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Two decades of blackbox optimization applications

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ABSTRACT

This article reviews blackbox optimization applications of direct search optimization methods over the past twenty years. Emphasis is placed on the Mesh Adaptive Direct Search (MADS) derivative-free optimization algorithm. The main focus is on applications in three specific fields: energy, materials science, and computational engineering design. Nevertheless, other applications in science and engineering, including patents, are also considered. The breadth of applications demonstrates the versatility of MADS and highlights the evolution of its accompanying software NOMAD as a standard tool for blackbox optimization.

1. Introduction

The general form of an optimization problem is

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

where Ω 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 Ω dictates what optimization methods and algorithms can 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 non-existent, unknown, or impossible to detect. This article surveys a significant number of applications from a wide variety of disciplines of direct search methods for such problems over the past two decades.

1.1. Blackbox optimization

Blackbox optimization (BBO) considers the design and analysis of algorithms for problems where the structure of the objective function f and/or the constraints defining the set Ω is unknown, unexploitable, or non-existent.

The most frequent BBO situation arises when the evaluation of the objective and /or constraint functions involve the execution of a computer code or simulation. The code receives a vector x and outputs values in $\overline{\mathbb{R}}$. In many engineering applications, 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 a helicopter rotor blade failed in 60% of the calls (Booker et al., 1999) and the ASPEN (Aspentech, Accessed: 2020-11-06) chemical engineering simulator failed in 43% of the calls during the optimization of a process to treat a toxic byproduct in aluminum production (Audet et al., 2008a).

BBO situations do not always involve computer simulations. A less frequent situation occurs when the output is the result of a physical or laboratory experiment rather than a simulation. For example, developing the best cookie recipe is considered in Solnik et al. (2017), where the objective function is a subjective score submitted by participants who taste different cookies.

Audet and Hare define all of the above-mentioned situations as *blackbox optimization problems* (Audet and Hare, 2017). There are no explicit formulations that can be readily exploited.

The simulation or process returning the objective and constraint functions may be time-consuming. For example, automotive valve train design (Choi et al., 2000) requires seconds, sample size identification

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for bioequivalence studies in the pharmaceutical industry (Xu et al., 2016) requires minutes, hyperparameter optimization (Audet and Orban, 2006) requires hours, and airfoil trailing-edge noise reduction (Marsden et al., 2007) requires days of CPU time for each execution of the associated computer code or simulation.

High computational cost is not the only challenge. Simulations may provide insufficient significant digits or return different output when executed using the same input more than once. In a calibration context of computationally intensive hydrological models (Huot et al., 2019a), the output of the simulation is rounded to 10^{-3} to avoid over-optimizing and to trigger the stopping criteria more rapidly. An approach for solving stochastic optimization problems is presented in Characklis et al. (2006) to identify portfolios of permanent rights, options, and leases that minimize the expected costs of meeting a city's annual demand within a pre-specified reliability. A Monte Carlo simulation is used in portfolio selection using real data from the Shanghai–Shenzhen stock market (Chen et al., 2018). A CPU time-related objective function involving numerical fluid dynamics for a lid-driven cavity problem (Griebel et al., 1998) (where a fluid in a rectangular container is subject to forces imposed by the top boundary) is considered in Abramson et al. (2012).

Another difficulty associated with BBO problems is that the number of variables may be itself an optimization variable. These are a particular type of categorical variables. In Abramson (2004), Kokkolaras et al. (2001), 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 nonordinal. The optimal design of a small apparatus for magnetic resonance is studied in Lucidi et al. (2005), 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 (Lakhmiri et al., 2021).

1.2. The MADS algorithm and the NOMAD software

In BBO problems, functions are often nondifferentiable; automatic differentiation may thus produce false and misleading results. Direct search methods (Lewis et al., 2000) 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. BBO and DFO methods have been developed and continuously improved since the mid-1990s. Their maturity is reflected by the existence of two textbooks. The first one dates from 2009 (Conn et al., 2009) and the second one was published in 2017 (Audet and Hare, 2017). In addition, several surveys on the methodology and evolution of BBO and DFO algorithms are available (Audet, 2014; Custódio et al., 2017; Kolda et al., 2003; Larson et al., 2019; Xi et al., 2020). However, none of those are devoted exclusively to applications of BBO and DFO.

This article focuses on the mesh adaptive direct search (MADS) algorithm, first introduced in 2006 (Audet and Dennis, Jr., 2006). The reasons of focusing on this specific algorithm include:

(i) its simplicity: the pseudocode in the original paper (Audet and Dennis, Jr., 2006) takes only 12 lines; the algorithm alternates between a flexible global exploration phase called the *search* and a rigorously defined local exploration phase called the *poll*;

(ii) Its capability to handle many types of constraints: bounds, nonquantifiable, and hidden constraints by the extreme barrier (Audet et al., 2020a; Audet and Dennis, Jr., 2006), quantifiable and relaxable constraints by the progressive barrier (Audet and Dennis, Jr., 2009), and explicit linear equalities (Audet et al., 2015);

(iii) its ability to treat various types of variables: continuous (Audet and Dennis, Jr., 2006), integer and categorical variables (discrete variables that cannot be ordered) (Abramson et al., 2009a; Audet et al., 2019), as well as periodical (e.g., angles in $[0, 2\pi]$) (Audet and Le Digabel, 2012);

(iv) its exploitation of static and dynamic surrogate models (Audet and Côté-Massicotte, 2019; Audet et al., 2018b; Booker et al., 1999; Conn and Le Digabel, 2013; Talgorn et al., 2018);

(v) its rigorous hierarchical convergence analysis (Audet and Dennis, Jr., 2006; Vicente and Custódio, 2012) based on nonsmooth calculus (Clarke, 1983); the analysis exploits the rigorously defined poll step and the main result ensures, under a local Lipschitz hypothesis, that the method produces a subsequence of iterates converging to some point $\hat{x}$ for which the Clarke generalized derivative

$$f^{\circ}(\hat{x}; d) \;:=\; \limsup_{y \to \hat{x}, t \searrow 0} \frac{f(y+td) - f(y)}{t}$$

of the objective function $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ is nonnegative in every direction d in the hypertangent cone (Jahn, 2007) to the domain at $\hat{x}$ (the hypertangent cone is a generalization of the tangent cone for a domain defined by non-smooth functions);

(vi) 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 evolved considerably since its introduction, and may handle groups of variables (these are discussed at the end of Section 2.1) (Alarie et al., 2013), badly-scaled problems (Audet et al., 2016), grey box monotonic problems (Audet et al., 2020b), and multiobjective problems (Audet et al., 2008d; 2010). MADS allows the incorporation of various heuristic search strategies including VNS (Audet et al., 2008b) and Nelder-Mead (Audet and Tribes, 2018), and its local exploration strategies are diversified (Abramson et al., 2009b; Adjengue et al., 2014; Audet et al., 2014; Selvan et al., 2013; Van Dyke and Asaki, 2013). The above extensions inherit from the theoretical convergence guarantees of the MADS class of algorithm. Extensions involving stochastic problems have been developed (Alarie et al., 2019; Audet et al., 2021a; 2018a; Sankaran et al., 2010) but do not benefit from the same convergence guarantees.

The MADS algorithm and its various extensions are coded in C++ under the LGPL license and are available in the public domain through the NOMAD software package (Le Digabel, 2011). Version 1 of NOMAD was initiated in 2001 (based on the pattern search algorithm (Audet and Dennis, Jr., 2001; 2004; Torczon, 1997), the ancestor of MADS) and Version 4 was released in 2021 (Audet et al., 2021b). The original version of the MADS algorithm is part of the official MATLAB distribution in the `patternsearch` function.[3]

For clarity, the different variants of MADS that are mentioned throughout this review are summarized in Table 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 2 and in Fig. 1. The table was generated using Web of Science (WoS) and the citations of Le Digabel (2011) (328 references as of October 27, 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 (Le Digabel, 2011). WoS categories are grouped in fields with the corresponding overall number of references. The proportions of these WoS occurrences are illustrated in Fig. 1.

[3] The MATLAB version of MADS was distributed before the actual article (Audet and Dennis, Jr., 2006) was published in 2006. Coding was done from the 2004 associated technical report.

Table 1
Description of the different acronyms related to MADS and NOMAD.

Acronyms	Description	References
MADS	The Mesh Adaptive Direct Search class of algorithms	Audet and Dennis, Jr. (2006)
BIMADS	Extension of MADS to biobjective optimization	Audet et al. (2008d)
ROBUST-MADS	Adaptation of MADS for robust optimization	Audet et al. (2018a)
PSD-MADS	Parallel version of MADS for large problems	Audet et al. (2008c)
COOP-MADS and P-MADS	Two other parallel MADS versions	Le Digabel et al. (2010)
DDS-MADS	Hybrid method combining MADS and the global search algorithm DDS	Huot et al. (2019a)
NOMAD	A C+ MADS implementation that includes all algorithms from this table except DDS-MADS	Audet et al. (2021b), Le Digabel (2011)

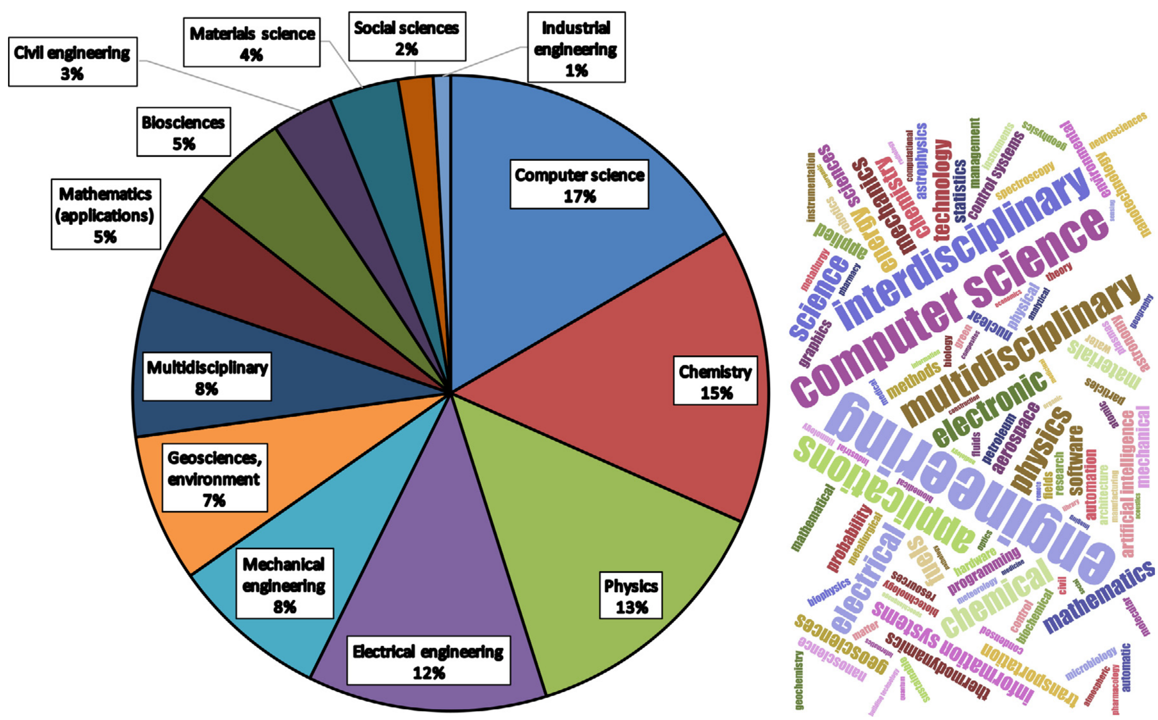

Fig. 1. Left: Distribution of the application fields that cite (Le Digabel, 2011), based on the data of Table 2. Right: "Word cloud" graph of all WoS categories from Table 2, generated with the Word Cloud Generator of https://www.jasondavies.com/wordcloud.

The present survey contains a large selection of applications where the MADS algorithm (via NOMAD, or another implementation, or a custom variant) was used during the last twenty years; this selection is far from being exhaustive, but highlights different areas in which it was successfully applied. It is also important to note that MADS and NOMAD have been improved throughout the years, mainly thanks to the lessons learned by their utilization in different applications.

The main part of this survey is composed of Section 2 (energy applications at Hydro-Québec), Section 3 (applications in materials science), and Section 4 (applications in computational engineering design). Section 5 considers other application domains where direct search methods have been used, including patents.

2. Energy applications at Hydro-Québec

Hydro-Québec (HQ) is a public utility company that manages the generation, transmission, and distribution of electricity in the province of Québec, Canada (Hydro-Québec, 2019). This section describes several optimization problems solved at HQ using NOMAD.

2.1. Apparatus positioning

One of the first projects using NOMAD at HQ involved optimal positioning of Gamma-ray MONitoring devices (GMON) (Alarie et al., 2013). A GMON (Choquette et al., 2010) is a monitoring apparatus that measures the attenuation of gamma rays emanating from the ground to infer snow water equivalent (SWE) in remote locations. Kriging is applied to SWE measurements 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 kriging error estimates. Since the GMONs cannot be installed anywhere (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 guess. 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. This feature allows the method to group the xy-coordinates of each GMON, and to force movement of only one GMON at a time. Introducing one group of two variables for each GMON helped to generate better solutions. More generally, this feature allows the user to indicate which set of variables are related with each other. These sets need not be disjoint. The algorithm generates directions in each subset associated to the groups, rather than generating directions in the entire space spanned by all variables.

Table 2
Application fields of the NOMAD software.

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

(*continued on next page*)

Table 2 (*continued*)

Field	#	Category in WoS	#
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

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 microwave satellite data and near-infrared satellite images (Alarie and Leclaire, 2013).

2.2. Hydrological model calibration

A group of projects involving NOMAD considered 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 (Fortin, 1999). The model is said to be conceptual because the relationships between the hydrological variables are described by simplified empirical equations. EAUptim uses NOMAD as its optimization library (Minville et al., 2014). 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 (Guay et al., 2015). The variables of interest are streamflow, snow accumulation, and actual evapotranspiration. The model was calibrated with the constraint of correctly rendering the annual cycle. Results indicate that the annual streamflow will increase in the entire province of Québec, but the distribution will vary : streamflow will be higher in the winter and lower in the summer, while spring floods will occur earlier.

Concurrently with this work, EAUptim was deployed on a computing cluster to allow parallel evaluations beyond the native $2n$ polling directions of MADS (Leclaire, 2015) (where n is the number of variables in the optimization problem). The aim was to be able to use efficiently as many as 1000 cores for exploring the design space. Three parallel implementations (P-MADS, COOP-MADS, and PSD-MADS Audet et al., 2008c; Le Digabel et al., 2010) were integrated with EAUptim's cluster version. The results showed that using several direction generators (P-MADS) or several independent searches (COOP-MADS and PSD-MADS) to generate multiple $2n$ evaluations (up to the number of available cores) was not sufficient to improve performance proportionally. This work led to the conclusion that a new (fourth) version of NOMAD had to be developed.[4]

HYDROTEL (Fortin et al., 2001) is another hydrological model used at HQ. As opposed to HSAMI, which is a conceptual model, HYDROTEL is physics-based; therefore, while simulating with the former requires a few seconds, the latter takes minutes. By comparing different algorithms to calibrate HYDROTEL, it appeared that the performance of the *dynamically dimensioned search* method (DDS Tolson and Shoemaker, 2007) and NOMAD is complementary (Huot et al., 2014). DDS, which adapts its search to a given simulation budget, seems to have the ability to identify quickly promising basins of solutions, while NOMAD is able to refine nearby solutions. An hybrid algorithm, called DDS-MADS, combining the global search of DDS with the local search of MADS, is proposed in Huot et al. (2019a). Computing time is reduced significantly without sacrificing the robustness and stability of calibrations.

A reduced-fidelity physics-based model was developed to be used as a surrogate model for improving the efficiency of DDS-MADS (Huot, 2019; Huot et al., 2019b). The reduced model was obtained by reducing the simulation period, the number of virtual meteorological stations, and the discretization of watershed into sub-basins. These reductions resulted in poor speed-up when applied individually, but combined, they reduced the computational time by a factor of at least 15 compared to the complete model. The best results were obtained by first applying the DDS-MADS algorithm to the reduced model and next applying NOMAD to the complete model with the remaining evaluation budget (Huot, 2019; Huot et al., 2019c). Compared to directly applying DDS-MADS to the complete model, this strategy reduced the overall computational time from 40% to 64% depending on the watershed.

2.3. Parameter tuning

HQ uses three-dimensional models to study the behavior of water moving in canals toward hydroelectric power stations. Such studies are performed with OpenFOAM (Group, Accessed: 2020-11-06), an open-source simulation software for parallel computational fluid dynamics. The efficiency of calculations depends on the simulation domain decomposition. OpenFOAM uses single-processor methods to accomplish this, which requires a large amount of local memory. This is particularly limiting when the 3D model contains millions of cells. An alternative method was developed at HQ to address these issues (Beaudoin, 2013). It is based on a library (Laboratories, Accessed: 2020-11-06) of 10 parallel decomposition algorithms, each with their own set of parameters. Some of these parameters are continuous variables, others are integer, and some are categorical, as they are not subject to any meaningful ordering. Moreover, the optimal choice of algorithms and parameters varies from one model to another. The selection of an appropriate algorithm and adequate parameters was formulated as a blackbox parameter tuning problem (Audet and Orban, 2006) and was solved using NOMAD's categorical variables option (Audet and Dennis, Jr., 2001) 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 model of 7 million cells with 120 partitions.

HQ developed the Simscape Power Systems (SPS) electrical simulator to model and simulate electric power systems within the MATLAB Simulink environment (Delavari et al., 2018). SPS can estimate electrical parameters of asynchronous machines based on manufacturer specifications (MathWorks, 2018a), which is similar to a model calibration problem. HQ decided to replace the MATLAB optimization toolbox by a trust-region approach (Bellavia et al., 2004). Although the new method was fast enough, the proposed default settings were inappropriate to generate high-quality solutions. This turned out to be a parameter tuning problem and NOMAD was used to adjust the calibra-

[4] This version has been released in 2021 (Audet et al., 2021b).

tion model parameters. A set of 115 asynchronous machines was used as a test problem. The parameter optimization improved the quality of calibrations by 33%. The resulting implementation is available as MATLAB's `power_AsynchronousMachineParams` function since the R2018a release (MathWorks, 2018b).

Tuning problems do not only arise with computer models and simulators, but also with physical control devices such as power system stabilizers (PSSs). 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 margins must be specified for each oscillation mode. Their performance can be evaluated by simulation, as with SPS, against fault scenarios. NOMAD has been applied for tuning PSSs by considering several generators (Alarie et al., 2015) simultaneously rather than sequentially (Gérin-Lajoie et al., 1999). By using the groups of variables feature (Alarie et al., 2013) (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

HQ's grid infrastructure equipment involved in the production, transport, and delivery of electricity is referred to as *assets*. Optimization problems also arise in grid asset management, i.e., in all the activities carried out to ensure long term proper functioning of the power grid. HQ has set up an important project for its transmission system, named PRIAD, in order to optimize its maintenance and asset management strategies (Komljenovic et al., 2021). To achieve this, models predicting asset reliability based on maintenance strategies need to be developed. Such models are built from expert knowledge, but they need to be calibrated using historical failure data, which was accomplished using NOMAD (Côté et al., 2020). In case of inconsistency, the approach identified bias in the data. It also allowed the questioning of experts on some of their previous assessments and to revise them based on calibration results.

Given an asset model, it is possible to feed a reliability simulator with failure rates corresponding to any variant of a given maintenance strategy. Such simulators rely on stochastic Monte Carlo methods, where the output can vary for the same input. This led to new research initiatives to adapt MADS to stochastic blackboxes (Alarie et al., 2019). Using a reliability simulator called VME (Lonchampt, 2017), developed by the R&D division of *Électricité de France* (EDF), numerical experiments are conducted on a small problem of determining five investment dates in asset management (Browne et al., 2016). They show that NOMAD with its ROBUST-MADS option (Audet et al., 2018a) is too computationally expensive. The approach proposed in Alarie et al. (2019) takes into account the standard deviation of the Monte Carlo simulations directly into the internal mechanisms of MADS and reduces the calculation time drastically from several days to a few hours.

2.5. Isolated power grids

Most inhabited areas of the province of Québec are connected by a large electricity system that links different power producers to consumers. There are however some isolated regions that solely depend on local power grids. HQ owns 21 such isolated power grids, mostly located in Northern Québec. Using a one-minute time-step isolated grid simulator, NOMAD was employed to minimize diesel consumption by optimizing the set of rules governing when a generator is turned on and off (Barris et al., 2015). The challenge of this problem lies in that there are several types of rules to start and stop the generators; depending on their parameter values, some rules prevail over the others. This introduces discontinuities in the solution domain, which can lead to ineffective searches. The use of groups of variables (Alarie et al., 2013) helps to restore efficiency by grouping the parameters by rules. Optimizing of the rules according to their type allows the handling of discontinuities.

Using the same simulator, NOMAD was also employed to study the integration of renewable energy sources (wind, solar, storage) to reduce diesel consumption and greenhouse gases in its isolated power grids (Brochu, 2017). 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, assuming that they are replaced only once during this time period.

3. Applications in materials science

During the last decade, the design of materials based on integrated computational materials engineering (ICME) attracted attention considerably in the R&D of several industrial branches. This section presents examples on how MADS can be used in conjunction with ICME methods to assist engineers and scientists in materials and industrial processes.

The MADS algorithm and the NOMAD software package were successfully applied to different fields of materials science to (i) optimize materials performance, (ii) optimize industrial processes, and (iii) design new materials. A goal in alloys design is to determine a set of compositions, temperature, and pressure that optimize a set of functions that describes the material properties under certain constraints. These functions depend on the amount, type, and structure of phases. Note that in the thermodynamic context, a phase is a region throughout which all physical properties of a material are uniform; in general a solid phase has a unique crystallographic structure, while a liquid or gas phase are homogeneous mixtures. The material properties (mechanical, thermodynamic, structural, dynamics, thermal transport, surface properties) depend on the phase volume fractions and the temperature. Phase volume fractions depend on both temperature and composition. Closed-form expressions of material properties as functions of composition and temperature are not known. Optimization of industrial processes 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 (Bale et al., 2016) 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 information on thermodynamic properties such as functions of temperature, pressure, and composition for over 7000 pure substances (compounds) and hundreds of multi-component solid and liquid solutions for a large variety of materials, including steels, light metals, rare earths, noble metals, oxides, salts, semiconductors, and refractory materials.

Equilibrium calculations in multi-component systems may be used to 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. Aside from equilibrium calculations, FactSage can be used to simulate para-equilibrium and the cooling effect upon the phase composition of solid systems for microstuctures.

Combining the 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, aluminum, and copper. This combination also allowed the screening of potential multi-component alloys, searching for compositions having desired properties and phase assemblages within a reasonable amount of time. In multi-component systems, an evaluation of a given property by FactSage can be time-consuming, as it ranges from a few seconds up to a 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. Optimizing the performance of materials

From a practical point of view, the design of materials consists of minimizing, maximizing, or targeting specific properties. Targeting values is achieved by minimizing the (square of the) norm of the difference between a property and its target value. Optimization problems with more than two objectives are handled by a sequence of biobjective problems, in which all but two objective functions are treated as constraints. For some material design problems, this approach is preferable to applying multiobjective optimization (Gheribi et al., 2016).

In materials science, the properties depend on the amount of each phase, i.e., compounds (e.g., Fe_3C or Al_3Ni) or solutions constituting the system. However, in multi-component 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 multi-component systems is one of the most difficult problems to solve in alloy 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 twelve components is predicted in Gheribi et al. (2012, 2013, 2018) for different problems. This is the most remarkable achievement of NOMAD in terms of alloy design. The robustness of NOMAD in the determination of phase stability in multi-component systems is partially due to using Latin hypercube sampling and Variable Neighborhood Search (Audet et al., 2008b) strategies.

3.2. Optimizing industrial processes

The design of many industrial processes involves the design of materials. In general, finding alloys or mixtures with optimal specific properties is highly desirable. For instance, obtaining Pareto-optimal solutions of a biobjective optimization problem, which consists of determining a set of alloy's compositions that simultaneously minimize the liquidus temperature and target a specific freezing range (region of co-existence between the liquid and solid phases) under constraints on composition, density, thermal expansion, and shrinkage ratio, is highly desirable in many metallurgical applications. But, most importantly, the structure and amount of precipitates (that can be compounds and/or solutions) needs to be optimized in order to control the mechanical thermal, electrical, and physical properties.

Case studies (Gheribi et al., 2012; 2013) reported the improvement of the mechanical properties of light metals alloys by maximizing the volume fraction of several specific aluminum (Al) rare earth (RE = La, Ce, Pr, Nd, Pm, Sm) intermetallics of type Al_nRE_m ($n > m$) under constraints related to liquidus temperature, density, and heat capacity.

Managing the constraints on the liquidus temperature is 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. Management of the constraints on compositions, heat capacity, and density is simpler. Many alloys have been identified as potential low-cost candidates for the next generation of light metal alloys for lighter automotive applications.

Predicting the global and subsequent local minima on the liquidus temperature hypersurface is a real challenge in several materials science applications. A local minimum upon the liquidus surface is characterized by the chemical reaction $Liquid \rightarrow S_1+S_2+\cdots+S_n$ where the S_i are the solids (compounds and solutions) constituting the systems. In other words, a local minimum of the liquidus temperature corresponds to a null freezing range.

A phase change material (PCM) is a local minimum of the liquidus surface of critical importance to thermal solar energy (Shukla et al., 2009). In the context of global warming, identifying sustainable and low-cost PCMs with good performance in terms of heat storage capacity is a real challenge. A methodology to determine local minima of the liquidus surface is presented in Gheribi et al. (2011). The technique consists of minimizing the freezing range. When a PCM solution x^0 is identified, an additional constraint $\|x - x^0\|^2 \geq \epsilon$ is added, where $\epsilon > 0$ is a small adjustable parameter. Then, the minimization procedure is restarted again including the above constraint. This is repeated until no additional PCM solutions can be found. This method has be proven to be reliable, as it predicted with considerable accuracy the global minimum of the liquidus temperature in an eight-components salts system, for which the liquidus temperature was measured experimentally (Renaud et al., 2011). More recently (Gheribi et al., 2020), the same procedure produced 30 new potential low-cost PCM materials with excellent heat storage capacity.

Finally, NOMAD was applied to optimize energetic efficiency and therefore reduce greenhouse gas emissions of key industrial processes for the production of primary metals (Gheribi et al., 2016; Harvey and Gheribi, 2014).

3.3. Designing new materials

NOMAD was also applied to design innovative materials. The most notable example is that of so-called *high entropy alloys*. High entropy alloys have more than five constituents, consisting of a single face centred cubic (FCC) or body centred cubic (BCC) solid solution, or in some cases, a dual FCC-BCC phase solid solution (Miracle and Senkov, 2017). 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 phases are stable. The main challenge in the identification of entropy alloys is the predictability of the stability range of single or dual phase. A methodology using NOMAD was proposed in Gheribi et al. (2018) to predict the stability range. According to 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 NOMAD 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 NOMAD (Gheribi et al., 2018), thereby opening the door to new potential sustainable applications, in particular for the automotive industry.

Finally, NOMAD was used for metamaterials in Audet et al. (2013), Diest (2013). 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 (Moré and Wild, 2014). In these cases, DFO and BBO algorithms are the only option (Kokkolaras, 2020). Because of their simplicity, the most popular DFO algorithms in the engineering design community are

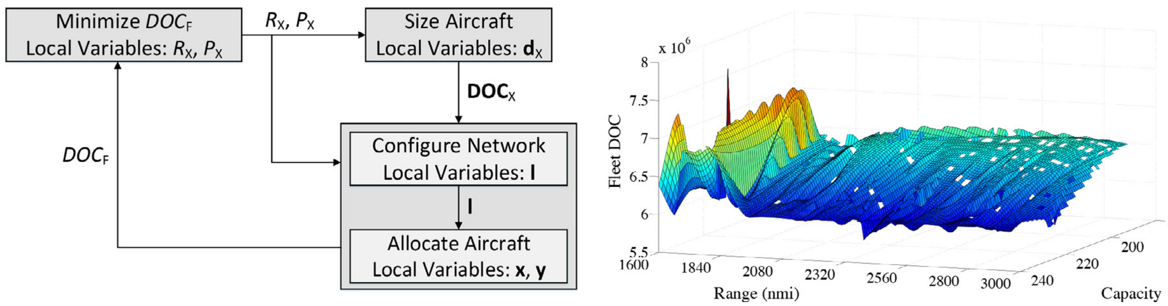

Fig. 2. Nested blackbox optimization problem (left) and blackbox response surface for 15 network nodes (right) (Marwaha and Kokkolaras, 2015).

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 (Audet and Hare, 2017).

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 (Kolda et al., 2003). The first engineering design application reported in the literature utilized the direct ancestor of MADS with mixed variable programming (Audet and Dennis, Jr., 2001); 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 (Kokkolaras et al., 2001). 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 Kokkolaras et al. (2001) were enhanced by Abramson (2002, 2004), which led to even larger performance improvements.

A particularly challenging engineering design problem (Marwaha and Kokkolaras, 2015) was solved using NOMAD. 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. Fig. 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; previous results from the literature were limited to seven nodes, and NOMAD solved problems up to 15 nodes.

NOMAD was also used to optimize an electro-thermal wing anti-icing system (Pourbagian et al., 2015). 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. Therefore, the authors made use of both quadratic and statistical surrogates based on the work presented in Talgorn et al. (2015). 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 Tournemenne et al. (2017a,b) 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 (2018) developed a mechanistic model of nanoparticle-mediated drug delivery in a two-dimensional vascularized tumor and used NOMAD to determine optimal nanoparticle size and aspect ratio. A biobjective optimization problem was formulated and solved by NOMAD and its implementation of the BIMADS algorithm (Audet et al., 2008d) 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. NOMAD was used to solve a sequential optimization problem, increasing the dead tumor area by 16% without the need of additional drugs (Chamseddine and Kokkolaras, 2020). Chamseddine et al. (2018) considered 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.

Design optimization of nanoparticles was performed in Chamseddine et al. (2020) 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.

Finally, in a recent study published in *Nature*, NOMAD was used to tune the parameters of a mathematical transmission model to demonstrate the under-detection of COVID-19 cases in France (Pullano et al., 2021).

4.3. Multidisciplinary design optimization

MADS has been also used in multidisciplinary design optimization (MDO) and multimodel management. MDO problems include so-called “consistency” constraints, whose violations quantify discrepancies among coupled subproblems related to different disciplines. Talgorn and Kokkolaras (Talgorn, 2016) developed a user-friendly compact implementation of an augmented Lagrangian algorithm for coordinating distributed MDO problems (Talgorn and Kokkolaras, 2017). 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. (2017) considered both NOMAD and gradient-based algorithms to solve the subproblems formulated by an interdisciplinary feasible architecture known as non-hierarchical analytical target cascading. Results show that NOMAD yields higher-consistency solutions (i.e., solutions with smaller discrepancies among disciplinary subproblems), but with greater variance than the MATLAB implementation of an interior point gradient-based algorithm.

Bayoumy and Kokkolaras (2020a) 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 NOMAD as the optimization solver. 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 (Bayoumy and Kokkolaras, 2020b; 2020c) extends the RAF for MDO by utilizing NOMAD for monolithic, distributed, and time-dependent problems. When using the RAF to solve multidisciplinary feasible problem formulations, the key arguments for using NOMAD are: (1) MADS is the only algorithm that offers the (optional) search step where surrogate models 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 and NOMAD have also been used in assembly optimization problems and remanufacturing-based design strategies. Lupuleac et al. (2020) considered the problem of optimizing temporary fastener patterns in aircraft assembly and compared NOMAD 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 NOMAD yielded good results; however, the former obviously required many more function evaluations than the latter. Al-Handawi et al. (2020) 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 (Bahrami et al., 2017; 2016).

Aircraft engine blade 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 (Lainé et al., 2019). 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. Other applications of direct search methods

The MADS algorithm and its implementation in NOMAD have also been used in a variety of other applications, as illustrated in Table 2 and Fig. 1. This section summarizes some of them associated with significant amount of publications and patents.

5.1. Road design optimization

There has been considerable 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 three related subproblems. First, the horizontal alignment optimization determines the number and position of horizontal intersection points and corresponding curve radii. NOMAD is the recommended solver according to Li et al. (2019, 2016). Second, the vertical alignment optimization determines vertical position with specified rates of curvature and bounded grades. NOMAD is recommended for presetting control points (Li et al., 2017). Finally, the earthwork optimization minimizes the total cost of hauling, excavation and embankment. Bi-level approaches resulting in potentially millions of dollars of savings are proposed in Mondal et al. (2015), Vázquez-Méndez et al. (2018) and multi-fidelity direct search algorithms are studied in Aziz et al. (2020) for problems that take from 20 to 24 h to run.

5.2. Cardiovascular geometries

Marsden provides an historical perspective on the development of simulation-based cardiac surgery and links between engineering, medicine, and optimization that facilitated clinical advances (Marsden, 2013). The author also discusses the application of these tools to two clinically relevant examples in pediatric cardiology.

A framework for coupling optimal shape design to time-accurate 3D blood flow simulations in idealized cardiovascular geometries is presented in Marsden et al. (2008). The optimization of a Y-graft design for the Fontan procedure (a surgery used to treat single ventricle heart defects) is conducted in Yang et al. (2010, 2013) under pulsatile rest and exercise flow conditions. Stent implantation for the treatment of coronary artery disease is studied in Gundert et al. (2012a,b). 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 Drews et al. (2020), Ramachandra et al. (2017), Sankaran et al. (2013), Szafron et al. (2019), and surrogate-based direct search optimization techniques are used to accelerate parameter estimation. Shape optimization problems motivated by hemodynamically-driven surgical design are studied in Verma et al. (2020).

5.3. Astrophysics

There are numerous applications of direct search methods in astrophysics. In a paper with more than 700 co-authors (Aasi et al., 2013), 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

Table 3
Patents associated with the MADS algorithm or with the NOMAD software.

Context	Origin	References
Analysis of radiographic images	Los Alamos National Laboratory	Temple et al. (2015)
Calibrating parameters in a patterning process	ASML Netherlands BV	Ypma et al. (2018)
Controlling the readhesion of a flow	INRIA	Feingesicht et al. (2018)
Cone beam CT image scattering correction	Shenzhen Institutes of Advanced Technology	Liang et al. (2020)
Designing narrowband light filters	California Institute of Technology	Fleischman and Atwater (2018a,b)
Heat exchanger design	Hamilton Sundstrand Corporation	Bollas et al. (2019)
Maintaining vascular connections	Imp Innovations Ltd	Vincent et al. (2017)
Optimization processes in aeronautic design	The Boeing Company	Abramson et al. (2017), Drumheller (2010), Erignac and Drumheller (2010), Heidari et al. (2016)

to observed kinematics (Mehrgan et al., 2019), and to compute mass distributions (Neureiter et al., 2020).

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 (Hibberd et al., 2020).

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 (Rossi, 2017; Rossi et al., 2016).

Kinematics analysis of galaxies are performed in Ramakrishnan et al. (2019), 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 with direct search methods

In addition to research papers, there have been many patents 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 3.

6. Conclusion

This review focused on three particular application domains of blackbox optimization. Over the past two decades, direct search methods and algorithms such as MADS evolved through research motivated by a vast variety of applications. Since its introduction in 2006, MADS can now consider continuous and discrete, (including categorical) variables, handle blackbox constraints and multiple objectives, tackle increasingly larger problems (partially through parallelism), and, even solve stochastic blackbox problems.

These improvements, along with the availability of greater and better computing resources, allow practitioners to solve a large variety of problems for which blackbox optimization is the only applicable approach.

A particularly interesting emerging field of artificial intelligence and machine learning applications is the optimization of the hyperparameters of deep neural networks, for which MADS and NOMAD are natural candidates.

It can be argued that the variety and number of BBO and DFO applications has not only grown considerably in the past two decades, but will continue to grow in future years.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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