A numerical exploration of recursive multiscale unconstrained optimization

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Unconstrained optimization

The unconstrained nonlinear programming problem:

$$\text{minimize} f(x)$$

for $x \in \mathbb{R}^n$, f smooth.

Main applications:

- surface design
- nonlinear least-squares (parameter estimation)

Plan

→ ***Introduction***

- Problem
- Algorithm
- Model coherence
- Taylor iterations
- Iter. structure
- TR radius
- Initial point
- Test problems
- Some results
- Perspectives

Hierarchy of problem descriptions

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Can we use a structure of the form:

Finest problem description	
Restriction $\downarrow R$	$P \uparrow$ Prolongation
Fine problem description	
Restriction $\downarrow R$	$P \uparrow$ Prolongation
$\cdots$	
Restriction $\downarrow R$	$P \uparrow$ Prolongation
Coarse problem description	
Restriction $\downarrow R$	$P \uparrow$ Prolongation
Coarsest problem description	

Sources for such problems

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- parameter estimation in
  - discretized ODEs
  - discretized PDEs
- optimal control problems
- surface design
  (optics, shape optimization)
- weather prediction
  (level of physics in the model)
- Proper Orthogonal Decomposition
  (snapshots) (Sachs *et al.*)
- . . .

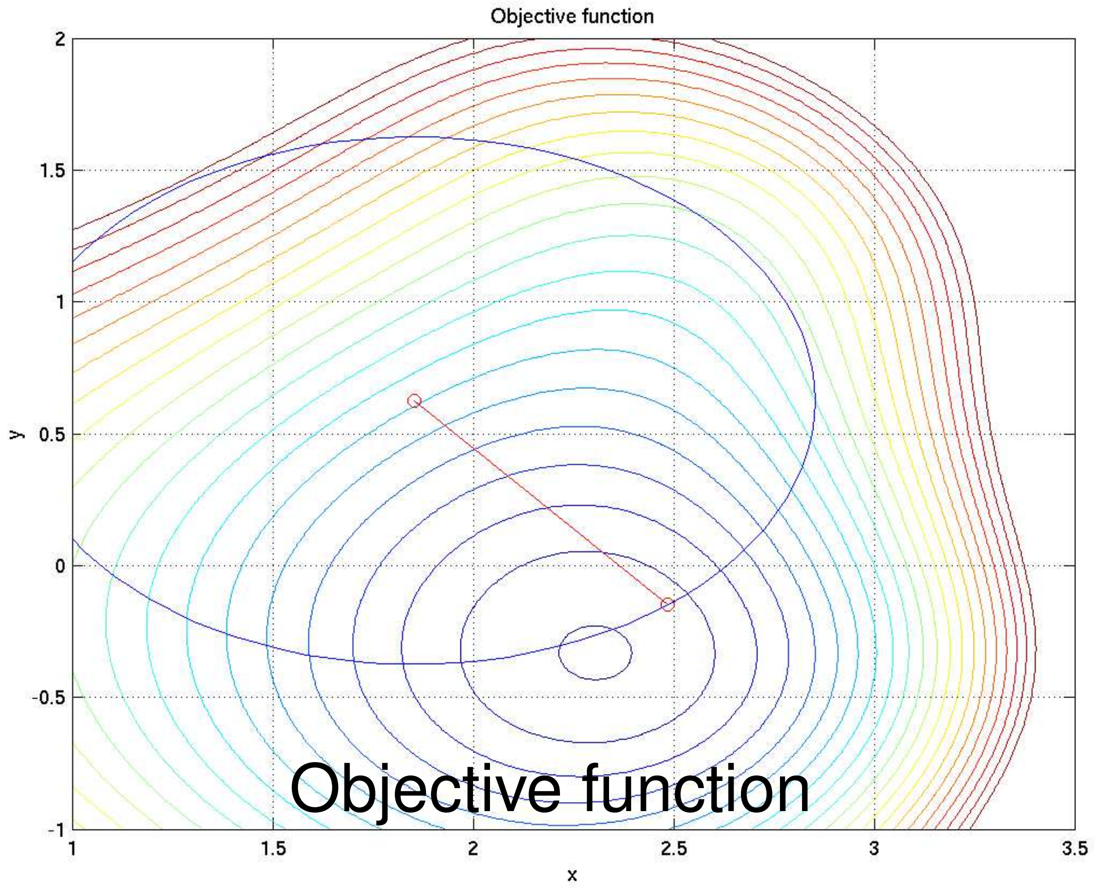
Basic trust-region algorithm

Until convergence:

- Choose a local model of the objective f
- Compute a trial point that decreases this model within the trust region
- Evaluate change in the objective function
- If achieved reduction $\approx$ predicted reduction,
  - accept trial point as new iterate
  - (possibly) enlarge the trust region

  else
  - reject the trial point
  - shrink the trust region

Model and objective comparison



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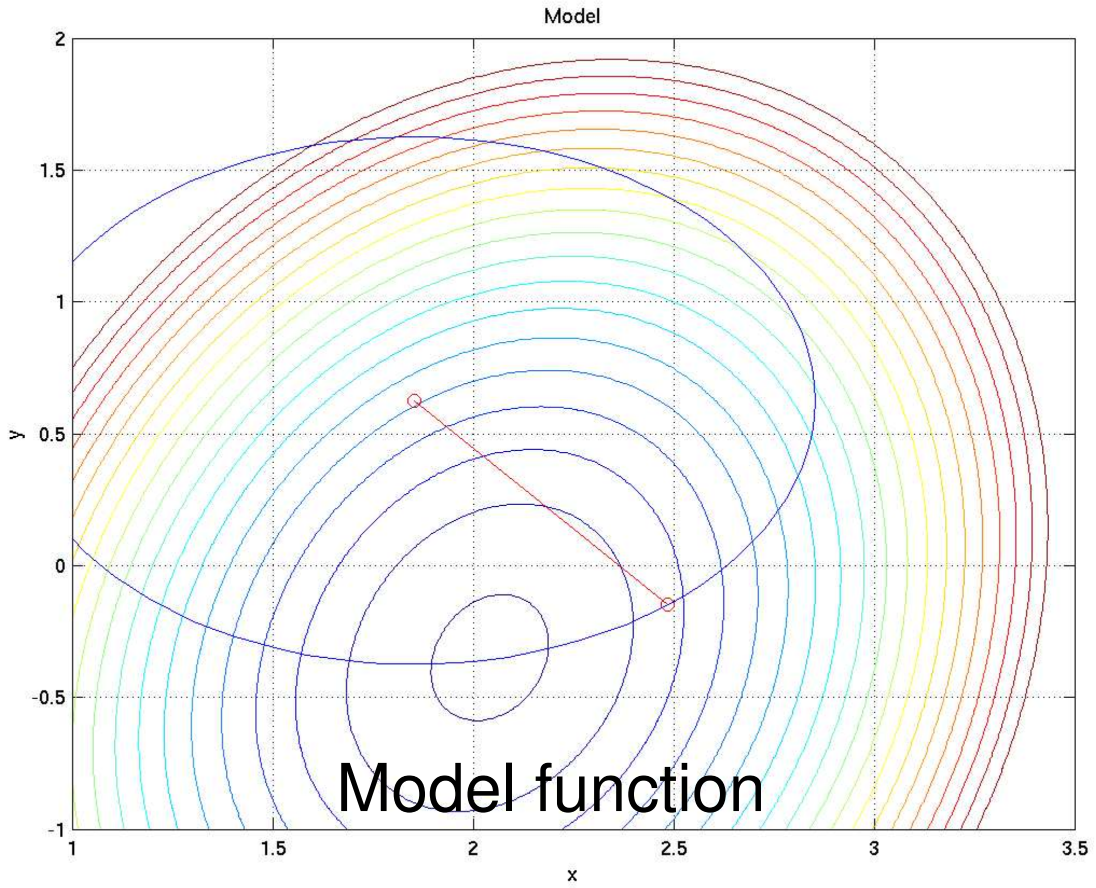

Trust-Region methods

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Example (Conn, Gould, Toint 2000):

$$\min_{x,y} -10x^2 + 10y^2 + 4\sin(xy) - 2x + x^4$$

Trust-Region methods

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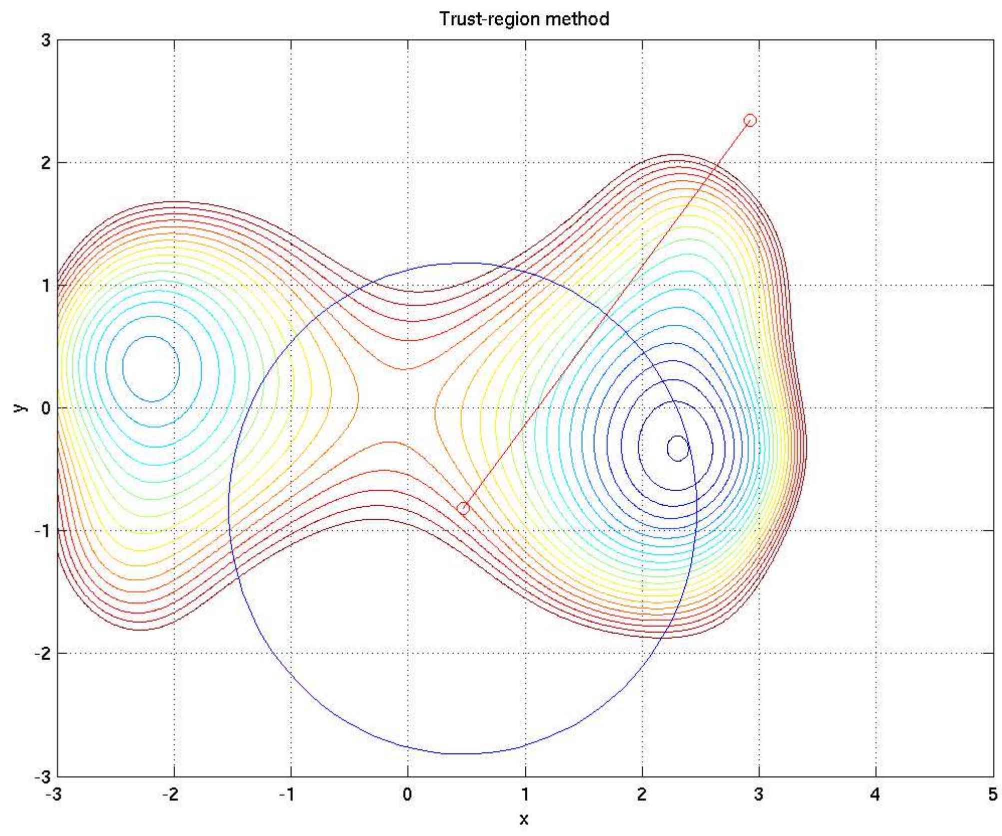

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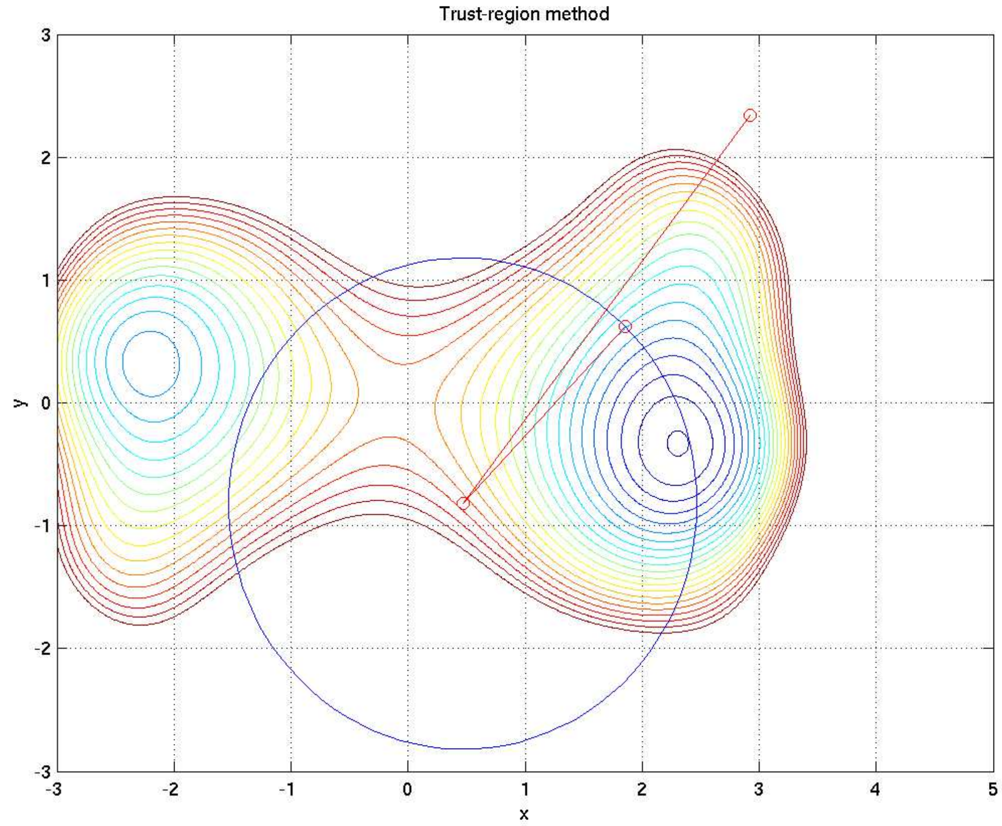

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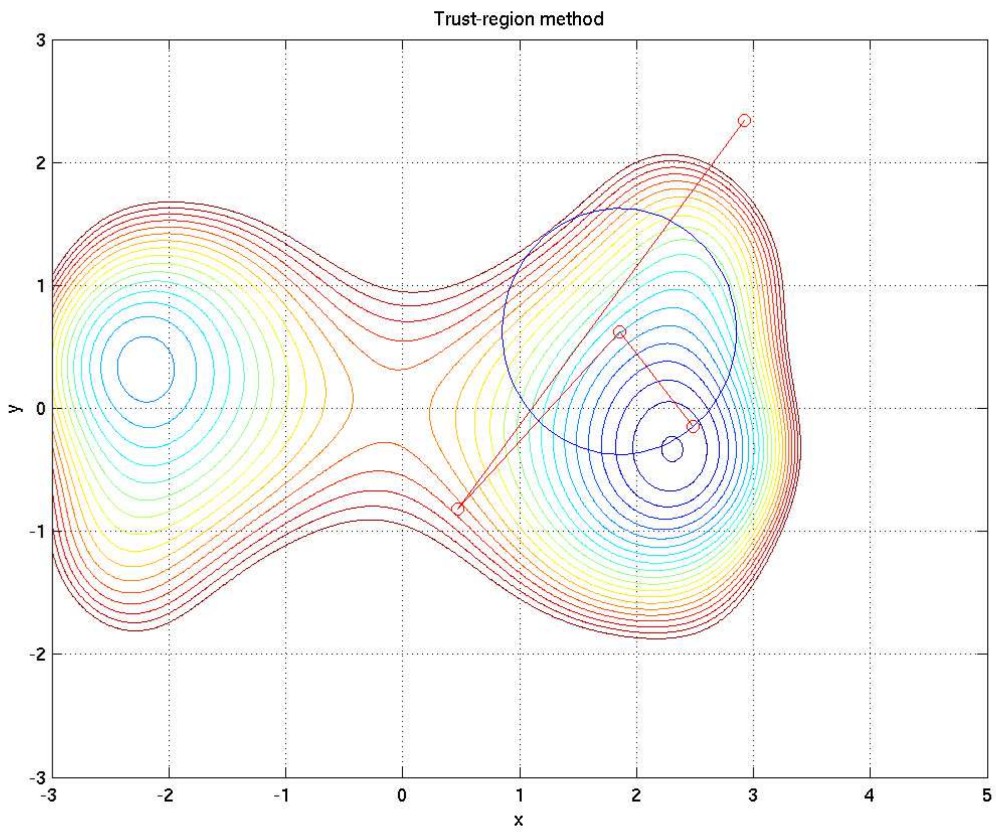

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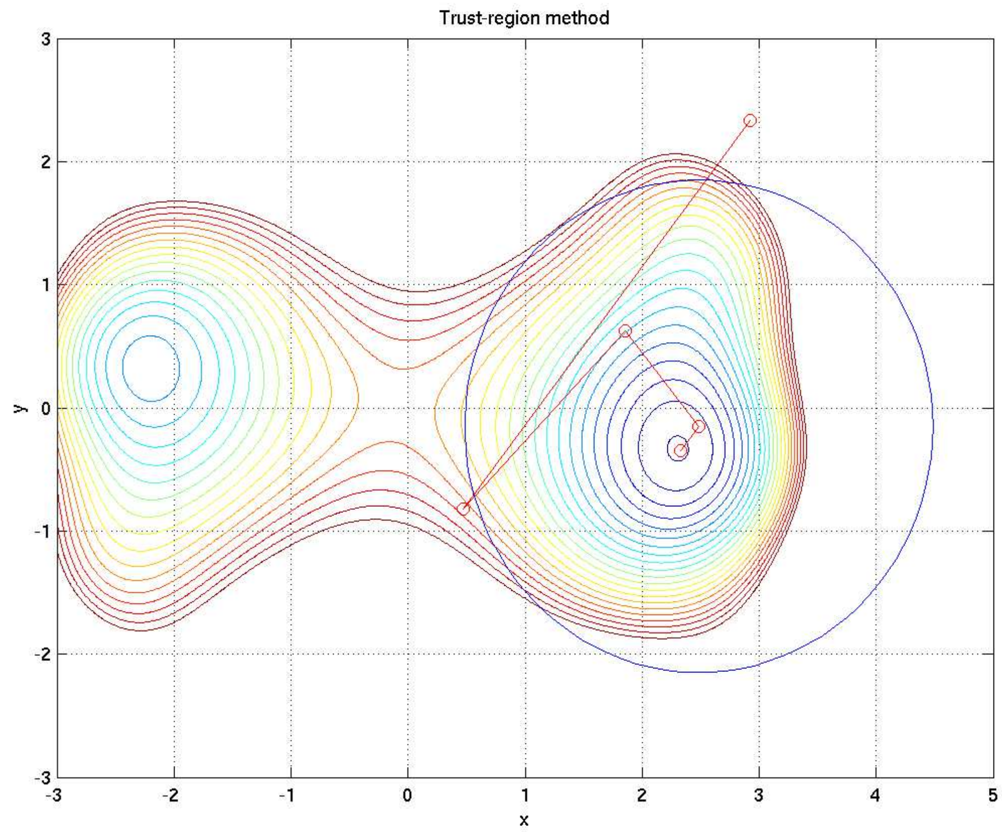

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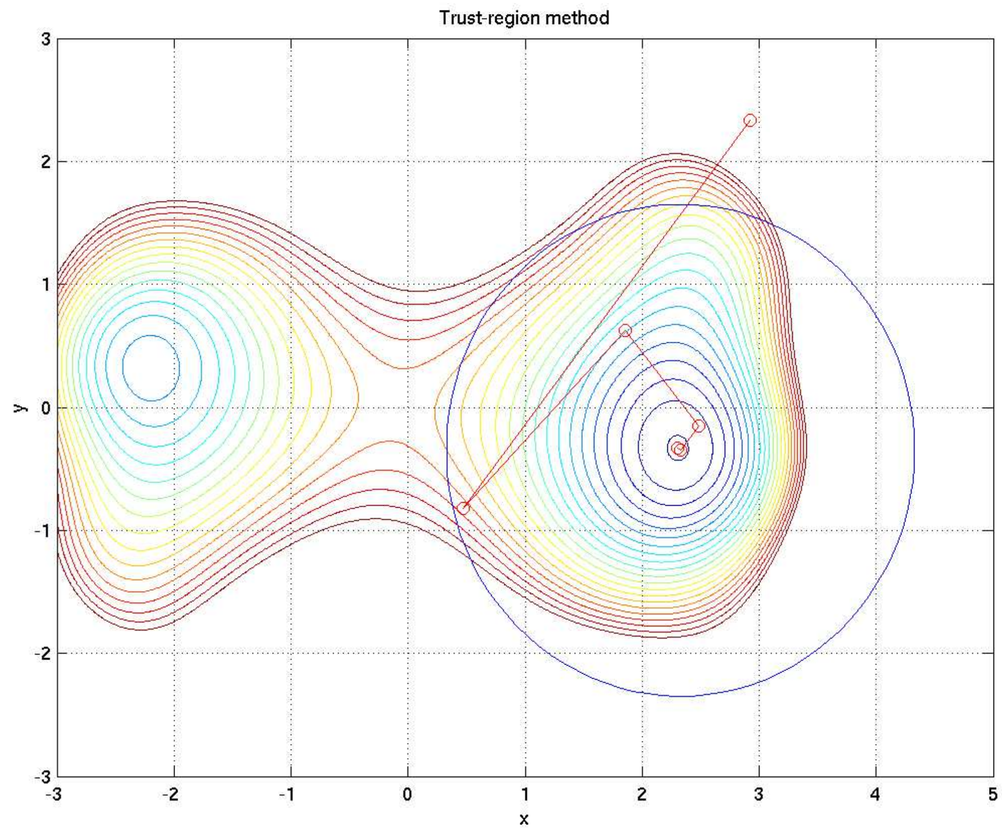

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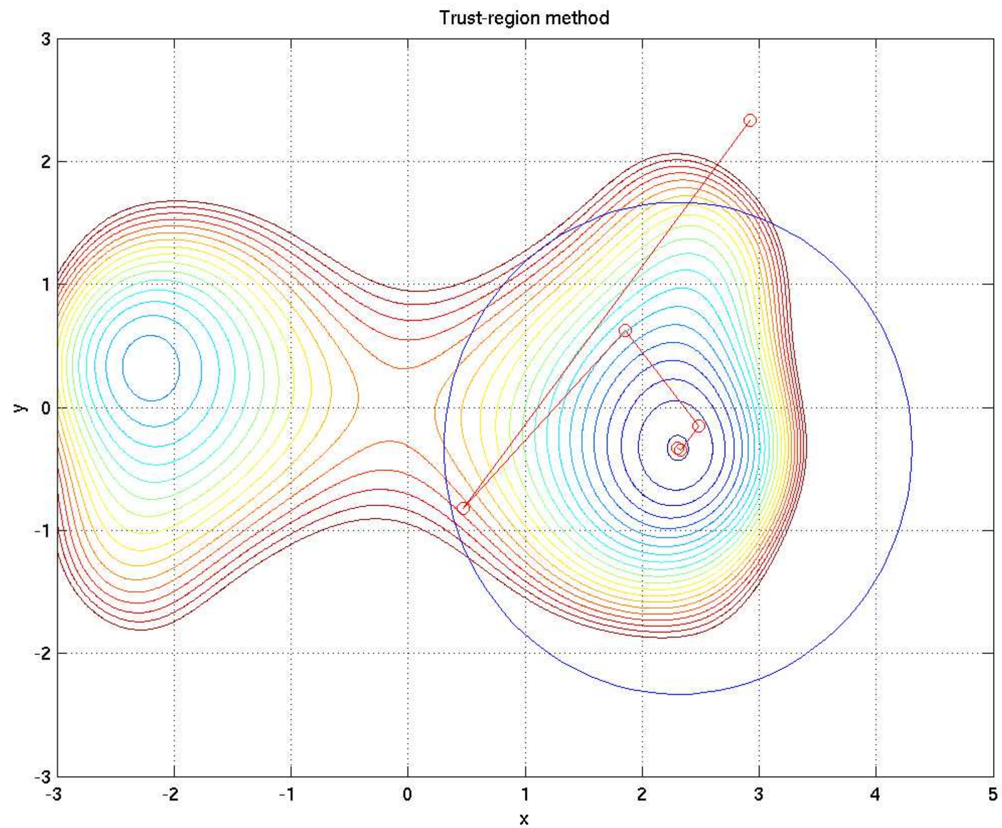

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Advantages of the BTR algorithm

(A probably biased view)

- robust, reliable and efficient
  - ensures globalization
  - allows fast convergence
  - good implementations
- very adaptable:
  - free choice of the model
  - flexible algorithmic variants
- well understood:
  - sound convergence theory
  - finite and infinite dimensional versions

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Conditions on the model

Requirements on model choice:

- smoothness
- (asymptotic) first-order coherence with the objective function (second-order better)
- bounded curvature

Subproblem: find step s and trial point $x+s$ from:

$$\min_{\|s\|\leq\Delta} \text{model}(x+s)$$

Structured model choice

Consider minimizing at topmost (finest) level.
At each iteration, choose the model as

- a local Taylor expansion (classical)
  $\longrightarrow$ Taylor iteration
- the immediately coarser problem description
  $\longrightarrow$ recursive iteration:

compute fine g (and H) | step and trial point

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

minimize the *coarse* model within the *fine* TR

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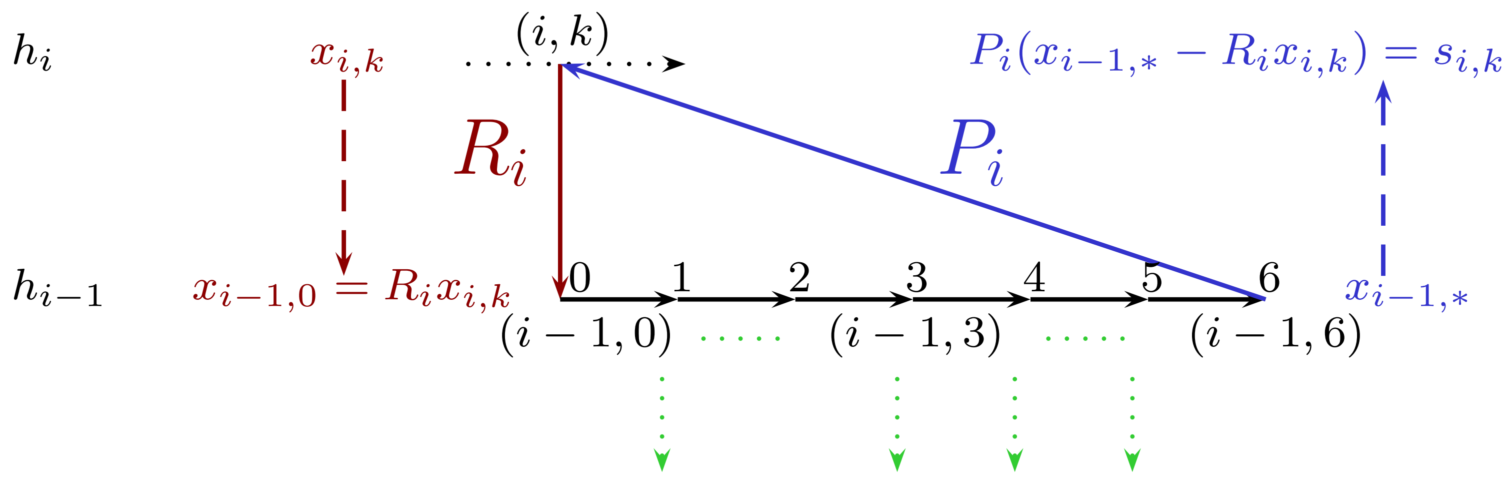
Performing the recursion



Additional ingredients:

- only useful if $\|R_i g_{i,k}\| \geq \kappa \|g_{i,k}\|$
- first-order coherence (see below)
- TR constraint preservation

Lower level TR radius update

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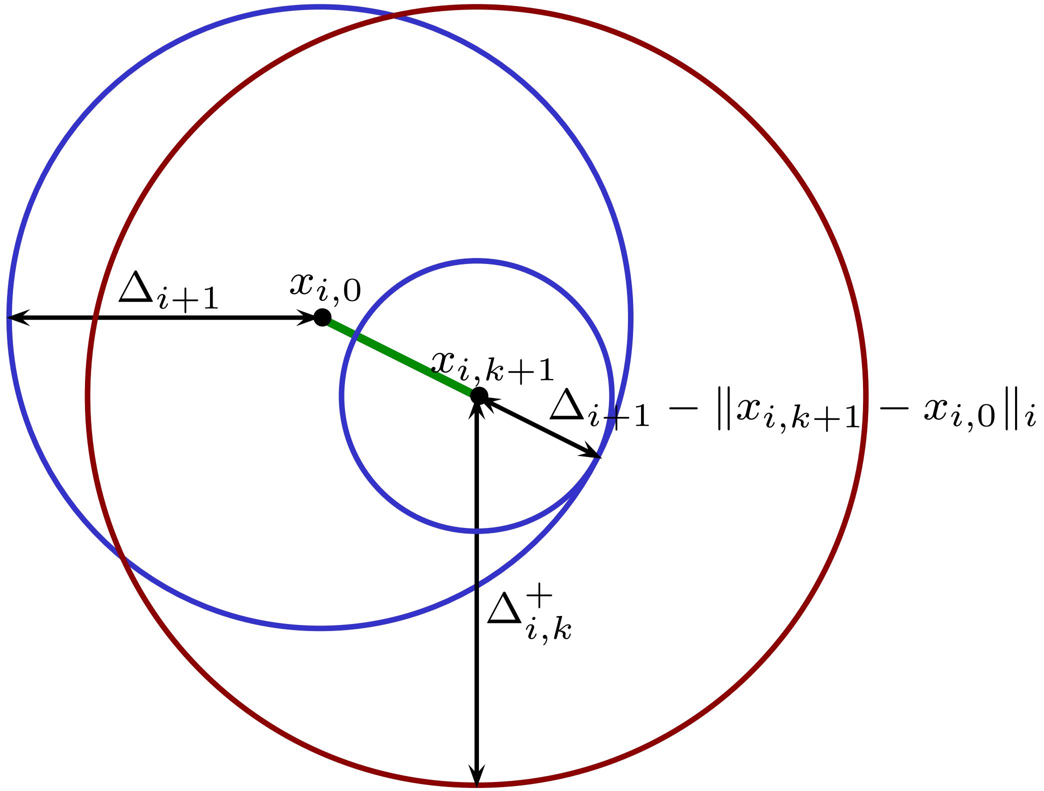

Trust-region radius update:

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

A recursive multi-scale algorithm

Until convergence:

- Choose either a Taylor or recursive model
  - Taylor model: compute a Taylor step
  - Recursive: apply the Algo recursively
- Evaluate change in the objective function
- If achieved reduction $\approx$ predicted reduction,
  - accept trial point as new iterate
  - (possibly) enlarge the trust region

  else
  - reject the trial point
  - shrink the trust region
- Impose: current TR $\subseteq$ upper level TR

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Still unspecified. . .

The main design questions:

- what information to “pass down” at lower recursion levels?
- what Taylor iteration should we use? (must enforce sufficient model decrease condition)
- trust-region radius management
- what structure for recursive iterations?
- computation of the initial point $x_{r,0}$
- dynamic accuracy threshold management

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Linear Model coherence

At level i, model fo level $i+1$:

$$h_i(x) = f_i(x) + \langle v_i, x - x_{i,0} \rangle$$

with $x_{i,0} = R_{i+1} x_{i,k}$ and

$$v_i = R_{i+1} \nabla_x h_{i+1}(x_{i+1,k}) - \nabla_x f_i(x_{i,0})$$

Hence

$$\boxed{\nabla_x h_i(x_{i,0}) = R_{i+1} \nabla_x h_{i+1}(x_{i+1,k})}$$

(required by the first-order convergence theory)

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Quadratic model coherence (1)

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At level i,

$$h_i(x) = f_i(x) + \langle v_i, x - x_{i,0} \rangle + \tfrac{1}{2} \langle x - x_{i,0}, W_i (x - x_{i,0}) \rangle$$

with (additionally)

$$W_i = R_{i+1} \nabla_{xx} h_{i+1}(x_{i+1,k}) R_{i+1}^T - \nabla_{xx} f_i(x_{i,0})$$

Hence

$$\nabla_x h_i(x_{i,0}) = R_{i+1} \nabla_x h_{i+1}(x_{i+1,k})$$
$$\nabla_{xx} h_i(x_{i,0}) = R_{i+1} \nabla_{xx} h_{i+1}(x_{i+1,k}) R_{i+1}^T$$

Quadratic model coherence (2)

Notes on the quadratic case:

- also covered by the theory:

$$h_i(x) = \left[f_i(x) + \tfrac{1}{2}\langle x - x_{i,0}, W_i(x - x_{i,0})\rangle\right] + \langle v_i, x - x_{i,0}\rangle$$

- quadratic model coherence implies second-order convergence properties ? (currently under study)
- ...but additional cost of computing and using the correction matrix W_i!
- can use $f_i(x) = 0$!

(Simple) Taylor iterations

Which solver for the (approximate) solution of the (same level) trust-region subproblem?

Simple answer:

- for low(est) level(s) (small dimension): the exact Moré-Sorensen method
- for higher levels (high dimension): a truncated conjugate gradient (Steihaug-Toint or GLTR)

But. . .

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Multigrid technology...

Multigrid techniques for PDE problems indicates:

- the high-frequency components of residual only visible in fine mesh (high levels)
- need two different methods:
  - reduce high frequency components on the fine mesh

    Smoothing

  - reduce low frequency components on the coarse mesh

    Damping

…adapted to optimization

In unconstrained optimization,

residual $\longrightarrow$ gradient

- gradient smoothing:
  - TCG not very efficient!
  - adapt Gauss-Seidel smoothing
    $\longrightarrow$ cyclic coordinate search
    (on Taylor's model)
- low frequency damping:
  full solution (MS) in low dimension

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Cyclic coordinate search (CCS)

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From $s_0 = 0$ and for $i = 1, \ldots, n$, solve:

$$s_i \Leftarrow \min_{\alpha} m(s_{i-1} - \alpha e_i)$$

Cost: 1 cycle $\approx$ 1 matrix-vector product

Two difficulties:

- need to require sufficient decrease?
- how to impose the trust-region constraint?

The dogleg CCS (1)

- compute s_0 by coordinate search along the largest gradient component
- while inside the TR and at most p times, update the step with 1 full CCS cycle
- if s lies outside the TR:
  - if s is gradient-related ($\langle g, s \rangle \leq -\kappa \|s\| \, \|g\|$) then backtrack,
  - else compute dogleg step along the piecewise curve $[0, s_0, s]$

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The dogleg CCS (2)

- efficient gradient smoothing:
  as Gauss-Seidel in multigrid for PDE systems
- ensures sufficient decrease
  (the modified Cauchy condition of CGT 2000)
- reasonable arithmetic cost:
  $\approx p$ matrix-vector products
  (or less if less than p cycles leads outside the TR)

In practice: dogleg extremely rare

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Structure of the recursive iterations

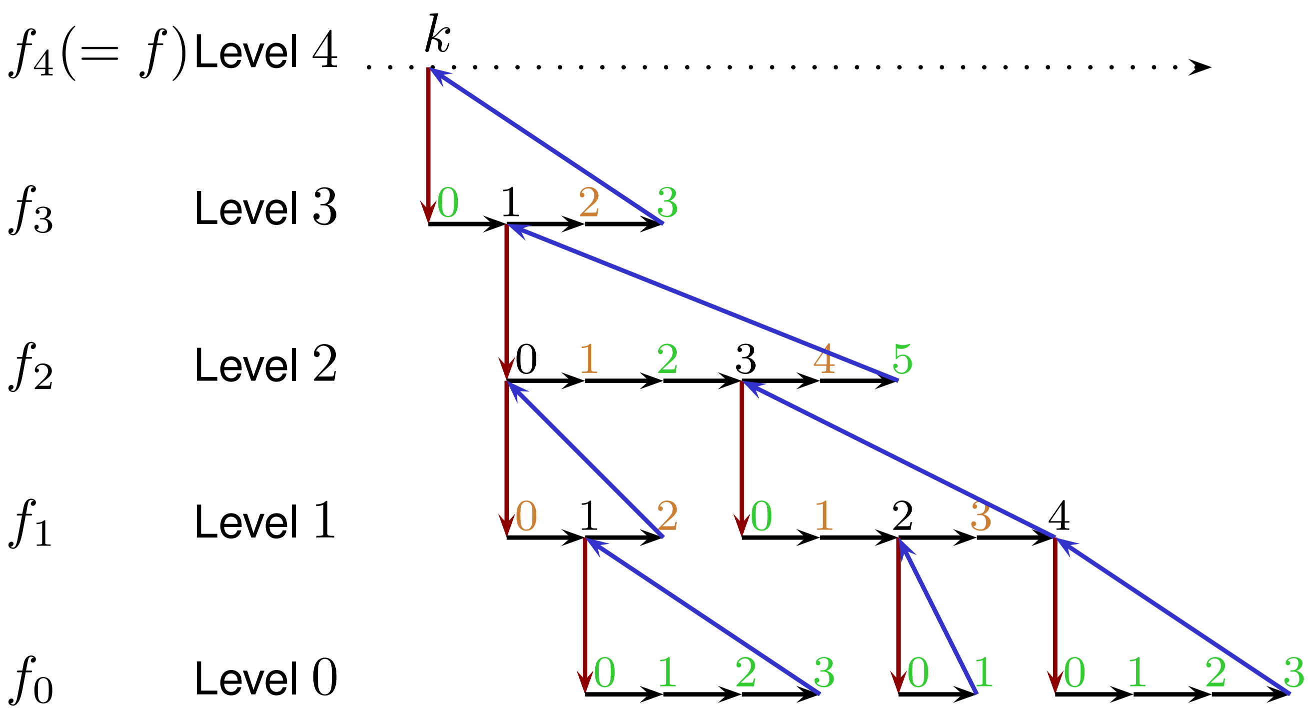
Decision to stop solving the lower-level subproblem based on

- subproblem criticality → free form (gradient accuracy + TR constraint activity)
- fixed form cycles (possibly truncated)
  - V cycles
  - W cycles
  - Wq cycles ($q > 2$)

At least one successful iteration per level

Free form iterations (1)

The “iteration view” for an example of free form recursion (5 levels, all iterations successful):



Prolongation Restriction Damping Smoothing

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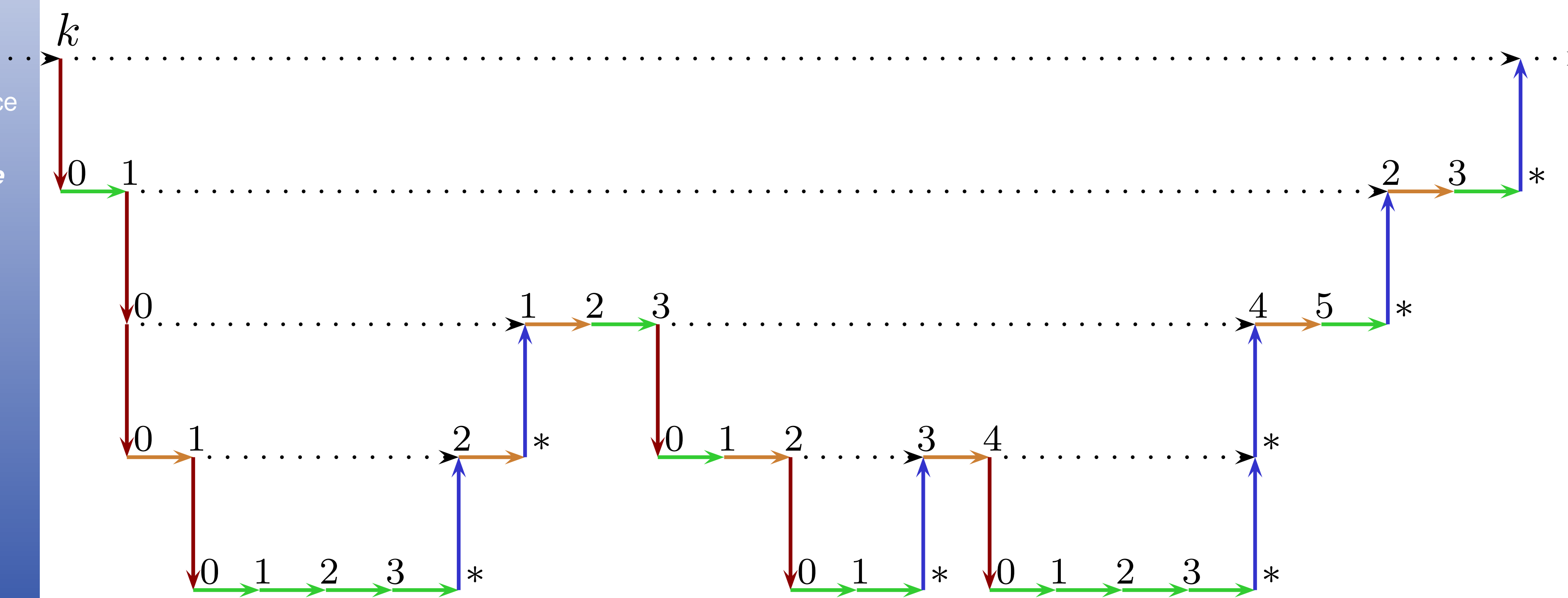
Free form iterations (2)

The “iterates view” for the same example:



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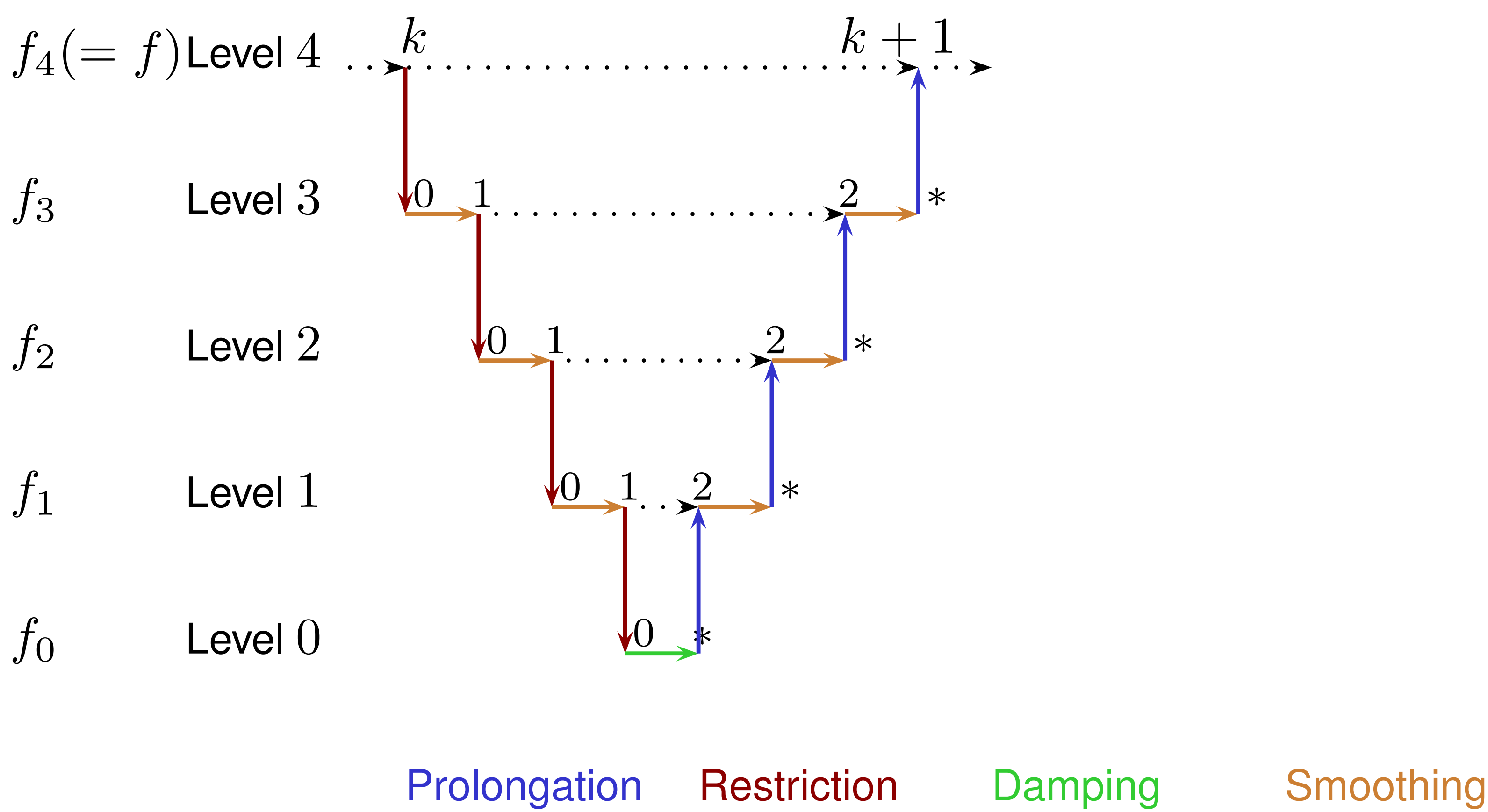
V cycles

The "iterates view" for a V cycle recursion (5 levels, all iterations successful):



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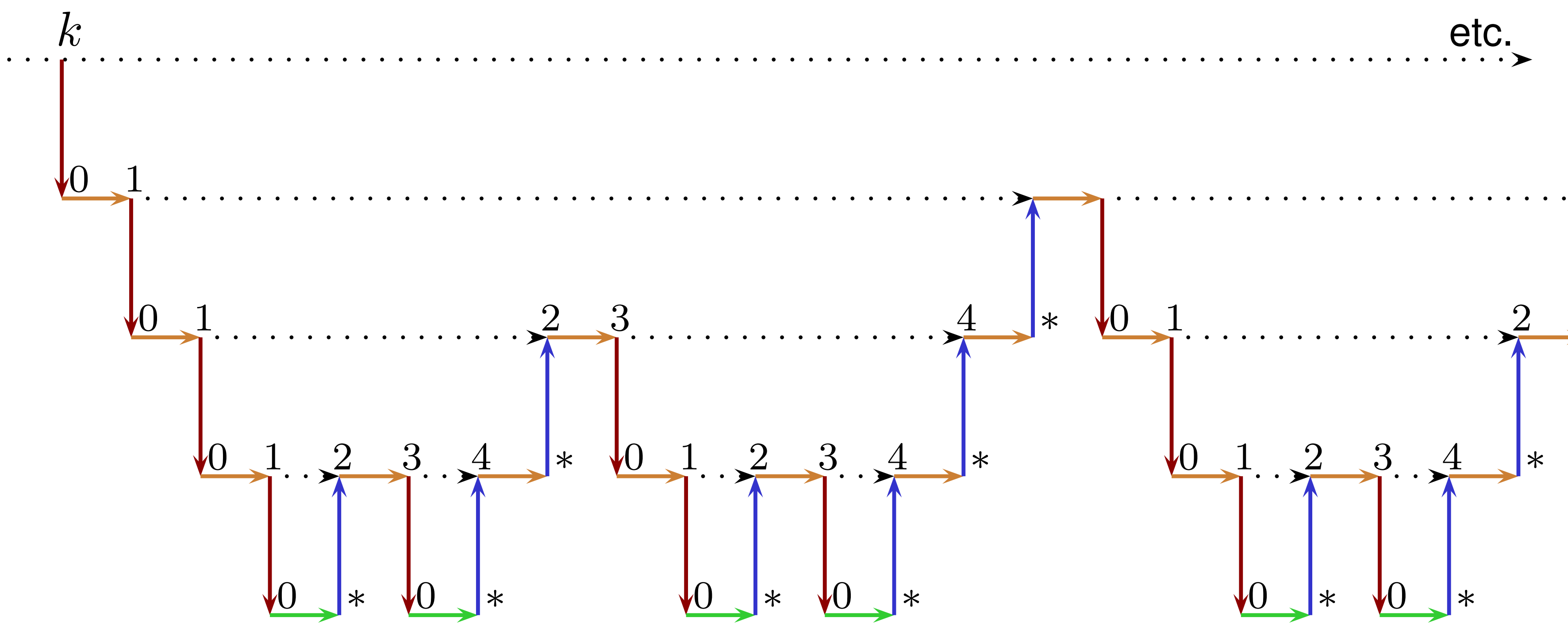
W cycles

2 3

An example of W cycle recursion
(5 levels, all iterations successful):



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Trust-region radius management

Scaling could differ between $h_i(x)$ and $h_{i-1}(x)$...
Use the same TR radius ???

Use a different radius for Taylor iterations and recursive iterations

- exploits theoretical freedom (bounded rescaling admitted)
- (maybe) not meaningful when $f_i(x) = 0$

In practice: radii ratio ≤ 5

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Computing the initial point

Need $x_{r,0}$ (starting point at topmost level):
$\rightarrow$ use a mesh refinement technique.

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

- apply the recursive algorithm to solve

$$\min_x f_i(x)$$

(with increasing accuracy)

- apply the prolongation to obtain the initial point at next level

- reminiscent of the full multigrid scheme
- approach of the solution at coarse levels

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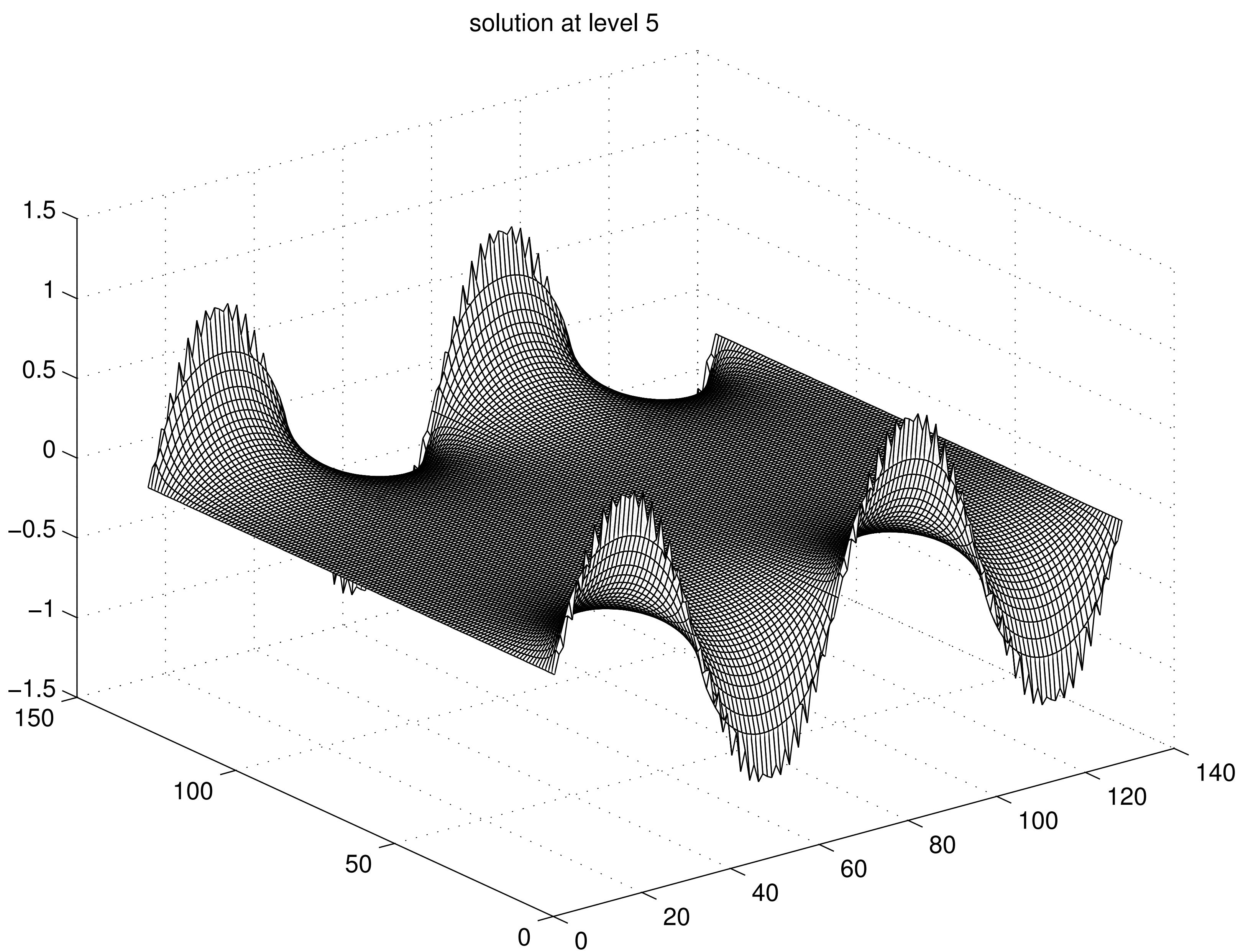
A minimum surface problem



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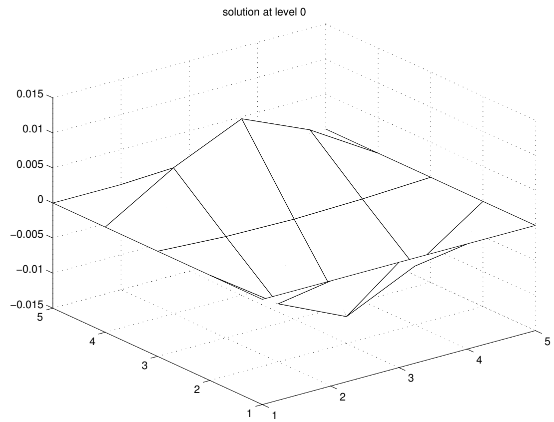
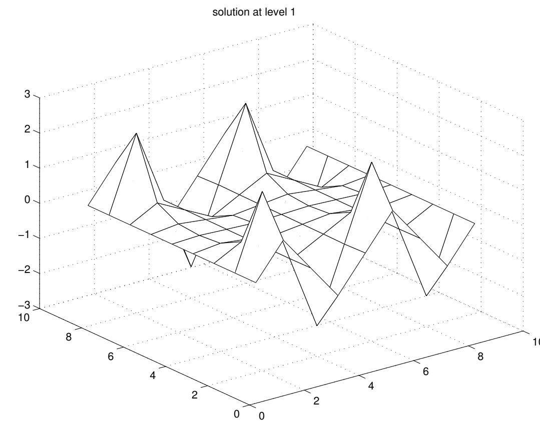
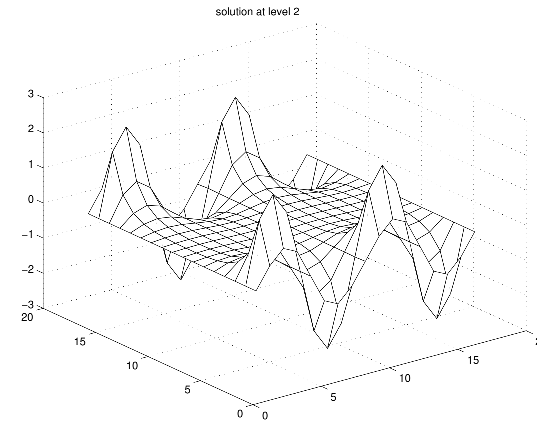
The level structure



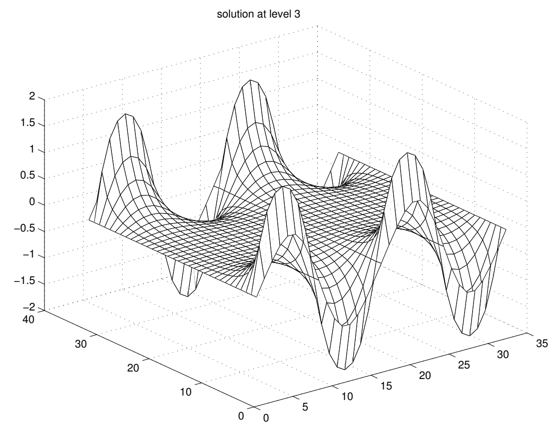
$n = 3^2 = 9$



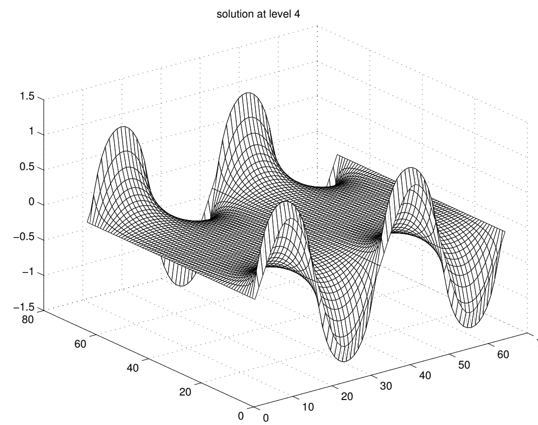
$n = 7^2 = 49$



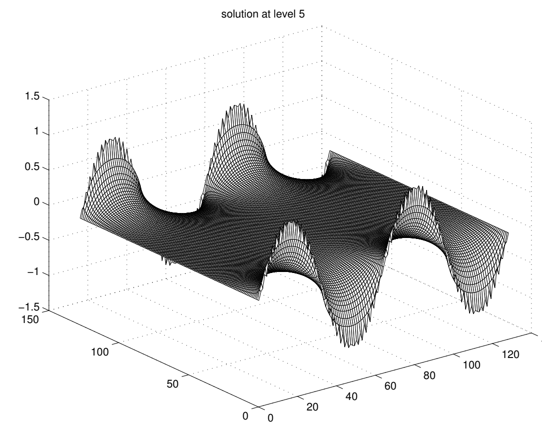
$n = 15^2 = 225$



$n = 31^2 = 961$



$n = 63^2 = 3969$



$n = 127^2 = 16129$

Further problem details

- structured level transfer operators
  - $P =$ full weighting interpolation operator
  - $R =$ normalized P^T
- handling the boundary condition
  - boundary condition not forced
  - additional smoothing "just inside"
- random starting point (at coarsest level)

Contact me for a live demo . . .

Other test problems (1)

- 2D Laplacian (check) problem (5 points FD pencil, unit square)

$$\min -\tfrac{1}{2}x^T \Delta x - f^T x$$

$$f = \sin[x_1 * (1 - x_1)] * \sin[x_2 * (1 - x_2)]$$

- 2D nonconvex quartic nonlinear least-squares (5 points FD pencil, unit square)

$$\min \int (u - f)^2 + 10^{-2} \int (\gamma - f)^2 + \int (-\Delta u + u\gamma - g)^2$$

$$g = -\Delta f + f^2$$

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Other test problems (2)

- Lewis and Nash Dirichlet to Neumann transfer problem:

$$\min_{a\,:\,[0,\pi]\to\mathbb{R}} \int_0^\pi \left(\frac{\partial u}{\partial x_2}(x_1, 0) - \phi(x_1) \right)^2 dx_1$$

with
$$S = \{(x_1, x_2), 0 \le x_1 \le \pi, 0 \le x_2 \le \pi\}$$
$$\Gamma = \{(x_1, x_2), 0 \le x_1 \le \pi, x_2 = 0\}.$$
$$\phi(x) = \sum_{i=1}^{15} \sin(i\,x) + \sin(40\,x)$$

subject to the boundary value problem

$$\begin{cases} \Delta u = 0 \\ u(x,y) = a(x_1) \text{ on } \Gamma, \quad u(x,y) = 0 \text{ on } \partial S \backslash \Gamma \end{cases}$$

A typical run

V style, pure quadratic recursion,
2 smoothing cycles, gradient accuracy: 1e-07

level	3	7	15	31	63	127	255
Tayl. its	26	0	0	0	0	0	0
smooth cyc	0	214	285	286	223	141	83
prolong	0	20	36	36	31	23	11
restric	0	41	72	73	63	48	25
evals f	12	8	12	13	19	36	66
evals g	6	8	12	13	19	29	37
evals H	6	3	4	4	6	8	17

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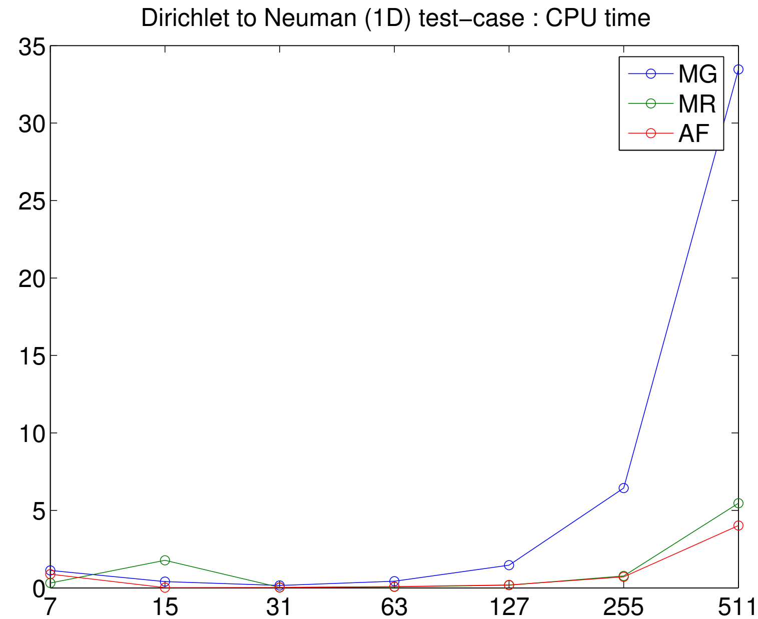
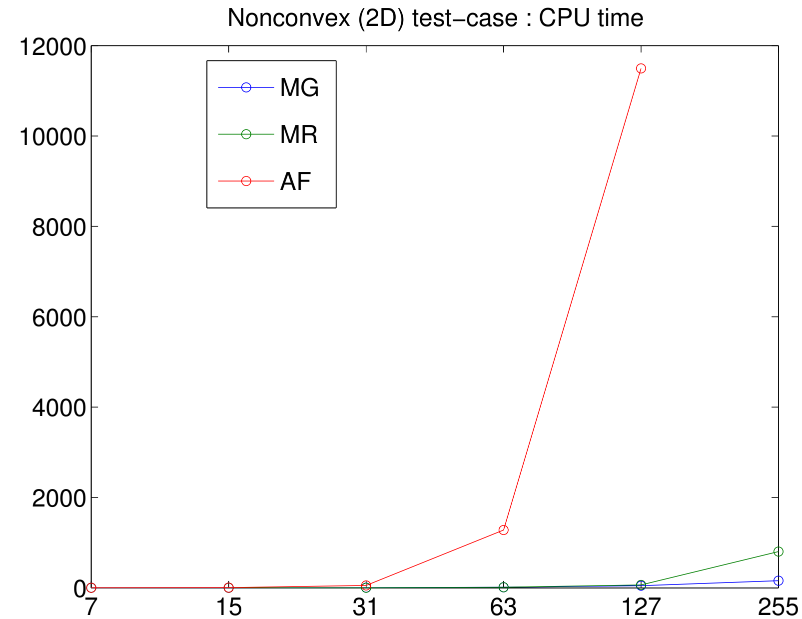
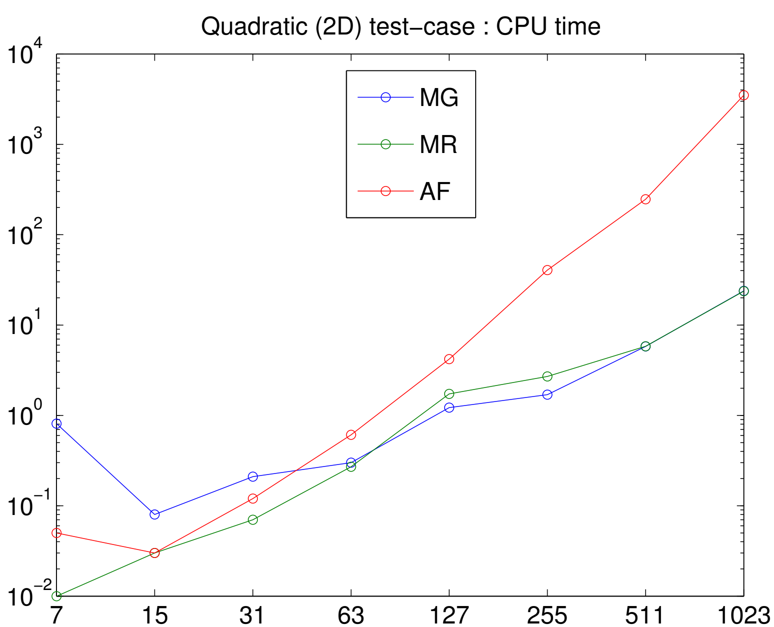
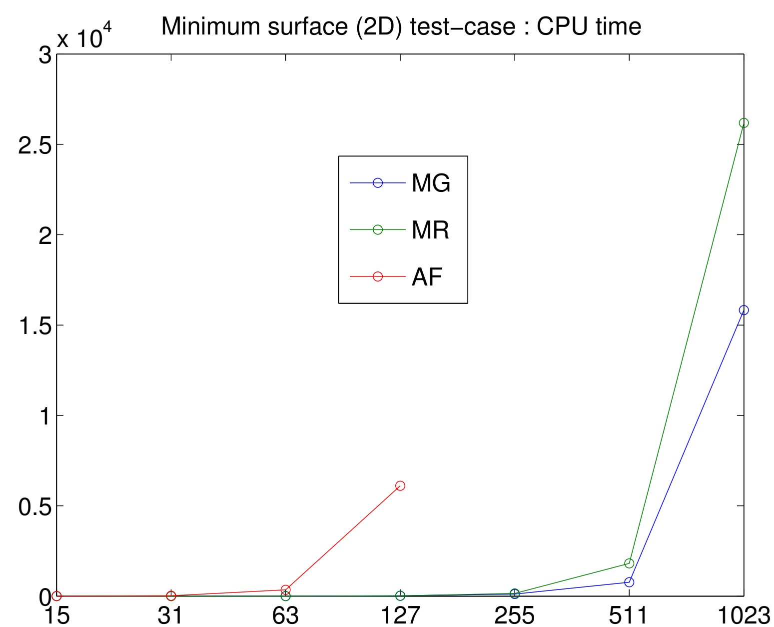
Problem size and CPU









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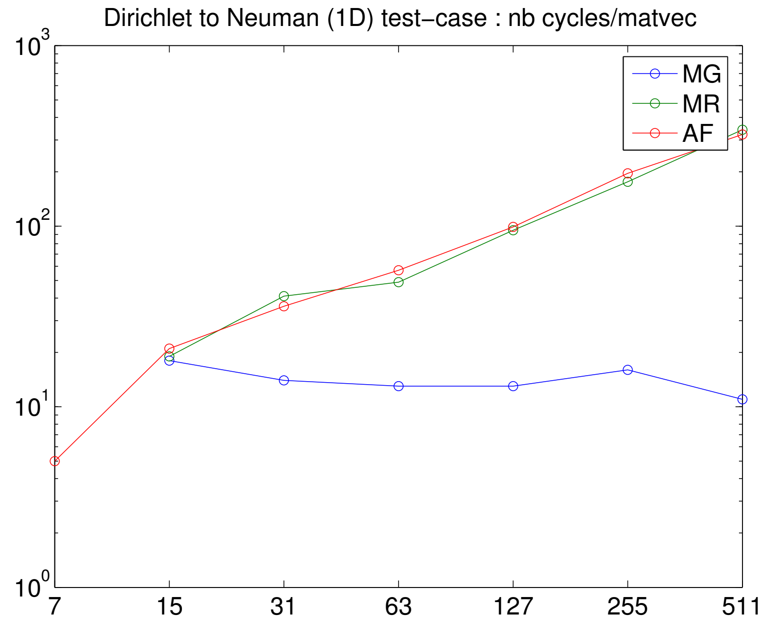
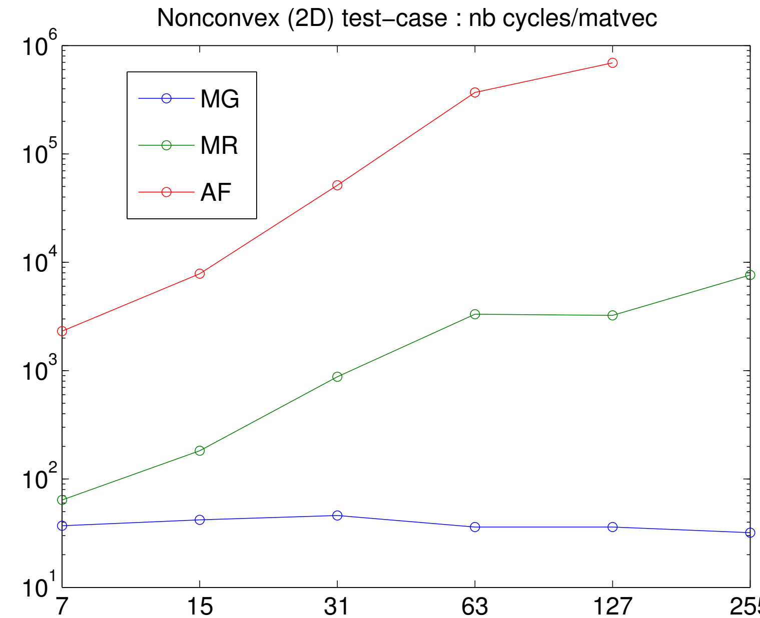
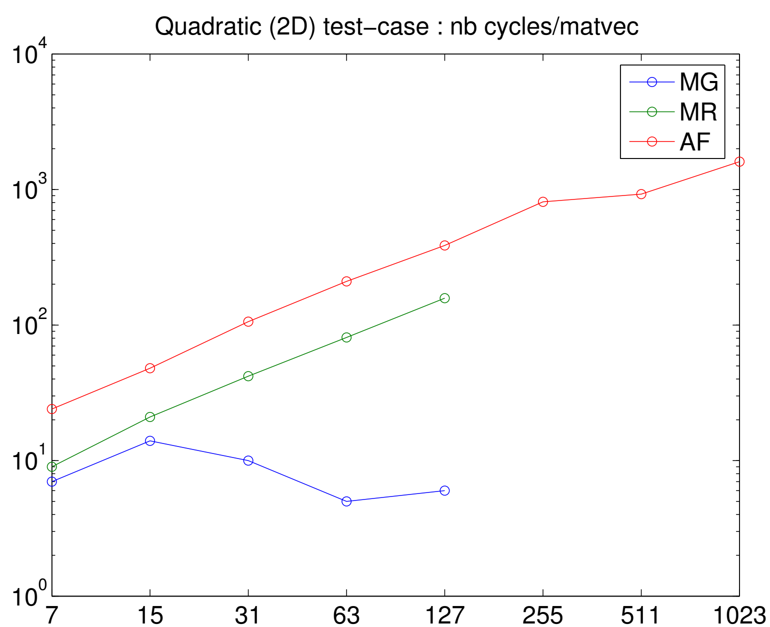
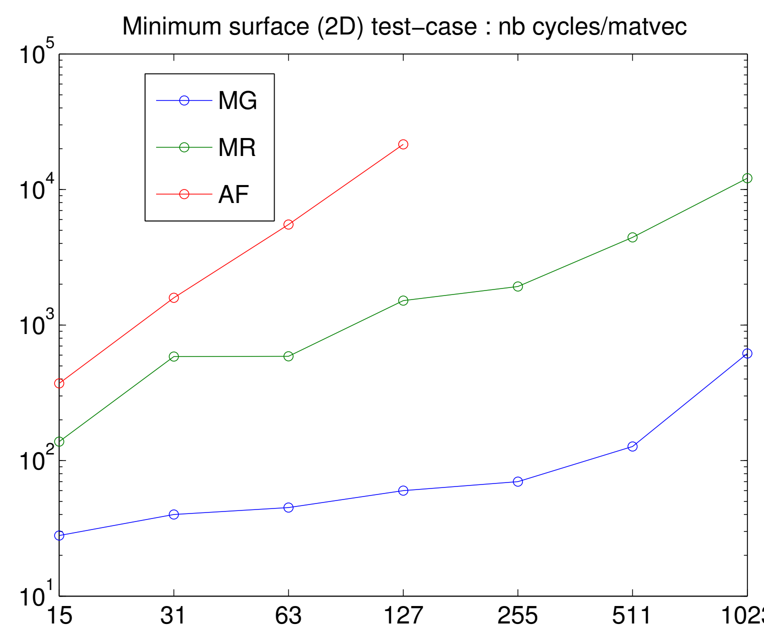
Problem size and linear algebra









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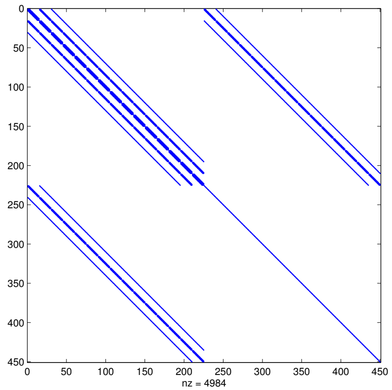
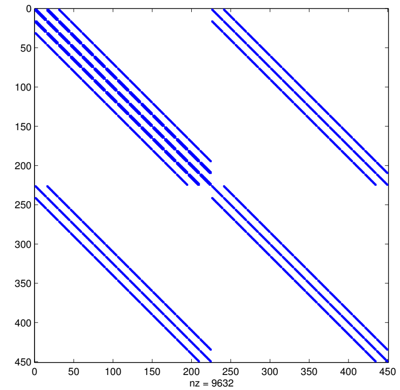
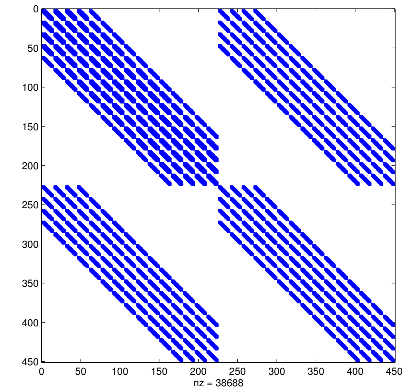
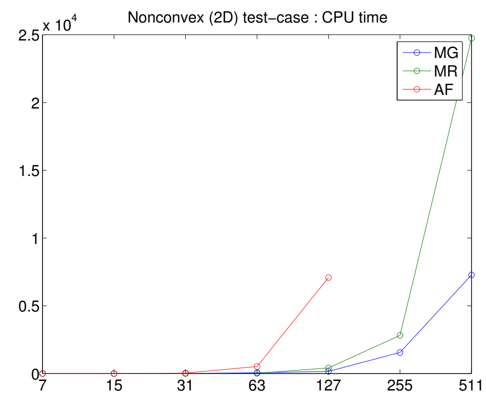
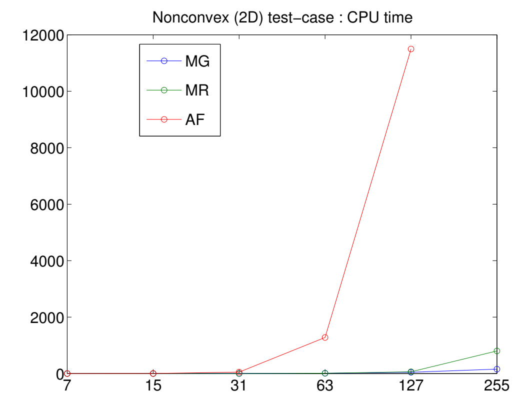
Interpolation and fill-in

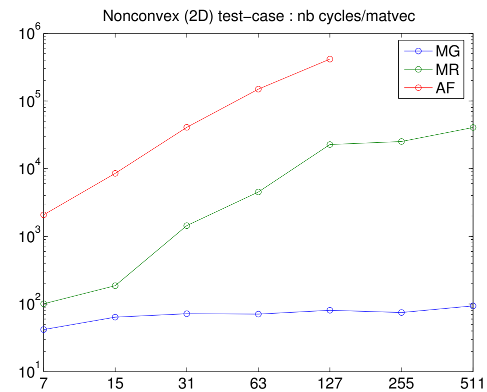


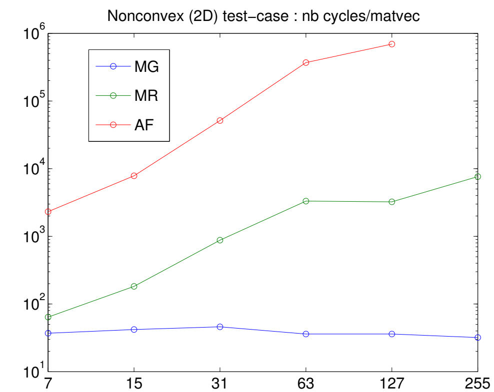












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Current conclusions

- more efficient than mesh refinement for large instances
- pure quadratic recursion ($f_i = 0$, Galerkin) very efficient
- interpolation degree crucial
- V cycles most efficient

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Perspectives

Encouraging (so far)

- more numerical experiments!
- second-order convergence theory
- multigrid-type developments:
  (semi-coarsening, algebraic multilevel, . . .)
- constrained problems
  (bounds, equalities, general)
- non-monotone (filter) techniques
- . . . and much more!

Thank you for your attention

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