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A hybrid optimization approach for efficient calibration of computationally intensive hydrological models

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Abstract: The calibration of hydrological models is here formulated as a Blackbox optimization problem where the only information available to the optimization algorithm is the objective function value. In the case of distributed hydrological models, the calibration process is often known to be hampered by computational efficiency issues. Running a single simulation may take several minutes, and the optimization process may require thousands of model simulations; the computational time can thus easily expand to several hours or days. A new hybrid optimization algorithm for the calibration of computationally-intensive hydrological models is introduced. It merges both the convergence analysis and robust local refinement from the Mesh Adaptive Direct Search (MADS) algorithm with the global exploration capabilities from the heuristic strategies used by the Dynamically Dimensioned Search (DDS) algorithm. The new hybrid method is applied to the calibration of the distributed and computationally-intensive HYDROTEL model on three different river basins located in the province of Québec (Canada). Results show that the hybrid DDS-MADS method can reduce the total number of required model simulations without compromising the quality of the final objective function value.

Keywords: Distributed hydrological model, computationally intensive simulation models, optimization algorithm, efficient calibration, Dynamically Dimensioned Search algorithm, Mesh Adaptive Direct Search algorithm

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1 Introduction

Hydrological catchment models are simulation tools built with a sequence of mathematical equations to represent hydrological processes such as rainfall, snow accumulation and melt, evapotranspiration, infiltration and runoff at a catchment-area scale (Singh & Woolhiser, 2002). Hydrological models are used to reproduce the relations between water inflows, such as precipitation, and the discharge at the catchment outlet. They require long-term meteorological time series and a good knowledge of catchment characteristics to adequately simulate streamflow (Singh & Woolhiser, 2002; Moradkhani & Sorooshian, 2008). All of these characteristics, meteorological data time series and hydrological processes can be integrated within the models according to different spatialization scales, corresponding to the level of a territory's subdivisions. Hydrological models can be classified into three main categories according to their level of spatial discretization: global models that represent the catchment area as a single spatial entity; semi-distributed models that roughly divide the catchment area into sub-watersheds/catchments; and distributed models where the area is organized into fine mesh elements with reduced size (Singh & Woolhiser, 2002; Das et al., 2008; Moradkhani & Sorooshian, 2008; Pechlivanidis et al., 2011).

Hydrological models are fundamental tools for many engineering applications: hydroelectricity production, water supply, delineation of flood zones, etc. (Beven, 2006). For all these fields of application, distributed modeling provides a better representation of spatial variability in the catchment than either global or semi-distributed models. The distributed models have the advantage of representing some hydrological processes that are impossible to assess otherwise, such as the spatial distribution of snow accumulation on the catchment, or the transport of pollutants and sediments in the water system (Moradkhani & Sorooshian, 2008). They are also particularly useful for glacier coverage analysis over mountainous catchments and for the analysis of hydrological response in ungauged watersheds when a fine mesh scale is required (Verbunt et al., 2003; Moradkhani & Sorooshian, 2008; Lei et al., 2011; Huang et al., 2014).

Hydrological models need to be adapted to each watershed by adjusting the internal parameters of the equations governing the hydrological processes' simulation. The adjustment of these parameter values is referred to as calibration. This process leads to the identification of a parameter set minimizing a measure of the difference between observed and predicted/simulated variables, generally the discharge at the catchment outlet (Duan et al., 1994; Singh & Woolhiser, 2002; Moriasi et al., 2007; Moradkhani & Sorooshian, 2008; Pechlivanidis et al., 2011; Pushpalatha et al., 2012). Various combinations of parameter sets are explored during the calibration process. The use of an objective criterion makes it possible to find a combination of parameters that satisfy the user's needs (Moriasi et al., 2007). Good calibration is critical; as it is key to users' confidence in the model. The calibrated model will then be used as a tool to support management decisions on water resources or infrastructures built in/around water environment.

2 Literature review and research objectives

Hydrological calibration belongs to the class of "Blackbox Optimization" problems (Audet, 2014) in which the function to be optimized and the functions that define the feasible region of the parameter space (delimited by user-defined boundaries) are not analytically known. These functions are evaluated by launching a computer simulation, which can be time-consuming, mainly in the case of distributed models. Due to the complexity of the simulation, these functions are nonsmooth, discontinuous, and contaminated by some numerical noise. The term "Blackbox" refers to the fact that the exploitation of the internal structure of the optimization problem is difficult, inefficient or simply impossible. The only information used by the optimization process is the value of the objective criterion estimated from hydrological simulations. Consequently, a combination of multiple hydrological simulations and sufficiently efficient optimization strategies is essential to obtain a fine-tuned model (Audet et al., 2014; Shan & Wang, 2010; Conn et al., 2009; Boukouvala et al., 2016).

In recent decades, important developments have been made in hydrological modeling, including growth in computational power. However, the use of distributed models still generates an intensive computational cost, especially for the calibration process. For example, running a single simulation may take several minutes, and the calibration process may require more than thousands of simulations. The time consumed

by a simulation (and the calibration) depends on the mathematical equations governing the hydrological processes, the level of spatial discretization, the input data size and the number of internal parameters to be calibrated (Mungunthan et al., 2005; Zhang et al., 2009; Razavi et al., 2010). Examples of time-consuming hydrological models can be found in the recent scientific literature: a single simulation of the Dipole Flow and Reactive Tracer Test – Interpretation Model (DFRIT-IM; Roos, 2009) takes about 37 minutes on average on a 2.8 GHz Intel Premium processor (Razavi et al., 2012b) and the Soil and Water Assessment Tool, version 2000 (SWAT2000; Neitsch et al., 2002) consumes 1.8 minutes on average for a single simulation on a 2.8 GHz Pentium processor (Razavi et al., 2012b).

Various optimization algorithms are based on standard metaheuristic methods, such as the “Shuffled Complex Evolution method of the University of Arizona” (SCE-UA; Duan et al., 1993), the “Adaptive Simulated Annealing” (ASA; Ingber, 1993), the “Particle Swarm Optimization” (PSO; Eberhart & Kennedy, 1995), the “Covariance Matrix Adaptation Evolution Strategy” (CMAES; Hansen, 2006) or the “Dynamically Dimensioned Search” (DDS; Tolson & Shoemaker, 2007), to name just a few popular ones. There is also a wide range of direct-search methods (Torczon, 1997; Audet & Dennis, 2006) that can be used to optimize Blackbox problems. All these algorithms provide a “state-of-the-art” for hydrological model optimization; in the past few decades, hydrologists have studied their optimization strategies, evaluated their efficiency, applied them in many case studies and adopted them in operational contexts. The efficiency of many of these optimizers has been shown when used for the calibration of non-computationally intensive hydrological models (e.g. Duan et al., 1994; Madsen, 2003; Tolson & Shoemaker, 2007; Arsenault et al., 2014; Minville et al., 2014). However, the development of these optimizers is not always oriented towards a high computational time issue, and so efficient optimizers must be chosen for this kind of problem.

According to Razavi et al. (2010), there are four types of approaches for dealing with the issue of computationally-intensive problems: 1) the development of more computationally efficient optimization algorithms; 2) the use of parallel computing networks for running several simulations simultaneously; 3) the use of model preemption (evading model simulations that are identified as being of poor quality); and 4) the use of surrogate models inside the optimization process. These approaches are complementary and can either be combined (Razavi et al., 2010; Regis & Shoemaker, 2013; Audet et al., 2008) or used separately (Booker et al., 1999; Shoemaker et al., 2007; Razavi et al., 2010; Razavi et al., 2012a; Regis & Shoemaker, 2013; Razavi & Tolson, 2013; Huang et al., 2014).

The present study aims to develop a new computationally efficient optimization algorithm to significantly reduce the computational time consumed by an optimization process on computationally intensive hydrological models. This work is based on the first types of approaches identified by Razavi et al. (2010). A preliminary step assesses the efficiency of three benchmark optimization algorithms for the calibration of a distributed and computationally intensive hydrological model. Those results and a preliminary discussion highlight the optimization strategies used by the algorithms that show real potential for reducing the computational time. The main objective of this study is realised by its proposal of a hybrid approach consisting of an operating framework exploiting the previously identified efficient strategies. This new hybrid method is able to reduce the number of model simulations necessary for calibration while achieving good-quality optimization results.

The paper is organized as follows. Section 3 presents the hydrological model HYDROTEL (Fortin et al., 2001a, b), followed by the optimization problem and the modeled watersheds of this study. Section 4 benchmarks the three optimization algorithms using computational tests to identify which optimization strategies can potentially best reduce the computational time. Section 5 proposes the operating framework of the hybrid calibration approach, followed by a summary of the numerical results. Discussion and proposed future work conclude the paper.

3 The calibration problem

This section describes the hydrological models used and their problem formulation. The three studied watersheds’ characteristics are also presented.

3.1 Model description

The distributed and physically-based computationally intensive hydrological model HYDROTEL (Fortin et al., 2001a, b) is considered for this study. The spatial discretization of the territory is represented by several simulation units named RHHUs (Relatively Homogenous Hydrological Units), and all hydrological processes are simulated on each RHHU. This hydrological model is mainly designed to account for the spatial variability of hydrological processes and to exploit Geographic Information System (GIS) and/or remote sensing data providing topography, land cover, land use, natural waterways and soil type, to name just a few examples.

HYDROTEL has 27 internal parameters, but according to some studies (Fortin et al., 2001a, b; Turcotte et al., 2007; Poulin et al., 2011; Ricard et al., 2012), some can be fixed at first, as they generally have a low sensitivity impact on simulation results or they are purely additive or corrective factors. Therefore, two optimization problems were designed, one with 10 parameters and one with 19 parameters (hereafter referred to as HYDROTEL 10 and HYDROTEL 19, respectively). Both problems allow the assessment of the impacts of different dimensionalities, levels of complexity and levels of equifinality, and these will be treated in this study. Table 1 shows the selected parameters for both optimization problems and the boundaries for each parameter included within HYDROTEL 10 and HYDROTEL 19.

Table 1: Summary of selected parameters and boundaries for HYDROTEL 10 and HYDROTEL 19

Submodel Used	N ^o	HYDROTEL Model Parameter	Units	10 Parameters ¹	19 Parameters ¹	Lower Bound	Upper Bound
Take-off Program	1	Initial Rainfall Coefficient	mm/d		X	0	2
	2	Initial Rainfall Coefficient	%/d		X	0.0	0.1
	3	Initial Rainfall Coefficient	%	X	X	0	∞
	4	Initial Rainfall Coefficient	mm/d		X	0.0	1.0
	5	Initial Rainfall Coefficient	mm		X	0.0	0.01
Soil Water Capacity and Infiltration	6	Soil Water Capacity	mm/d	X	X	0.0	0.01
	7	Soil Water Capacity	mm/d	X	X	0.0	0.01
	8	Soil Water Capacity	mm/d	X	X	0.0	0.01
	9	Soil Water Capacity	mm/d	X	X	0.0	0.01
	10	Soil Water Capacity	mm/d	X	X	0.0	0.01
	11	Soil Water Capacity	mm/d	X	X	0.0	0.01
	12	Soil Water Capacity	mm/d	X	X	0.0	0.01
Soil Water Method	13	Soil Water Method	mm	X	X	0.0	1.0
	14	Soil Water Method	mm	X	X	0.0	1.0
Soil	15	Soil Water Method	mm	X	X	0.0	1.0
	16	Soil Water Method	mm	X	X	0.0	1.0
	17	Soil Water Method	mm	X	X	0.0	1.0
Kinematic Wave Method	18	Kinematic Wave Method	mm	X	X	0.000001	0.0001
	19	Kinematic Wave Method	mm	X	X	0.0001	0.01

¹ Marked with an asterisk (*) indicates that the parameter is fixed at 1.0.

² Marked with a double asterisk (**) indicates that the parameter is fixed at 0.0.

3.2 Problem formulation

To assess the quality of each model simulation, the objective function (to be minimized) is computed between simulated and observed streamflows as 1 minus the Nash-Sutcliffe Efficiency criterion ($1 - NSE$), described as follows:

$$1 - NSE = \frac{\sum_{i=1}^N (O_i - S_i)^2}{\sum_{i=1}^N (O_i - \bar{O})^2} \tag{1}$$

where O_i is the i^{th} observed streamflow value, S_i is the i^{th} simulated streamflow value, \bar{O} is the mean of observed streamflows and n is the total number of observations. $1 - NSE$ is a normalized statistic that determines the relative magnitude of the residual variance to the measured data variance (Moriassi et al., 2007). $1 - NSE$ ranges from 0 to ∞ , with $1 - NSE = 0$ indicating a perfect fit between observed and simulated values.

3.3 Studied watersheds

As part of this research, both hydrological models have been applied to three different watersheds with dissimilar characteristics and located in different regions of the province of Québec (Canada). The meteorological

data required as input to the hydrological models includes daily minimum temperature, daily maximum temperature, and daily precipitation. Daily observed streamflows at the outlets of the three studied watersheds were also required to assess the quality of simulations. The watersheds are:

- **Cowansville:** an upstream sub-basin of the Yamaska River. Located on the south shore of the St. Lawrence River in the Montérégie region (in the south of the province), Cowansville has a small area (215 km) and is mainly covered by forest and agriculture. Meteorological data were obtained from a gridded dataset at a 20-km resolution from DEH (*Direction de l'expertise hydrique* - see the acknowledgment section) and the calibration period spans from October 1, 2000 to September 30, 2005. Daily observed streamflows for the same period were also obtained from DEH.
- **Ceizur:** an upstream sub-basin of the Gatineau River basin in the Outaouais region (western sector of province), which is mainly forested and contains a large area (6,928 km). Hydro-Québec provided a meteorological gridded dataset at a 10-km resolution and daily observed streamflows at the outlet of the sub-basin (see the acknowledgment section). The calibration period is from October 1, 1988 to September 30, 1992.
- **Toulnustouc.** This is part of the Manicouagan River basin located in the Côte-Nord region (Central-East sector of the province), one of the most important rivers for hydroelectric production in Québec. It is an upstream sub-basin and has the largest forested area (8,109 km). The calibration periods span from October 1, 1984 to September 30, 1988, and denoted by a meteorological gridded dataset at a 20-km resolution derived from a NLWIS (National Land and Water Information Service - www.agr.qc.ca) dataset and daily observed streamflows from Hydro-Québec (see the acknowledgement section).

4 Preliminary studies

The preliminary studies were used to identify the effective optimization strategies of each benchmark optimization algorithm. Each benchmark method is presented, followed by a discussion of the results on computational tests.

4.1 Benchmark optimization algorithms

Three algorithms are considered in this study:

- **SCE-UA.** This algorithm, the “Shuffled Complex Evolution”, was developed at the University of Arizona (SCE-UA; Duan et al., 1993). It is an evolutionary algorithm that generates a first population of parameter sets (solutions) and makes them evolve in the solution space through “Competitive Complex Evolution” (CCE). This is a heuristic method that performs some reflections of the lower-quality solutions according to a reflection axis drawn through a centroid formed by higher-quality solutions, hence leading the optimization process to good-quality zones. The SCE-UA works by grouping solutions into complexes that are mixed on subsequent algorithm iteration to explore different zones of the solutions space. The extensive use of SCE-UA for hydrological model calibration in the last three decades makes it a “state-of-the-art” algorithm for comparison with other optimization algorithms (Yapo et al., 1996; Vrugt et al., 2003; Mugunthan et al., 2005; Arsenault et al., 2013; Huang et al., 2014). Provided by the authors, the release that was used in this study includes updates as of September 2004.
- **DDS.** The second algorithm is the “Dynamically Dimensioned Search” (DDS) approach introduced by Tolson and Shoemaker (2007). The main feature of DDS is its ability to automatically scale the search dimension on a user-specified simulations budget. At the beginning of the optimization, it perturbs a large number of parameters (search dimensions), and as the optimization progresses it gradually reduces the number of dimensions to be searched, to finally perturb only one dimension at a time. This single-solution based algorithm always searches from the current best solution; all of the worse solutions are rejected and never influence the optimization process. Previous studies (Razavi et al., 2010; Arsenault et al., 2014) have shown that the global search strategies used by DDS perform efficiently for the calibration of hydrological models, quickly targeting a high-quality solution. Provided by the authors, release DDS 1.2, which includes updates as of February 2015 was used here.

- **MADS.** The last algorithm is the “Mesh Adaptive Direct Search” (MADS; Audet & Dennis, 2006; Abramson et al., 2009). MADS is a direct search method that uses a discretization of the solution space, called the mesh. It performs an adaptive search on the mesh, including controlling refinement and expansion. Each iteration of the algorithm generates $2N$ trial points on the mesh according to orthogonal directions from the current best solution (N being the number of calibration parameters). When iterations fail to improve the solution (after testing the $2N$ trial points), the next iteration is initiated on a finer mesh. On successful iterations, the mesh is coarsened, which may occur as soon as a trial point appears to be better than the current best solution. Unlike the previous two methods, MADS treats general constraints and is supported by a rigorous convergence analysis, guaranteeing that the final solution will satisfy some necessary optimality conditions (Audet & Dennis, 2006). These conditions involve the nonsmooth calculus theory and allow MADS to stop as soon as they are satisfied. This is a quite interesting feature since it may reduce the number of unnecessary model simulations. The NOMAD 3.5 implementation of MADS is used for the present numerical experiments (Le Digabel, 2011).

All algorithm parameters are set to the default values as recommended by the authors of each method (Duan et al., 1994; Tolson & Shoemaker, 2007; and Le Digabel, 2011) in the interest of fair comparison.

4.2 Computational time

HYDROTEL’ spatial discretization, when combined with a long simulation time period and watershed with a high number of meteorological stations, leads to an intensive computational time for a single simulation. In daily operational conditions, calibrating such models is simply unpractical. Table 2 presents the computational times required for calibrating each combination of the “Watershed-Optimization Problem” with the algorithms detailed in section 4.1. The experiments were carried out on a 3.40 GHz Intel Core i7 processor with 12 Go of RAM. Based on Poulin et al. (2011) and recent works from the authors (Huot et al., 2014), the calibration process is limited to 2,000 model simulations, which is reached here by all three of the considered algorithms, whatever the problem. The $1 - NSE$ values obtained are also reported in Table 2. As mentioned in Huot et al. (2014), the three algorithms provide equally accurate calibrations after 2,000 model simulations are completed. Although they work differently, the computational times are identical for all, since it is the number of simulations that is decisive.

Table 2: Summary of computational times and $1 - NSE$ results from automatic optimization for each “Watershed-Optimization Problem” combination

Watershed	Area (km ²)	Simulated Period	HYDROTEL - 10 Parameters		HYDROTEL - 19 Parameters	
			Computational Times ^a	Standard 1-NSE ^b	Computational Time ^a	Standard 1-NSE ^b
Cowansville	213	5 years	37 hours	0.38	41 hours	0.30
Ceizur	6,098	4 years	54 hours	0.15	62 hours	0.13
Toulousonne	8,108	4 years	63 hours	0.14	77 hours	0.27

^a Computational time based on a 2,000 evaluations calibration budget

^b Standard 1-NSE value (Structure Efficiency (NSE)) result from an automatic calibration

4.3 Performance comparison

Only the Cowansville and Ceizur watersheds are considered at this stage for the purpose of performance analysis. Given that hydrological model calibration is characterized by equifinality (Beven, 2006), each method is used to perform 32 calibration trials for a better statistical representativeness of the results. Each calibration trial is given a budget of 2,000 model simulations.

Figure 1 shows boxplots of the $1 - NSE$ values that summarize results obtained for the Ceizur watershed for both optimization problems (HYDROTEL 10 and HYDROTEL 19). The results are shown at four checkpoints along the optimization process, i.e., at 250, 500, 1,000 and 2,000 simulations. Similar results were obtained for the Cowansville watershed (not shown).

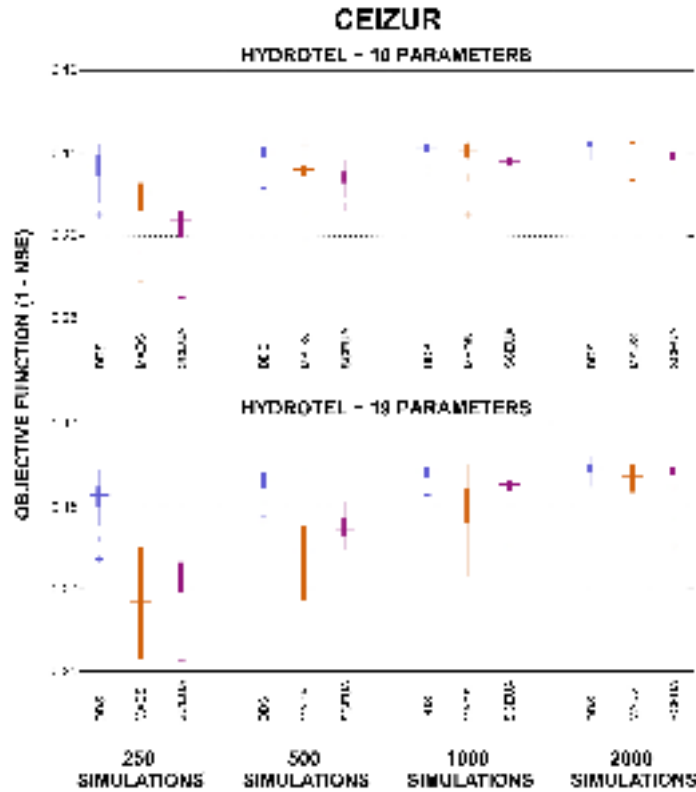


Figure 1: Final NSE results from optimizations by DDS, MADS and SCE-UA for the calibrations of HYDROTEL 10 and HYDROTEL 19 on the Ceizur watershed at 250, 500 and 1,000 simulations, and at the end of the optimization

Firstly, Figure 1 shows that the DDS algorithm stands out over the course of the calibration, and demonstrates a high potential for reducing the computational time since it finds good-quality parameter sets very quickly, in only a low number of simulations. After only 250 simulations, the 32 DDS optimization trials are already in a good-quality zone of the solution space for both HYDROTEL versions. For the remaining 1750 simulations, the DDS method reduces the distance between the upper and lower quartiles and it slightly improves the median value. The MADS and SCE-UA algorithms are much slower. They need 1,000 simulations to get solutions that are generated by the DDS in some 250 simulations. However, from a hydrological perspective, all three methods converge on solutions of similar quality at the end. The median is within a 0.02 interval and the interquartile ranges are of the same order of magnitude for both HYDROTEL models. Although the DDS definitely shows a better efficiency during the optimization sequence, MADS and SCE-UA still provide high-quality final results after 2,000 simulations.

The results presented in Figure 1 highlight some important questions regarding the optimization strategies used by each method. The DDS algorithm offers significant potential for reducing the number of model simulations, as it identifies good-quality solutions very quickly in comparison with MADS and SCE-UA. Its ability to properly explore the solution space reveals interesting optimization strategies that differentiate it from the others. SCE-UA works with a population of parameter sets that evolves in the solution space and consequently, it wastes a significant number of model simulations because it needs to transport the whole population to good-quality zones, not just a single point as with DDS. In some ways, MADS also wastes model simulations when converging, since it must proceed through $2N$ simulations before decreasing the mesh size of the grid. However, this inefficiency remains limited because MADS stops as soon as it reaches a local optimal solution. For the HYDROTEL 10 problem, 65% over the 32 MADS optimization trials were completed before reaching the 2,000 simulations budget, and 15% in the case of HYDROTEL 19.

5 Proposed hybrid calibration approach

Two important factors need to be considered when choosing or developing optimization methods. First, the method must be able to perform a global exploration of the space of variables in order to identify a promising region containing good-quality solutions. Second, the method needs to perform a local descent within the region to approach the locally-optimal solution. Among the three optimization methods tested, DDS was shown to outperform the other two in the global exploration phase, while MADS was shown to be the most efficient for the local descent. Based on these complementary features, the following hybrid approach is proposed.

5.1 A hybrid DDS-MADS calibration approach

The hybrid DDS-MADS calibration approach aims to exploit the most efficient optimization strategies of both methods for reducing the overall computational time. A two-step approach is considered (a DDS step and a MADS step), with the effective strategies consisting of: 1) the global exploration ability of the DDS algorithm; 2) the local refinement process of the MADS algorithm; and 3) the automatic stopping criterion of MADS, relative to the convergence process.

In order to adequately merge the two methods, five simple transition features were attached to the source codes of the two optimization algorithms. Despite the broad availability of source codes, no changes were made in an effort to maintain a high level of simplicity and to respect the original optimization strategies of both algorithms. For more details on the optimization strategies used, see Tolson & Shoemaker (2006) and Le Digabel (2011) for the DDS and MADS algorithms, respectively. These transition features are described below. Figure 2 presents the pseudocode of the hybrid DDS-MADS calibration, highlighting in blue the five added transition features.

1. Cache

A first transition feature is the addition of a cache file C over the link between the Blackbox simulation and the feedback sent to the optimization algorithm. After each call to the simulation, the objective function value $F(X_{new})$ and its associated parameter sets X_{new} are registered in a cache file. This cache contains the historical record of the optimization process. Its implementation serves two purposes: 1) to avoid launching the simulation with the same parameter sets; and 2) to provide information on the sensitivity of the objective function to each calibration parameter.

2. Fine-tuning of the initial mesh size

The MADS algorithm requires an initial value of the mesh size parameter Δ_{k0} . Instead of using the default value, the hybrid method analyzes the results from the DDS step to propose a more appropriate value of Δ_{k0} . This parameter dictates the initial step lengths performed by MADS. If a good-quality solution X^{DDS}_{best} is provided to the MADS step, the initial mesh size Δ_{k0} must be tuned on a local domain. Alternately, if a poor-quality solution is provided to the MADS step, the initial mesh size Δ_{k0} must be tuned on a larger domain to allow the method to escape from it. In both situations, the Δ_{k0} fine-tuning is achieved using a spatial variability analysis from the parameter sets found in the cache file C . The initial mesh size Δ_{k0} is determined according to the two following steps.

The first step deals with selecting the parameter sets from the cache memory C . All parameter sets X having an objective function value $F(X)$ within a prescribed tolerance gap with $F(X^{DDS}_{best})$ are selected to be part of the lower-quality cache C^* serving the fine-tuning process. This gap is set to 10% of the difference between the worst X in C and the value of X^{DDS}_{best} . This gap leads to a local domain selection when X^{DDS}_{best} is already in a good-quality zone, and to a larger domain selection when the quality of X^{DDS}_{best} is poorer. This strategy opens up the possibility to include more than one good-quality zone if C^* is composed of lower-level good-quality solutions positioned inside other good-quality zones far from the value of X^{DDS}_{best} .

The second step concerns the spatial variability analysis of X in the lower-quality cache C^* . Since the range of values may vary greatly from one calibration parameter to another, the initial mesh size Δ_{k0}

must be fine-tuned anisotropically, i.e., differently for each parameter. The maximum and minimum values of each calibration parameter j are used for setting the initial parameter mesh size Δ_{k0}^j . Three different situations are possible. The first is that the value of j is the same for all X in C^* . The mesh size is then set to its default value, i.e., 10% of the interval defined by the upper and lower bounds on the allowed values of j . The second is that the values of j mostly cover the interval defined by the bounds. In this case, the mesh size is set to 50% of the bound interval to maintain an efficient size of the mesh. In all other cases, the initial mesh size is set as the ratio between the length covered by the values of assumed by j and the interval length defined by the bounds on j .

3. Stagnation parameter

With a two-step calibration approach, identifying the appropriate timing for interrupting the DDS step and initiating the MADS step becomes a major issue to assure efficient calibration. When the DDS reaches a zone of good-quality solutions, its optimization strategies become less efficient for local improvement. Stagnation occurs and often results in several hundreds of simulations that do not improve the quality of the objective function value. Such stagnation suggests the exhaustion of the DDS step optimization strategies and indicates the starting point for the MADS step. To ensure the transition between the two calibration steps, a stopping criterion represented by the stagnation parameter *stag* is inserted to limit the number of consecutive unsuccessful simulations.

The stagnation parameter *stag* must be set to a threshold value that allows a smooth transition to the MADS step without being premature or late. The proposed value is $2N$, where N is the number of calibration parameters. There are two justifications for this choice: 1) the local search strategy of the MADS algorithm proceeds to the refinement of the mesh size after $2N$ unsuccessful simulations; and 2) a sensibility analysis was performed on some HYDROTEL calibration problems, and has validated that $2N$ is an appropriate threshold for the stagnation parameter *stag*. In this way, the DDS step benefits from the same opportunity to improve the quality of the objective function value as the MADS step does for the refinement of the mesh size.

After each completed simulation, the value $F(X_{new})$ is compared to the best current value F_{best} in order to update the number of consecutive unsuccessful simulations s . Three scenarios may occur: 1) if $F(X_{new})$ improves the objective function value, the stagnation counter is reset to $s = 1$ and $F_{best} = F(X_{new})$; 2) if $F(X_{new})$ equals F_{best} , the stagnation counter remains unchanged; and 3) if F_{best} remains superior to $F(X_{new})$, then the simulation is declared unsuccessful and the stagnation counter increases to $s = s + 1$. When the stagnation counter s reaches the threshold of the stagnation parameter *stag*, the DDS step is stopped and the MADS step takes the lead for the calibration process.

4. Total simulation budget

The user must provide the total simulation budget m , which determines the overall allowed computational time for the optimization process. The two-step approach is designed to allow the optimization strategies of both methods consume the necessary simulation budget in terms of their own capacity to decrease the objective function value. The DDS step is initially set with the total simulation budget b_t to globally explore the solution space until the stagnation threshold *stag* is reached. The MADS step then continues the optimization process with the remaining budget $b_2 = b_t - b_1$, where b_1 represents the number of simulations consumed by the DDS step. It is important to keep in mind that the remaining budget b_2 is not necessarily reached if the MADS step terminates the optimization process according to its own stopping criterion (see Figure 2).

5. Rounding the objective function value

The last feature addresses the attenuation of the numerical noise on the objective function surface by rounding the values. A very desirable property of the MADS algorithm is its capacity to adapt the mesh size to nonsmooth objective functions, regardless of the noise level. The calibration of hydrological models is certainly a noisy problem. Nevertheless, from a hydrological perspective, a difference of 0.01 between two values of $1 - NSE$ does not allow for any differentiation of the quality of the parameter sets on a validation or operational simulation. A continuous adaption from refinement to expansion of the mesh size for slight gains less than a 0.01 interval of $1 - NSE$ would lead to unnecessary computational

efforts. To avoid this situation, the noise level is attenuated with an appropriate rounding process to reflect the hydrological perspective. Rounding the objective function values conservatively to 3 digits ensures a faster convergence to a satisfactory optimum. By handling this directly through the $F(X)$ values returned by the hydrological model simulation, both the DDS and MADS steps can take advantage of this rounding.

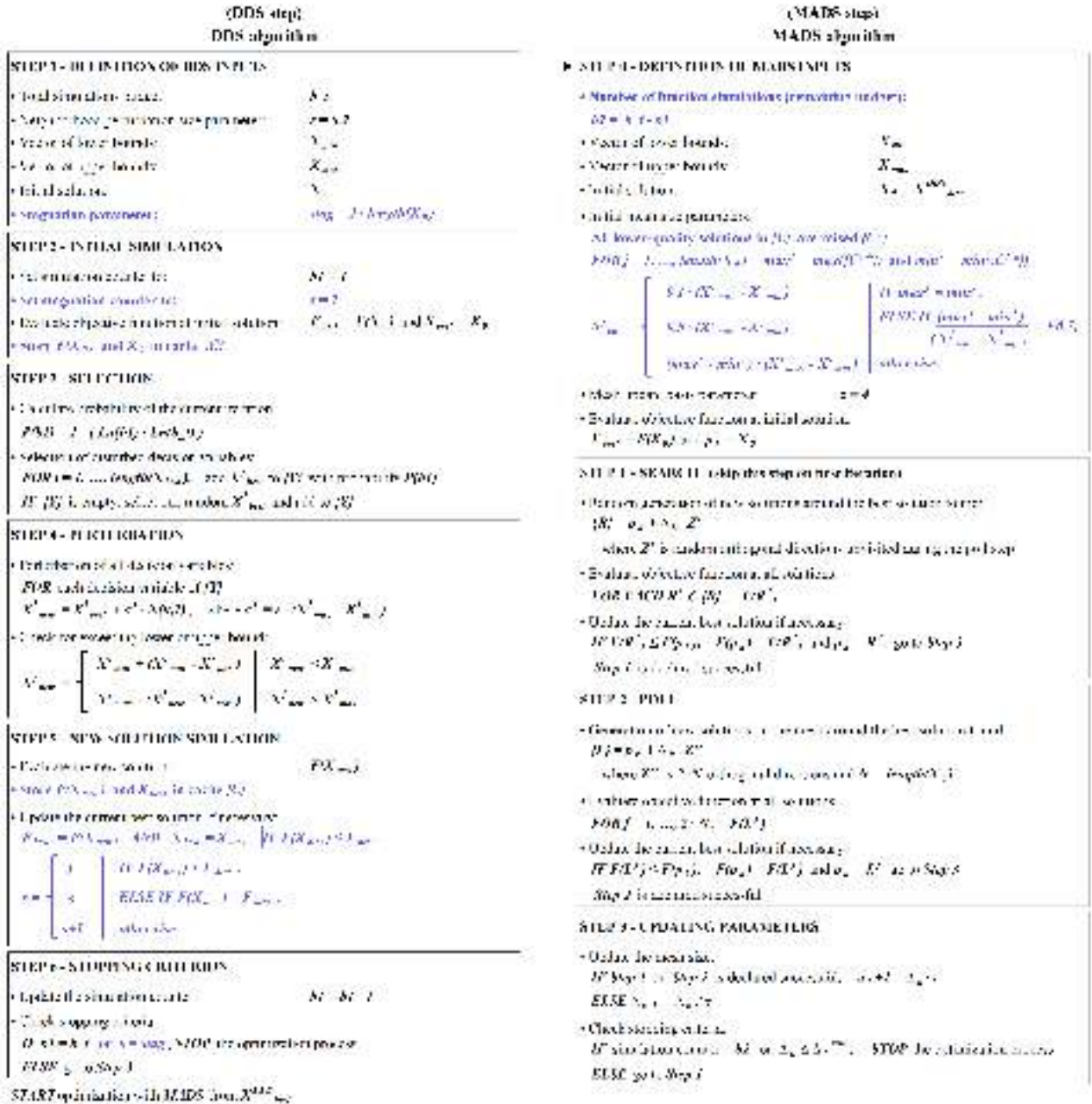


Figure 2: Pseudocode of the hybrid DDS-MADS calibration approach

5.2 Numerical results

Figure 3 presents the final results from 32 calibration trials using the hybrid DDS-MADS approach for the Cowansville watershed modeled by HYDROTEL 10 and 19, in comparison with the benchmark DDS

algorithm set with a 2,000 total simulations budget (hereafter called DDS-Bench). DDS-Bench is used for comparison because it provided the best performance in preliminary studies (Section 4). The hybrid method and DDS-Bench both start with the same 32 random parameter sets. In Figure 3, the grey curves in the background represent results obtained with DDS-Bench. The blue curves represent the DDS optimization step within the hybrid DDS-MADS approach, while orange curves represent the MADS optimization step. The blue dots are the endpoints of the DDS step and the starting points of the MADS step. The orange points correspond to the final objective function obtained at the end of the hybrid approach. This section exclusively presents the results from the Cowansville watershed, but similar results were obtained for Ceizur for both HYDROTEL optimization problems.

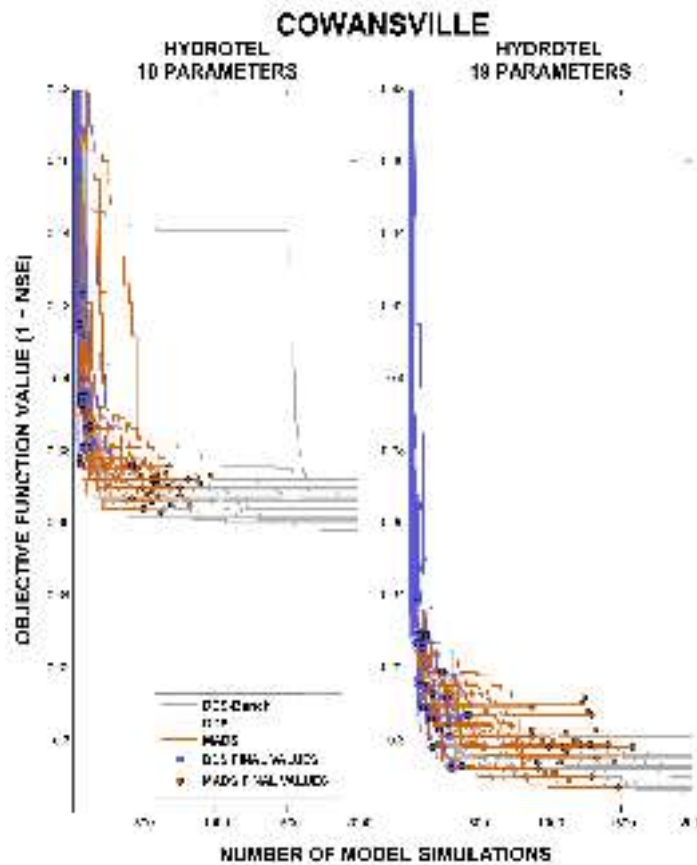


Figure 3: Evolutions of the best objective function values obtained ($1 - NSE$) with the hybrid DDS-MADS approach compared to DDS-Bench values. Optimization was performed for the HYDROTEL 10 and 19 problems on the Cowansville watershed

Figure 3 shows that the evolutions of the best objective function values of the hybrid approach are comparable to those obtained with DDS-Bench. However, each calibration trial of DDS-MADS stopped before reaching the 2,000 total simulations budget, providing a reduction in computational time. It can be observed that the DDS optimization step tends to greatly reduce the value of the objective function within a very limited number of simulations. As discussed in Section 4.3, the DDS step demonstrates remarkable efficiency in global exploration of the solution space, quickly locating good-quality zones. Then, when the DDS optimization strategies are dwindling, the MADS step takes over and continues to decrease the objective function value. The MADS step allows the calibration process to finish quickly, while ensuring that a local optimum can be obtained on a limited area of the solution space. Note that there is no slow-down in the decreasing curve when the MADS optimization step takes the lead, an indication that the initial mesh size is a good fit based on the historical results of the DDS step. This scenario provided an efficient profitability for all of the simulations performed by offering significant reductions in computational time while providing final solutions that satisfy some necessary optimality conditions.

Figure 4 shows the same results as those in Figure 3 but with the focus on the final objective function values. This figure shows that the range between the final values of DDS-Bench (grey box plots) and those of the hybrid DDS-MADS approach (orange box plots) is less than 0.02 of the NSE. In a context of hydrological modelling, this range is too small to favor one optimization method or the other. A final calibration value that is only slightly better than another one cannot ensure better quality on a validation or operational simulation. A low variability of the 32 final solutions obtained with DDS-MADS provides an indication of the robustness of the calibration approach.

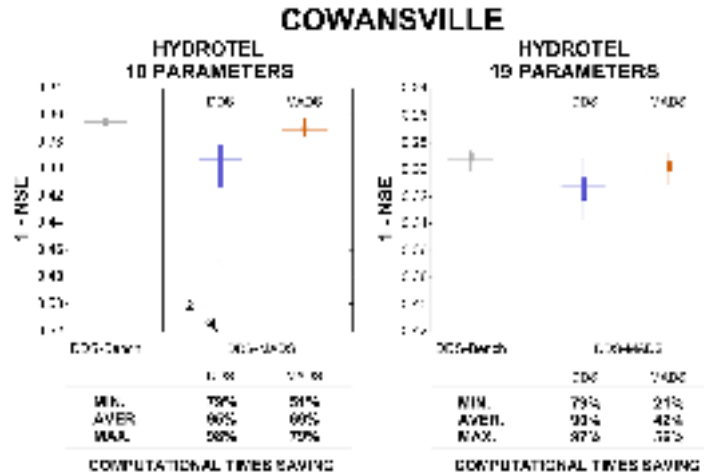


Figure 4: Final NSE optimization results and computational time savings of DDS-MADS (separated into DDS and MADS steps) compared to DDS-Bench results. Optimization was performed for the HYDROTEL 10 and 19 problems on the Cowansville watershed

It is also important to observe the wider variability obtained by the DDS step (blue box plots) in comparison with that of the MADS step (orange box plots). This wide variability suggests that it is not a good strategy to terminate the calibration immediately after the DDS step when the stagnation parameter threshold has been reached. The MADS step demonstrates the capacity to reduce the variability of the objective function values, indicating its value as a complementary method to the efficiency of the global exploration capacity of the DDS step.

The computational time savings realized are significant for both optimization problems. Using the hybrid DDS-MADS approach offers a computational time reduction of 69% on average compared to the DDS-Bench results for the calibration of HYDROTEL 10, and of 42% on average for HYDROTEL 19. This result is a reduction of 25 and 18 hours, respectively, on the computational times in Table 2 for the two Cowansville HYDROTEL problems. Increasing the number of parameters from $N = 10$ to $N = 19$ almost doubles the computational time. This is mostly due to the fact that each iteration of MADS launches $2N$ simulations at each iteration in order to eventually refine the mesh size and converge to a nearby local optimum. Similar interesting results were obtained on the Ceizur watershed, i.e., 70% on average for the calibration of HYDROTEL 10 and 38% on average for HYDROTEL 19, representing a reduction of 37 and 23 hours respectively on the computational times in Table 2.

5.3 Validation

Since the Toulmustouc watershed was not considered for designing the hybrid DDS-MADS calibration approach, it is used here to validate the performance obtained on the Cowansville and Ceizur watersheds. This choice was motivated by the objective of validating the versatility of the hybrid approach while also proving a non-overfit to some specific optimization problems. Figure 5 shows the same type of results as in Figure 3, but for the Toulmustouc watershed. The performance of the hybrid approach is equally effective as it was on the other two watersheds. The quality of the final objective function values is comparable to those obtained with DDS-Bench, and the variability of final solutions is within the 0.02 range of the objective function. All

calibration trials are stopped before the 2,000 total simulations budget. Based on Table 2, the computational time savings is slightly higher on these validation problems; 75%, corresponding to 45 hours on average on HYDROTEL 10, and 45%, corresponding to 35 hours on average on HYDROTEL 19. The results on the Toulnostouc watershed show robustness in terms of the quality of the final solutions, and computational time efficiency is preserved.

The HYDROTEL 19 results in Figure 5 show that two calibration trials by DDS were trapped in a zone of poor quality with a value of $1 - NSE$ superior to 0.39. A similar observation was possible on one calibration trial in Figure 3 for DDS-Bench on HYDROTEL 10. Such a situation is likely to occur when multiple calibrations are conducted. The authors of the DDS algorithm (Tolson & Shoemaker, 2007) propose starting multiple simultaneous calibrations to reduce the likelihood of being trapped in a poor quality zone. It can observe that the addition of the MADS step to the hybrid approach prevents this kind of situation and maintains the optimization process on one single calibration.

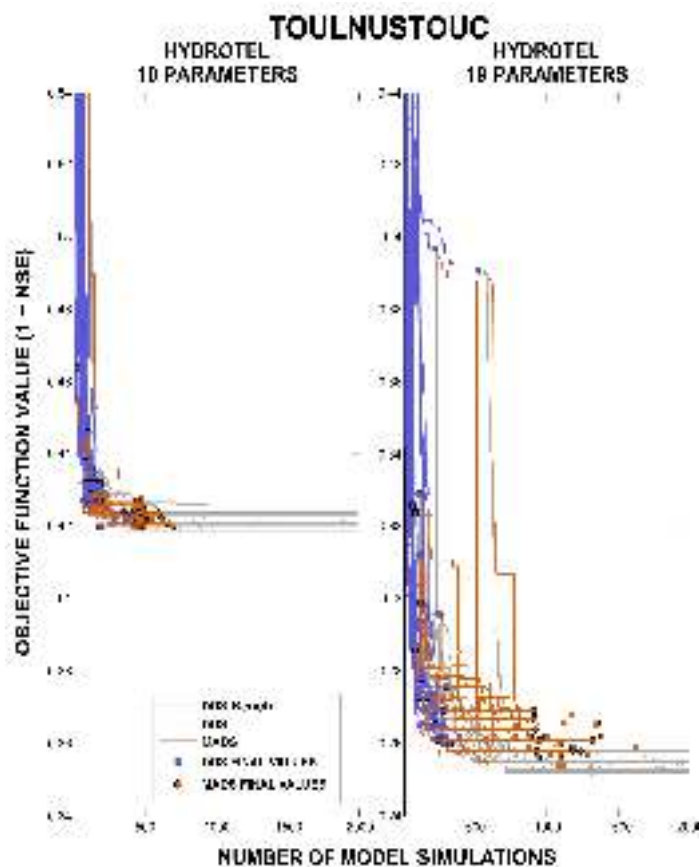


Figure 5: Evolutions of the best objective function values obtained ($1 - NSE$) with the hybrid DDS-MADS approach compared to DDS-Bench values. Optimization performed for the HYDROTEL 10 and 19 problems on the Toulnostouc watershed

5.4 Discussion and future works

Figures 3 to 5 and preliminary studies clearly show that the DDS-Bench algorithm performs effectively at the beginning of the calibration, but consumes many unnecessary simulations after having found a good-quality solution. In several of these runs, more than 1,000 simulations (unnecessary) improve the quality of the final solution by only a marginal amount. This behaviour suggests beginning the calibration process using the DDS algorithm and then to terminate it as soon as a good-quality solution is found. However, this approach requires constant monitoring by the user in order to cut off the process with good timing. A good knowledge of the modeled watershed is crucial to halting the calibration process when a satisfying solution has been obtained.

Another possibility is to use the DDS algorithm with a lower budget of simulations. The capacity to adapt the optimization to the user-specified budget is an interesting feature of the DDS algorithm. The authors of this algorithm (Tolson & Shoemaker, 2007) prove that a lower total simulations budget normally leads to a faster decrease of the objective function value. However, the probability of being trapped in a poor quality zone increases when the number of simulations dedicated to the global exploration is reduced due to the adaptive process. As mentioned in Section 5.3, multi-start strategies and parallelism may help in preventing trapping issues, but that would involve the use of a multi-core processor.

The hybrid DDS-MADS calibration approach does not require any parameters. First of all, DDS-MADS has a strategy to stop the calibration automatically related to the quality of the objective function value. No constant monitoring and no manual cut-off are needed. A good knowledge of the modeled watershed is not mandatory to evaluate what is a good or satisfying solution. Secondly, the hybrid approach is designed to run on a single-core processor without monopolizing all the computational power of a standard laptop. These two functionalities provide for a simplified implementation for operational usage and for research purposes.

The results presented in Sections 5.2 and 5.3 show that DDS-MADS is an efficient and robust hybrid approach combining the best optimization strategies of two existing algorithms. The capacity to globally explore the solution space of DDS quickly leads to a good-quality zone. Then, when stagnation occurs in the global exploration step, MADS ensures local tuning of the parameter set and converges to a nearby local optimum. This hybrid calibration approach provides straightforwardness and robustness in terms of the quality of the final solution. The main feature of this hybrid calibration approach is its significant reduction in computational time. For the three watersheds combined, an average time savings of 70% on HYDROTEL 10 and 40% on HYDROTEL 19 was achieved. These results translate into saving many computational hours.

Another important point about optimization tools is the accessibility of the source codes and the technical support offered. In both cases, these optimization algorithms are freely and easily available on the authors' websites. Matlab source codes for the DDS algorithm are available in open source by emailing the first author (Tolson & Shoemaker, 2007). Releases are updated and technical support is always available. The latest release allows solving box-constrained optimization problems with continuous, integer or mixed decision parameters. With the large community around the MADS algorithm, the authors service a website dedicated to this optimization tool. The MADS algorithm is downloadable from the Matlab OPTI Toolbox (open source code), as well as in C++ for multi-platform applications. Multiple functionalities are continuously added to MADS and it is accompanied by a clear user guide. Different types of decision parameters including categorical variables, Variable Neighborhood Search (VNS) and quadratic and surrogate models are just a short list of the additional functionalities.

Another significant point about DDS-MADS is the possibility to transpose the hybrid approach on biobjective and/or parallel computing networks optimization. The authors of both methods propose different versions or modalities offering these possibilities. The DDS authors propose the multi-objective "Pareto Archived Dynamically Dimensioned Search" (PADDS; Asadzadeh & Tolson; 2009) version, the "Asynchronous Parallel Dynamically Dimensioned Search" (PDDS; Tolson et al.; 2007), a parallel computing networks method, and the "Parallel Pareto Archived Dynamically Dimensioned Search" (ParaPADDS; Tolson et al.; 2015), combining multi-objective and parallel computing networks. The NOMAD software package also provides tools for biobjective optimization (Audet et al., 2010) as well as for its utilization in a parallel environment (Audet et al., 2008).

Razavi et al. (2010) introduced four different approaches for dealing with the issue of computationally intensive problems. Future research efforts will be focused on the last one: the implementation of surrogate models within the optimization process. Working on intensive computational hydrological models, two broad families of surrogate models will be analysed: 1) the lower-fidelity physically based surrogates, which are a simplification of the original model; and 2) the response surface surrogates, which are statistical or empirical data-driven models reproducing the response of the original model (Razavi et al., 2012a). Retaining the goal of reducing the computational time, future research will evaluate the representativeness of a wide range of surrogate models built from the original HYDROTEL model. The representative surrogate models will then be implemented inside different optimization algorithms or calibration approaches. Mixing surrogate models and more computationally-efficient optimization approaches is not ruled out.

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