# Two decades of blackbox optimization applications

Stéphane Alarie* Charles Audet† Aïmen E. Gheribi‡
Michael Kokkolaras§ Sébastien Le Digabel¶

October 30, 2020

**Abstract:** This work reviews blackbox optimization applications over the last twenty years, addressed using direct search optimization methods. Emphasis is placed on the Mesh Adaptive Direct Search (MADS) derivative-free optimization algorithm. The core of the document describes applications in three specific fields: Energy, materials science, and computational engineering design. Other applications in science and engineering as well as patents are also mentioned. This selection highlights the versatility and the evolution of MADS and its accompanying software, NOMAD, that became over the years the baseline solver in blackbox optimization.

**Keywords:** Blackbox optimization, Derivative-free optimization, Mesh adaptive direct search, Applications.

**AMS subject classifications:** 90C30, 90C56, 90C90.

## 1 Introduction

The most general form of an optimization problem is

$$\min_{x \in \Omega} \quad f(x) \,, \tag{1}$$

where $\Omega$ is the feasible region and $f : \Omega \to \overline{\mathbb{R}}$ (with $\overline{\mathbb{R}} = \mathbb{R} \cup \{+\infty\}$) is the objective function. The nature of $f$ and $\Omega$ restricts which optimization method may be used to solve a given problem. Exploiting specificities of the problem such as linearity, convexity or differentiability lead to efficient algorithms. There are numerous optimization problems in which such characteristics are either inexistent, unknown, or impossible to detect. The

*Hydro-Québec and IREQ, alarie.stephane@hydroquebec.com.
†GERAD and Polytechnique Montréal, www.gerad.ca/Charles.Audet.
‡CRCT and Polytechnique Montréal, aimen.gheribi@polymtl.ca.
§GERAD and McGill University, michael.kokkolaras@mcgill.ca.
¶GERAD and Polytechnique Montréal, www.gerad.ca/Sebastien.Le.Digabel.

present work surveys an important number of applications of direct search methods for such problems over the past two decades. The applications reported in this survey are chosen from a wide variety of domains.

## 1.1 Blackbox optimization

Blackbox optimization (BBO) is the study of design and analysis of algorithms for optimization problems in which the structure of the objective function $f$ and/or the constraints defining the set $\Omega$ is unknown, unexploitable or non-existant.

The most frequent BBO situation arises when the evaluation of the objective and constraint functions involve launching a computer code or simulation. The code receives a vector $x$ and outputs values in $\overline{\mathbb{R}}$. In many real engineering situations, the code occasionally exits due to internal errors and fails to produce valid output. This is the reason that the output may take values in $\overline{\mathbb{R}}$ rather than $\mathbb{R}$. Invalid output values are flagged by assigning them the $+\infty$ value. In a minimization context, the value $f(x) = +\infty$ corresponds to an unacceptable trial point $x$. Similarly, for the inequality constraint $c(x) \leq 0$, the value $c(x) = +\infty$ indicates an infinite violation of the constraint. For example, the simulation used for the design of an helicopter rotor blade failed on 60% of the calls [51] and the ASPEN [14] chemical engineering simulator failed on 43% of the call for the optimization of a spent potliner treatment process [16]. The output may also be the result of an experiment. For example, the question of developing the best cookie recipe is analyzed in [139], when the objective function was a subjective score entered by participants who tasted different cookies. The above-mentioned situations are called *blackbox optimization problems* [28]. There are no explicit formulation that can be readily exploited.

The simulation that returns the objective and constraint functions may be time consuming. For example, valve train design [60] requires seconds for each call to the simulation, adaptive sequential designs for crossover bioequivalence studies in the pharmaceutical industry [157] requires minutes, hyperparameter optimization [36] requires hours and trailing-edge noise reduction [120] requires days of CPU time for each call to the simulation.

Expensive computational costs are not the only difficulties. The simulation may provide few significant digits, or may return different output when given twice the same input. In a calibration of computationally intensive hydrological models context [96], the output of the simulation is rounded to $10^{-3}$ to account for undesirable imprecision. A stochastic optimization approach is presented in [58] to identify portfolios of permanent rights, options, and leases that minimize the expected costs of meeting a city's annual demand with a specified reliability. A Monte Carlo simulation is used in portfolio selection [59] using real data from the Shanghai-Shenzhen stock market. A CPU time related objective function involving the lid-driven cavity problem [83] from numerical fluid dynamics is analyzed in [4].

Another difficulty related to BBO problems is that the number of variables may be itself an optimization variable. These are a particular type of categorical variables. In [3, 99], a thermal insulation problem involves a variable dictating the number of heat intercepts,

and each of these intercepts is parameterized through other variables, some of them being non-ordinal. The optimal design of a small apparatus for magnetic resonance is studied in [116], in which the number of variables and constraints are affected by the values of some discrete variables. More recently, the number of layers of a deep neural network is analyzed in an hyperparameter optimization setting [105].

## 1.2 The MADS algorithm and the NOMAD software

For BBO problems, the functions are often nondifferentiable, and automatic differentiation may produce false results. Direct search methods [110] are designed to interact directly with the blackbox output, without needing to compute or estimate derivatives. Derivative-free optimization (DFO) is closely related to BBO. In DFO, derivatives are not explicitly available, but are usually assumed to exist. Therefore, they may be estimated through various strategies, and exploited to guide the algorithm toward locally optimal solutions. Both BBO and DFO are in constant progression since the mid nineties. These fields are mature to a point where two books exist, a first one dates from 2009 [64] and a second was published in 2017 [28]. In addition, many surveys on the methodology and evolution of the algorithms are now available [15, 65, 101, 106, 156], but none are devoted exclusively to applications of BBO and DFO.

Amongst all direct search optimization methods, the present paper focuses on the MADS algorithm first introduced in 2006 [23]. The reasons why we are interested in this specific algorithm are for

i- its simplicity;

ii- its ability to handle constraints [18, 23, 24, 33] as well as continuous, integer and categorical variables [5, 35];

iii- its exploitation of static and dynamic surrogate models [20, 31, 51, 63, 142];

iv- its rigorous hierarchical convergence analysis [23, 154] based on nonsmooth calculus [62];

v- its ability to deal with a wide range of optimization problems, as illustrated by the numerous applications detailed in the next sections.

The MADS algorithm has considerably evolved since its introduction, and may handle periodical variables [32], groups of variables [12], badly-scaled problems [34], grey box monotonic problems [19], multiobjective problems [37, 38], stochastic or noisy problems [11, 30, 27, 135], it incorporates various heuristic search strategies including VNS [17] and Nelder-Mead [39], and its local exploration strategies are diversified [6, 8, 29, 137, 151].

The MADS algorithm and its various extensions are coded in C++ under the LGPL license and are freely available as the NOMAD software [107]. Version 1 of NOMAD was initiated in 2001 (with the pattern search algorithm [21, 22, 148], the ancestor of MADS)

and the Beta of Version 4 was released in 2020. The `patternsearch` function of the official MATLAB distribution has an option to select MADS polling directions.[1]

## 1.3 Motivation and structure of the survey

Solving real problems is the main motivation for the development of MADS and NOMAD. Over the years, the algorithm and its implementation have been employed in a broad variety of fields, as illustrated in Table 1 and Figure 1. The table was generated using Web of Science (WoS) and the citations of [107] (328 references as of October 27th, 2020). For each citation, the citing journal has been examined with the "Journal Citation Reports" tool of WoS, and the corresponding application categories have been counted. For example, the entry "Engineering, biomedical: 2" indicates that WoS reports two papers published in biomedical engineering journals citing the NOMAD paper [107]. WoS categories are grouped in fields with the corresponding overall number of references.

| Field | # | Category in WoS | # |
|---|---|---|---|
| Computer science | 75 | Computer science, interdisciplinary applications | 33 |
| | | Computer science, information systems | 14 |
| | | Computer science, artificial intelligence | 9 |
| | | Computer science, software engineering | 6 |
| | | Computer science, software, graphics, programming | 6 |
| | | Computer science, hardware & architecture | 4 |
| | | Computer science, theory & methods | 3 |
| Chemistry | 68 | Engineering, chemical | 30 |
| | | Energy & fuels | 19 |
| | | Chemistry, physical | 5 |
| | | Engineering, petroleum | 5 |
| | | Chemistry, analytical | 2 |
| | | Chemistry, multidisciplinary | 2 |
| | | Chemistry | 1 |
| | | Chemistry, applied | 1 |
| | | Chemistry, inorganic & nuclear | 1 |
| | | Chemistry, medicinal | 1 |
| | | Chemistry, organic | 1 |
| Physics | 61 | Thermodynamics | 9 |
| | | Physics, applied | 6 |
| | | Astronomy & astrophysics | 6 |
| | | Nanoscience & nanotechnology | 6 |
| | | Physics, nuclear | 4 |
| | | Physics, particles & fields | 4 |
| | | Spectroscopy | 4 |
| | | Physics, atomic, molecular & chemical | 3 |
| | | Physics, condensed matter | 3 |
| | | Physics, fluids & plasmas | 3 |
| | | Instruments & instrumentation | 3 |
| | | Physics, mathematical | 2 |
| | | Physics, multidisciplinary | 2 |
| | | Optics | 2 |
| | | Quantum science & technology | 1 |
| | | Nuclear science & technology | 1 |
| | | Acoustics | 1 |
| | | Remote sensing | 1 |
| Electrical engineering | 55 | Engineering, electrical & electronic | 28 |
| | | Telecommunications | 16 |
| | | Automation & control systems | 7 |
| | | Robotics & automatic control | 4 |
| Mechanical engineering | 36 | Mechanics | 17 |
| | | Engineering, mechanical | 9 |
| | | Engineering, aerospace | 6 |
| | | Aerospace engineering & technology | 4 |
| Geosciences, environment | 34 | Geosciences, interdisciplinary | 12 |
| | | water resources | 4 |
| | | Engineering, environmental | 3 |
| | | Environmental sciences | 3 |
| | | Geochemistry & geophysics | 3 |
| | | Green & sustainable science & technology | 3 |
| | | Limnology | 2 |
| | | Meteorology & atmospheric sciences | 2 |
| | | Geography | 1 |
| | | Geography, physical | 1 |
| Multidisciplinary | 34 | Engineering, multidisciplinary | 24 |
| | | Engineering | 6 |
| | | Multidisciplinary sciences | 4 |
| Mathematics (applications) | 24 | Mathematics, interdisciplinary applications | 16 |
| | | Statistics & probability | 8 |
| Biosciences | 23 | Biochemical research methods | 4 |
| | | Neurosciences | 3 |
| | | Biophysics | 3 |
| | | Biotechnology & applied microbiology | 3 |
| | | Engineering, biomedical | 2 |
| | | Pharmacology & pharmacy | 2 |
| | | Mathematical & computational biology | 2 |
| | | Radiology, nuclear medicine & medical imaging | 1 |
| | | Medical informatics | 1 |
| | | Biology | 1 |
| | | Audiology & speech-language pathology | 1 |
| Civil engineering | 14 | Transportation science & technology | 6 |
| | | Transportation | 4 |
| | | Engineering, civil | 3 |
| | | Construction & building technology | 1 |
| Materials science | 16 | Materials science | 4 |
| | | Materials science, composites | 1 |
| | | Materials science, multidisciplinary | 8 |
| | | Metallurgy & metallurgical engineering | 3 |
| Social sciences | 8 | Management | 5 |
| | | Information science & library science | 1 |
| | | Social sciences, mathematical methods | 1 |
| | | Economics | 1 |
| Industrial engineering | 4 | Engineering, industrial | 2 |
| | | Engineering, manufacturing | 2 |

Table 1: Application fields of the NOMAD software.

[1]The MATLAB version of MADS was distributed before the actual paper [23] paper was published in 2006. Coding was done from the 2004 associated technical report.

The proportions of these WoS occurrences are illustrated in Figure 1.

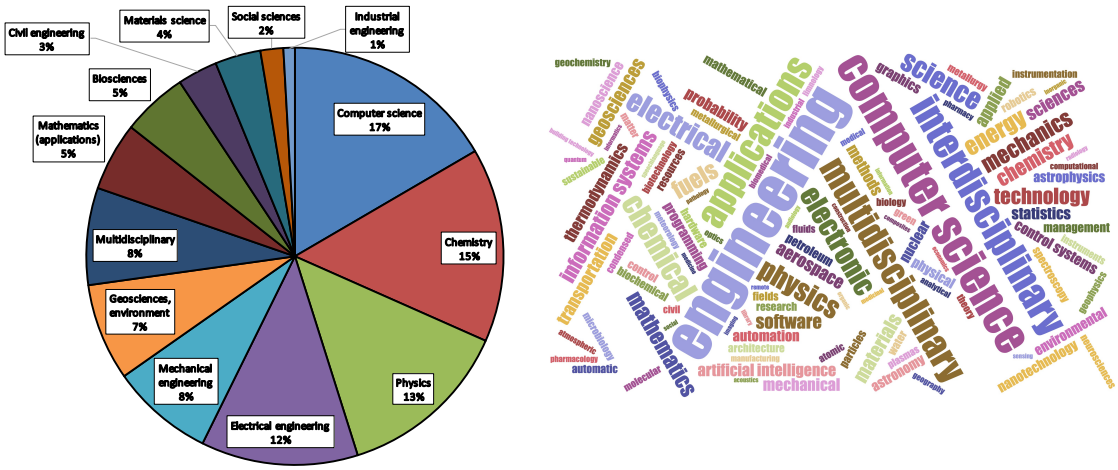


Figure 1: Left: Distribution of the application fields that cite [107], based on the data of Table 1. Right: "Word cloud" graph of all WoS categories from Table 1, generated with the Word Cloud Generator of `https://www.jasondavies.com/wordcloud`.

The present survey contains a selection of applications that have been addressed using the MADS algorithm or the NOMAD software over the last twenty years. It is far from being exhaustive. Rather, we prefer to illustrate different areas in which MADS was successfully applied. For each of these areas, we provide a global perspective. Such a general vision is only possible because of the expertise gained by the development and utilization of direct search methods over a long time period. It is also important to note that both MADS and NOMAD were greatly improved during these years, mainly thanks to the lessons learned with their usage in these areas.

The core of this survey is composed of Section 2 on applications at Hydro-Québec, Section 3 on applications in materials sciences and Section 4 on selected applications in engineering design. Section 5 lists other areas in which direct search methods were applied, and also mentions some patents using it.

# 2 Applications in energy at Hydro-Québec

Hydro-Québec (HQ) is a public utility that manages the generation, transmission and distribution of electricity in Québec [97]. This section describes many optimization problems addressed by HQ using NOMAD.

## 2.1 Apparatus positionning

One of the first project using NOMAD at HQ involved optimal positioning of GMON devices [12]. A GMON [61] is a monitoring apparatus that measures the attenuation of

gamma rays emanating from the ground to infer snow water equivalent (SWE) in remote locations. SWE measurements are kriged to obtain a grid of estimates over the territory, which is used to forecast the inflows that reservoirs will receive during the snowmelt. The areas of the studied territories range from 24,000 to 90,000 km$^2$. The GMONs must be positioned to minimize the estimate errors from the kriged values. Since the GMONs cannot be installed everywhere (not over water, urban or agricultural areas, the surrounding vegetation should not be too dense, the soil needs to be sufficiently rich in gamma radiation, etc.), the positioning domain is highly fragmented and prevented NOMAD from exploring beyond the initial solution. To overcome this difficulty, two strategies have been developed. The first one mapped the fragmented domain to a continuous one. The second led to the development of groups of variables in NOMAD. The feature allows to link the $xy$-coordinates of GMONs, which forces to only move one GMON at a time, and consequently, helped to generate better solutions.

The positioning of the GMONs was also considered to have SWE measurements on the ground to improve and/or complete the snow maps generated from satellite data (SSM/I and AVHRR) [13].

## 2.2 Hydrological model calibration

A group of projects involving NOMAD revolves around the tuning of hydrological forecast models. Hydrologists at HQ have developed the model parameter optimization software EAUptim to calibrate the 23 parameters of the conceptual model HSAMI [76]. EAUptim uses NOMAD as optimization library [125]. By adding threshold constraints on internal hydrological variables to the calibration process, EAUptim improves the model response in validation, which is suitable for hydrological forecasts, but also allows robust hydrological projections. EAUptim was used to calibrate HSAMI over 305 watersheds ranging from 10 to 69,000 km$^2$ to study the impact of climate change on hydrological regimes for the province of Québec at the 2050 horizon [85]. The variables of interest are streamflow, snow accumulation and actual evapotranspiration (AET). The model was calibrated with the constraint of correctly rendering the AET annual cycle. The results indicate that the annual streamflow will increase for all the province, but the distribution varies: higher in winter, lower in summer and earlier spring floods.

Concurrently with this work, EAUptim was deployed on a computing cluster to allow paralleling evaluations beyond the native $2n$ polling directions of MADS [109] (where $n$ is the number of variables in the optimization problem). The aim is to be able to use as much as 1,000 cores and to feed them efficiently to explore the space of variables. The parallel implementations P-MADS, COOP-MADS and PSD-MADS [25, 108] have been integrated as solvers to the cluster version of EAUptim. The results showed that using several direction generators (P-MADS) or several independent searches (COOP-MADS, PSD-MADS) to generate multiple $2n$ evaluations (up to the number of cores) was not sufficient to proportionally improve performance. This work led to a reflection that ended with the need to develop a fourth version of NOMAD.

HYDROTEL [75] is another hydrological model used at HQ. While HSAMI is a con-

ceptual model, HYDROTEL is a distributed physically-based one, and hence, while simulating with the former requires a few seconds, it may take minutes with the latter. The DDS [147] and NOMAD optimization methods have complementary features [93]. DDS showed abilities to quickly identify promising basins of solutions and NOMAD was able to refine nearby solutions. An hybrid algorithm, denoted DDS-MADS, in which the global search of DDS is combined to the local search of MADS, is proposed in [96]. Computing time are significantly reduced without sacrificing robustness and stability of calibrations.

Reduced-fidelity physic-based models have been next developed to be used as surrogate models for improving the performances of DDS-MADS [92, 94]. To do so, the number of points with meteorological data was reduced by 87.5%, the simulation period reduced to 12 month and coarse discretization of watershed into sub-basins. These reductions bring poor speed-up when applied individually, but together, they reduce the computational time by a factor of 15 or more.

The proposed reduced-fidelity models were then integrated into DDS-MADS [92, 95]. Among the different frameworks tested, the best results have been obtained when DDS-MADS is only executed with reduced-fidelity models and if there are any evaluations left to spend, to pursue with MADS with a local search on the full and complete model. Compared to running DDS-MADS with the complete model, this reduces the overall computing time by a factor ranging from 40% to 64%.

## 2.3 Parameter tuning

For security reasons, three-dimensional modeling of open channel flows is regularly used to study the behavior of control structures under unobserved situations. Such studies can be performed with OpenFOAM [84], an open-source simulation software for computational fluid dynamics that decomposes the simulation domain for parallel computing. Unfortunately, these studies mostly rely on one processor and require an important amount of local memory, which is particularly limiting when the mesh contains millions of cells. A new method was developed at HQ to address these issues [48] and is based on the Zoltan library [103], which offers 10 parallel decomposition algorithms, each with quantity of parameters. Their meaning and how they interact are not easy to understand in practice. Moreover, the optimal choice of algorithms and parameters could vary from one mesh to another. This was addressed by a blackbox parameter tuning approach [36] with NOMAD using categorical variables [21]. The algorithm and its parameters were selected to minimize the communication volume between the processors. Compared to the best mono-processor decomposition algorithm, the proposed approach reduced the decomposition time by a factor of 36 for a mesh of 7 million cells with 120 partitions.

HQ develops the electrical simulator Simscape Power Systems (SPS), which allows to model and simulate electric power systems within the MATLAB Simulink environment [67]. SPS has a functionality to estimate electrical parameters of asynchronous machines based on manufacturer specifications [122], which is similar to a model calibration problem. To avoid additional charges to the users, it was decided to no longer rely on MATLAB Optimization Toolbox for this particular function and instead use a trust

region approach based on [49]. Although the new method was fast enough to maintain the customer experience, the proposed default setting appeared inappropriate to generate quality solutions. This turned out to be a parameter tuning problem and NOMAD was used to adjust the parameters to maximize the model calibration. A set of 115 asynchronous machines was used as test problem. The parameter optimization brought an improvement of 33% on the quality of calibrations. The resulting implementation is integrated to the `power_AsynchronousMachineParams` function from MathWorks release R2018a [123].

Tuning problems do not only arise with computer models and simulators, but also with physical control devices such as power system stabilizers (PSS). NOMAD has been applied for tuning PSS considering several generators simultaneously [10] instead of in sequence [88]. PSSs are installed on generators to protect them against faults on the network by damping inter-area, inter-plant and inter-machine oscillations. Damping and gain margin must be specified for each oscillation mode. Their performance can be evaluated by simulation, as with SPS, against fault scenarios. By using the groups of variables feature [12] (one group per generator), the trajectory of improvements has provided a feasible solution for implementing the new optimal values in the PSSs (the sequence of adjustments to be made without decreasing overall performance at any moment).

## 2.4 Asset management strategies

Optimization problems also arise in asset management. HQ has set up an important project for its transmission system, named PRIAD, in order to optimize its maintenance and asset management strategies [102]. The optimizations will rely on a power grid reliability simulator coupled with a power flow software. The former to generate failure events and the latter to establish the resulting power interruptions or reductions of transmission capacity (if any). To achieve this, models predicting asset reliability based on maintenance strategies are needed. These models are built from expert knowledge and calibrated with NOMAD to reproduce historical failure data [66]. In case of inconsistency, the approach identified biases in the data, and proposed corrections to improve their collection. The approach also allowed to question the experts on some of their previous assessments and to revise them based on calibration results. Hence, by iterating on the data and with the experts, a proper predictive model was obtained.

Given an asset model, it is now possible to feed the reliability simulator with failure rates corresponding to any variant of the maintenance strategy. The simulator relies on Monte Carlo simulations, which means it is doubly noisy: Noisy between neighboring points, but also at each point of the domain since simulating twice a same point produces different results. This led to new research activities to adapt MADS to stochastic blackboxes [11]. Numerical experiments with VME [115], a reliability simulator developed by EDF R&D, on a small problem of determining five investment dates in asset management [53] showed that MADS and ROBUST-MADS [30] were too expensive in computational time. The approach proposed in [11] explicitly considers the standard deviation from the Monte Carlo simulations into the internal mechanisms of MADS and drastically

reduces the calculation time from several days to a few hours.

### 2.5 Isolated power grids

HQ owns 21 isolated power grids, mostly located in northern Québec. NOMAD was used to minimize diesel consumption in those grids by optimizing the start and stop thresholds of gensets [44]. A 1-minute time step isolated grid simulator was used to compute the consumption of gensets resulting from modified thresholds. The difficulty is that one rule prevails over the applicable ones. This brings discontinuities in the solution domain, which leads to ineffective search. The use of groups of variables [12] helps to restore efficiency and fixed variables to remove discontinuities (by deactivating the rules alternately).

Using the same simulator as above, NOMAD was also used to study the integration of renewable energies (wind, solar, storage) to reduce diesel consumption and greenhouse gases in its isolated power grids [52]. The best mix of renewable energies must be identified, including the choice, size and number of equipment to be installed. Simulations were conducted over a period of 20 years to capture the degradation of batteries, allowing only one replacement of cells after 10 years [44].

## 3 Applications in materials science

The MADS algorithm and the NOMAD software package were successfully applied in different fields of materials science to (i) optimize material performances, (ii) optimize industrial processes and (iii) to design new materials. A goal in alloys design is to determine a set of compositions, temperature and pressure that maximizes functions which depend on phases, volume fractions and on the thermodynamic, structural, dynamics, thermal transport and surface properties. The industrial processes optimization either involves the determination of an optimal material or optimal process conditions such as temperature, pressure, weight fraction between different chemical constituents, etc.

The FactSage software [43] consists of a suite of programs and databases to perform chemical equilibrium calculations on isolated closed and open systems by means of Gibbs energy minimization techniques. The FactSage database contains thermodynamic information as functions of temperature, pressure and composition for over 7,000 pure substances (compounds) and hundreds of multicomponent solid and liquid solutions for a large variety of materials including steels, light metals, rares earth, noble metals, oxides, salts, semiconductors, refractory.

Equilibrium calculations in multicomponent systems can predict quantities such as phase volume fractions, freezing ranges, segregation of alloying elements, phase formation, accompanying volumes, enthalpy changes and the amounts of various precipitates during subsequent annealing. An accurate knowledge of these properties is of critical importance in the understanding and description of mechanical, electrical and corrosion resistance properties. Beside equilibrium calculations, FactSage may be used to simulate

para-equilibrium and the cooling effect upon the phases constitution of solid systems for microstuctures.

Combining FactSage software and database with NOMAD has lead to the design of several innovative materials and the optimization of important industrial processes for the production of primary metals such as iron, aluminium and copper. This combination also allows alloys to screen potential multicomponent alloys, searching for compositions having desired properties and phase assemblages within a reasonable amount of time. In multicomponent systems, an evaluation of a given property by FactSage can be time consuming from few seconds up to few minutes depending on the system size and the calculation type. Determining optimal alloys under a given set of constraints by calculating the properties over a grid of compositions is almost impossible for a system with more than four constituents.

## 3.1 Material performance optimization

From a practical point of view, the design of material consists in either minimizing, maximizing or targeting specific properties. Targeting values is achieved by minimizing the norm of the difference between a function and its target value. When dealing with optimization problems with more than two objectives, decomposing the problem into several sequential phased biobjective problems (where the third, fourth and higher order objectives are treated as more and more restrictive constraints) is preferable to applying multiobjective optimization [78].

In materials science, the properties depend on the amount of each phases, i.e. compounds (e.g. $Fe_3C$ or $Al_3Ni$) or solutions, constituting the system. However, in a multicomponent systems, a given phase may be stable in a narrow range of composition, temperature and pressure. The identification of the range of stability of a given phase assemblage in multicomponent systems is one of the most difficult problem to solve in the alloys design. FactSage can calculate the phase stability at a specific temperature pressure and composition, but cannot directly determine the range of stability of a given phase. The range of phase stability in systems with up to 12 components are predicted in [77, 79, 80] for different problems. This is the most remarkable achievement of MADS in term of alloys design. The robustness of MADS in the determination of phase stability in multicomponent system lies in the use of Latin hypercube sampling and Variable Neighborhood Search [17] strategies.

## 3.2 Optimal industrial processes

In many applications, it is desirable to find alloys with minimum liquidus (melting) temperature, target a specific freezing range (region of coexistence between the liquid and solid phases), desired density range and shrinkage ratio and but most importantly the type and amount of precipitates which can be compounds and/or solutions. Case studies [77, 79] lead to improvement of mechanical properties of light metals alloys by maximizing the volume fraction of several specific Aluminium (Al) rare earth (RE = La, Ce, Pr, Nd, Pm,

Sm) intermetallics of type $Al_nRE_m$ ($n > m$) under constraints on liquidus temperature, density and heat capacity. Managing the constraints on the liquidus temperature is in general not trivial. Even though liquidus temperature is a continuous function of composition, the liquidus temperature has no analytically exploitable structure and it possesses several local minima and saddle points even in a narrow composition range. The management of the constraints on compositions, heat capacity and density is simpler. Many alloys have been identified to be potential low cost candidates for the next generation of light metals alloys for lighter automotive applications.

Predicting the global and subsequent local minima upon the liquidus temperature hypersurface is a real challenge in several materials science applications. A local minima upon the liquidus surface is characterized by the chemical reaction $Liquid \rightarrow S_1 + S_2 + \ldots + S_n$ where the $S_i$ are the solids (compounds and solutions) constituting the systems. In other words, a local minima upon the liquidus temperature corresponds to a null freezing range. A Phase Change Materials (PCM) is a local minima upon the liquidus surface, and have numerous application in thermal solar energy [138]. In the context of fight against the global warming, identifying sustainable and low cost PCM with good performance in terms of heat storage capacity is a real challenge. A methodology to determine all local minima upon the liquidus surface is presented in [82]. The technique consists in minimizing the freezing range up to zero. When a PCM solution $x^0$ is identified, an additional constraint $\|x - x^0\|^2 \geq \epsilon$ is added, where $\epsilon > 0$ is small adjustable parameter. Then, the minimization procedure is restarted again with the above constraint and so one and so forth until no more PCM solutions are found. This method has be proven to be reliable, as it predicted with an appreciable accuracy the global minimum upon the liquidus temperature in an 8 components salts systems for which the liquidus temperature was measured experimentally [132]. More recently [81], the same procedure produced 30 new potential low cost PCM materials with excellent heat storage capacity.

Lastly, MADS was applied to optimize energetic efficiency and therefore reducing the greenhouse gas emissions of key industrial processes for the production of primary metals [78, 89].

## 3.3 Design of new materials

The MADS algorithm was also applied to design innovative materials. The most notable example is that of so-called *high entropy alloys*. High entropy alloys are a system with more than 5 constituents consisting in a single Face Centred Cubic (FCC) or Body Centred Cubic (BCC) solid solution or in some case in a dual FCC+BCC phase solid solution [126]. High entropy alloys have remarkable mechanical and corrosion resistance properties. The main limiting factor in the large scale industrial production is the relatively high cost of raw materials and the high temperature range where the single or dual phase are stable. The main challenge in the identification of entropy alloys is the predictability of the stability range of single or dual phase. In order to predict it, a methodology using MADS was proposed [80]. According to the thermodynamics principles, when the activity of a given phase equals 1, this phase is formed. Thereafter, starting from the composition where the

activity is equal to 1, the amount of FCC and/or BCC is maximized until the amount of all other phases is null. For economical and industrial processes issues constraints on cost and on the temperature stability range of FCC and/or BCC phase are added. The capability of MADS to identify high entropy alloys according to this procedure was clearly demonstrated. More than 100 low cost high entropy alloys with a reasonable temperature stability range have been identified by MADS [80] thereby opening the door to new potential sustainable applications in particular for the automotive industry.

Finally, the MADS algorithm was used for metamaterials in [26, 68]. More specifically, these works aim to adapt the spectral response and near-field interactions of split ring resonator metamaterials, by tuning the spectral position of resonant reflection peaks and near-field interactions within the metamaterial, over the near-infrared spectrum.

# 4 Applications in computational engineering design

Computer-aided engineering has revolutionized the engineering design process: computational models are now used to assess design alternatives rapidly and enable conducting elaborate optimization studies. A major challenge of this simulation-based design optimization paradigm is that the gradients of the objective and constraint functions evaluated by means of computational models either are not guaranteed to exist theoretically or, when they do exist theoretically, cannot be approximated with reliable accuracy without unreasonably large computational effort [128]. In these cases, DFO and BBO algorithms are the only option [98]. Because of their simplicity, the most popular DFO algorithms in the engineering design community are based on heuristics (e.g., genetic algorithms, simulated annealing, particle swarm optimization, etc). These algorithms are designed to always yield results, which largely explains their popularity. However, the design engineer cannot characterize the optimality (or lack thereof) of the obtained results as these heuristics are not supported by a useful convergence analysis [28].

## 4.1 First uses of MADS in engineering design

The advent of modern direct search methods has offered an invaluable toolkit to design engineers for conducting derivative-free optimization whose results are supported by convergence theory [101]. The first engineering design application reported in the literature utilized the direct ancestor of MADS with mixed variable programming [21]; a thermal insulation system was optimized with respect to categorical variables (number and material type of heat shields), resulting to a 65% improvement in performance relative to the best design known until then [100]. An interesting feature of the design optimization problem was that the number of optimization variables was a function of one of the optimization variables. The analysis models and constraint handling procedure used in [100] were enhanced by Abramson [2, 3], which led to even larger performance improvements.

A particularly challenging engineering design problem [121] was solved using MADS. Three optimization problems corresponding to aircraft sizing, route network configuration,

and aircraft allocation were integrated into a blackbox representing an air transportation system of systems, which was then optimized to minimize fleet operation cost. Figure 2 depicts the nested optimization problem on the left and the response surface of the blackbox on the right; the white "pixels" on the response surface denote areas of the design space where the blackbox did not return a function value. MADS did particularly well handling such so called hidden constraints. The size and complexity of this mixed variable programming problem grows rapidly with increasing number of network nodes; results from the literature with only 7 nodes were improved to 15.

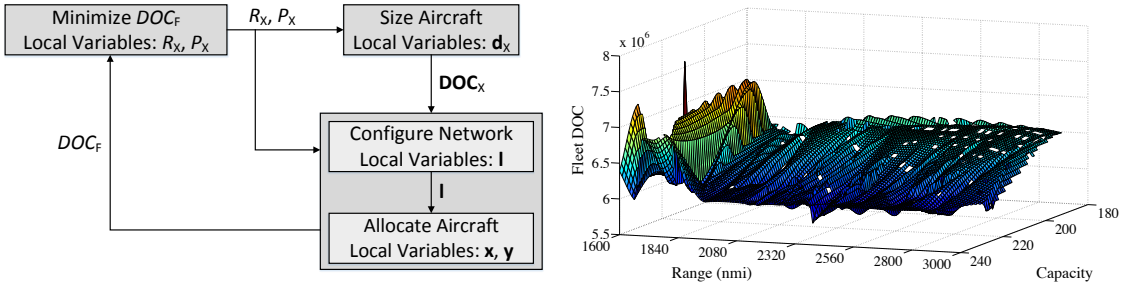


Figure 2: Nested blackbox optimization problem (left) and blackbox response surface for 15 network nodes (right) [121].

MADS was also used to optimize an electro-thermal wing anti-icing system [129]. Evaluating the performance of the anti-icing system required the numerical solution of a conjugate heat transfer problem between the fluid and solid domains in both running-wet and evaporative regimes, which is computationally expensive. are presented. Therefore, the authors made use of both quadratic and statistical surrogates based on the work presented in [143]. Computationally expensive simulations were also necessary to model sound regimes in order to optimize the design of a trumpet's bore in order to improve intonation. Results were reported in [150] and [149] for unconstrained and constrained problem formulations, respectively.

## 4.2 Biomedical applications

The use of numerical optimization has been recently introduced to the field of mathematical oncology with a focus on cancer nanotherapy, where drugs are safely carried to tumors via nanoparticles. The design of these nanoparticles highly influences treatment efficacy, thus creating a need to search throughout large design spaces for the optimal nanoparticle structural variables.

Chamseddine and Kokkolaras [56] developed a mechanistic model of nanoparticle-mediated drug delivery in a two-dimensional vascularized tumor and used MADS to determine optimal nanoparticle size and aspect ratio. A bi-objective optimization problem was formulated and solved by BIMADS [37] to quantify the tradeoff between two competing objectives: maximizing nanoparticle vascular binding and maximizing dead tumor

area. Based on the findings of that work, the authors developed a dual delivery strategy, in which two different nanoparticle designs formulate one regimen. MADS was used to solve a sequential optimization problem, increasing the dead tumor area by 16% without the need of additional drugs [57]. Chamseddine et al. [54] considered then a dynamic model to evaluate tumor size after treatment in order to minimize its size while maximizing targeting. The optimization problem was extended to consider the properties of nanoparticle surface binding proteins and exploring new traits of nanoparticle biodistribution. In addition, multiple treatment cycles were simulated, where nanoparticles were re-optimized along the treatment in a form of adaptive therapy.

Finally, design optimization of nanoparticles was performed in [55] for a cohort of tumors which vary in size – an important clinical covariate. In this paper, the authors also optimized the drug diffusivity along with the nanoparticle size. The results suggested that integrating the selection of the drug and the nanoparticle size in practice may lead to better treatment outcomes.

## 4.3 Multidisciplinary design optimization

MADS has been also used as the main tool for multidisciplinary design optimization (MDO) and multimodel management. Talgorn and Kokkolaras [141] developed a user-friendly compact implementation of an augmented Lagrangian algorithm for coordinating distributed MDO problems [144]. An associated publicly available MATLAB-based software package offers MADS as the default optimization algorithm although the user can link any other algorithm as they see fit (one of the advantages of distributed MDO formulations is that different algorithms can be used for different subproblems depending on their features and properties). Talgorn et al. [145] considered both MADS and gradient-based algorithms to solve the subproblems formulated by an interdisciplinary feasible architecture known as non-hierarchical analytical target cascading. Results show that MADS yields higher-consistency solutions, but with greater variance than the MATLAB implementation of an interior point gradient-based algorithm.

Bayoumy and Kokkolaras [45] developed a relative adequacy framework (RAF) for multimodel management in design optimization and implemented their strategy by means of a trust-region management framework that utilizes MADS as the optimization algorithm. The RAF is used to quantify and utilize relative errors among available models to enhance the predictive capability of models associated with lower computational cost, and use them in certain areas of the design space as the latter is being explored during the optimization process. Specifically, the MADS search step is used to solve a surrogate optimization problem. In this problem, surrogates are not built for the optimization functions, but for model errors. The purpose is to mitigate discrepancy among available models to approach the adequacy level of a reference model while favoring the utilization of inexpensive models. In the MADS poll step, models are selected based on trust-region principles.

A pair of papers [46, 47] extends the RAF for MDO by utilizing MADS for monolithic, distributed, and time-dependent problems. When using the RAF to solve multidisciplinary feasible problem formulations, the key arguments for using MADS are: (1) MADS is the

only algorithm that offers the (optional) search step where SM for relative errors can be trained and/or selected; (2) the optimization process does not stall if a multidisciplinary analysis fails to return a value. For distributed MDO workflows, results show that penalizing surrogate errors among available models using trust-region principles in each subproblem contributes to mitigating the computational cost of the MDO process compared with the high-fidelity MDO one while ensuring adequate accuracy.

### 4.4 Other applications in mechanical engineering

MADS has also been used in assembly optimization problems and remanufacturing-based design strategies. Lupuleac et al. [117] considered the problem of optimizing temporary fastener patterns in aircraft assembly and compared MADS to a local exhaustive search and simulated annealing for several problems including a real Airbus A350-900 wing-to-fuselage assembly. The results indicated that simulated annealing did not provide repeatable results and required large numbers of function evaluations. Both the local exhaustive search and MADS yielded good results; however, the former obviously required many more function evaluations than the latter. Al-Handawi et al. [9] considered remanufacturing as a strategy to address changing requirements in design problems.

Sets of optimal design solutions, as opposed to single-point designs, are obtained using MADS. Parametric studies are then conducted to obtain optimal solutions for different parameter values, which are used to build a response surface providing a map from the design space to the parameter space. In the parameter space, a manufacturing transition rule is formulated to identify sets of design solutions that are scalable by additive manufacturing. Scalable design solutions are then mapped back to the design space to obtain the corresponding design variable values.

The design of Francis hydraulic turbine runner –moving blades– plays an important role in the energy production efficiency of an hydraulic dam. NOMAD was used to redesign an existing runner achieving high performance for new operating conditions, using multi-fidelity computational fluid dynamics analyses and a multiobjective approach for optimizing the blades shape [41, 42].

Aircraft engine blades geometries are optimized to account for structural contact interactions between the blades and the casing. NOMAD is used to solve a constrained problem where only the three-dimensional properties of the blade are allowed to vary [104]. The objective function is a simplified criteria describing the clearance between the top of the blade and the casing for one of the free-vibration mode of the blade. Contact simulations are conducted on both initial and optimized blades and show that the vibration level of optimized blades following the contact interaction are significantly reduced.

## 5 Applications of direct search methods in various fields

The MADS algorithm and its implementation in NOMAD has also been used in a variety of fields, as illustrated in Table 1 and Figure 1. The survey [15] lists applications in

shape optimization, positioning problems, parameter estimation, tuning of algorithms and engineering design. Section 5.1 of the present work discusses recent applications in road design, Section 5.2 enumerates applications in cardiovascular geometry applications, Section 5.3 mentions many uses of NOMAD in astrophysics, and Section 5.4 discusses patents associated to direct search optimization.

## 5.1 Road design optimization

There has been important progress over the last five years in road design optimization. This research addresses the question of finding the shape of a curve describing a road that minimizes the construction cost while satisfying many design specifications. The problem is divided into 3 related subproblems First, the horizontal alignment optimization that determines the number and position of horizontal intersection points and corresponding curve radii. NOMAD is the recommended solver according to [111, 113]. Second, the vertical alignment optimization that determines vertical position with specified rates of curvature and bounded grades. NOMAD is recommended for presetting control points [112]. Third the earthwork optimization that minimizes the total cost of hauling, excavation and embankment. Bi-level approaches resulting in potentially millions of dollars of savings are proposed in [127, 152] and multi-fidelity direct search algorithms are studied in [40] for problems that take 20 to 24 hours to run.

## 5.2 Cardiovascular geometries

The paper [118] provides an historical perspective on the development of cardiac surgery and links between engineering, medicine and surrogate-based direct search optimization that facilitated clinical advances. The paper discusses the application of these tools to two clinically relevant examples in pediatric cardiology.

In [119], a framework for coupling optimal shape design to time-accurate 3D blood flow simulations in idealized cardiovascular geometries is presented. The optimization of a Y-graft design for the Fontan procedure, a surgery used to treat single ventricle heart defects is studied in [159, 158] under pulsatile rest and exercise flow conditions. Stent implantation for the treatment of coronary artery disease is studied in [86, 87]. These papers analyse idealized stent geometries using a derivative-free optimization algorithm coupled with computational fluid dynamics. Vein graft failure is a prevalent problem in vascular surgeries, due to severe changes in pressure and flow. Models of venous growth and remodelling are proposed in [69, 136, 130, 140] and surrogate-base direct search optimization techniques are used to accelerate parameter estimation. Shape optimization problems motivated by hemodynamically-driven surgical design are studied in [153].

## 5.3 Astrophysics

There are numerous applications of direct search methods in astrophysics. In a paper with more than 700 co-authors [1], NOMAD was used for a computationally intensive search

for periodic gravitational waves carried out with the Einstein@Home volunteer distributed computing project.

In the context of black hole observation, NOMAD was used to find the set of parameters of a Monte Carlo model that yields the best fit to observed kinematics [124].

The first interstellar object within our solar system, now called 1I/'Oumuamua, was discovered in 2017. Trajectory analyses were conducted using NOMAD, revealing characteristics that have never before been observed in a celestial body [91].

Hall Effect thrusters are flown in space missions. They incorporate a magnetic circuit that generate a specific electromagnetic flux distribution inside and near the outlet of a plasma channel. The design of this type of structure requires a specific magnetic topography in the thruster channel with given magnetic field radial component values and a certain inclination of this field lines. NOMAD was used to solve the inverse magnetostatic problem to obtain a new low-erosion magnetic configuration [133, 134].

Kinematics analysis of galaxies are performed in [131], revealing various deviations from pure circular rotation in the inner kiloparsec of seven galaxies, including kinematic twists, decoupled and counter-rotating cores. That paper states that the MADS algorithm is *becoming quite indispensable in practice*.

## 5.4 Patents associated to direct search methods

In addition to research papers, there have been many patent filed related to direct search methods. A query for patents referring to the MADS algorithm or to the NOMAD software package generated the entries listed in Table 2.

| Context | Origin | References |
|---|---|---|
| Analysis of radiographic images | Los Alamos National Laboratory | [146] |
| Calibrating parameters in a patterning process | ASML Netherlands BV | [160] |
| Controlling the readhesion of a flow | INRIA | [72] |
| Cone beam CT image scattering correction | Shenzhen Institutes Of Advanced Technology | [114] |
| Designing narrowband light filters | California Institute of Technology | [73, 74] |
| Heat exchanger design | Hamilton Sundstrand Corporation | [50] |
| Maintaining vascular connections | Imp Innovations Ltd | [155] |
| Optimization processes in aeronautic design | The Boeing Company | [7, 70, 71, 90] |

Table 2: Patents associated to the MADS algorithm or to the NOMAD software.

# 6 Discussion

This review mainly focuses on three particular fields of applications of blackbox optimization. Over the past two decades, direct search methods such as MADS greatly evolved

through algorithmic research motivated by a vast variety of applications. Since its introduction in 2006, MADS can now treat continuous and discrete variables including categorical variables, blackbox constraints, multiple objectives, parallelism, larger and larger problems, and more recently stochastic blackboxes. These improvements, along with the availability of greater and better computing resources, allow to address problems for which the blackbox approach is the only applicable possibility. In particular, one emerging field of applications is the optimization of the hyperparameters of deep neural networks, for which MADS and NOMAD are natural candidates.

The variety of application fields of BBO and DFO has considerably grown in the past two decades and will certainly continue to grow at a rapid pace in future years.

**Acknowledgments** The authors would like to thank Martin Beaudoin, Patrice Brunelle, Patrick Jeandroz, Solène Kojtych, Dragan Komljenovic, Louis-Alexandre Leclaire, Marie Minville, Christophe Tribes and Walid Zegal for discussing some applications.

# References

[1] J. Aasi et al. Einstein@Home all-sky search for periodic gravitational waves in LIGO S5 data. *Physical Review D*, 87:042001, February 2013.

[2] M.A. Abramson. *Pattern Search Algorithms for Mixed Variable General Constrained Optimization Problems*. PhD thesis, Department of Computational and Applied Mathematics, Rice University, August 2002.

[3] M.A. Abramson. Mixed variable optimization of a Load-Bearing thermal insulation system using a filter pattern search algorithm. *Optimization and Engineering*, 5(2):157–177, 2004.

[4] M.A. Abramson, T.J. Asaki, J.E.Dennis, Jr., R. Magallanez, Jr., and M.J. Sottile. An Efficient Class of Direct Search Surrogate Methods for Solving Expensive Optimization Problems with CPU-time-related Functions. *Structural Multidisciplinary Optimization*, 45(1):53–64, 2012.

[5] M.A. Abramson, C. Audet, J.W. Chrissis, and J.G. Walston. Mesh Adaptive Direct Search Algorithms for Mixed Variable Optimization. *Optimization Letters*, 3(1):35–47, 2009.

[6] M.A. Abramson, C. Audet, J.E. Dennis, Jr., and S. Le Digabel. OrthoMADS: A Deterministic MADS Instance with Orthogonal Directions. *SIAM Journal on Optimization*, 20(2):948–966, 2009.

[7] M.A. Abramson, A.J. Booker, E.J. Cramer, and J.P. Simonis. Search and poll method for solving multifidelity optimization problems. Patent US 2017/0011143 A1, 2017.

[8] L. Adjengue, C. Audet, and I. Ben Yahia. A variance-based method to rank input variables of the Mesh Adaptive Direct Search algorithm. *Optimization Letters*, 8(5):1599–1610, 2014.

[9] K. Al-Handawi, P. Andersson, M. Panarotto, O. Isaksson, and M. Kokkolaras. Scalable set-based design optimization and remanufacturing for meeting changing requirements. *ASME Journal of Mechanical Design*, 143(42), 2020.

[10] S. Alarie, N. Amaioua, and C. Cyr. Global Optimization with NOMAD for the Simultaneous Tuning of Several Power System Stabilizers. In *CORS/INFORMS International Conference*, Montreal, June 2015.

[11] S. Alarie, C. Audet, P.-Y. Bouchet, and S. Le Digabel. Optimization of noisy blackboxes with adaptive precision. Technical Report G-2019-84, Les Cahiers du GERAD, 2019.

[12] S. Alarie, C. Audet, V. Garnier, S. Le Digabel, and L.-A. Leclaire. Snow water equivalent estimation using blackbox optimization. *Pacific Journal of Optimization*, 9(1):1–21, 2013.

[13] S. Alarie and L.-A. Leclaire. Positionnement de stations GMON avec inversion du modèle HUT. In *Optimization Days*, Montreal, May 2013. GERAD.

[14] Aspentech. Aspen chemical engineering simulator. https://www.aspentech.com.

[15] C. Audet. A survey on direct search methods for blackbox optimization and their applications. In P.M. Pardalos and T.M. Rassias, editors, *Mathematics without boundaries: Surveys in interdisciplinary research*, chapter 2, pages 31–56. Springer, New York, NY, 2014.

[16] C. Audet, V. Béchard, and J. Chaouki. Spent potliner treatment process optimization using a MADS algorithm. *Optimization and Engineering*, 9(2):143–160, 2008.

[17] C. Audet, V. Béchard, and S. Le Digabel. Nonsmooth optimization through Mesh Adaptive Direct Search and Variable Neighborhood Search. *Journal of Global Optimization*, 41(2):299–318, 2008.

[18] C. Audet, G. Caporossi, and S. Jacquet. Tuning Runge-Kutta parameters on a family of ordinary differential equations. *Operations Research Letters*, 48(4):467–471, 2020.

[19] C. Audet, P. Côté, C. Poissant, and C. Tribes. Monotonic grey box optimization. *Optimization Letters*, 14(1):3–18, 2020.

[20] C. Audet and J. Côté-Massicotte. Dynamic improvements of static surrogates in direct search optimization. *Optimization Letters*, 13(6):1433–1447, 2019.

[21] C. Audet and J.E. Dennis, Jr. Pattern search algorithms for mixed variable programming. *SIAM Journal on Optimization*, 11(3):573–594, 2001.

[22] C. Audet and J.E. Dennis, Jr. A pattern search filter method for nonlinear programming without derivatives. *SIAM Journal on Optimization*, 14(4):980–1010, 2004.

[23] C. Audet and J.E. Dennis, Jr. Mesh Adaptive Direct Search Algorithms for Constrained Optimization. *SIAM Journal on Optimization*, 17(1):188–217, 2006.

[24] C. Audet and J.E. Dennis, Jr. A Progressive Barrier for Derivative-Free Nonlinear Programming. *SIAM Journal on Optimization*, 20(1):445–472, 2009.

[25] C. Audet, J.E. Dennis, Jr., and S. Le Digabel. Parallel Space Decomposition of the Mesh Adaptive Direct Search Algorithm. *SIAM Journal on Optimization*, 19(3):1150–1170, 2008.

[26] C. Audet, K. Diest, S. Le Digabel, L.A. Sweatlock, and D.E. Marthaler. Metamaterial Design by Mesh Adaptive Direct Search. In *Numerical Methods for Metamaterial Design*, volume 127 of *Topics in Applied Physics*, pages 71–96. Springer, Dordrecht, 2013.

[27] C. Audet, K.J. Dzahini, M. Kokkolaras, and S. Le Digabel. StoMADS: Stochastic blackbox optimization using probabilistic estimates. Technical Report G-2019-30, Les Cahiers du GERAD, 2019.

[28] C. Audet and W. Hare. *Derivative-Free and Blackbox Optimization*. Springer Series in Operations Research and Financial Engineering. Springer, Cham, Switzerland, 2017.

[29] C. Audet, A. Ianni, S. Le Digabel, and C. Tribes. Reducing the Number of Function Evaluations in Mesh Adaptive Direct Search Algorithms. *SIAM Journal on Optimization*, 24(2):621–642, 2014.

[30] C. Audet, A. Ihaddadene, S. Le Digabel, and C. Tribes. Robust optimization of noisy

blackbox problems using the Mesh Adaptive Direct Search algorithm. *Optimization Letters*, 12(4):675–689, 2018.

[31] C. Audet, M. Kokkolaras, S. Le Digabel, and B. Talgorn. Order-based error for managing ensembles of surrogates in mesh adaptive direct search. *Journal of Global Optimization*, 70(3):645–675, 2018.

[32] C. Audet and S. Le Digabel. The mesh adaptive direct search algorithm for periodic variables. *Pacific Journal of Optimization*, 8(1):103–119, 2012.

[33] C. Audet, S. Le Digabel, and M. Peyrega. Linear equalities in blackbox optimization. *Computational Optimization and Applications*, 61(1):1–23, 2015.

[34] C. Audet, S. Le Digabel, and C. Tribes. Dynamic scaling in the mesh adaptive direct search algorithm for blackbox optimization. *Optimization and Engineering*, 17(2):333–358, 2016.

[35] C. Audet, S. Le Digabel, and C. Tribes. The Mesh Adaptive Direct Search Algorithm for Granular and Discrete Variables. *SIAM Journal on Optimization*, 29(2):1164–1189, 2019.

[36] C. Audet and D. Orban. Finding optimal algorithmic parameters using derivative-free optimization. *SIAM Journal on Optimization*, 17(3):642–664, 2006.

[37] C. Audet, G. Savard, and W. Zghal. Multiobjective Optimization Through a Series of Single-Objective Formulations. *SIAM Journal on Optimization*, 19(1):188–210, 2008.

[38] C. Audet, G. Savard, and W. Zghal. A mesh adaptive direct search algorithm for multiobjective optimization. *European Journal of Operational Research*, 204(3):545–556, 2010.

[39] C. Audet and C. Tribes. Mesh-based Nelder-Mead algorithm for inequality constrained optimization. *Computational Optimization and Applications*, 71(2):331–352, 2018.

[40] M. Aziz, W. Hare, M. Jaberipour, and Y. Lucet. Multi-fidelity algorithms for the horizontal alignment problem in road design. *Engineering Optimization*, 52(11):1848–1867, 2020.

[41] S. Bahrami, M. Khelghatibana, C. Tribes, S.Y. Lo, S. von Fellenberg, J-Y. Trépanier, and F. Guibault. Application of a territorial-based filtering algorithm in turbomachinery blade design optimization. *Engineering Optimization*, 49(2):216–234, 2017.

[42] S. Bahrami, C. Tribes, C. Devals, T.C. Vu, and F. Guibault. Multi-fidelity shape optimization of hydraulic turbine runner blades using a multi-objective mesh adaptive direct search algorithm. *Applied Mathematical Modelling*, 40(2):1650 – 1668, 2016.

[43] C.W. Bale, E. Bélisle, P. Chartrand, S.A. Decterov, G. Eriksson, A.E. Gheribi, K. Hack, I.-H. Jung, Y.-B. Kang, J. Melançon, A.D. Pelton, S. Petersen, C. Robelin, J. Sangster, P. Spencer, and M-A. Van Ende. Reprint of: Factsage thermochemical software and databases, 2010–2016. *Calphad*, 55:1 – 19, 2016. Christopher W. Bale Symposium - Thermodynamic Applications, Optimizations and Simulations in High Temperature Processes.

[44] N. Barris, S. Alarie, and M.F. Anjos. Simulation-Based Optimization of the Control Strategy for Isolated Power Grids via Blackbox Software. In *CORS/INFORMS International Conference*, Montreal, June 2015.

[45] A. Bayoumy and M. Kokkolaras. A relative adequacy framework for multi-model management in design optimization. *ASME Journal of Mechanical Design*, pages 1–22, 2019.

[46] A. Bayoumy and M. Kokkolaras. Multi-model management for time-dependent multidisciplinary design optimization problems. *Structural and Multidisciplinary Optimization*, 61(5):1821–1841, 2020.

[47] A. Bayoumy and M. Kokkolaras. A relative adequacy framework for multimodel manage-

ment in multidisciplinary design optimization. *Structural and Multidisciplinary Optimization*, 62(4):1701–1720, 2020.

[48] M. Beaudoin. DecomposeZoltan: Doing domain decomposition in parallel. In *8th International OpenFOAM Workshop*, Jeju, South Korea, 2013.

[49] S. Bellavia, M. Macconi, and B. Morini. STRSCNE: A scaled trust-region solver for constrained nonlinear equations. *Computational Optimization and Applications*, 28:31–50, 2004.

[50] G.M. Bollas, K. Palmer Kyle, D. Prasad, C.A. Jacobson, J.M. Maljanian Jr, R.A. Poisson, and Y.K. Park. Plate-fin heat exchanger fouling identification. Patent US 10495547 B2, 2019.

[51] A.J. Booker, J.E. Dennis, Jr., P.D. Frank, D.B. Serafini, V. Torczon, and M.W. Trosset. A Rigorous Framework for Optimization of Expensive Functions by Surrogates. *Structural and Multidisciplinary Optimization*, 17(1):1–13, 1999.

[52] J. Brochu. Enjeux reliés à l'intégration des énergies renouvelables en réseaux autonomes. In *Atelier Technique d'Automne – Intégration des énergies renouvelables dans les micro-réseaux autonomes*, Montreal, November 2017. TechnoCentre Éolien.

[53] T. Browne, B. Iooss, L. Le Gratiet, J. Lonchampt, and E. Remy. Stochastic simulators based optimization by Gaussian process metamodels - Application to maintenance investments planning issues. *Quality and Reliability Engineering International*, 32(6):2067–2080, 2016.

[54] I.M. Chamseddine, H.B. Frieboes, and M. Kokkolaras. Design optimization of tumor vasculature-bound nanoparticles. *Scientific Reports*, 8, 2018.

[55] I.M. Chamseddine, H.B. Frieboes, and M. Kokkolaras. Multi-objective optimization of tumor response to drug release from vasculature-bound nanoparticles. *Scientific Reports*, 10, 2020.

[56] I.M. Chamseddine and M. Kokkolaras. Nanoparticle optimization for enhanced targeted anticancer drug delivery. *ASME Journal of Biomechanical Engineering*, 140(4), 2018.

[57] I.M. Chamseddine and M. Kokkolaras. A dual nanoparticle delivery strategy for enhancing drug distribution in cancerous tissue. *ASME Journal of Biomechanical Engineering*, 142(12), 2020.

[58] G.W. Characklis, B.R. Kirsch, J. Ramsey, K.E.M. Dillard, and C.T. Kelley. Developing portfolios of water supply transfers. *Water Resources Research*, 42(5):W05403, 2006.

[59] X. Chen, C.T. Kelley, F. Xu, and Z. Zhang. A smoothing direct search method for monte carlo-based bound constrained composite nonsmooth optimization. *SIAM Journal on Scientific Computing*, 40(4):A2174–A2199, 2018.

[60] T.D. Choi, O.J. Eslinger, C.T. Kelley, J.W. David, and M. Etheridge. Optimization of automotive valve train components with implicit filtering. *Optimization and Engineering*, 1(1):9–27, 2000.

[61] Y. Choquette, P. Lavigne, P. Ducharme, A. Houdayer, and J.-P. Martin. Apparatus and Method for Monitoring Snow Water Equivalent and Soil Moisture Content Using Natural Gamma Radiation, September 2010. US Patent No. 7800051 B2.

[62] F.H. Clarke. *Optimization and Nonsmooth Analysis*. John Wiley and Sons, New York, 1983. Reissued in 1990 by SIAM Publications, Philadelphia, as Vol. 5 in the series Classics in Applied Mathematics.

[63] A.R. Conn and S. Le Digabel. Use of quadratic models with mesh-adaptive direct search for constrained black box optimization. *Optimization Methods and Software*, 28(1):139–158, 2013.

[64] A.R. Conn, K. Scheinberg, and L.N. Vicente. *Introduction to Derivative-Free Optimization*. MOS-SIAM Series on Optimization. SIAM, Philadelphia, 2009.

[65] A.L. Custódio, K. Scheinberg, and L.N. Vicente. Methodologies and software for derivative-free optimization. In T. Terlaky, M.F. Anjos, and S. Ahmed, editors, *Advances and Trends in Optimization with Engineering Applications*, MOS-SIAM Book Series on Optimization, chapter 37. SIAM, Philadelphia, 2017.

[66] A. Côté, O. Blancke, S. Alarie, A. Dems, D. Komljenovic, and D. Messaoudi. Combining historical data and domain expert knowledge using optimization to model electrical equipment reliability. In *2020 International Conference on Probabilistic Methods Applied to Power Systems (PMAPS)*, pages 1–6, Liege, Belgium, 2020.

[67] A. Delavari, I. Kamwa, and P. Brunelle. Simscape power systems benchmarks for education and research in power grid dynamics and control. In *2018 IEEE Canadian Conference on Electrical Computer Engineering (CCECE)*, pages 1–5, 2018.

[68] K. Diest. *Numerical Methods for Metamaterial Design*, volume 127 of *Topics in Applied Physics*. Springer, Netherlands, 2013.

[69] J.D. Drews, V.K. Pepper, C.A. Best, J.M. Szafron, J.P. Cheatham, A.R. Yates, K.N. Hor, J.C. Zbinden, Y-C. Chang, G.J.M. Mirhaidari, A.B. Ramachandra, S. Miyamoto, K.M. Blum, E.A. Onwuka, J. Zakko, J. Kelly, S.L. Cheatham, N. King, J.W. Reinhardt, T. Sugiura, H. Miyachi, Y. Matsuzaki, J. Breuer, E.D. Heuer, T.A. West, T. Shoji, D. Berman, B.A. Boe, J. Asnes, M. Galantowicz, G. Matsumura, N. Hibino, A.L. Marsden, J.S. Pober, J.D. Humphrey, T. Shinoka, and C.K. Breuer. Spontaneous reversal of stenosis in tissue-engineered vascular grafts. *Science Translational Medicine*, 12(537), 2020.

[70] M. Drumheller. Constraint-based method of designing a route for a transport element. Patent US 7647211 B2, 2010.

[71] C.A. Erignac and M. Drumheller. Adaptive distance field constraint for designing a route for a transport element. Patent US 7668700 B2, 2010.

[72] M. Feingesicht, A. Polyakov, F. Kerherve, and J.-P. Richard. Device for active control of the readhesion of a flow on a profile. Patent WO 2018/229442 A1, 2018.

[73] D. Fleischman and H.A. Atwater. Narrowband light filters. Patent US 2018/0308888 A1, 2018.

[74] D. Fleischman and H.A. Atwater. Narrowband light filters. Patent WO 2018/200593 A1, 2018.

[75] J.-P. Fortin, R. Turcotte, S. Massicotte, R. Moussa, J. Fitzback, and J.-P. Villeneuve. Distributed Watershed Model Compatible with Remote Sensing and GIS Data. I: Description of Model. *Journal of Hydrologic Engineering*, 6(2):91–99, 2001.

[76] V. Fortin. Le Modèle Météo-Apport HSAMI: Historique, Théorie et Application. Technical Report IREQ-1999-0255, Institut de recherche d'Hydro-Québec, Varennes, Qc, 1999.

[77] 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 properties databases, the FactSage software and the Mesh Adaptive Direct Search algorithm. *CAL-*

*PHAD: Computer Coupling of Phase Diagrams and Thermochemistry*, 36:135–143, 2012.

[78] A.E. Gheribi, J.-P. Harvey, E. Bélisle, C. Robelin, P. Chartrand, A.D. Pelton, C.W. Bale, and S. Le Digabel. Use of a biobjective direct search algorithm in the process design of material science applications. *Optimization and Engineering*, 17(1):27–45, 2016.

[79] 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*, 559(0):107–110, 2013.

[80] A.E. Gheribi, A.D. Pelton, E. Bélisle, S. Le Digabel, and J.-P. Harvey. On the prediction of low-cost high entropy alloys using new thermodynamic multi-objective criteria. *Acta Materialia*, 161:73–82, 2018.

[81] A.E. Gheribi, A.D. Pelton, and J.-P. Harvey. Determination of optimal compositions and properties for phase change materials in a solar electric generating station. *Solar Energy Materials and Solar Cells*, 210:110506, 2020.

[82] 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*, 43(9):1323–1330, 2011.

[83] M. Griebel, T. Dornseifer, and T. Neunhoeffer. *Numerical Simulation in Fluid Dynamics*. Society for Industrial and Applied Mathematics, 1998.

[84] ESI Group. OpenFOAM - The open source CFD toolbox. https://www.openfoam.com/.

[85] C. Guay, M. Minville, and M. Braun. A global portrait of hydrological changes at the 2050 horizon for the province of Québec. *Canadian Water Resources Journal / Revue canadienne des ressources hydriques*, 40(3):285–302, 2015.

[86] T.J. Gundert, A.L. Marsden, W. Yang, and J.F. LaDisa, Jr. Optimization of Cardiovascular Stent Design Using Computational Fluid Dynamics. *Journal of biomechanical engineering*, 134:011002, 2012.

[87] T.J. Gundert, A.L. Marsden, W. Yang, D.S. Marks, and J.F. LaDisa, Jr. Identification of Hemodynamically Optimal Coronary Stent Designs Based on Vessel Caliber. *IEEE Transactions on Biomedical Engineering*, 59(7):1992–2002, 2012.

[88] L. Gérin-Lajoie, D. Lefebvre, M. Racine, L. Soulières, and I. Kamwa. Hydro-Québec experience with PSS tuning. In *1999 IEEE Power Engineering Society Summer Meeting. Conference Proceedings (Cat. No.99CH36364)*, volume 1, pages 88–95, Edmonton, 1999.

[89] J.-P. Harvey and A.E. Gheribi. Process Simulation and Control Optimization of a Blast Furnace Using Classical Thermodynamics Combined to a Direct Search Algorithm. *Metallurgical and Materials Transactions B*, 45(1):307–327, 2014.

[90] M.A. Heidari, M.D. Druckman, and O.B. Nakhjavani. Methods for optimized engine balancing based on flight data. Patent US 9347321 B2, 2016.

[91] A. Hibberd, A.M. Hein, and T.M. Eubanks. Project Lyra: Catching 1I/'Oumuamua - Mission opportunities after 2024. *Acta Astronautica*, 170:136–144, 2020.

[92] P.-L. Huot. *Développement d'approches de calage efficaces pour les modèles hydrologiques coûteux en temps de calcul, au moyen du modèle HYDROTEL*. PhD thesis, École de Technologie Supérieure, 2019.

[93] P.-L. Huot, A. Poulin, and S. Alarie. Assessment Of Blackbox Optimization Methods For Efficient Calibration Of Computationally Intensive Hydrological Models. In *11th International Conference on Hydroinformatics*, New York City, 2014. CUNY Academic Works.

[94] P.-L. Huot, A. Poulin, C. Audet, and S. Alarie. Low-cost and representative surrogate hydrological models. Part I – Construction of surrogates. Technical Report G-2019-07, Les Cahiers du GERAD, 2019.

[95] P.-L. Huot, A. Poulin, C. Audet, and S. Alarie. Low-cost and representative surrogate hydrological models. Part II – Use within calibration frameworks. Technical Report G-2019-08, Les Cahiers du GERAD, 2019.

[96] P.L. Huot, A. Poulin, C. Audet, and S. Alarie. A hybrid optimization approach for efficient calibration of computationally intensive hydrological models. *Hydrological Sciences Journal*, 64(10):1204–1222, 2019.

[97] Hydro-Québec. Setting new sights with our clean energy, annual report. https://www.hydroquebec.com/about/financial-results/annual-report.html, 2019.

[98] M. Kokkolaras. When, why, and how can derivative-free optimization be useful to computational engineering design? *ASME Journal of Mechanical Design*, 142(1), 2020.

[99] M. Kokkolaras, C. Audet, and J.E. Dennis, Jr. Mixed variable optimization of the Number and composition of heat intercepts in a thermal insulation system. *Optimization and Engineering*, 2(1):5–29, 2001.

[100] M. Kokkolaras, C. Audet, and J.E. Dennis Jr. Mixed variable optimization of the number and composition of heat intercepts in a thermal insulation system. *Optimization and Engineering*, 2(1):5–29, 2001.

[101] T.G. Kolda, R.M. Lewis, and V. Torczon. Optimization by direct search: New perspectives on some classical and modern methods. *SIAM Review*, 45(3):385–482, 2003.

[102] D. Komljenovic, D. Messaoudi, A. Côté, M. Gaha, L. Vouligny, S. Alarie, and O. Blancke. Asset Management in Electrical Utilities in the Context of Business and Operational Complexity. In *World Congress on Resilience, Reliability and Asset Management*, Singapore, 2019.

[103] Sandia National Laboratories. Zoltan: Parallel Partitioning, Load Balancing and Data-Management Services . https://cs.sandia.gov/Zoltan/.

[104] J. Lainé, E. Piollet, F. Nyssen, and A. Batailly. Blackbox Optimization for Aircraft Engine Blades With Contact Interfaces. *Journal of Engineering for Gas Turbines and Power*, 141(6), 02 2019. 061016.

[105] D. Lakhmiri, S. Le Digabel, and C. Tribes. HyperNOMAD: Hyperparameter optimization of deep neural networks using mesh adaptive direct search. Technical Report G-2019-46, Les Cahiers du GERAD, 2019.

[106] J. Larson, M. Menickelly, and S.M. Wild. Derivative-free optimization methods. *Acta Numerica*, 28:287–404, 2019.

[107] S. Le Digabel. Algorithm 909: NOMAD: Nonlinear Optimization with the MADS algorithm. *ACM Transactions on Mathematical Software*, 37(4):44:1–44:15, 2011.

[108] S. Le Digabel, M.A. Abramson, C. Audet, and J.E. Dennis, Jr. Parallel Versions of the MADS Algorithm for Black-Box Optimization. In *Optimization days*, Montreal, May 2010.

GERAD.

[109] L.-A. Leclaire. Massive Distribution of Black Box Calculation for Model Calibration. In *CORS/INFORMS International Conference*, Montreal, June 2015.

[110] R.M. Lewis, V. Torczon, and M.W. Trosset. Direct search methods: Then and now. *Journal of Computational and Applied Mathematics*, 124(1–2):191–207, 2000.

[111] W. Li, H. Pu, P. Schonfeld, Z. Song, L. Wang, J. Wang, X. Peng, and L. Peng. A Method for Automatically Recreating the Horizontal Alignment Geometry of Existing Railways. *Computer-Aided Civil and Infrastructure Engineering*, 34(1):71–94, 2019.

[112] W. Li, H. Pu, P. Schonfeld, J. Yang, H. Zhang, L. Wang, and J. Xiong. Mountain Railway Alignment Optimization with Bidirectional Distance Transform and Genetic Algorithm. *Computer-Aided Civil and Infrastructure Engineering*, 32(8):691–709, 2017.

[113] W. Li, H. Pu, P. Schonfeld, H. Zhang, and X. Zheng. Methodology for optimizing constrained 3-dimensional railway alignments in mountainous terrain. *Transportation Research Part C: Emerging Technologies*, 68:549–565, 2016.

[114] X. Liang, Y. Xie, Z. Zhang, and T. Niu. Method and apparatus for optimizing blocking grating for cone beam ct image scattering correction. Patent US 10722205 B2, 2020.

[115] J. Lonchampt. VME a tool for probabilistic models valuation in engineering asset management. In *Risk, Reliability and Safety: Innovating Theory and Practice – Walls, Revie & Bedford (Eds)*, pages 1158–1164, London, 2017. CRC Press, Taylor & Francis Group. Proceedings of ESREL 2016 (Glasgow, Scotland, 25-29 September 2016).

[116] S. Lucidi, V. Piccialli, and M. Sciandrone. An Algorithm Model for Mixed Variable Programming. *SIAM Journal on Optimization*, 15(4):1057–1084, 2005.

[117] S. Lupuleac, T. Pogarskaia, M. Churilova, M. Kokkolaras, and E. Bonhomme. Optimization of fastener pattern in airframe assembly. *Assembly Automation*, 40(5):723–733, 2020.

[118] A.L. Marsden. Simulation based planning of surgical interventions in pediatric cardiology. *Physics of fluids (1994)*, 25(10):101303, 2013.

[119] A.L. Marsden, J.A. Feinstein, and C.A. Taylor. A computational framework for derivative-free optimization of cardiovascular geometries. *Computer Methods in Applied Mechanics and Engineering*, 197(21–24):1890–1905, 2008.

[120] A.L. Marsden, M. Wang, J.E. Dennis, Jr., and P. Moin. Trailing-edge noise reduction using derivative-free optimization and large-eddy simulation. *Journal of Fluid Mechanics*, 572:13–36, 2007.

[121] G. Marwaha and M. Kokkolaras. System-of-systems approach to air transportation design using nested optimization and direct search. *Structural and Multidisciplinary Optimization*, 51(4):885–901, 2015.

[122] MathWorks. power_AsynchronousMachineParams. https://www.mathworks.com/help/releases/R2018a/physmod/sps/powersys/ref/power_asynchronousmachineparams.html.

[123] MathWorks. Simscape Power Systems Release Notes. https://www.mathworks.com/help/releases/R2018a/physmod/sps/release-notes.html.

[124] K. Mehrgan, J. Thomas, R. Saglia, X. Mazzalay, P. Erwin, R. Bender, M. Kluge, and M. Fabricius. A 40 Billion Solar-mass Black Hole in the Extreme Core of Holm 15A, the Central Galaxy of Abell 85. *Astrophysical Journal*, 887(2):195, 2019.

[125] M. Minville, D. Cartier, C. Guay, L.-A. Leclaire, C. Audet, S. Le Digabel, and J. Merleau. Improving process representation in conceptual hydrological model calibration using climate simulations. *Water Resources Research*, 50:5044–5073, 2014.

[126] D.B. Miracle and O.N. Senkov. A critical review of high entropy alloys and related concepts. *Acta Materialia*, 122:448 – 511, 2017.

[127] S. Mondal, Y. Lucet, and W. Hare. Optimizing horizontal alignment of roads in a specified corridor. *Computers and Operations Research*, 64:130–138, 2015.

[128] J.J. Moré and S.M. Wild. Do you trust derivatives or differences? *Journal of Computational Physics*, 273:268–277, 2014.

[129] M. Pourbagian, B. Talgorn, W.G. Habashi, M. Kokkolaras, and S. Le Digabel. Constrained problem formulations for power optimization of aircraft electro-thermal anti-icing systems. *Optimization and Engineering*, 16:663–693, 2015.

[130] A.B. Ramachandra, J.D. Humphrey, and A.L. Marsden. Gradual loading ameliorates maladaptation in computational simulations of vein graft growth and remodelling. *Journal of The Royal Society Interface*, 14:20160995, 2017.

[131] V. Ramakrishnan, N.M. Nagar, C. Finlez, T. Storchi-Bergmann, R. Slater, A. Schnorr-Muller, R.A. Riffel, C.G. Mundell, and A. Robinson. Nuclear kinematics in nearby AGN - I. An ALMA perspective on the morphology and kinematics of the molecular CO(2–1) emission. *Monthly Notices of the Royal Astronomical Society*, 487(1):444–455, 2019.

[132] E. Renaud, C. Robelin, A.E. Gheribi, and P. Chartrand. Thermodynamic evaluation and optimization of the Li, Na, K, Mg, Ca, Sr // F, Cl reciprocal system. *Journal Of Chemical Thermodynamics*, 43(8):1286–1298, 2011.

[133] A. Rossi. *Développement d'outils d'optimisation dédiés aux circuits magnétiques des propulseurs à effet Hall*. PhD thesis, Université de Toulouse, 2017.

[134] A. Rossi, F. Messine, and C. Henaux. Parametric optimization of a hall effect thruster magnetic circuit. *Transactions of the Japan Society for Aeronautical and Space Sciences, Aerospace Technology Japan*, 14(ists30):Pb 197–Pb 202, 2016.

[135] S. Sankaran, C. Audet, and A.L. Marsden. A method for stochastic constrained optimization using derivative-free surrogate pattern search and collocation. *Journal of Computational Physics*, 229(12):4664–4682, 2010.

[136] S. Sankaran, J.D. Humphrey, and A.L. Marsden. An efficient framework for optimization and parameter sensitivity analysis in arterial growth and remodeling computations. *Computer methods in applied mechanics and engineering*, 256:200–210, 2013.

[137] S.E. Selvan, P.B. Borckmans, A. Chattopadhyay, and P.-A. Absil. Spherical mesh adaptive direct search for separating quasi-uncorrelated sources by range-based independent component analysis. *Neural Computation*, 25(9):2486–2522, 2013.

[138] A. Shukla, D. Buddhi, and R.L. Sawhney. Solar water heaters with phase change material thermal energy storage medium: A review. *Renewable and Sustainable Energy Reviews*, 13(8):2119–2125, 2009.

[139] B. Solnik, D. Golovin, G. Kochanski, J.E. Karro, S. Moitra, and D. Sculley. Bayesian Optimization for a Better Dessert. In *Proceedings of the 2017 NIPS Workshop on Bayesian Optimization*, Long Beach, USA, 2017.

[140] J. Szafron, A. Ramachandra, C. Breuer, A. Marsden, and J. Humphrey. Optimization of

tissue engineered vascular graft design using computational modeling. *Tissue Engineering Part C: Methods*, 25:561–570, 06 2019.

[141] B. Talgorn. NoHiMDO, a Non Hierarchical Solver for MDO problems. https://github.com/bastientalgorn/NoHiMDO, 2016.

[142] B. Talgorn, C. Audet, M. Kokkolaras, and S. Le Digabel. Locally weighted regression models for surrogate-assisted design optimization. *Optimization and Engineering*, 19(1):213–238, 2018.

[143] B. Talgorn, S. Le Digabel, and M. Kokkolaras. Statistical surrogate formulations for simulation-based design optimization. *ASME Journal of Mechanical Design*, 137(2), 2015.

[144] B. Talgorn and M. Kokkolaras. Compact implementation of non-hierarchical analytical target cascading for coordinating distributed multidisciplinary design optimization problems. *Structural and Multidisciplinary Optimization*, 56(6):1–6, 2017.

[145] B. Talgorn, M. Kokkolaras, A. DeBlois, and P. Piperni. Numerical investigation of non-hierarchical coordination for distributed multidisciplinary design optimization with fixed computational budget. *Structural and Multidisciplinary Optimization*, 55(1):205–220, 2017.

[146] B.A. Temple, J.C. Armstrong, K.L. Bueschern, and J.A. Favorite. Radiograph and passive data analysis using mixed variable optimization. Patent US 9047397 B1, 2015.

[147] B.A. Tolson and C.A. Shoemaker. Dynamically dimensioned search algorithm for computationally efficient watershed model calibration. *Water Resources Research*, 43(1), 2007.

[148] V. Torczon. On the convergence of pattern search algorithms. *SIAM Journal on Optimization*, 7(1):1–25, 1997.

[149] R. Tournemenne, J.-F. Petiot, B. Talgorn, J. Gilbert, and M. Kokkolaras. Optimization of brass wind instruments based on sound simulations. *Journal of the Acoustical Society of America*, 145(6):3795–3804, 2017.

[150] R. Tournemenne, J.-F. Petiot, B. Talgorn, and M. Kokkolaras. Brass instruments design using physics-based sound simulation models and surrogate-assisted derivative-free optimization. *ASME Journal of Mechanical Design*, 139(4), 2017.

[151] B. Van Dyke and T.J. Asaki. Using QR Decomposition to Obtain a New Instance of Mesh Adaptive Direct Search with Uniformly Distributed Polling Directions. *Journal of Optimization Theory and Applications*, 159(3):805–821, 2013.

[152] M.E. Vázquez-Méndez, G. Casal, D. Santamarina, and A. Castro. A 3D Model for Optimizing Infrastructure Costs in Road Design. *Computer-Aided Civil and Infrastructure Engineering*, 33(5):423–439, 2018.

[153] A. Verma, K. Wong, and A.L. Marsden. A concurrent implementation of the surrogate management framework with application to cardiovascular shape optimization. *Optimization and Engineering*, 21(4):1487–1536, 2020.

[154] L.N. Vicente and A.L. Custódio. Analysis of direct searches for discontinuous functions. *Mathematical Programming*, 133(1-2):299–325, 2012.

[155] P. Vincent, L. Grechy, and R. Corbett. A device for maintaining vascular connections. Patent WO 2017/148836 A1, 2017.

[156] M. Xi, W. Sun, and J. Chen. Survey of derivative-free optimization. *Numerical Algebra, Control and Optimization*, 10(4):537–555, 2020.

[157] J. Xu, C. Audet, C.E. DiLiberti, W.W. Hauck, T.H. Montague, A.F. Parr, D. Potvin, and

D.J. Schuirmann. Optimal adaptive sequential designs for crossover bioequivalence studies. *Pharmaceutical Statistics*, 15(1):15–27, 2016.

[158] W. Yang, J.A. Feinstein, and A.L. Marsden. Constrained optimization of an idealized Y-shaped baffle for the Fontan surgery at rest and exercise. *Computer Methods in Applied Mechanics and Engineering*, 199(33):2135–2149, 2010.

[159] W. Yang, J.A. Feinstein, S.C. Shadden, I. Vignon-Clementel, and A.L. Marsden. Optimization of a Y-Graft Design for Improved Hepatic Flow Distribution in the Fontan Circulation. *Journal of biomechanical engineering*, 135(1):011002, 2013.

[160] A. Ypma, M. Van Der Schaar, G. Tsirogiannis, L.J. Karssemeijer, and C.-H. Fan. Apparatus and method for inferring parameters of a model of a measurement structure for a patterning process. Patent US 2018/0239851 A1, 2018.