

JOPT 2010

Ecole Polytechnique de Montréal

Parallel Versions of the MADS Algorithm for Black-Box Optimization

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2010-05-10

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Black-box optimization problems

We consider the nonsmooth optimization problem:

$$\begin{aligned} & \text{Minimize} && f(x) \\ & \text{subject to} && x \in \Omega, \end{aligned}$$

where evaluation of the functions are usually the result of a computer code (a black-box).

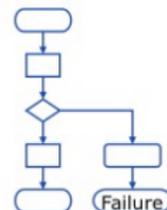
Black-boxes as illustrated by J. Simonis [ISMP 2009]



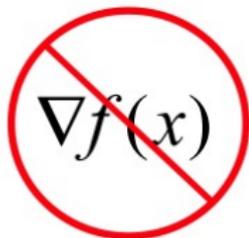
Long runtime



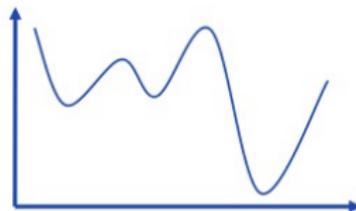
Large memory
requirement



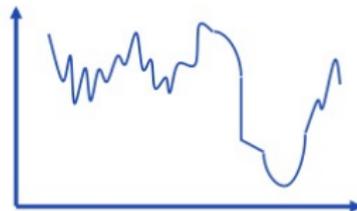
Software
might fail



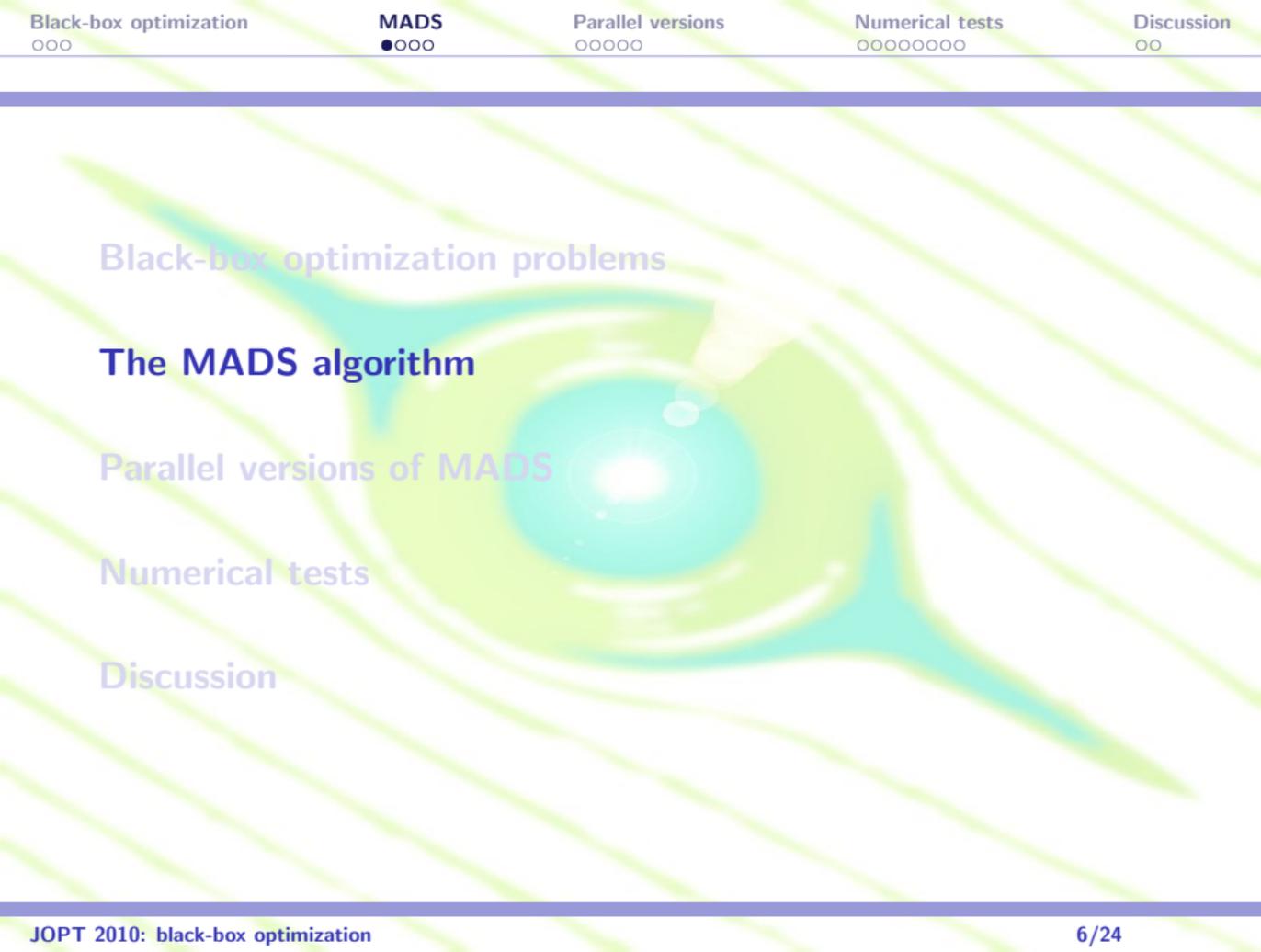
No derivatives
available



Local
optima



Non-smooth,
noisy



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Mesh Adaptive Direct Search (MADS)

- ▶ Iterative algorithm that evaluates the black-box functions at some **trial points** generated on the **mesh**

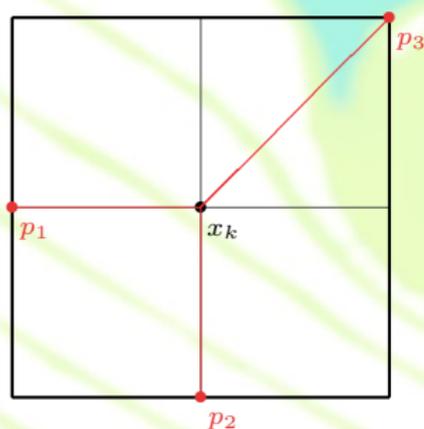
$$M(\Delta_k) = \{x_k + \Delta_k D z : z \in \mathbb{N}^{n_D}\} \subset \mathbb{R}^n$$

where x_k is the current iterate, $\Delta_k \in \mathbb{R}^+$ is the mesh size parameter, and D a fixed set of n_D directions in \mathbb{R}^n .

- ▶ **Search step:** trial points can be generated anywhere on the mesh. It is typically user-provided but can also be generic.
- ▶ **Poll step:** **directions** are used to generate poll trial points. The normalized directions become dense in the unit sphere.
- ▶ **Updates step:** the mesh size is reduced if no new iterate is found.
- ▶ Algorithm backed by a **convergence analysis** based on the Clarke Calculus for nonsmooth functions.

Poll illustration (successive fails and mesh shrink)

$$\Delta_k = 1$$

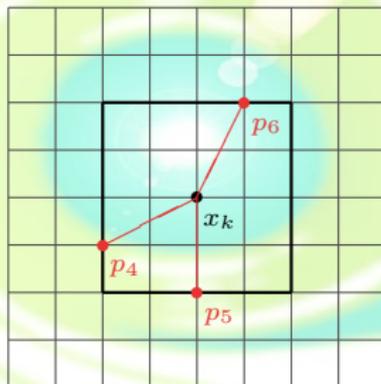
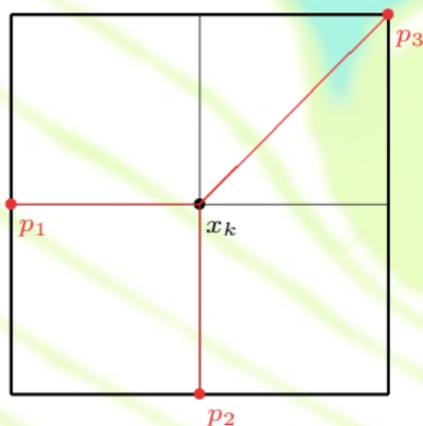


trial points = $\{p_1, p_2, p_3\}$

Poll illustration (successive fails and mesh shrink)

$$\Delta_k = 1$$

$$\Delta_{k+1} = 1/4$$

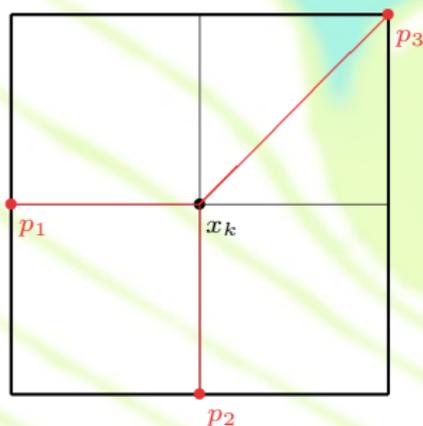


trial points = $\{p_1, p_2, p_3\}$

= $\{p_4, p_5, p_6\}$

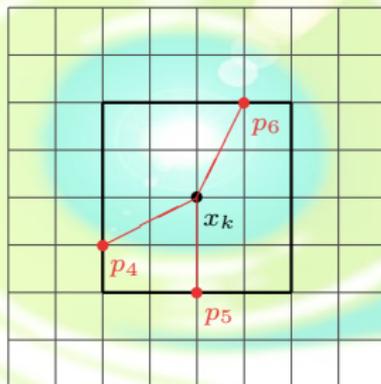
Poll illustration (successive fails and mesh shrink)

$$\Delta_k = 1$$



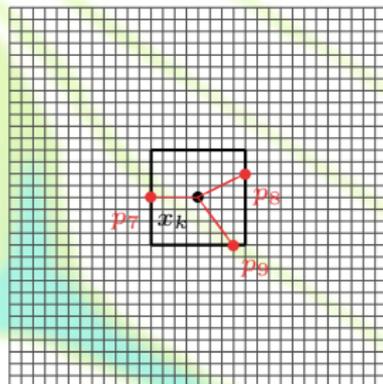
trial points = $\{p_1, p_2, p_3\}$

$$\Delta_{k+1} = 1/4$$



= $\{p_4, p_5, p_6\}$

$$\Delta_{k+2} = 1/16$$



= $\{p_7, p_8, p_9\}$

Two ways of generating dense sets of poll directions

- ▶ LTMADS:
 - ▶ Random directions.
 - ▶ **Random seed.**
- ▶ OrthoMADS:
 - ▶ Deterministic directions.
 - ▶ Orthogonal directions with a better space coverage.
 - ▶ Default polling method in the NOMAD software.
 - ▶ \simeq coordinate directions for initial values of Δ_k^m .
 - ▶ **Halton seed.**



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pMADS

- ▶ Idea: simply evaluate the trial points in parallel.
- ▶ Synchronous version **pMADS-S**:
 - ▶ The iteration is over only when all the evaluations in progress are terminated.
 - ▶ Processes can be idle between two evaluations.
 - ▶ The algorithm is identical to the scalar version.
- ▶ Asynchronous version **pMADS-A**:
 - ▶ If a new best point is found, the iteration is terminated even if there are evaluations in progress. New trial points are then generated.
 - ▶ Processes never wait between two evaluations.
 - ▶ 'Old' evaluations are considered when they are finished.
 - ▶ The algorithm is slightly reorganized.

PSD-MADS

- ▶ **PSD**: Parallel Space Decomposition.
- ▶ Idea: each process executes a MADS algorithm on a subproblem and has responsibility of small groups of variables.
- ▶ Based on the block-Jacobi method [Bertsekas, Tsitsiklis 1989] and on the Parallel Variable Distribution [Ferris, Mangasarian 1994].
- ▶ Objective: solve larger problems ($\simeq 50 - 500$ instead of $\simeq 10 - 20$).
- ▶ (Almost) asynchronous method.
- ▶ Convergence analysis.
- ▶ Audet, Dennis, Le Digabel [SIOPT 2008].

PSD-MADS: processes

► Master

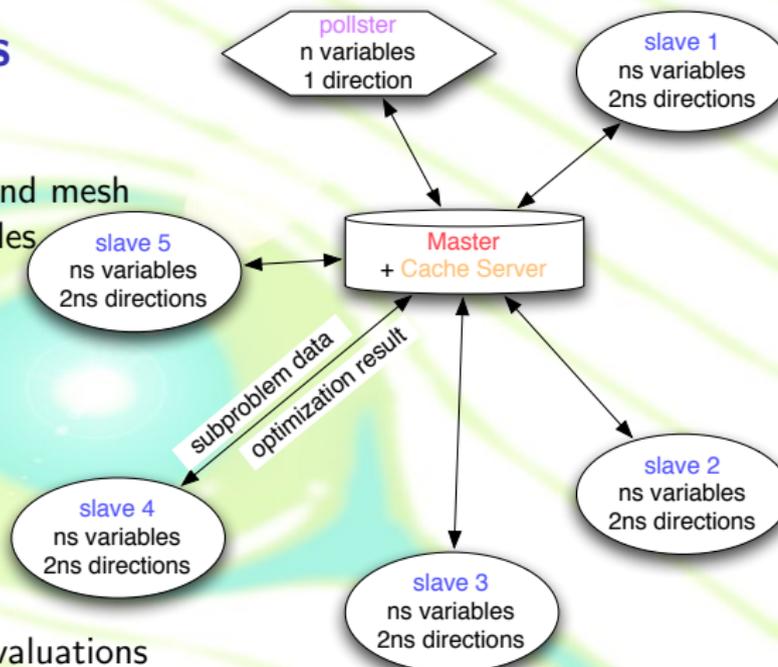
- receives all slave's signals
- updates current solution and mesh
- decides subproblem variables
- sends subproblem data

► Slaves

- receive subproblem data
- optimize subproblem
- send optimization data

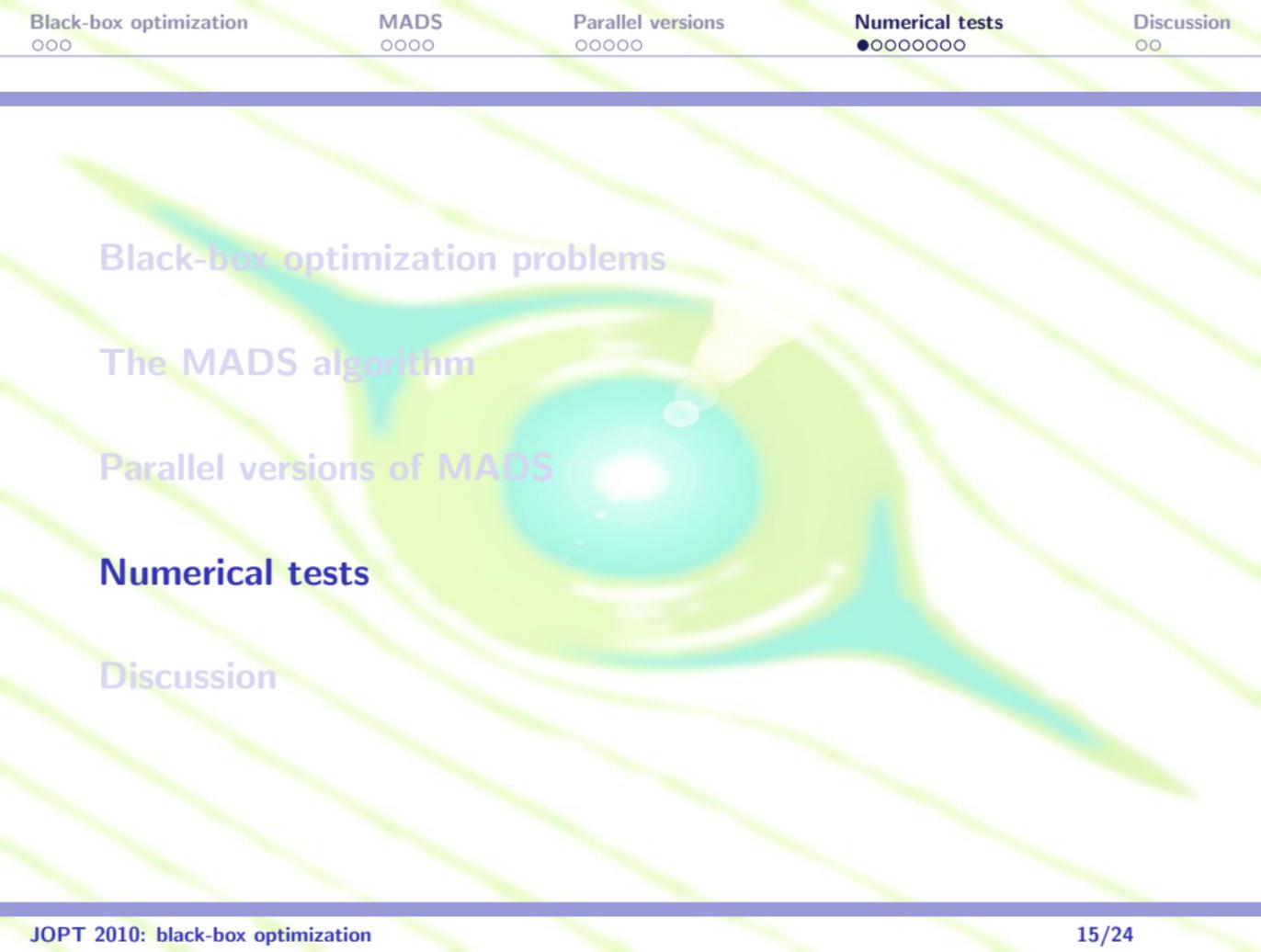
► Cache server

- memorizes all black-box evaluations
- allows the “cache search” in the pollster



COOP-MADS

- ▶ Uses a simplified version of the PSD-MADS parallel framework.
- ▶ Processes run in parallel on the original problem with different seeds in order to produce different behaviours.
- ▶ The cache server allows to share evaluations and the cache search is performed by all processes.
- ▶ (Almost) asynchronous method.



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- ▶ NOMAD: **N**onsmooth **O**ptimization with **MADS**:
 - ▶ MADS, pMADS-A/S, COOP-MADS and PSD-MADS (release 3.4 in May).
 - ▶ Parallelism with MPI.
 - ▶ <http://www.gerad.ca/nomad> (LGPL).

- ▶ Computer: 6 cores with Hyper-Threading \simeq 12 processors.

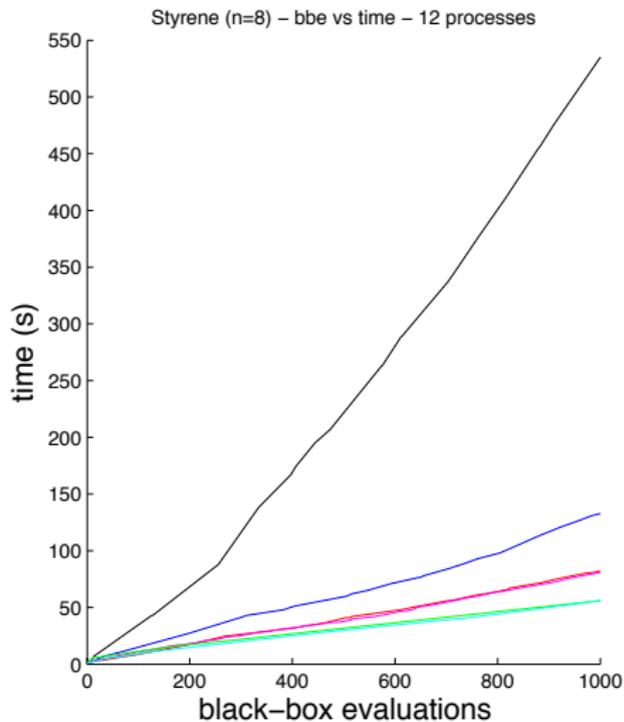
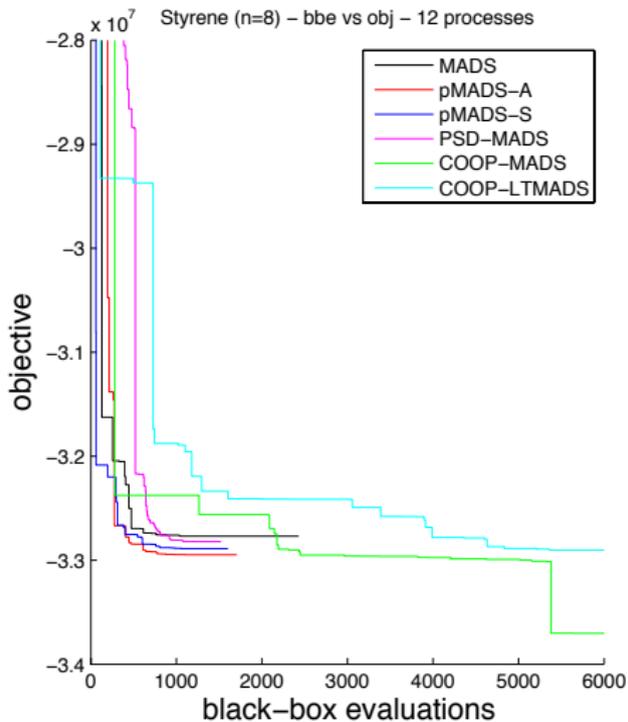
Algorithms parameters

- ▶ MADS and pMADS-A/S: default parameters, $np=13$ (1 master+12 slaves).
- ▶ PSD-MADS with the SIOPT paper settings:
 - ▶ $np=14$: 1 master + 1 cache server + 1 pollster slave + 11 regular slaves.
 - ▶ Max. number of evaluations for each regular slave: 10.
 - ▶ Number of free variables for each regular slave: 2.
 - ▶ Groups of variables: randomly chosen.
- ▶ COOP-MADS, $np=13$ (1 cache server+12 workers).
 - ▶ COOP-MADS: each process uses OrthoMADS polling directions with different Halton seeds.
 - ▶ COOP-LTMADS: LTMADS with different random seeds.
- ▶ Stopping criteria: maximum number of black-box evaluations or a minimal mesh size.

Styrene production simulation [JOGO 2008]

- ▶ Maximize the net present value while satisfying industrial and environmental regulations.
- ▶ Written by a chemical engineer.
- ▶ Uses some common methods such as Runge-Kutta, Newton, fixed points, secant, bisection, and many other chemical engineering related solvers.
- ▶ 8 bound constrained variables,
4 boolean unrelaxable constraints,
7 relaxable constraints.
- ▶ 14% of trial points violate a hidden constraint.
- ▶ Evaluations can take different evaluation times (up to $\simeq 3$ seconds).

Styrene, n=8, 6,000 evaluations



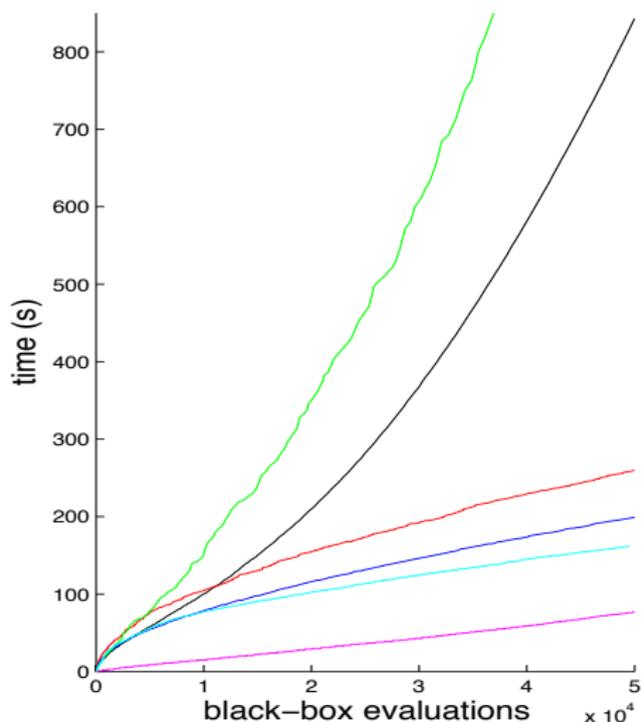
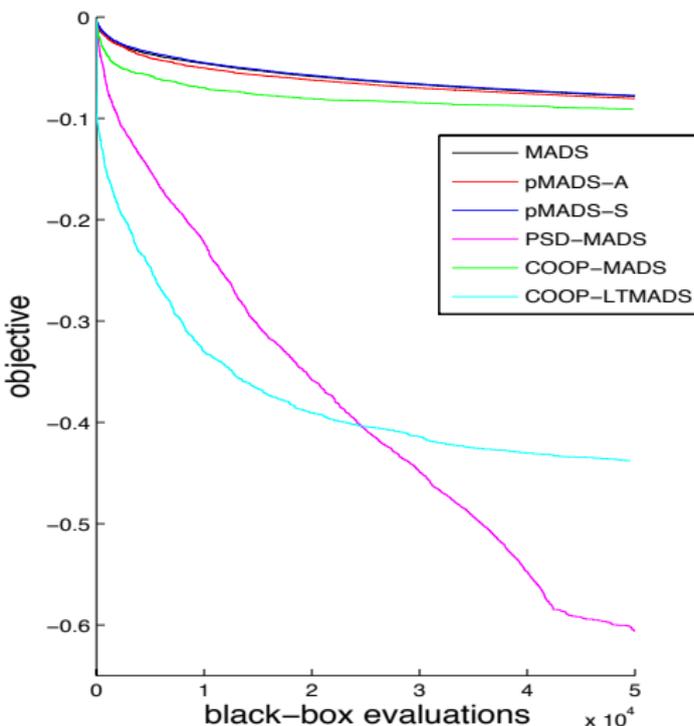
Test Problem G2 [Hedar & Fukushima, JOGO 2006]

$$\min_{x \in \mathbb{R}^n} f(x) = \left| \frac{\sum_{i=1}^n \cos^4 x_i - 2 \prod_{i=1}^n \cos^2 x_i}{\sqrt{\sum_{i=1}^n i x_i^2}} \right|$$

$$s.t. \begin{cases} g_1(x) = - \prod_{i=1}^n x_i + 0.75 \leq 0 \\ g_2(x) = \sum_{i=1}^n x_i - 7.5n \leq 0 \end{cases}$$

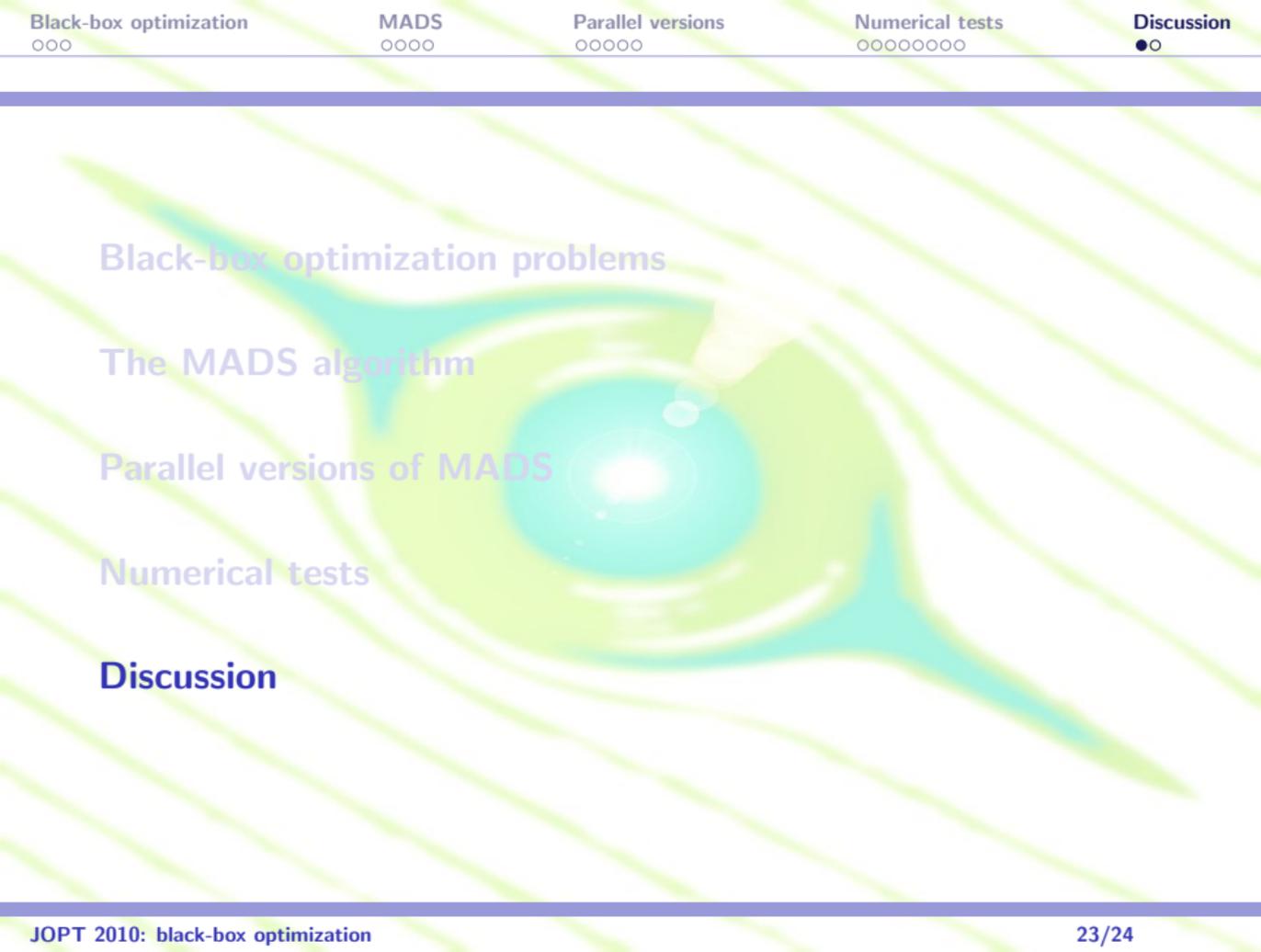
$$n = 500, 0 \leq x \leq 10, x_0 = [5 \ 5 \ \dots \ 5]^T$$

Problem G2, $n=500$, 50,000 evaluations



Results analysis

- ▶ PSD-MADS is much more efficient on the large problem.
- ▶ COOP-MADS gives the best result on the Styrene problem, and COOP-MADS is better than COOP-LTMADS.
- ▶ The bad behaviour of COOP-MADS on the large problem is due to the fact that processes never go to small meshes where OrthoMADS directions are different even for different Halton seeds: all processes are evaluating almost exactly the same points and the cache server makes them wait.
- ▶ MADS and pMADS seem equivalent. In fact, many other tests suggest that MADS gives better solutions than pMADS. This is due to the **opportunistic strategy** that the scalar version exploits better.



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- ▶ Parallel versions of MADS seem efficient and allow to solve black-box optimization problems faster and sometimes better.
- ▶ The basic parallel method pMADS gives similar results than the scalar version, but much faster.
- ▶ More evolved parallel strategies are needed to improve the method's efficiency.
- ▶ COOP-MADS seems a good method for small problems, and PSD-MADS for larger ones.
- ▶ The current PSD-MADS algorithm is based on random subproblems: statistic methods identifying the important variables should improve its efficiency even more.