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Engineering applications treated with the MADS algorithm

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Collaborators

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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

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Blackbox optimization problems

We consider the optimization problem:

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

where evaluations of $f$ and the functions defining $\Omega$ 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

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

![GMON device image]
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?
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 $\approx 2$ 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.
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  - 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.
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The Water Cycle

Evaporation + Transpiration = Evapotranspiration.

credit: NASA.
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

\[
\frac{T}{\sum_{t=1}^{T} (Q^o_t - Q^s_t)^2}
\]

- 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
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**Biobjective optimization of aircraft takeoff trajectories**

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Aircraft takeoff trajectories


- 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 (*)

Acceleration and thrust reduction can occur in any order.
The blackbox: MCDP: Multi-Criteria Departure Procedure

DATA
Scenario configuration
(Aircraft, weather, airport, etc.)

NADP Trajectory

Multi-Criteria Departure Procedure

→ Noise
→ NOx Emissions
→ Consumption
→ Constraints

One evaluation ≈ 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.
- \( \sim 3000 \) evaluations for \( \sim 30 \) undominated points.
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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.

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 $\beta$-phase volume fraction and the amounts of Al$_2$Ca and Mg$_2$Si:
  - Volume fraction of $\beta$(Mg$_{17}$Al$_{12}$) phase $\leq$ 5.5%.
  - $0.45 \leq$ wt. % Al$_2$Ca $\leq$ 0.85.
  - $0.25 \leq$ wt. % Mg$_2$Si $\leq$ 0.45.
  - $0 \leq$ wt. % Mg $\leq$ 1.
- And bounds on the 6 variables:

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<th>Mn</th>
<th>Al</th>
<th>Zn</th>
<th>Ce</th>
<th>Ca</th>
<th>Si</th>
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<td>2.00</td>
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<td>0.75</td>
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</tbody>
</table>
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):

There are two regions of the Pareto front, in one region $\text{Mg}_{12}\text{RE}$ precipitates are observed, while $\text{Mg}_{41}\text{RE}_5$ is the stable phase in the other region.

$\sim 1000$ 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
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.


