ICCOPT 2013

Engineering applications treated with the MADS algorithm

Sébastien Le Digabel, École Polytechnique de Montréal

2013–07–31

Collaborators

- École Polytechnique de Montréal:
  - Charles Audet
  - Dominique Cartier
  - Vincent Garnier
  - Aimen Gheribi
  - Bastien Talgorn
- Hydro-Québec:
  - Stéphane Alarie
  - Louis-Alexandre Leclaire
  - Marie Minville

Presentation outline

The MADS algorithm

Snow Water Equivalent estimation

Calibration of a Hydrologic Model

Biobjective optimization of aircraft takeoff trajectories

Alloy design using the FactSage software

The MADS algorithm

Snow Water Equivalent estimation

Calibration of a Hydrologic Model

Biobjective optimization of aircraft takeoff trajectories

Alloy design using the FactSage software

Blackbox optimization problems

We consider the optimization problem:

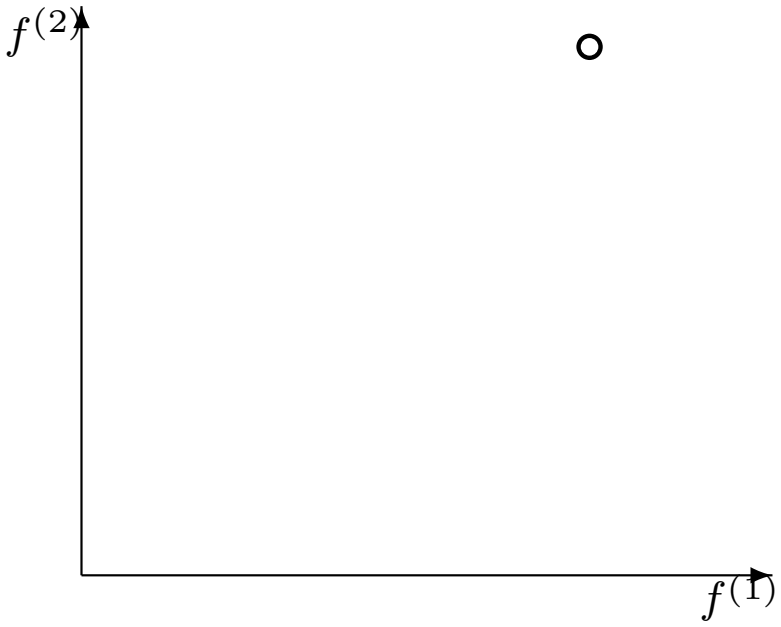
$$\min_{x \in \Omega} \quad f(x)$$

where evaluations of f and the functions defining Ω are usually the result of a computer code (a blackbox).

Mesh Adaptive Direct Search (MADS)

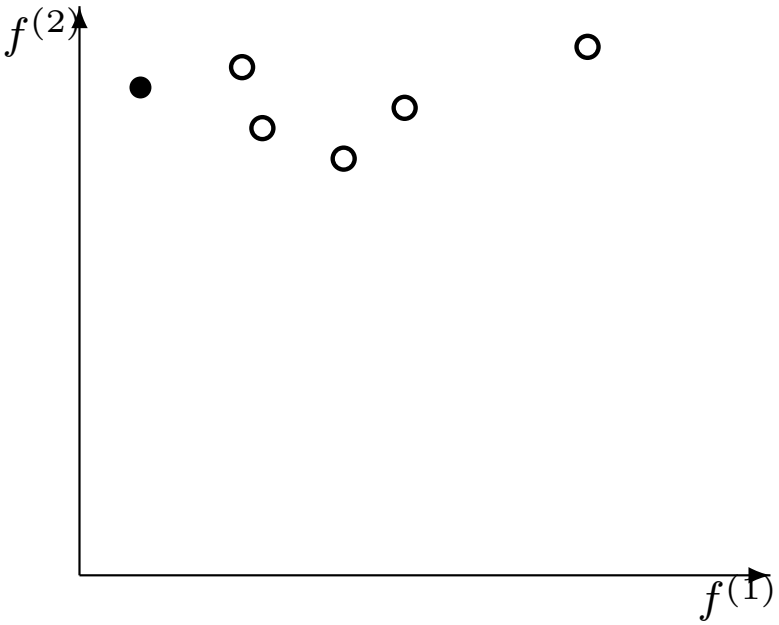
- Audet and Dennis [SIOPT, 2006]
- Iterative algorithm that evaluates the blackbox at some trial points on a spatial discretization called the mesh.
- One iteration = search and poll.
- The search allows trial points generated anywhere on the mesh.
- The poll consists in generating a list of trial points constructed from poll directions. These directions grow dense.
- At the end of the iteration, the mesh size is reduced if no new iterate is found.
- Algorithm is backed by a convergence analysis based on the Clarke Calculus for nonsmooth functions.
- MADS is available via the NOMAD free software package at www.gerad.ca/nomad.

Biobjective optimization: successive MADS runs



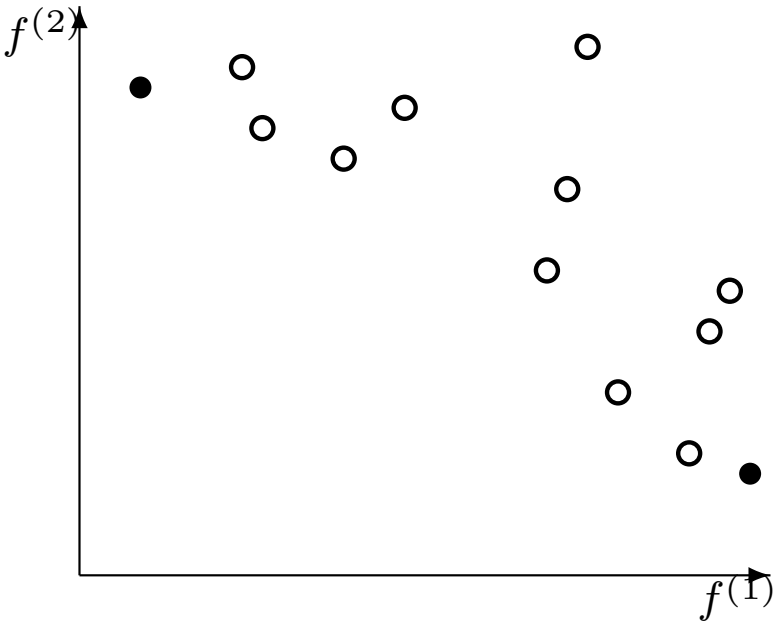
- INITIALIZATION:
  Solve $\min_{x \in \Omega} f^{(q)}(x)$ for $q \in \{1, 2\}$.

Biobjective optimization: successive MADS runs



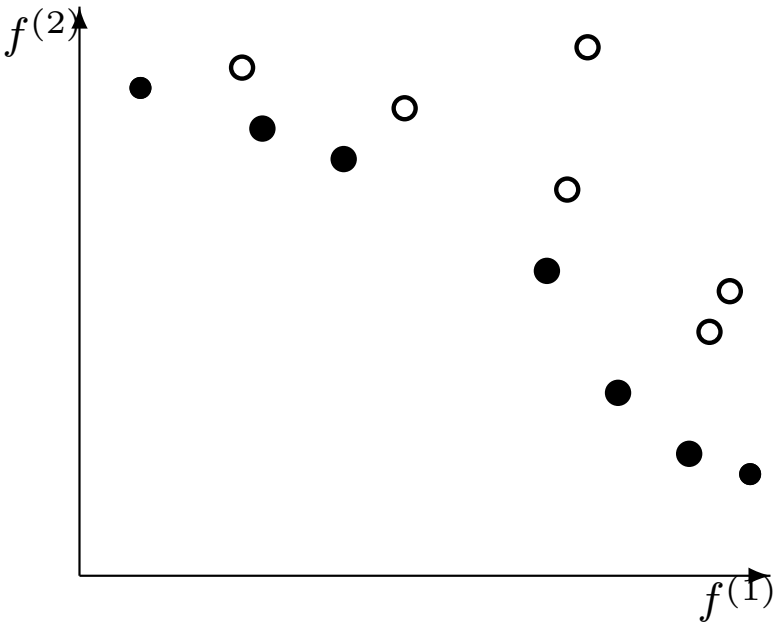
- INITIALIZATION:
  Solve $\min_{x \in \Omega} f^{(q)}(x)$ for $q \in \{1, 2\}$.

Biobjective optimization: successive MADS runs



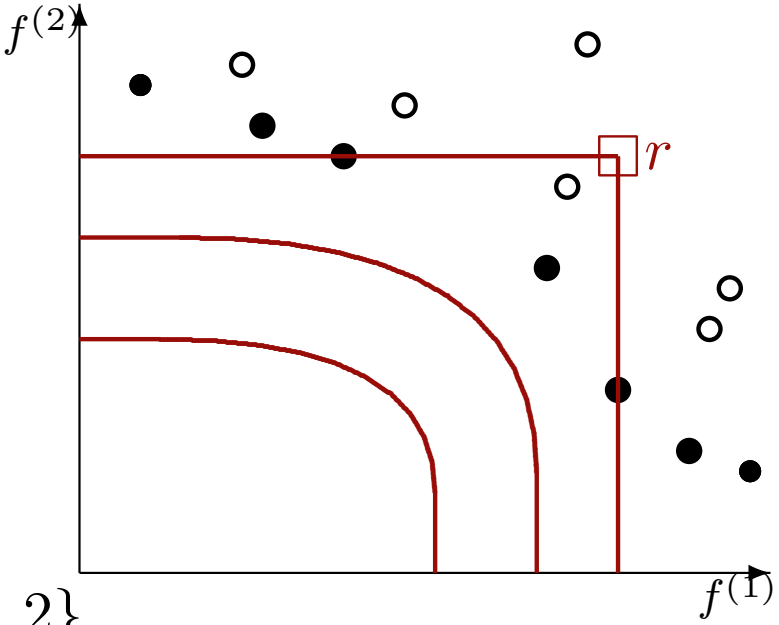
- INITIALIZATION:
  Solve $\min_{x \in \Omega} f^{(q)}(x)$ for $q \in \{1, 2\}$.

Biobjective optimization: successive MADS runs



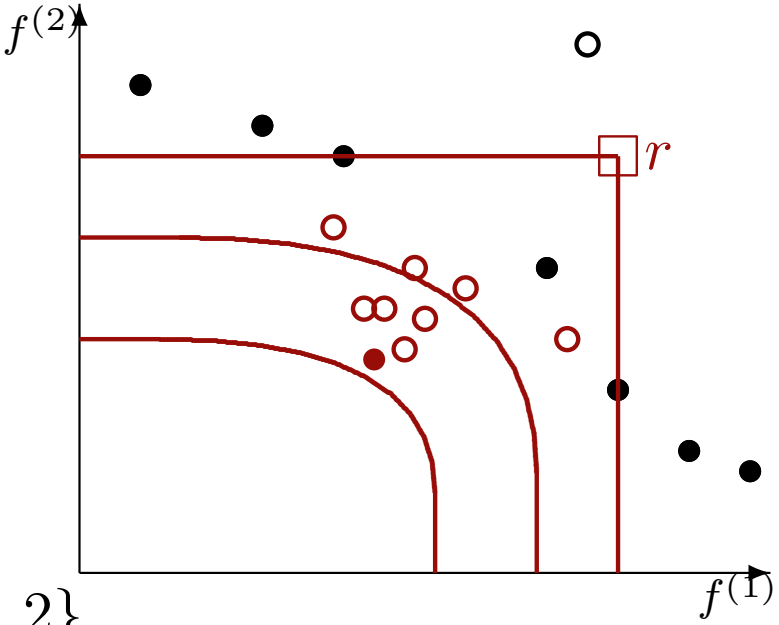
- INITIALIZATION:
  Solve $\min_{x \in \Omega} f^{(q)}(x)$ for $q \in \{1, 2\}$.
- MAIN ITERATIONS:
  - REFERENCE POINT DETERMINATION:
    Use the set of feasible ordered undominated points generated so far to generate a reference point r.

Biobjective optimization: successive MADS runs



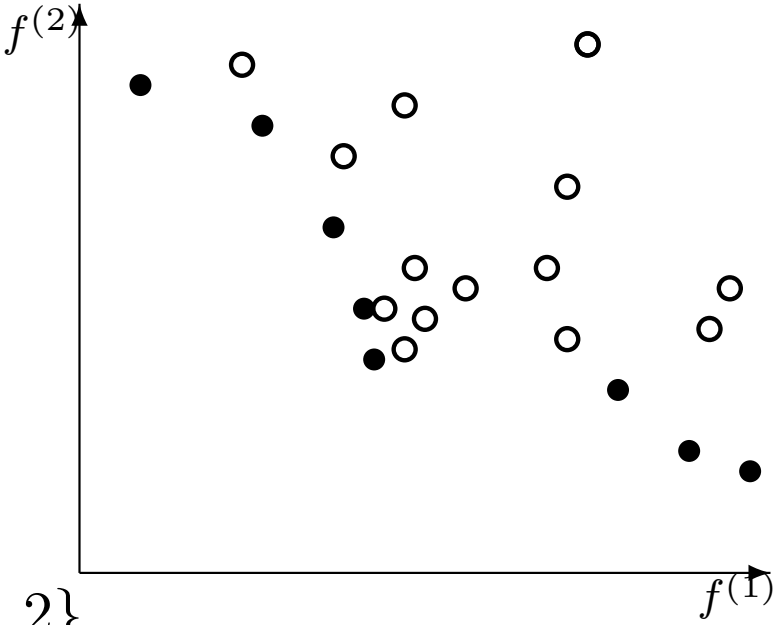
- Initialization:
  Solve $\min_{x \in \Omega} f^{(q)}(x)$ for $q \in \{1, 2\}$.
- Main iterations:
  - Reference point determination:
    Use the set of feasible ordered undominated points generated so far to generate a reference point r.
  - Single-objective minimization:
    Solve the problem $\max_{x \in \Omega} (r_1 - f^{(1)}(x))_+^2 (r_2 - f^{(2)}(x))_+^2$.

Biobjective optimization: successive MADS runs



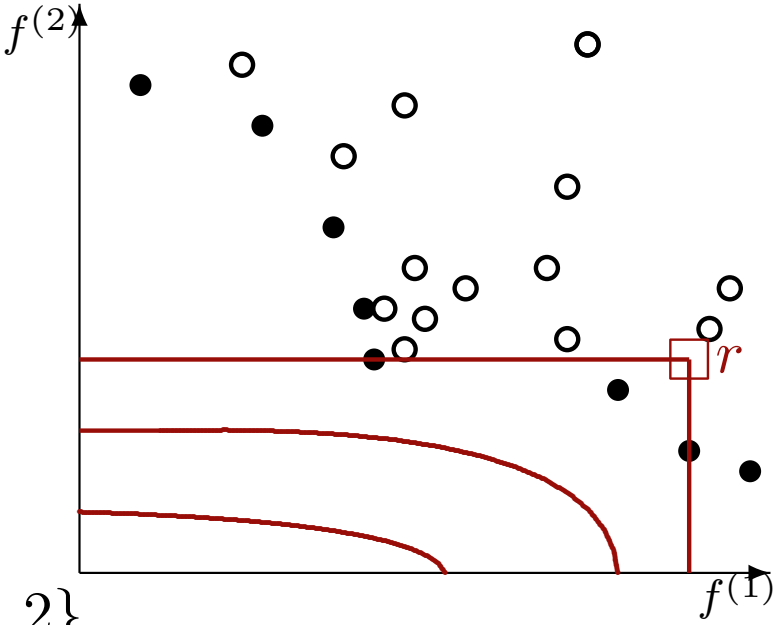
- Initialization:
  Solve $\min_{x \in \Omega} f^{(q)}(x)$ for $q \in \{1, 2\}$.
- Main iterations:
  - Reference point determination:
    Use the set of feasible ordered undominated points generated so far to generate a reference point r.
  - Single-objective minimization:
    Solve the problem $\max_{x \in \Omega} (r_1 - f^{(1)}(x))_+^2 (r_2 - f^{(2)}(x))_+^2$.

Biobjective optimization: successive MADS runs



- INITIALIZATION:
  Solve $\min_{x \in \Omega} f^{(q)}(x)$ for $q \in \{1, 2\}$.
- MAIN ITERATIONS:
  - REFERENCE POINT DETERMINATION:
    Use the set of feasible ordered undominated points generated so far to generate a reference point r.
  - SINGLE-OBJECTIVE MINIMIZATION:
    Solve the problem $\max_{x \in \Omega} (r_1 - f^{(1)}(x))_+^2 (r_2 - f^{(2)}(x))_+^2$.

Biobjective optimization: successive MADS runs



- Initialization:
  Solve $\min_{x \in \Omega} f^{(q)}(x)$ for $q \in \{1, 2\}$.
- Main iterations:
  - Reference point determination:
    Use the set of feasible ordered undominated points generated so far to generate a reference point r.
  - Single-objective minimization:
    Solve the problem $\max_{x \in \Omega} (r_1 - f^{(1)}(x))_+^2 (r_2 - f^{(2)}(x))_+^2$.

The MADS algorithm

Snow Water Equivalent estimation

Calibration of a Hydrologic Model

Biobjective optimization of aircraft takeoff trajectories

Alloy design using the FactSage software

Importance of the Snow Water Equivalent (SWE)

- Accurate estimate of water stored in snow is crucial to optimize hydroelectric plants management.
- Exact snow measurement is impossible.
- SWE is measured at specific sites and next interpolated over the territory.
- Territory is huge: Hydro-Québec (HQ) operates 565 dams, 75 reservoirs, and 56 hydroelectric power plants, located over 90 watersheds and covering more than 550,000 km^2.



SWE estimation

- Presently, done manually by weighing snow cores at specific sites.
- Each measurement campaign requires 2 weeks.
- Missing measurements due to adverse meteorological conditions.

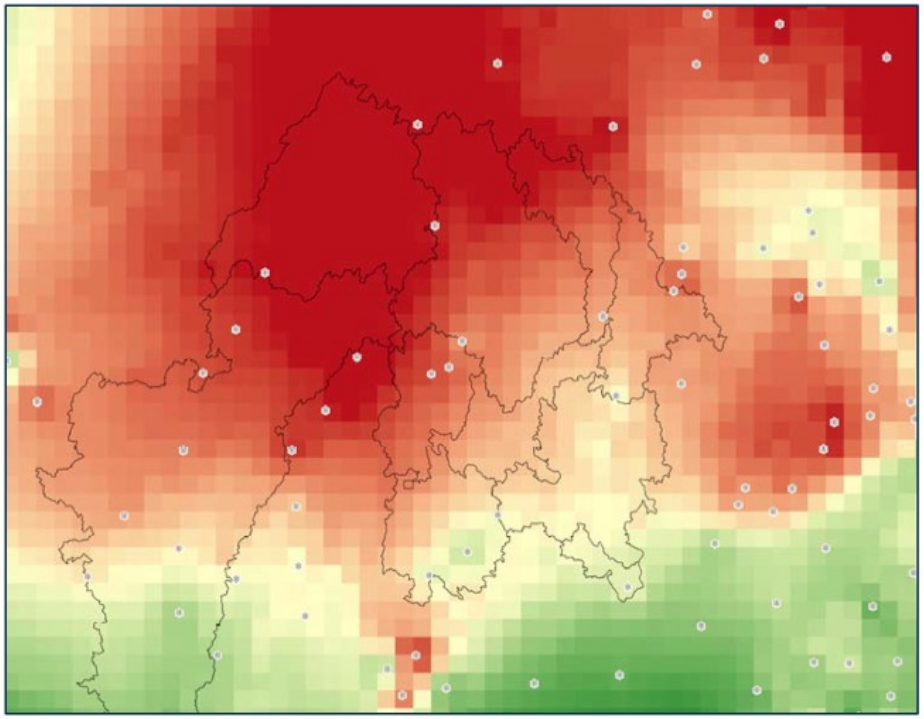
GMON device

- A new measuring instrument that provides daily automatic SWE.
- GMON for Gamma-MONitoring device: it measures the natural Gamma radiation emitted from the soil.
- Communicates via satellites.

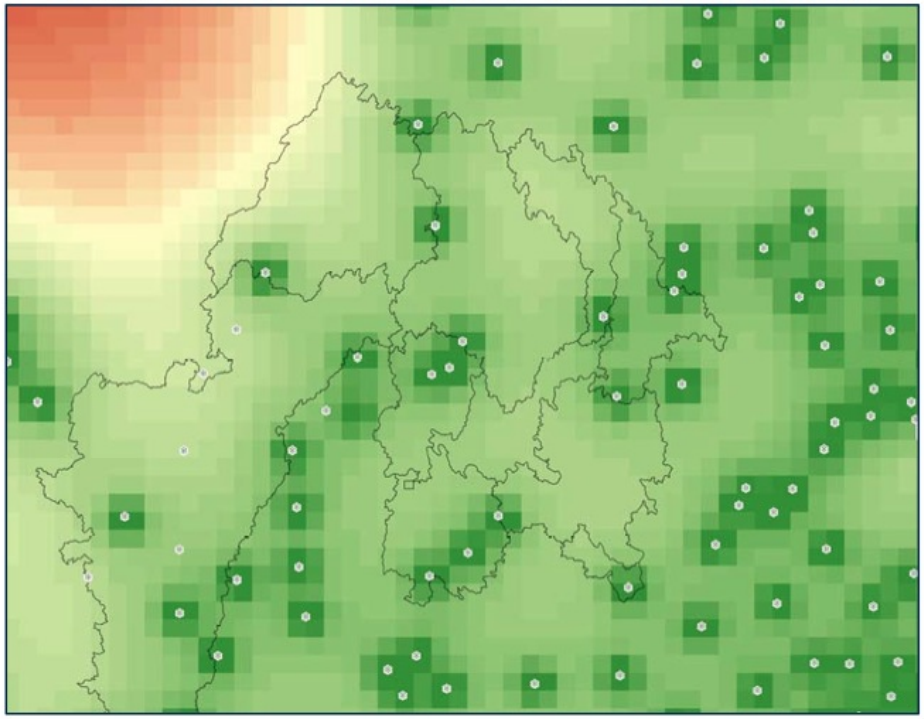
SWE estimation from GMON measures

- Kriging interpolation is used to obtain SWE estimation together with an error map.
- How to find the device locations that minimize the kriging interpolation error of the SWE?

SWE estimation



standard deviation of estimation

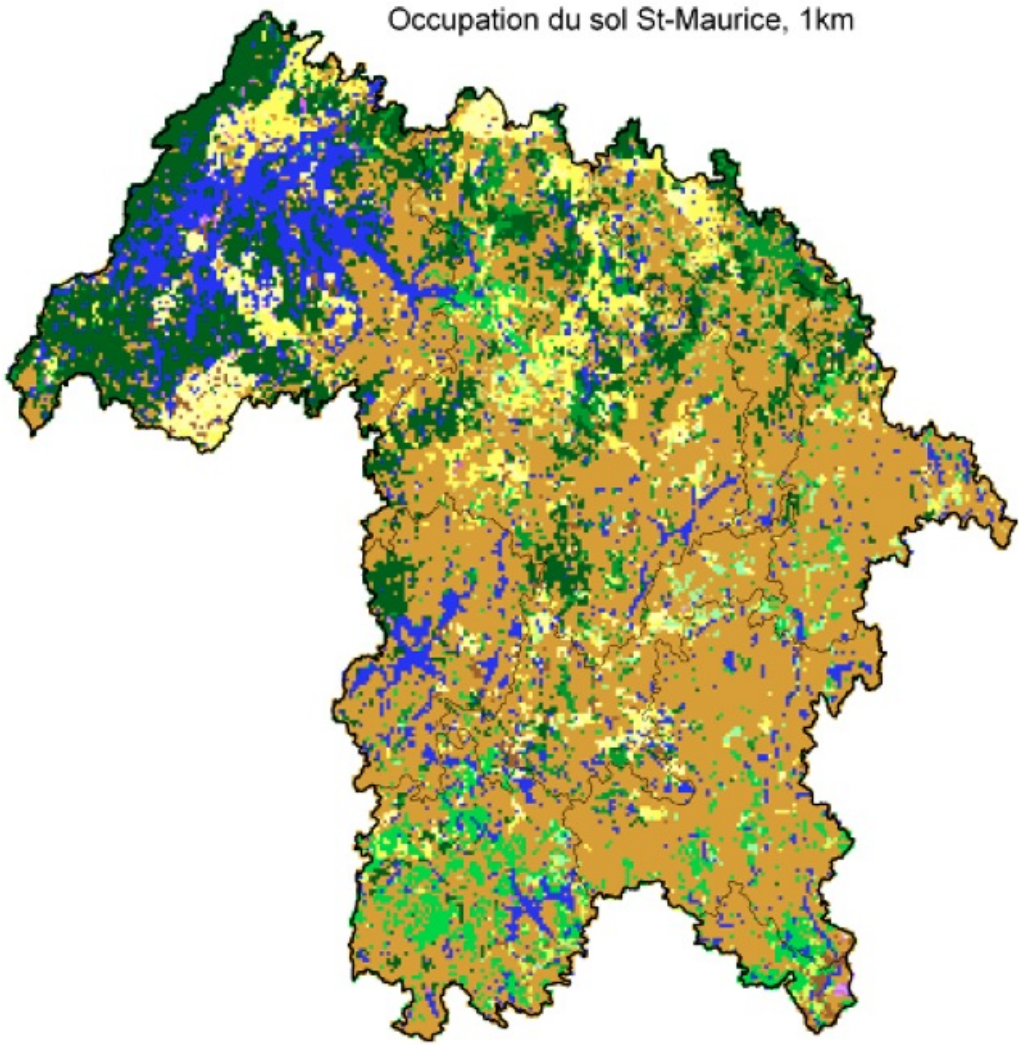


Problem formulation

- $x \in \mathbb{R}^{2N}$ are the locations of N stations.
- Typically, $N \leq 10$, so we do not consider it as a variable.
- $\Omega \subseteq \mathbb{R}^2$ is the feasible domain where the stations can be located.
- $f(x)$ is a score based on the standard deviation map obtained by the kriging simulation and is considered as a blackbox.
- Each simulation requires $\simeq 2$ seconds, and can only be launched within the Hydro-Québec research center.

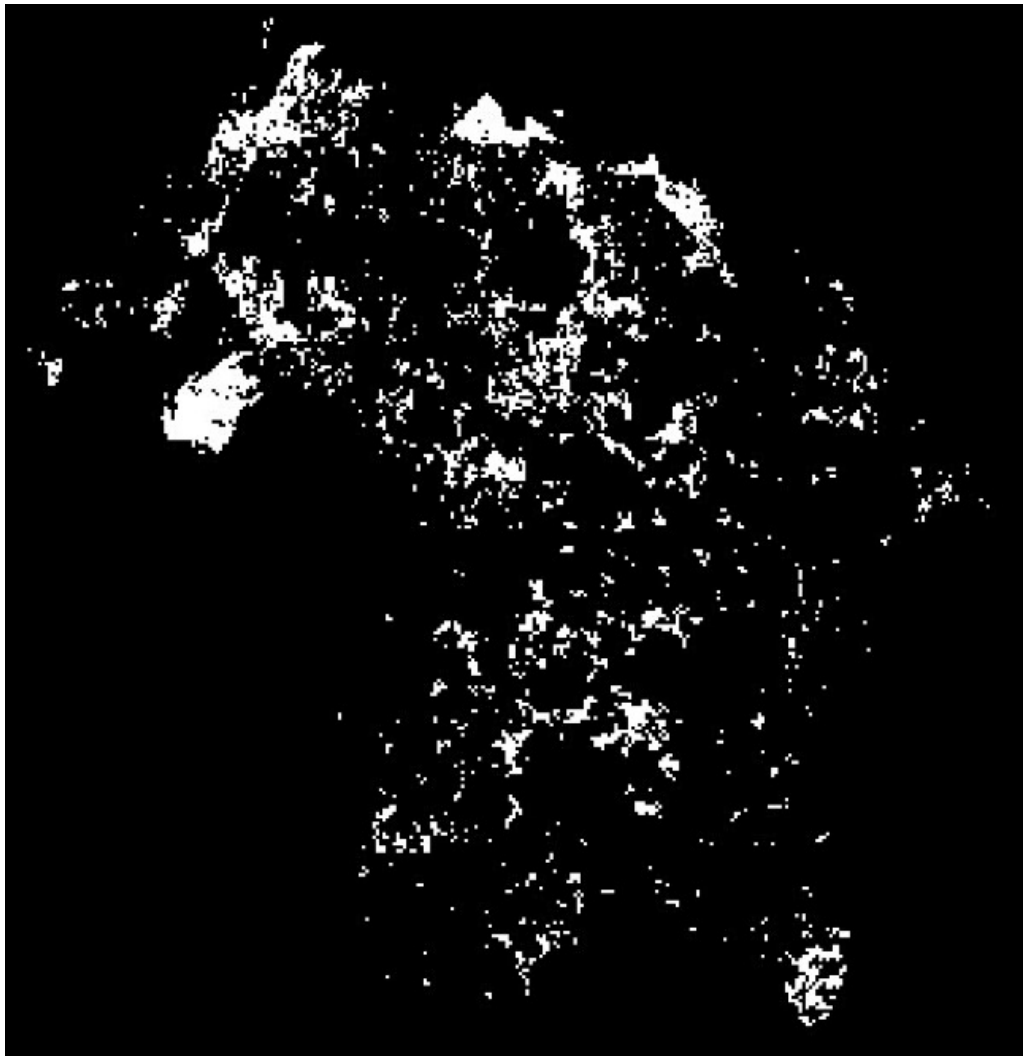
Constraints

- GMON stations cannot be located anywhere.
- Restrictions on:
  - subsoil properties,
  - slope,
  - vegetation,
  - exploitation,
  - etc.



Constraints

- GMON stations cannot be located anywhere.
- Restrictions on:
  - subsoil properties,
  - slope,
  - vegetation,
  - exploitation,
  - etc.
- Highly fragmented domain.



Special features

- Fragmented domain: Heuristic directly integrated in the simulator to identify the closest feasible location.
- Groups of variables:
  - Variables represent 2D locations.
  - Makes sense to simultaneously move both GMON coordinates.
  - Different grouping strategies are developed.
  - Some are dynamic: groups are changed during the optimization.
- Static surrogate:
  - Cheap replacement of the true function.
  - Simple analytic expression of the objective.
  - Allowed the algorithm design outside of Hydro-Québec.
  - Parameters defining the surrogate were chosen in collaboration with Hydro-Québec experts, by comparing corresponding error maps.

Results

- Three maps: Gatineau, Saint-Maurice and La Grande.
- The number of GMON stations varies from $N = 5$ to 10, for a total of 18 test instances.
- Dynamically regrouping the variables is preferable than either moving individual variables, or moving all variables simultaneously.
- Some strategies developed in this work are specific to positioning problems, other are generic.

The MADS algorithm

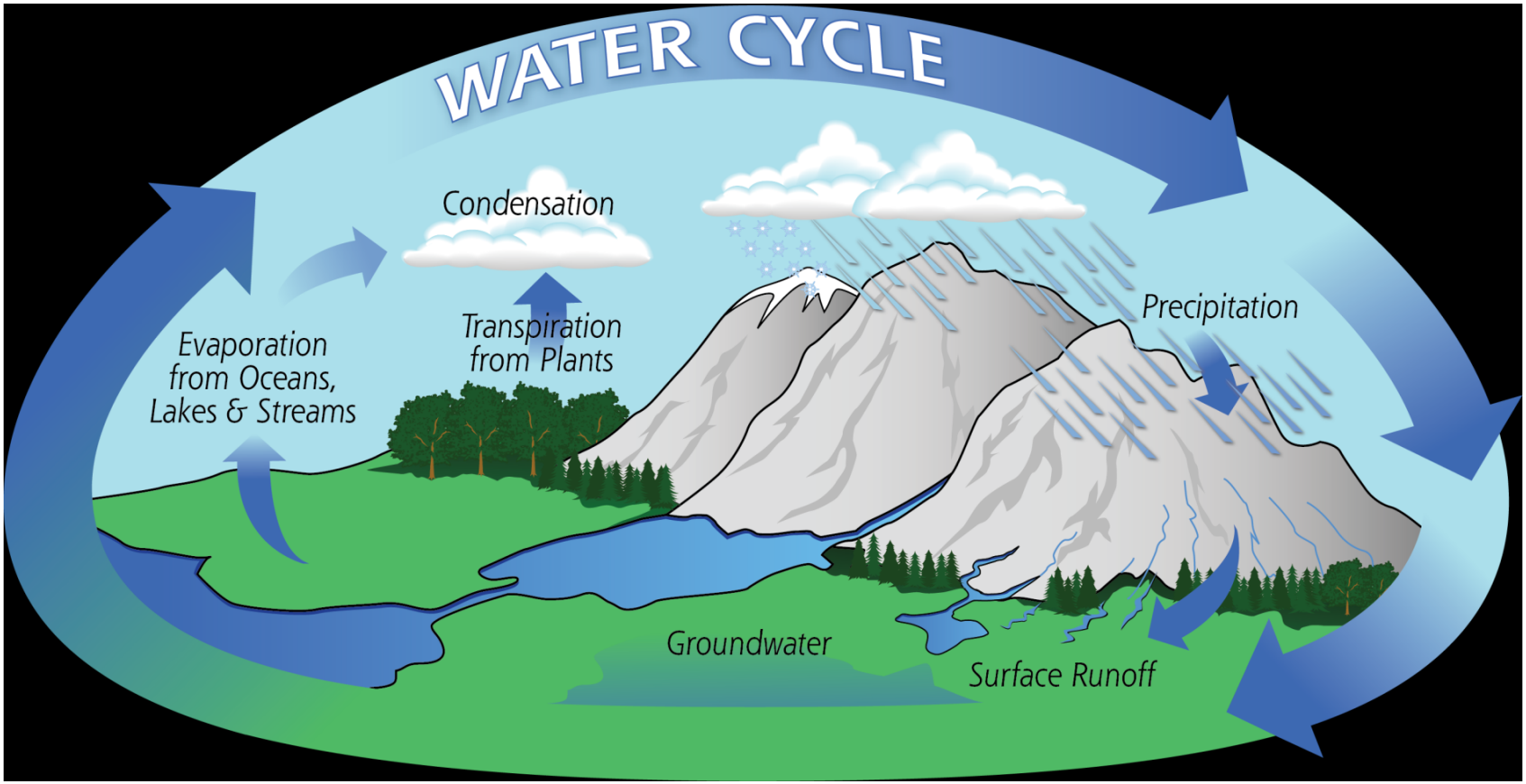
Snow Water Equivalent estimation

Calibration of a Hydrologic Model

Biobjective optimization of aircraft takeoff trajectories

Alloy design using the FactSage software

The Water Cycle



credit: NASA.

Evaporation + Transpiration = Evapotranspiration.

Objectives

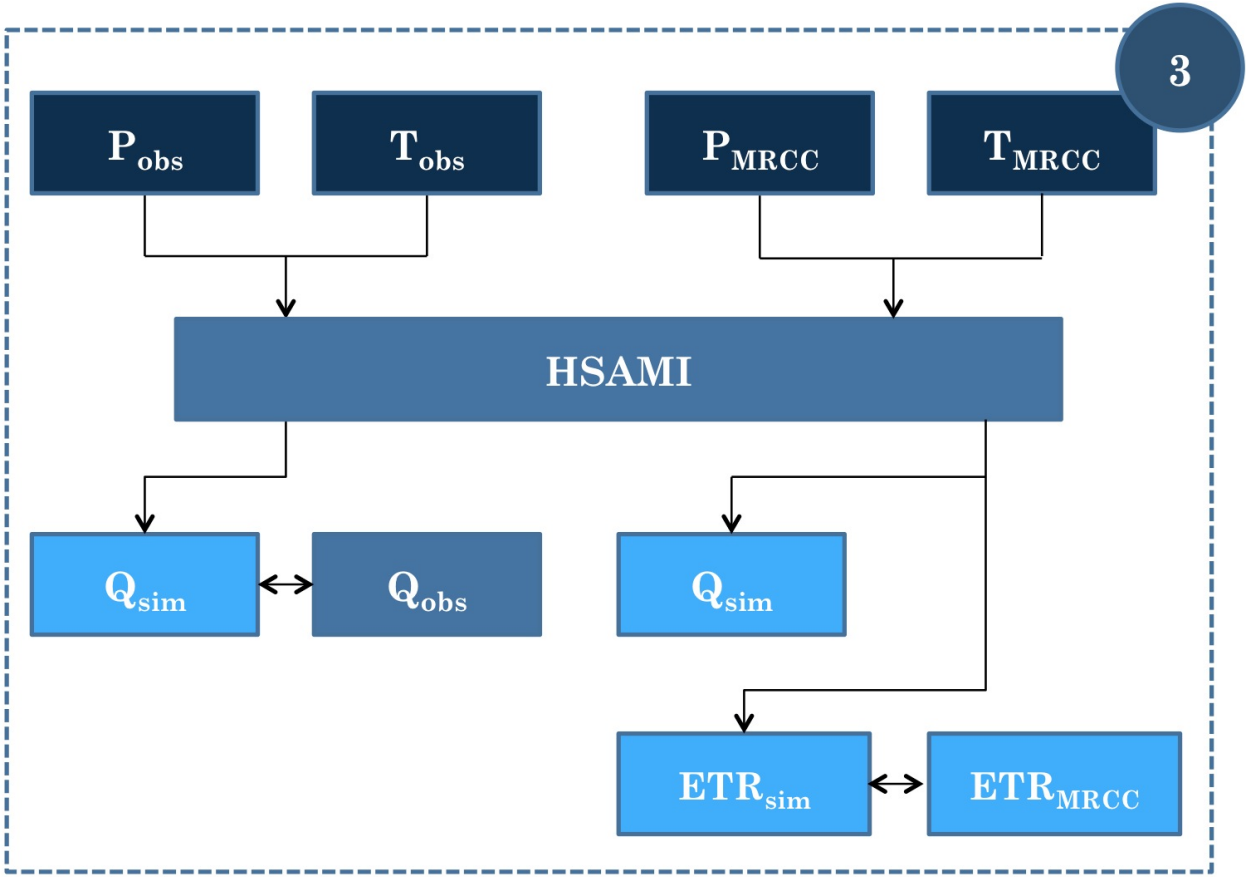
- Define a calibration (= parameters optimization) approach in order to improve the transposability of the hydrologic model.
- A transposable model should adequately reproduce hydrologic processes when they are employed with other data than those used to obtain the parameters (e.g. climate change).
- Emphasis on a realistic representation of evapotranspiration.
- Characteristics of the optimization problem: Nonsmoothness, multiple regions of attraction, and many local optima within each region of attraction.

The model

- HSAMI (*Service hydrométéorologique apports modulés intermédiaires*) [Bisson, Roberge, 1983] [Fortin, 1999].
- Hydrologic model developed and used at Hydro-Québec.
- 23 parameters: optimization variables.
- One evaluation takes $\simeq$ 1-2 seconds.
- We compare the simulated and observed streamflows and minimize the Nash-Sutcliffe criteria $\frac{\sum_{t=1}^{T}(Q_t^o - Q_t^s)^2}{\sum_{t=1}^{T}(Q_t^o - \overline{Q^o})^2}$.
- Cross-validation typically over half the data.

Definition of the evapotranspiration (ETR) constraint

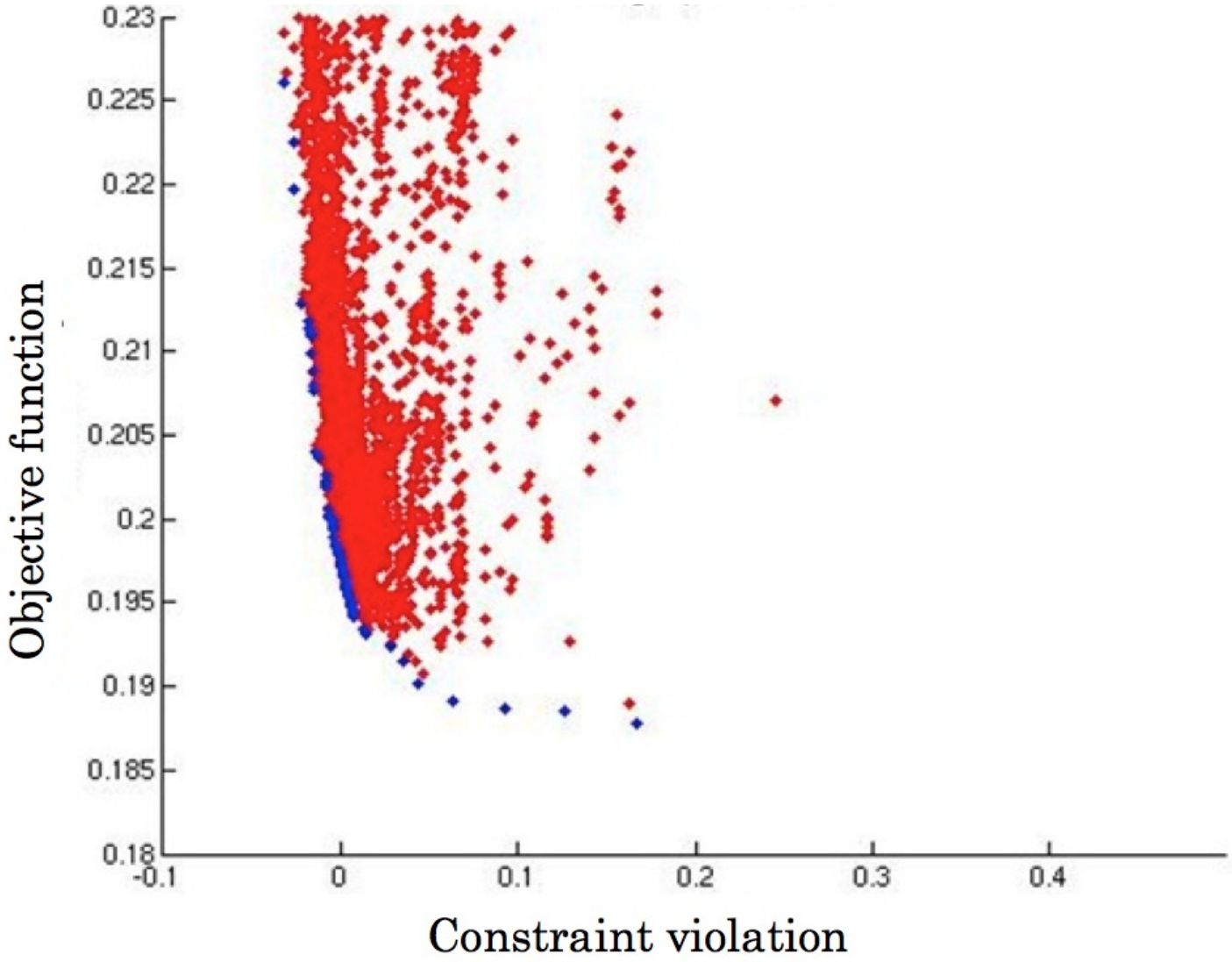
Calibration of the ETR is achieved by considering a climatic model (MRCC) for known values of P, T, and ETR.



Special features

- Progressive Barrier [SIOPT 2009] to treat the constraint.
- VNS (Variable Neighborhood Search) [JOGO 2008]: Useful in the presence of many local optima. Costs more evaluations but helps to achieve global optimization. For the present project, VNS gave improvements of up to 12%.
- Tool for the sensitivity analysis of the constraints [OMS 2012].

Sensitivity Analysis



The MADS algorithm

Snow Water Equivalent estimation

Calibration of a Hydrologic Model

Biobjective optimization of aircraft takeoff trajectories

Alloy design using the FactSage software

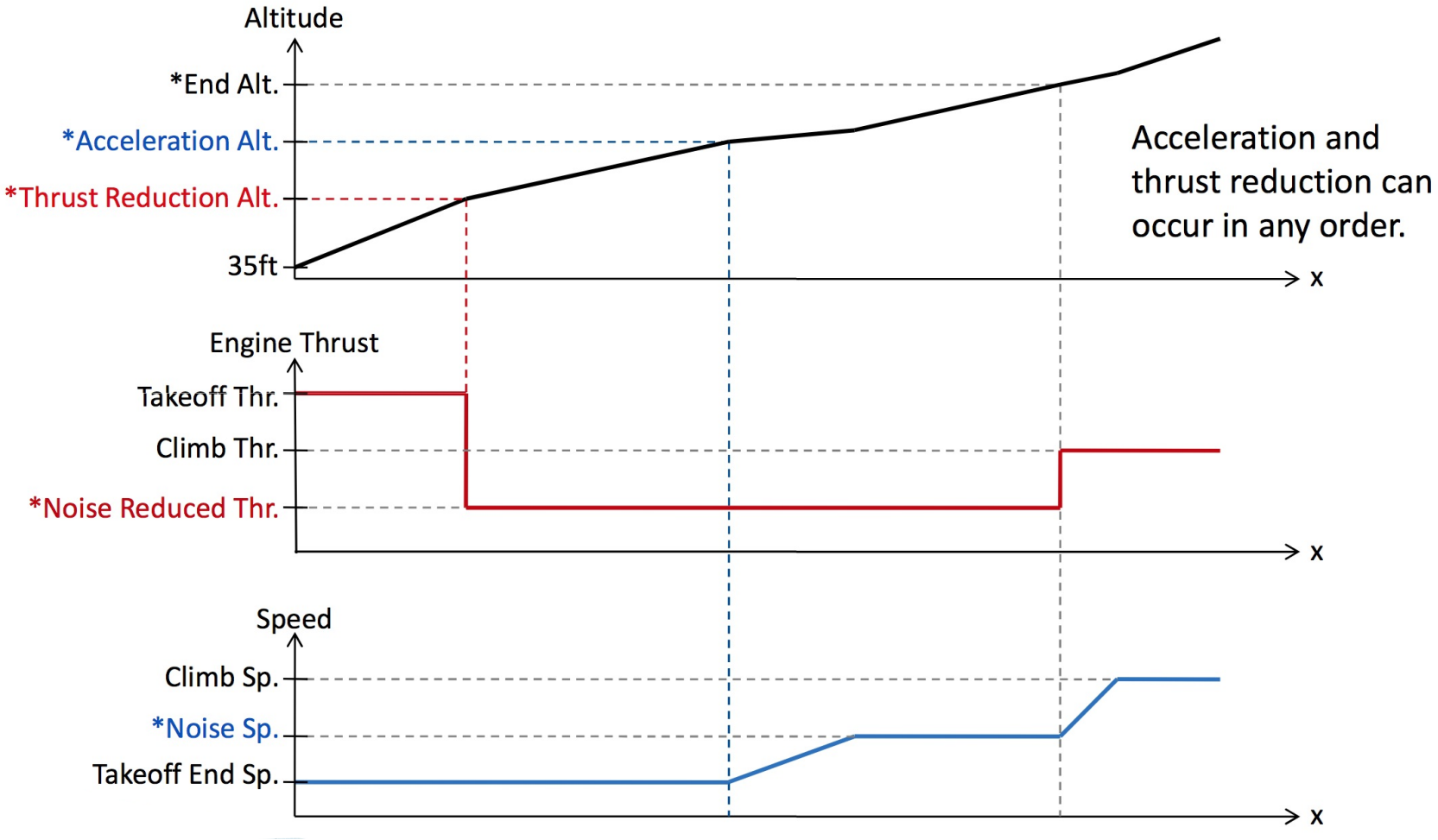
Aircraft takeoff trajectories

- AIRBUS problem involving (among others): O. Babando, C. Bes, J. Chaptal, J.-B. Hiriart-Urruty, B. Talgorn, B. Tessier, and R. Torres.
- Motivations for MADS/NOMAD:
  - A blackbox is involved.
  - Biobjective optimization.
  - Free software.
  - Must execute on different platforms including some old Solaris distributions.

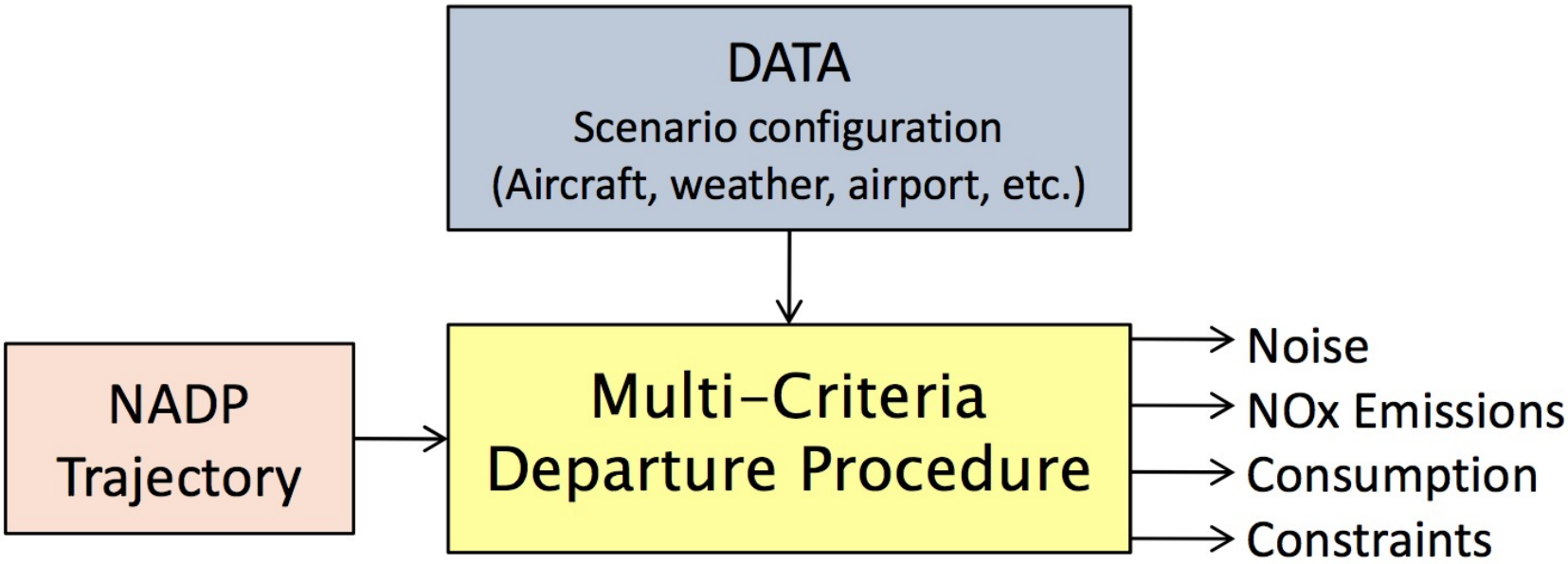
Definition of the optimization problem

- Concept : Optimization of vertical flight path based on procedures designed to reduce noise emission at departure to protect airport vicinity.
- Minimization of environmental and economical impact: Noise and Fuel consumption.
- During departure phase, the aircraft will target its climb configuration:
  - Increase the speed up to climb speed (acceleration phase).
  - Reduce the engine rate to climb thrust (reduction phase).
  - Gain altitude.

Parametric Trajectory: 5 optimization variables (*)



The blackbox: MCDP: Multi-Criteria Departure Procedure



One evaluation $\simeq$ 2 seconds.

Special features

- The best trajectory parameters are returned to the pilot who enters them in the aircraft system manually.
- Finite precision on optimization parameters: Discretization of optimization variables (100 to 1000 different values for each parameter).
- The variables have been defined as integers in NOMAD (minimum mesh size of 1 and rounding of directions).

Results

Detailed results are confidential. But we can say:

- Tested for the Munich airport.
- Aircraft: A321.
- $\simeq$ 3000 evaluations for $\simeq$ 30 undominated points.

The MADS algorithm

Snow Water Equivalent estimation

Calibration of a Hydrologic Model

Biobjective optimization of aircraft takeoff trajectories

Alloy design using the FactSage software

The basic tool: FactSage

- Objective: identify the low melting compositions (i.e. liquidus minima) in a multicomponent system.
- The experimental determination of these compositions can be very lengthy and expensive.
- The CALPHAD (calculation of phase diagrams) approach: databases are developed using an appropriate mathematical model for each phase which gives the thermodynamic properties as functions of temperature and of composition.
- The FactSage databases contain assessed model parameters for thousands of compounds and hundreds of solid and liquid solution phases of metallic, salt, oxide, etc. systems.

[Gheribi et al., J. Chem. Thermodynamics, 2011].

Improvement of properties of magnesium alloys

- We want to improve the mechanical, corrosion and texture properties of the AZ91 magnesium alloy.
- AZ91 is widely used because of its excellent castability and mechanical properties. However a disadvantage of AZ91 is its poor corrosion resistance.
- The addition of RE (rare earth) improves the corrosion resistance.
- The addition of RE and Ca improves the mechanical properties.
- The addition of RE and Ca could increase the freezing range of AZ91 and thus decrease significantly the castability.

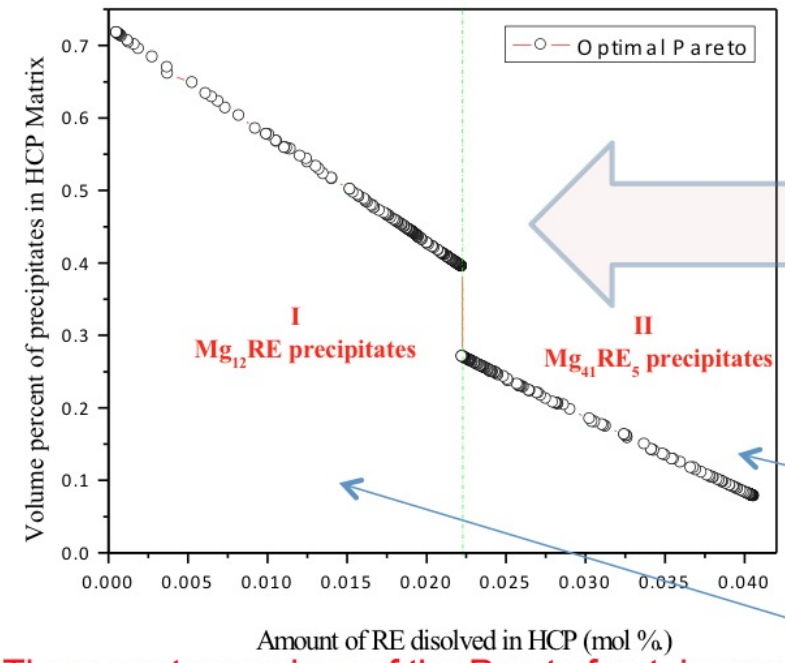
Improvement of properties of magnesium alloys

- This is a biobjective optimization problem, with:
  - Maximize the volume fraction of precipitates.
  - Maximize the atomic fraction of RE.
- The constraints are the β-phase volume fraction and the amounts of Al_2Ca and Mg_2Si:
  - Volume fraction of $\beta(Mg_{17}Al_{12})$ phase $\leq 5.5\%$.
  - $0.45 \leq$ wt. % $Al_2Ca \leq 0.85$.
  - $0.25 \leq$ wt. % $Mg_2Si \leq 0.45$.
  - $0 \leq$ wt. % $Mg \leq 1$.
- And bounds on the 6 variables:

	Mn	Al	Zn	Ce	Ca	Si	Mg
Min(Wt.%)	0	7.5	0.25	0	0	0	Bal.
Max(wt.%)	0.20	10.50	1.15	2.00	0.75	0.75	Bal.

Improvement of texture and mechanical properties of Mg-based alloys by addition of RE metals

Approximation of the Pareto front after 1000 FactSage calculations ($\simeq$ 3 hours):



~1000 FactSage calculations(3h00)

Pareto front representing optimal compositions of Mg-(La-Ce-Pr-Nd-Sm) alloys which maximize simultaneously

1- the volume fraction of precipitates in the Mg matrix

2-the atomic fraction of RE in the HCP solid solution.

Wt.%(RE)=0.3

There are two regions of the Pareto front, in one region $Mg_{12}RE$ precipitates are observed, while $Mg_{41}RE_5$ is the stable phase in the other region.

Discussion

- Four different engineering applications.
- Many special features of MADS / NOMAD have been exploited. The algorithm and the code are robust and mature enough to adapt to many different situations.
- NOMAD is now widely spread and used in industry.

- S. Alarie, C. Audet, V. Garnier, S. Le Digabel, and L.A. Leclaire: *Snow water equivalent estimation using blackbox optimization.* Pacific Journal of Optimization, 2013.
- M. Minville, D. Cartier, C. Guay, L.-A. Leclaire, C. Audet, S. Le Digabel, and J. Merleau: *New calibration approaches for conceptual hydrological models: incorporating external information for oriented parametrisations based on physical processes.* In revision for Water Resources Research.
- C. Audet, J.E. Dennis, Jr., and S. Le Digabel: *Trade-off studies in blackbox optimization.* Optimization Methods and Software, 27(4-5), 613-624, 2012.
- R. Torres, J. Chaptal, C. Bès, and J.-B. Hiriart-Urruty: *Optimal, Environmentally Friendly Departure Procedures for Civil Aircraft.* Journal of Aircraft, 2011.
- A.E. Gheribi, S. Le Digabel, C. Audet, and P. Chartrand: *Identifying optimal conditions for Magnesium based alloy design using the Mesh Adaptive Direct Search algorithm.* Thermochimica Acta, 2013.
- A.E. Gheribi, C. Audet, S. Le Digabel, E. Bélisle, C.W. Bale, and A.D. Pelton: *Calculating optimal conditions for alloy and process design using thermodynamic and property databases, the FactSage software and the Mesh Adaptive Direct Search algorithm.* CALPHAD, 2012.
- A.E. Gheribi, C. Robelin, S. Le Digabel, C. Audet, and A.D. Pelton: *Calculating all local minima on liquidus surfaces using the FactSage software and databases and the Mesh Adaptive Direct Search algorithm.* The Journal of Chemical Thermodynamics, 2011.