_{i,k} + s_{i,k}) \geq \tfrac{1}{2} |\mu_{i,k}| \Delta_{i,k}^2$$

$\longrightarrow$ Asymptotic positive curvature:

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

$\longrightarrow$ "Weak" minimizers

Outline

DN: a Dirichlet-to-Neumann transfer problem

(Lewis and Nash, 2005)

$$\min_{a\,:\,[0,\pi]\to\mathbb{R}} \int_0^\pi \left(\partial_y u(x,0) - \phi(x)\right)^2 dx$$

where u is the solution of the boundary value problem

- $$\begin{cases} \Delta u(x,y) = 0 & \text{in } S, \\ u(x,y) = a(x) & \text{on } \Gamma, \\ u(x,y) = 0 & \text{on } \partial S \backslash \Gamma. \end{cases}$$

with

- $S = \{(x,y),\ 0 \le x \le \pi,\ 0 \le y \le \pi\}$
- $\Gamma = \{(x,y),\ 0 \le x \le \pi,\ y = 0\}$

- $\phi(x) = \sum_{i=1}^{15} \sin(i\,x) + \sin(40\,x)$

$\longrightarrow$ The discretized problem is a 1D linear least-squares problem

DN: a Dirichlet-to-Neumann transfer problem

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Q2: a simple quadratic example

$$\begin{aligned} -\Delta u(x,y) &= f \text{ in } S_2 \\ u(x,y) &= 0 \text{ on } \partial S_2 \end{aligned}$$

where

- f is such that the analytical solution to the problem is

$$u(x,y) = 2y(1-y) + 2x(1-x)$$

- $S_2 = \{(x,y),\ 0 \le x \le 1,\ 0 \le y \le 1\}$

$\longrightarrow$ 5-point finite-difference discretization:

$$A_i x = b_i \qquad (A_i \text{ sym pd})$$

at level i

$$\longrightarrow \min_{x \in \mathbb{R}^{n_r}} \tfrac{1}{2} x^T A_r x - x^T b_r$$

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Q3: a 3D quadratic example

$$\begin{array}{rcl} -(1+\sin(3\pi x)^2)\ \Delta u(x,y,z) & = & f \text{ in } S_3 \\ u(x,y,z) & = & 0 \text{ on } \partial S_3 \end{array}$$

where

- f is such that the analytical solution to the problem is

$$u(x,y,z) = x(1-x)y(1-y)z(1-z)$$

- $S_3 = [0,1] \times [0,1] \times [0,1]$

$\longrightarrow$ 7-point finite-difference discretization:

$$A_i x = b_i \qquad (A_i \text{ sym pd})$$

at level i (systems made symmetric)

$$\longrightarrow \min_{x \in \mathbb{R}^{n_r}} \tfrac{1}{2} x^T A_r x - x^T b_r$$

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Surf: the minimum surface problem

$$\min_{v} \int_0^1 \int_0^1 \left(1 + (\partial_x v)^2 + (\partial_y v)^2\right)^{\frac{1}{2}} \, dx \, dy$$

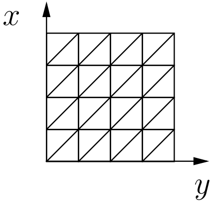
with the boundary conditions

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

where

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

$\longrightarrow$ Discretization using a finite element basis



$\longrightarrow$ Nonlinear convex problem

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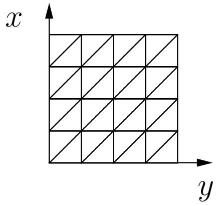

$\longrightarrow$ Nonlinear convex problem

Inv: an inverse problem from image processing

Image deblurring problem (Vogel, 2002)

$$\min \mathcal{J}(f) \quad \text{where} \quad \mathcal{J}(f) = \frac{1}{2}\|Tf - d\|_2^2 + TV(f)$$

where $TV(f)$ is the discretization of the total variation function

$\longrightarrow$ Same discretization scheme than for Surf

$$\int_0^1 \int_0^1 \left(1 + (\partial_x f)^2 + (\partial_y f)^2\right)^{\frac{1}{2}} \, dx\, dy$$

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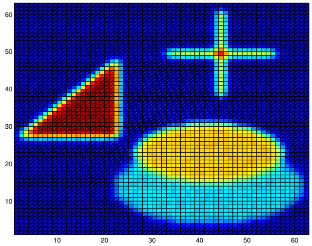
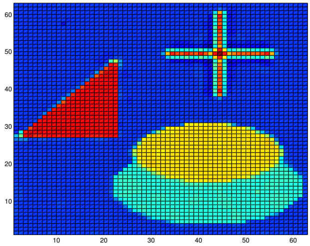
Vogel's problem data and result





Opt: an optimal control problem

Solid ignition problem (Borzi and Kunisch, 2006)

$$\min_f \mathcal{J}(u(f),f) = \int_{S_2} (u-z)^2 + \frac{\beta}{2}\int_{S_2} (e^u - e^z)^2 + \frac{\nu}{2}\int_{S_2} f^2$$

where

- $S_2 = \{(x,y),\ 0 \le x \le 1,\ 0 \le y \le 1\}$ $\longrightarrow$ Discretization by finite differences in S_2
- $\begin{cases} -\Delta u + \delta e^u = f & \text{in } S_2 \\ u = 0 & \text{on } \partial S_2 \end{cases}$ $\longrightarrow$ Nonlinear convex problem
- $\nu = 10^{-5}$, $\delta = 6.8$, $\beta = 6.8$, $z = \frac{1}{\pi^2}$

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NC: a nonconvex example

Penalized version of a constrained optimal control problem

$$\min_{u,\gamma} \mathcal{J}(u,\gamma) = \int_{S_2} (u-u_0)^2 + \int_{S_2} (\gamma-\gamma_0)^2 + \int_{S_2} f^2$$

where

- $S_2 = \{(x,y),\ 0 \le x \le 1,\ 0 \le y \le 1\}$
- $\left\{ \begin{array}{rcll} -\Delta u + \gamma u - f_0 & = & f & \text{in } S_2 \\ u & = & 0 & \text{on } \partial S_2 \end{array} \right.$
- $\begin{array}{rcl} \gamma_0(x,y) & = & u_0(x,y) \\ & = & \sin(x(1-x))\sin(y(1-y)) \end{array}$
- $-\Delta u_0 + \gamma_0 u_0 = f_0$

$\longrightarrow$ Discretization by finite differences

$\longrightarrow$ Nonconvex least-squares problem

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- $S_2 = \{(x,y),\ 0 \le x \le 1,\ 0 \le y \le 1\}$ ⟶ Discretization by finite differences
- $\begin{cases} -\Delta u + \gamma u - f_0 = f & \text{in } S_2 \\ u = 0 & \text{on } \partial S_2 \end{cases}$
- $\gamma_0(x,y) = u_0(x,y) = \sin(x(1-x))\sin(y(1-y))$ ⟶ Nonconvex least-squares problem
- $-\Delta u_0 + \gamma_0 u_0 = f_0$

Comparison of three algorithms

- **AF** ("All on Finest"): standard Newton trust-region algorithm (with TCG as subproblem solver) applied at the finest level

- **MR** ("Mesh Refinement"): discretized problems solved in turn from the coarsest level to the finest one, using the same standard Newton trust-region method

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

- **FM** ("Full Multilevel"): Algorithm RMTR

The default full multilevel (FM) algorithm

- Newton quadratic model at the finest level
- Galerkin models ($f_i = 0$) at coarse levels
- W-form recursion performed at each level
- Recursive iteration always attempted when allowed
- A single smoothing cycle allowed at SCM smoothing iterations

Comparison of computational kernels

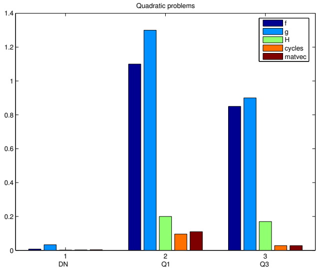
For the quadratic problems:

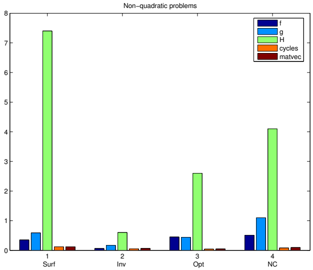
- Number of smoothing cycles (**FM**) vs number of matrix-vector products (**AF**, **MR**)

For the non-quadratic problems:

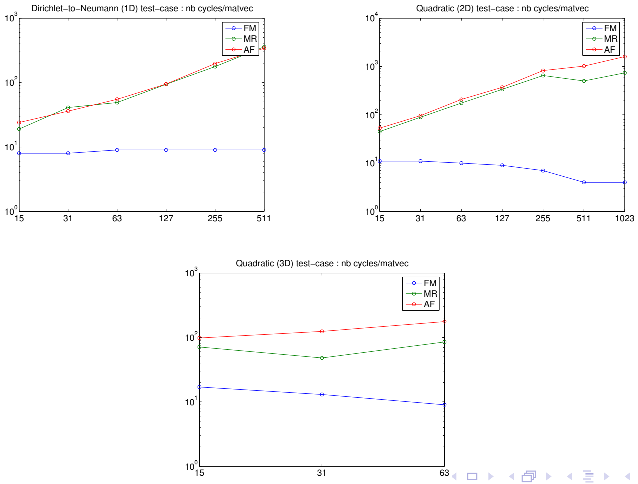
- Number of smoothing cycles (**FM**) vs number of matrix-vector products (**MR**)
- Number of f, g, and H evaluations

Time performance of computational kernels





Performance results on quadratic problems

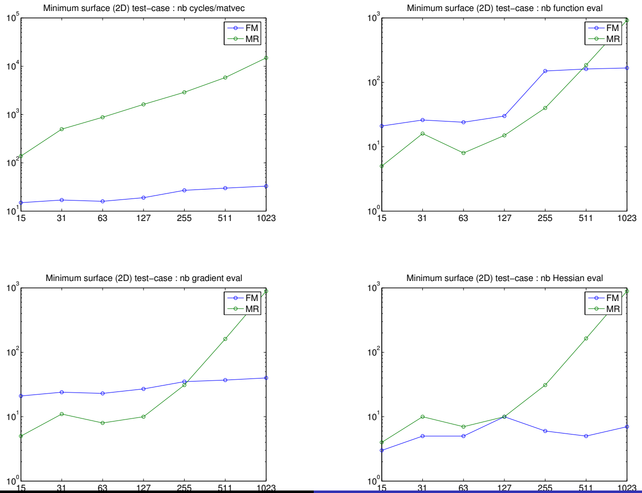


On quadratic problems: the number of smoothing cycles is fairly independent of the mesh size and dimension

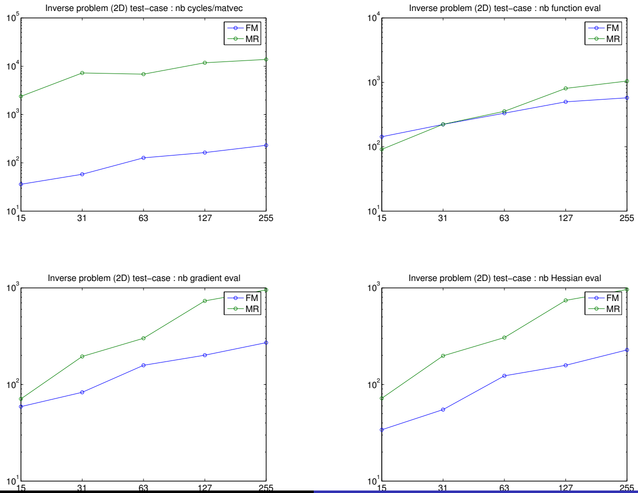
⟶ Similar behaviour as the linear multigrid approach

⟶ The trust-region machinery introduced in the multigrid setting does not alter the property

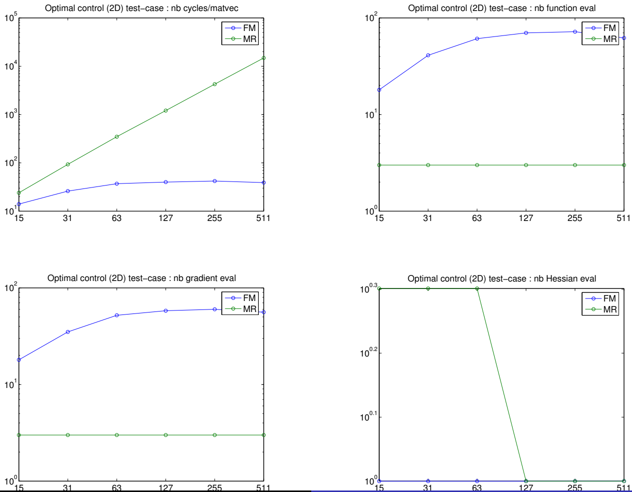
Performance results on Surf



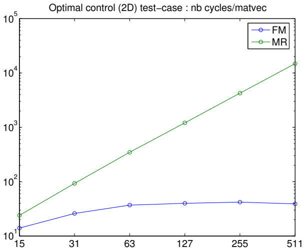
Performance results on Inv

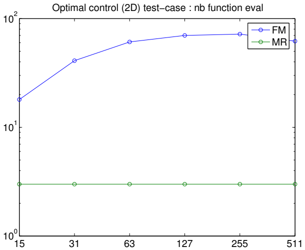


Performance results on Opt



Operations counts for Opt (at the finest level)



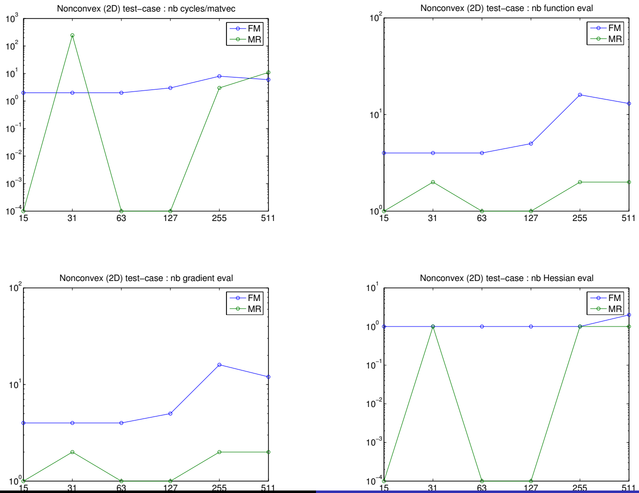


- One eval of $f = 14n_r$ flops
- One eval of $g = 56n_r$ flops
- One cycle/matvec $= 10n_r$ flops

- **FM**: 4394 flops
- **MR**: 148470 flops

$\longrightarrow$ **MR** much more expensive than **FM** because the gain in the number of smoothing cycles is much superior to the loss in f and g evaluations

Performance results on NC



Comparison of algorithmic variants

$\longrightarrow$ Sensibility investigation of **FM**

W2: two smoothing cycles per SCM smoothing iteration instead of one

W3: three smoothing cycles per SCM smoothing iteration instead of one

V1: V-form recursions instead of W-form recursions

F1: free form recursions instead of W-form recursions

LMOD: first-order coherent model rather than Galerkin model ($f_i = 0$)

QMOD: second-order coherent model rather than Galerkin model ($f_i = 0$)

LINT: linear rather than cubic interpolation in the initialization phase

Current comparative conclusions

$\longrightarrow$ Encouraging !

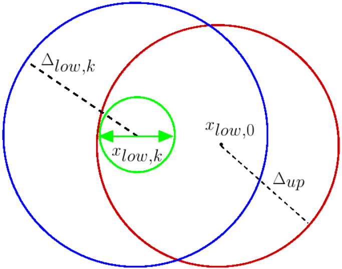
- Algorithm RMTR (default version **FM**) is more efficient than mesh refinement (**MR**) for large instances
- Pure quadratic recursion (Galerkin model) is very efficient
- W-form and free form recursions are most efficient

Outline

A (more natural) ℓ_∞ version

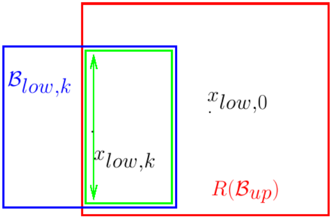
RMTR

- 2-norm criticality measure
- good results, but annoying trust region scaling problem (recursion)



RMTR-∞

- ∞-norm (bound constraints)
- new criticality measure
- new possibilities for step length



∞-norm in trust regions

- Possibility for asymmetric trust regions (more freedom)
- In lower levels, can be represented as a bound constrained subproblem
- We will impose that the lower level steps must remain inside the restriction of the upper level trust region: If

$$\mathcal{B}_{up} = \{x \,|\, l_{up} \leq x \leq u_{up}\}$$

then

$$\mathcal{B}_{low} = R\mathcal{B}_{up} = \{x \,|\, Rl_{up} \leq x \leq Ru_{up}\}$$

- The step $s_{up} = Ps_{low}$ will not necessarily be inside the upper level trust region! But: If $\Delta_{up} = \text{radius}(\mathcal{B}_{up})$, then

$$\|s_{up}\|_\infty \leq \|P\|_\infty \|R\|_\infty \Delta_{up}.$$

A new Criticality Measure

- Each lower level subproblem is constrained by the restriction of the upper level trust region; we can consider the lower level subproblem as a bound constrained optimization problem.
- Instead of evaluating g_{low} to check criticality, we will look at

$$\chi(x_{\text{low}}) = |\min_{\substack{d \in R\mathcal{B}_{\text{up}} \\ \|d\| \leq 1}} \langle g_{\text{low}}, d \rangle|.$$

- We only use recursion if:

$$\chi_{low} \geq \kappa_\chi \chi_{up}$$

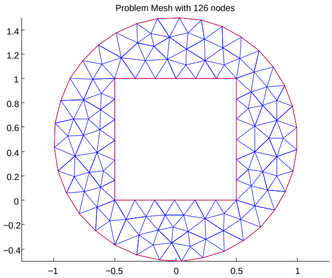
- We have found a solution to the current level i if

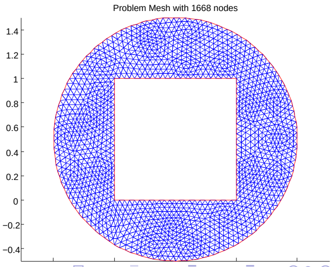
$$\chi < \epsilon_i^\chi.$$

Algebraic multigrid

No need for predefined grids; lower level information is obtained automatically through a preprocessing phase which can be expensive (but usually the resolution phase is faster for a single system).

1. Problem definition
2. Choice of smoothing operator (*smooth error* detection)
3. Construction of intergrid operators and subgrids.





P-multigrid

Need an initial grid (not necessarily uniform); Construct the finer grids by using higher level polynomials.

- Choice of the basis: shape functions, hierarchical basis, ... with different degrees at each level
- Same number of nodes for each level
- Construction of the intergrid operators that have to interpolate correctly the basis

Bound constrained problems

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \geq 0, \end{array}$$

Issues:

- Restriction of bound constraints $\neq$ bounds!
- Fast active set identification
- Bound compatible smoothing operator
- Criticality measure

Equality constrained problems

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & c(x) = 0, \end{array}$$

Issues:

- Error in the adjoint equation
- Inexactly tangential steps
- Iterative solvers
- (Filters?)

Perspectives

- More numerical experiments
- Hessian approximation schemes
- Combination with non-monotone techniques, filter methods, . . .
- Real applications in data assimilation . . .
- . . . and much more !