

Nomad user guide version 3.4.2

Sébastien Le Digabel

July 30, 2010

How to use this guide:

- New users of Nomad: Section 2 describes how to install the software. Section 3 describes the simplest usage of Nomad. Nomad has default values for all of its internal parameters.
- ADVANCED FEATURES OF NOMAD: The more experienced users will find in Section 4 and above ways to tailor the output files and to modify all internal parameters.

Contents

1	Inti	roduction		3
2	Inst	tallation and examples		4
	2.1	Installation procedure		4
	2.2	Setting environment variables		6
	2.3	Manual compilation of the code		6
		2.3.1 X systems: Linux, Unix, and Mac OS X		6
		2.3.2 Windows with minGW		6
		2.3.3 Windows with Visual C++		7
	2.4	Examples		7
		2.4.1 Advanced examples		7
		2.4.2 Interface examples		8
3	NO	OMAD batch mode		8
•	3.1	Creation of a basic parameters file		9
	3.2	Basic instructions on blackbox programs		9
	0.2	Danie interactions on brackbox programs		
4		OMAD library mode		4
	4.1	Definition of the problem		14
	4.2	The main function		17
		4.2.1 Parameters		۱7
		4.2.2 Evaluator declaration and algorithm run		۱7
		4.2.3 Access to the solution and to optimization data		18
	4.3	Other functionalities of the library mode		20
		4.3.1 Automatic calls to user-defined functions		20
		4.3.2 Create groups of variables		20
		4.3.3 Multiple runs	2	20
5	Par	rameters description	2	22
	5.1	Parameters describing the problem	2	22
		5.1.1 Basic		22
		5.1.2 Advanced	2	23
	5.2	Algorithmic parameters	2	24
		5.2.1 Basic	2	24
		5.2.2 Advanced		25
	5.3	Output parameters		26
		5.3.1 Basic		27
		5.3.2 Advanced		27
	5.4	Additional information for some parameters		27
		5.4.1 Executable parameters BB_EXE and SGTE_EXE		27
		5.4.2 Blackbox input parameter BB_INPUT_TYPE		28
		5.4.3 Blackbox output parameter BB_OUTPUT_TYPE		28
		5.4.4 Blackbox redirection parameter BB_REDIRECTION		29
		5.4.5 Bounds		-0 29
		5.4.6 Direction types		30
		5.4.7 Output parameters DISPLAY_STATS and STATS_FILE		30
		5.4.8 Fixed variables parameter FIXED_VARIABLE		32

		5.4.9 Mesh and poll size parameters	32 32 33
		5.4.11 Scaling parameter SCALING	33
		5.4.13 Group of variable parameter VARIABLE_GROUP	აა 33
			ээ 33
		5.4.14 Starting point parameter X0	33
6	Spe	cial functionalities	34
	6.1	Categorical variables	34
		6.1.1 Algorithm	34
		6.1.2 Categorical variables with NOMAD	35
	6.2	Biobjective optimization	36
	6.3	Sensitivity analysis	37
	6.4	Variable Neighborhood Search (VNS)	38
	6.5	Parallel versions	38
		6.5.1 The p-Mads method	39
		6.5.2 The Coop-MADS method	39
		6.5.3 The PSD-MADS method	40
7	Rele	ease notes	40
	7.1	Version 3.4	40
		7.1.1 Major changes	40
		7.1.2 Minor changes	41
		7.1.3 Specific changes for versions 3.4.1 and 3.4.2	41
		7.1.4 List of modified classes or methods	41
		7.1.5 List of main changes for programs using the NOMAD library	42
	7.2	Previous versions	42
		7.2.1 Version 3.3	42
		7.2.2 Version 3.2	42
		7.2.3 Version 3.1	43
	7.3	Future versions	43
Re	elate	l publications	46

1 Introduction

NOMAD (Nonsmooth Optimization by Mesh Adaptive Direct Search) is a C++ implementation of the Mesh Adaptive Direct Search (Mads) algorithm [6, 18, 20], designed for constrained optimization of blackbox functions in the form

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

where $\Omega = \{x \in X : c_j(x) \leq 0, j \in J\} \subset \mathbb{R}^n$, $f, c_j : X \to \mathbb{R} \cup \{\infty\}$ for all $j \in J = \{1, 2, ..., m\}$, and where X is a subset of \mathbb{R}^n . It is also possible to consider (2) as a biobjective version of (1). Biobjective optimization is described in Section 6.2.

Developers of the method behind Nomad include

• Mark A. Abramson (Mark.A.Abramson@boeing.com), The Boeing Company.

- Charles Audet (www.gerad.ca/Charles.Audet), GERAD and Département de mathématiques et de génie industriel, École Polytechnique de Montréal.
- J.E. Dennis Jr. (www.caam.rice.edu/~dennis), Computational and Applied Mathematics Department, Rice University.
- Sébastien Le Digabel (www.gerad.ca/Sebastien.Le.Digabel), GERAD and Département de mathématiques et de génie industriel, École Polytechnique de Montréal.

Version 3.0 (and above) of Nomad is developed by Sébastien Le Digabel. Previous versions were written by Gilles Couture (GERAD).

Nomad is designed to be used in two different modes: batch and library. The batch mode is intended for a basic and simple usage of the Mads method, while the library mode allows more flexibility. For example, in batch mode, users must define their separate blackbox program that will be called with system calls by Nomad. In library mode users may define their blackbox function as C++ code that will be directly called by Nomad without system calls and temporary files. This document explains how to get started with the batch mode in Section 3 and with the library mode in Section 4.

A new user of NOMAD can start to use it easily (see Section 3). NOMAD has default values for all of its internal parameters. The more experienced users will find in this document ways to tailor the output files and to modify the internal parameters.

NOMAD should be cited with references [4, 38]. Other relevant papers by the developers are accessible through the NOMAD website www.gerad.ca/nomad.

The project started in 2001, and was funded in part by AFOSR, CRIAQ, FQRNT, LANL, NSERC, the Boeing Company, and ExxonMobil Upstream Research Company.

2 Installation and examples

NOMAD is developed in C++ under Linux with the gcc compiler (g++), version 4. The parallel version uses the message passing interface (MPI [52]). In particular, the MPI implementations openMPI, LAM, MPICH, and the Microsoft HPC pack, have been considered.

NOMAD has also been tested on Unix, Mac OS X with Xcode (gcc 4), Windows XP with minGW (gcc for Windows), and Visual C++ 2008. NOMAD is freely distributed under the GNU Lesser General Public License that can be read in the file lgpl.txt provided in the package or at www.gnu.org/licenses.

There are two ways of installing NOMAD: execute the installation program corresponding to your system, or compile the source code. Three files containing the NOMAD package are available on the website. Download the one adapted to your system (Windows, Linux/Unix, or Mac OS X).

2.1 Installation procedure

For Windows, simply execute the downloaded file, and follow the instructions. The NOMAD executable and the NOMAD library included in the Windows package have been constructed with minGW. If you are using Visual C++, your programs will not link with this version of the library and you must compile the library yourself.

For Mac OS X, open the disk image and copy the NOMAD directory into your Applications folder. We suggest that the user chooses an installation directory without space in the name to ease the creation of environment variables. Also choose directories for which you have the adequate writing rights.

For X systems, decompress the downloaded zip file where you want to install NOMAD, go to the \$NOMAD_HOME/install directory, and execute the ./install command.

This script automatically compiles the code and generates the NOMAD executable in \$NOMAD_HOME/bin and the Nomad library in \$NOMAD_HOME/lib. The script also detects if MPI is installed by checking the existence of the command mpic++. If so, the parallel Nomad executable and library are generated in the same directories than for the scalar version. Note that this installation procedure may also be applied on Mac OS X if the gcc compiler is installed (if not, install Xcode). After installation, you should have the directory structure described by Figure 1.

```
$NOMAD_HOME
   I- bin
   |- doc
   |- examples
        I- advanced
              |- categorical
                   |- bi_obj
                   |- single_obj
              |- multi_start
              |- plot
              |- restart
              |- user_search
         |- basic
              |- batch
                   |- bi_obj
                   |- single_obj
              |- library
                   |- bi_obj
                   |- single_obj
           interfaces
              |- AMPL
              |- CUTEr
              |- DLL
              |- FORTRAN
              I- GAMS
              |- MATLAB
              |- NOMAD2
   |- install
   |- lib
   I- src
   I- tools
        I - COOP-MADS
        |- PSD-MADS
         I- SENSITIVITY
```

Figure 1: Directory structure of the Nomad package.

2.2 Setting environment variables

The installation programs do not set any environment variables. Defining such variables allows more convenient access to NOMAD. The first variable to be defined should be \$NOMAD_HOME, whose value is the directory where NOMAD has been installed. This variable is used by the makefiles provided in the examples and is assumed to be defined in this document. Another environment variable to set is the path variable where \$NOMAD_HOME/bin should be added. This way, you may just type nomad to execute NOMAD.

To create your environment variables, on X systems, if your shell is bash, add the following lines in the file .profile located in your home directory:

```
export NOMAD_HOME=YOUR_NOMAD_DIRECTORY
export PATH=YOUR_NOMAD_DIRECTORY/bin:$PATH
```

In case your shell is csh or tcsh, add the following lines to the file .login:

```
setenv NOMAD_HOME YOUR_NOMAD_DIRECTORY
setenv PATH YOUR_NOMAD_DIRECTORY/bin:$PATH
```

In order for your variables to be active, enter the command 'source .profile' or 'source .login', or simply log out and log in. If you use a different shell, please modify your environment variables accordingly.

On Windows, environment variables are accessible in the Control Panel|System|Advanced|Environment variables menu. Please note that environment variables are named differently and \$NOMAD_HOME corresponds to %NOMAD_HOME%. For the parallel version under Windows, you need also to define the %MPI_HOME% environment variable corresponding to the home directory of your MPI installation.

2.3 Manual compilation of the code

If the installation program failed, you need to compile the source code located in \$NOMAD_HOME/src to generate the NOMAD executables. We assume a basic knowledge of makefiles, which are provided for X and Windows systems.

2.3.1 X systems: Linux, Unix, and Mac OS X

Enter the command 'make all' from a terminal opened in directory \$NOMAD_HOME/src. This will create the executable file nomad located in \$NOMAD_HOME/bin and the library file nomad.a in \$NOMAD_HOME/lib. For the parallel version, type 'make allmpi', after ensuring that the command mpic++ works. The executable nomad.MPI and the library nomad.MPI.a should be generated after the compilation. If these 'make' commands fail, try 'gmake' instead of 'make'.

2.3.2 Windows with minGW

Apply the same procedure as in 2.3.1 except that for the parallel version the environment variable %MPI_HOME% must be defined depending on your MPI implementation. The executable are %NOMAD_HOME%\bin\nomad_MPI.exe, and the libraries %NOMAD_HOME%\lib\nomad_MPI.lib\nomad_MPI.lib\nomad_MPI.lib\.

2.3.3 Windows with Visual C++

For the scalar version, create a new console and empty project. Choose a name for your project ('project_name' for example), and create the project in %NOMAD_HOME%. Then, add all .cpp and .hpp source files to the project, and compile in release mode. This generates the executable file %NOMAD_HOME%\project_name\Release\project_name.exe, which can be copied in %NOMAD_HOME%\bin for convenience and to stay consistent with this document. Apply the same procedure to generate the library except that you must create an empty static library project and that you must not insert the file nomad.cpp into the project.

For the parallel version you must link your program with MPI. First, you must install a MPI implementation (MPICH or the Microsoft HPC pack, for example). Then, once your project is created, in the project properties, add your MPI library directory to 'Linker Additional Library Directories', and add the MPI library (typically mpi.lib) to 'Linker Input Additional Dependencies'. Finally, add the location of the MPI header file to 'Additional Include Directories'.

2.4 Examples

Examples are located in \$NOMAD_HOME/examples. Some of them use the batch mode described in Section 3 and some of them use the library mode of Section 4. For the library examples, a makefile is included which can be used to generate a scalar executable (command make), or a parallel executable (command make mpi). The examples are classified into 3 categories: basic examples, advanced examples, and examples illustrating interfaces between Nomad and various programing or modeling languages.

Basic examples are a good way to start out with NOMAD. The detailed description of the advanced examples is given next.

2.4.1 Advanced examples

- CATEGORICAL: Categorical variables on a simple portfolio selection problem. A singleobjective and a biobjective version are given.
- MULTI_START: Multistart program launching multiple instances of MADS. The different starting point are generated following a Latin-Hypercube sample strategy.
- **PLOT**: Illustration of the NOMAD::Evaluator::update_success() virtual function allowing to plot information during the NOMAD execution. This example has been developed by Quentin Reynaud.
- **RESTART**: How to make a Nomad restart and illustration of the user-defined function Nomad::Evaluator::update_iteration().
- USER_SEARCH: How users may code their own search strategy. This example corresponds to a search described in [24]. Other examples on how to design a search strategy can be found in files \$NOMAD_HOME/src/Speculative_Search.*pp, LH_Search.*pp, and VNS_Search.*pp. Please note that the MADS theory assumes that trial search points must be lying on the current mesh. Functions NOMAD::Point::project_to_mesh() and NOMAD::Double::project_to_mesh() are available to perform such projections.

2.4.2 Interface examples

Examples of interfaces inluded in the Nomad package are:

- AMPL: This interface to the AMPL format uses a library developed by Dominique Orban and available at www.gerad.ca/~orban/LibAmpl/. A readme.txt file is given with the example and describes the different steps necessary for the example to work. This example has been written with the help of Dominique Orban and Anthony Guillou.
- CUTEr: How to optimize CUTEr [43] test problems.
- **DLL**: Blackbox that is coded inside a dynamic library (a Windows DLL). Single-objective and biobjective versions are available.
- FORTRAN: Two examples. First a blackbox problem coded as a FORTRAN routine linked to the NOMAD library. Then a more elaborated example mixing FORTRAN and the NOMAD library where a FORTRAN program is used both to define the problem and to run NOMAD.
- GAMS: Optimization on a blackbox that is a GAMS [32] program.
- MATLAB: Optimization on a blackbox that is a MATLAB function. In order for this last example to work, the MATLAB MCC compiler must be present, allowing the creation of stand-alone executables from MATLAB functions.
- **NOMAD2**: Program to use NOMAD version 3 on a problem originally designed for the version 2 of the software. This example has been written by Quentin Reynaud.

3 NOMAD batch mode

This section explains how to get started with the NOMAD batch mode and describes all the steps to solve a blackbox problem. The NOMAD batch mode is launched with one argument that corresponds to the name of a parameters text file. The blackbox problem must be coded as a stand-alone program. The different steps are:

- 1. Install Nomad following the instructions in Section 2.
- 2. Create a directory for your problem. In this document, we use the notation \$PB_DIR to refer to this directory.
- 3. Create your problem blackbox, which corresponds to an executable located in \$PB_DIR (see Section 3.2). This program will output the objective and the constraints.
- 4. Create a parameters file, for example \$PB_DIR/param.txt, located in the problem directory (see Section 3.1). This file describes where NOMAD will find your problem and what parameters to use.
- 5. If the NOMAD executable corresponds to the file \$NOMAD_HOME/bin/nomad, launch the algorithm with '\$NOMAD_HOME/bin/nomad \$PB_DIR/param.txt'.

At any time, you can type 'nomad -h param_name' to have information on a specific parameter, as described in Section 7.2.2. Advanced usage of NOMAD is not described in this section: All parameters are described in Section 5 and other examples are given in \$NOMAD_HOME/examples/advanced.

3.1 Creation of a basic parameters file

The parameters file is a text file given as argument to the NOMAD executable with the command '\$NOMAD_HOME/bin/nomad \$PB_DIR/param.txt' where param.txt is the parameters file (which must be located in the problem directory) and nomad is the NOMAD executable.

For basic usage, the following parameters must be defined:

- The number of variables, n (DIMENSION).
- The name of the blackbox executable that outputs the objective and the constraints (BB_EXE).
- The output types of the blackbox executable: objective and constraints (BB_OUTPUT_TYPE).
- A starting point (X0).
- Some stopping criteria (MAX_BB_EVAL, for example).

Bounds on variables are defined with the LOWER_BOUND and UPPER_BOUND parameters. If no stopping criterion is specified, the algorithm will stop as soon as the mesh size reaches a given tolerance.

An example is given in Figure 2 that corresponds to the parameters file located in \$NOMAD_HOME/examples/basic/batch/single_obj. Any entry on a line is ignored after the character '#'. The order in which the parameters appear or their case is unimportant.

The two constraints defined in the parameters file in Figure 2 are of different types. The first constraint $c_1(x) \leq 0$ is treated by the progressive barrier approach (PB), which allows constraint violations. The second constraint, $c_2(x) \leq 0$, is treated by the extreme barrier approach (EB) that forbids violations.

See Section 5 for the detailed description of all parameters.

3.2 Basic instructions on blackbox programs

With the batch use of Nomad, the blackbox defining your problem corresponds to a program that will be system-called by the algorithm. It may be coded in any language (even scripts) but must respect certain conditions. It must be callable in a terminal as follows: If the blackbox executable is $PB_DIR/bb.exe$, one can execute it with the command ' $PB_DIR/bb.exe$ x.txt'. Here x.txt is a text file containing a total of n=DIMENSION values consisting of one value for each variable, separated by spaces.

The problem directory, where the parameters file is located, may have spaces in its name. The blackbox executable may be located in sub-directories of the problem directory, but the names of the sub-directories must be space-free.

The blackbox program returns the evaluation values by displaying them in the standard output. It also returns the value 0 to indicate that the evaluation went well (a simple 'return 0' instruction in C). Otherwise Nomad considers that the evaluation failed. The number of values displayed by the blackbox program corresponds to the number of constraints plus one (or two) representing the objective function value(s) that one seeks to minimize. The constraints values correspond to constraints of the form $c_j \leq 0$ (for example, the constraint $0 \leq x_1 + x_2 \leq 10$ will must be displayed with the two quantities $c_1(x) = -x_1 - x_2$ and $c_2(x) = x_1 + x_2 - 10$). The order of the displayed outputs corresponds to the order defined in the parameters file with parameters BB_EXE and BB_OUTPUT_TYPE. If variables have bound constraints, these are defined in the parameters file with parameters LOWER_BOUND and UPPER_BOUND. Bounds should not appear in the blackbox code.

In basic mode, your blackbox program cannot display other data than the objective and constraint values, but the advanced mode allows it to do so. Your code may generate temporary files but it is preferable to include tag numbers to the file names because of parallelism (see Section 6.5). The advanced parameters described in Section 5.2.2 allow you to include these tags in the blackbox input files. If you already have a blackbox program in a certain format, you need to interface it with a wrapper program to match the NOMAD specifications. If your blackbox program crashes in batch mode, it will not affect NOMAD: The point that caused this crash will simply be tagged as a blackbox failure.

A basic C++ program example is given in Figure 3 for the following problem with 5 variables and 2 constraints:

$$\min_{x \in \mathbb{R}^5} f(x) = x_5$$

$$\begin{cases}
c_1(x) = \sum_{i=1}^5 (x_i - 1)^2 - 25 & \leq 0 \\
c_2(x) = 25 - \sum_{i=1}^5 (x_i + 1)^2 & \leq 0 \\
x_i & \geq -6 & i = 1, 2, \dots, 5 \\
x_1 & \leq 5 \\
x_2 & \leq 6 \\
x_3 & \leq 7 .
\end{cases}$$

With gcc, you can compile this example with 'g++ -o bb.exe bb.cpp', and test it with the text file x.txt containing '0 0 0 0 0', by entering the command 'bb.exe x.txt'. This test should display '0 -20 20', which means that the point $x = (0\ 0\ 0\ 0)^T$ has an objective value of f(x) = 0, but is not feasible, since the second constraint is violated $(c_2(x) = 20 > 0)$.

```
DIMENSION
                              # number of variables
BB_EXE
               bb.exe
                              # 'bb.exe' is a program that
BB_OUTPUT_TYPE OBJ PB EB
                              # takes in argument the name of
                              # a text file containing 5
                              # values, and that displays 3
                              # values that correspond to the
                              # objective function value (OBJ),
                              # and two constraints values g1
                              # and g2 with g1 <= 0 and
                              # g2 <= 0; 'PB' and 'EB'
                              # correspond to constraints that
                              # are treated by the Progressive
                              # and Extreme Barrier approaches
                              # (all constraint-handling
                                 options are described in the
                                 detailed parameters list)
XΟ
               ( 0 0 0 0 0 ) # starting point
                              # all variables are >= -6
LOWER_BOUND
                              # x_1 <= 5, x_2 <= 6, x_3 <= 7
UPPER_BOUND
               (567 - -)
                              # x_4 and x_5 have no bounds
                              # the algorithm terminates when
MAX_BB_EVAL
               100
                              # 100 blackbox evaluations have
                              # been made
TMP_DIR
                              # indicates a directory where
               /tmp
                              # temporary files are put
                              # (increases performance by ~100%
                              # if you're working on a network
                              # account and if TMP_DIR is on a
                              # local disk).
```

Figure 2: Example of a basic parameters file. All parameters are detailed in Section 5 or with the command 'nomad -h param_name'.

```
#include <cmath>
#include <iostream>
#include <fstream>
#include <cstdlib>
using namespace std;
int main ( int argc , char ** argv ) {
  double f = 1e20, c1 = 1e20, c2 = 1e20;
  double x[5];
  if ( argc >= 2 ) {
    c1 = 0.0, c2 = 0.0;
    ifstream in ( argv[1] );
   for ( int i = 0 ; i < 5 ; i++ ) {
      in >> x[i];
      c1 += pow (x[i]-1, 2);
      c2 += pow (x[i]+1, 2);
    }
   f = x[4];
    if ( in.fail() )
      f = c1 = c2 = 1e20;
    else {
      c1 = c1 - 25;
      c2 = 25 - c2;
   }
    in.close();
  cout << f << " " << c1 << " " << c2 << endl;
  return 0;
}
```

Figure 3: Example of a basic blackbox program. This code corresponds to the file bb.cpp in \$NOMAD_HOME/examples/basic/batch/single_obj.

```
NOMAD - version 3.4.1 - www.gerad.ca/nomad
Copyright (C) 2001-2010 {
        Mark A. Abramson
                             - The Boeing Company
                             - Ecole Polytechnique de Montreal
        Charles Audet
        Gilles Couture
                             - Ecole Polytechnique de Montreal
        John E. Dennis, Jr. - Rice University
        Sebastien Le Digabel - Ecole Polytechnique de Montreal
Funded in part by AFOSR and Exxon Mobil.
         : '$NOMAD_HOME/src/lgpl.txt'
User guide: '$NOMAD_HOME/doc/user_guide.pdf'
Examples : '$NOMAD_HOME/examples'
          : '$NOMAD_HOME/tools'
Tools
Please report bugs to nomad@gerad.ca
MADS run {
        BBE
                OBJ
        3
        12
        34
                -2
        100
                -2
} end of run (max number of blackbox evaluations)
blackbox evaluations
best infeasible solution: (4.4\ 1.2\ 0\ -1\ -2)\ h=0.6\ f=-2
best feasible solution : ( 4.4 \ 1.2 \ 1.3 \ -1 \ -2 ) h=0 f=-2
```

Figure 4: Output given by NOMAD on the blackbox problem coded in Figure 3 with parameters file in Figure 2.

NOMAD is flexible enough so that blackbox codes can be coded differently and with more sophistication in the advanced mode (see Section 4).

Figure 4 shows the display that the execution of Nomad produces for the blackbox program in Figure 3 with the parameters file in Figure 2. Notice that the first feasible point has been found after 3 blackbox evaluations. In this case, the starting point $x = (0\ 0\ 0\ 0\ 0)^T$ violates the second constraint, which is treated by the extreme barrier approach. In such a situation, Nomad launches an initial optimization, called the *phase one step*, during which the value of the constraint violation is minimized. Once a feasible point is generated with this phase one, the original objective function is considered again.

4 Nomad library mode

This section explains how to create a C++ program able to call the NOMAD routines using the precompiled NOMAD static library. We suppose that the library is correctly installed and that the environment variable \$NOMAD_HOME is defined. If not, you must specify the installation directory of NOMAD in the makefile. Explanations are given for Linux and g++ and for the scalar library, but are similar for Windows and minGW or Visual C++, and for the parallel library. A basic knowledge of object oriented programmation with C++ is assumed.

The use of the standard C++ types for reals and vectors is of course allowed within your code, but it is suggested that you use the NOMAD types as much as possible. For reals, NOMAD uses the class NOMAD::Double, and for vectors, the class NOMAD::Point. A lot of functionalities have been coded for theses classes, which are visible in files Double.hpp and Point.hpp. All NOMAD class files are named like the classes and are located in the directory \$NOMAD_HOME/src. Other NOMAD types (essentially enumeration types) are also defined in defines.hpp. Some utility functions on these types can be found in utils.hpp. The namespace NOMAD is used for all NOMAD types, and you must type NOMAD:: in front of all types unless you type 'using namespace NOMAD;' at the beginning of your program.

The example shown in this section corresponds to files located in the directory \$NOMAD_HOME/examples/basic/library/single_obj. It is identical to the example shown in Section 3, except that no temporary files are used, and no system calls are made. For this example, just one C++ source file is used, but there could be a lot more. Other examples can be found in \$NOMAD_HOME/examples and in the main function of Nomad located in the file \$NOMAD_HOME/src/nomad.cpp which implements the Nomad batch mode. This illustrates the fact that even in library mode a parameters file may be used and system calls performed.

As a first task, a makefile needs to be created in the directory where your source code is located. An example of such a makefile is shown on Figure 5. Notice that each line after ':' has to begin with a tabulation. Such makefiles are given at various places inside the examples directory.

We now describe the other steps required for the creation of the source file basic_lib.cpp, which includes the header file nomad.hpp, and which is divided into two parts: a class for the description of the problem, and the main function. Once compiled with the makefile (type 'make'), the binary file basic_lib is created and can be executed.

4.1 Definition of the problem

Describing the blackbox problem directly in the code that calls NOMAD avoids the use of temporary files and system calls by the algorithm. This is achieved by defining a derived class My_Evaluator that inherits from the class NOMAD::Evaluator in single-objective optimization and from NOMAD::Multi_Obj_Evaluator in multi-objective mode (see header files Evaluator.hpp and Multi_Obj_Evaluator.hpp). An example of such a class is shown in Figure 7.

The objective of this user class is to redefine the virtual method eval_x() that will be automatically called by the algorithm. The prototype of eval_x() is given in Figure 6. Note that const and non-const versions of the method are available.

The argument x (in/out) corresponds to an evaluation point, i.e. a vector containing the coordinates of the point to be evaluated, and also the result of the evaluation. The coordinates are accessed with the operator [] (x[0] for the first coordinate) and outputs are set with the method NOMAD::Eval_Point::set_bb_output() ($x.set_bb_output(0,v)$) to set the objective function value to v if the objective has been defined at the first position). Constraints must be represented by values c_i for a constraint $c_i \leq 0$. Please refer to files Eval_Point.hpp and Point.hpp for details

```
EXE
           = basic_lib
COMPILATOR = g++
OPTIONS
           = -ansi -Wall -O3 -DGCC_X
L1
           = $(NOMAD_HOME)/lib/nomad.a
LIBS
           = $(L1) -lc -lm
INCLUDE
           = -I\$(NOMAD_HOME)/src -I.
           = $(COMPILATOR) $(OPTIONS) $(INCLUDE) -c
COMPILE
OBJS
           = basic_lib.o
$(EXE): $(OBJS)
        $(COMPILATOR) -o $(EXE) $(OBJS) $(LIBS) $(OPTIONS)
basic_lib.o: basic_lib.cpp $(L1)
        $(COMPILE) basic_lib.cpp
clean:
        @echo "
                   cleaning obj files"
        @rm -f $(OBJS)
```

Figure 5: Example of a makefile for a single C++ file linked with the NOMAD library.

Figure 6: Prototype of method NOMAD::Evaluator::eval_x(). A non-const version is also available.

about the classes defining Nomad vectors.

The second argument, the real h_max (in), corresponds to the current value of the barrier h_{max} parameter. It is not used in this example but it may interrupt an expensive evaluation if the constraint violation value h grows larger than h_{max} . See [20] for the definition of h and h_{max} and of the progressive barrier method for handling constraints.

The third argument, count_eval (out), needs to be set to true if the evaluation counts as a blackbox evaluation, and false otherwise (for example, if the user interrupts an evaluation with the h_{max} criterion before it costs some expensive computations, then set count_eval to false).

If a surrogate function is to be used, then its evaluation routine should be coded in the method $eval_x()$. First, to indicate that a surrogate can be computed, the user must set the parameter HAS_SGTE to yes, via the method NOMAD::Parameters::set_HAS_SGTE(). Then, in $eval_x()$, the test 'if (x.get_eval_type()==_SGTE_)' must be made to differentiate an evaluation with the true function f or with the surrogate. More notes on surrogates are given in Section 5.1.2.

Another possibility for the designer of eval_x() is the ability to define a priority for the trial point x via the method NOMAD::Eval_Point::set_user_eval_priority(). Points with higher priorities will be evaluated first. For more details, see the code in Priority_Eval_Point.*pp.

The function eval_x() should return true if the evaluation succeeded, and false if the evaluation failed.

Finally, note that the call to eval_x() inside the NOMAD code is inserted into a try block. This

means that if an error is detected by the user inside the eval_x() function, an exception should be thrown. The choice for the type of this exception is left to the user, but NOMAD::Exception is available (see Exception.*pp). If an exception is thrown by the user-defined function, then the associated evaluation is tagged as a failure and not counted unless the user explicitly set the flag count_eval to true.

```
class My_Evaluator : public NOMAD::Evaluator {
public:
  My_Evaluator ( const NOMAD::Parameters & p ) :
    NOMAD::Evaluator ( p ) {}
  ~My_Evaluator ( void ) {}
  bool eval_x ( NOMAD::Eval_Point
                const NOMAD::Double & h_max
                bool
                                    & count_eval
                                                   ) const {
    NOMAD::Double c1 = 0.0 , c2 = 0.0;
   for ( int i = 0 ; i < 5 ; i++ ) {
      c1 += (x[i]-1).pow2();
      c2 += (x[i]+1).pow2();
    }
    x.set_bb_output (0, x[4]); // objective value
    x.set_bb_output ( 1 , c1-25 ); // constraint 1
    x.set_bb_output (2, 25-c2); // constraint 2
    count_eval = true; // count a blackbox evaluation
                       // the evaluation succeeded
    return true;
  }
};
```

Figure 7: Example of a user class defining a hard-coded blackbox problem.

Of course, more elaborated NOMAD::Evaluator subclasses may be designed in order to consider some additional problem-related parameters. Such an example can be found in the source files Multi_Obj_Evaluator.*pp where some weights are defined to change the objective function of the problem between successive optimizations (this example correspond to the BIMADS algorithm [26]).

The virtual method update_success() can also be redefined in subclasses deriving from NOMAD::Evaluator. This method will be automatically invoked every time a new improvement is made. Note that the automatic calls to this method can be enabled/disabled with NOMAD::Evaluator_Control::set_call_user_update_success().

Another virtual method defined in the class NOMAD::Evaluator is compute_f(). This method allows the user to compute the value of the objective function directly from the blackbox outputs. This is used by the BIMADS algorithm. If compute_f() is not user-defined, then NOMAD simply takes the value of f as the first OBJ output from the blackbox.

4.2 The main function

Once your problem has been defined, the main function can be written. NOMAD routines may throw C++ exceptions, so it is recommended that you put your code into a try block. In addition, functions NOMAD::begin() and NOMAD::end() must be called at the beginning and at the end of the main function. NOMAD::Slave::stop_slaves() has also to be called at the end of the main function if parallelism is used.

4.2.1 Parameters

First, a NOMAD::Parameters object needs to be declared. Parameters are defined similarly as in batch mode and each parameter PNAME is set with the method NOMAD::Parameters::set_PNAME(). In order to see all the options, use the help 'nomad -h param_name', or refer to the detailed list of parameters in Section 5, or to the header file Parameters.hpp. NOMAD additional C++ types necessary for the calls to NOMAD::Parameters functions can be found in file defines.hpp. An example is given in Figure 8. This example is taken from file basic_lib.cpp located in \$NOMAD_HOME/examples/basic/library/single_obj and corresponds to the same parameters file example shown in Figure 2, except that no problem executable is used.

No parameters file is needed, but it is possible to take the parameters from such a file, with NOMAD::Parameters::read("param.txt") where param.txt is a valid parameters file. If a directory path is included in the name of the file, this path will be considered as the problem path instead of the default location './'. To display the parameters described by a Parameters object p, use the instruction 'cout << p << endl;'.

Once that all parameters are set, the method NOMAD::Parameters::check() must be invoked to validate the parameters. The algorithm will not run with a non-checked NOMAD::Parameters object. It is not even possible to access data from an object of this class while not checked. If parameters are changed, check() must be invoked again before a new run can be conducted. Notice that the call to check() may be bypassed by using NOMAD::Parameters::force_check_flag() but only advanced users should use it.

4.2.2 Evaluator declaration and algorithm run

The Mads algorithm is implemented with the NOMAD::Mads class. Objects of this class are created with a NOMAD::Parameters object and an NOMAD::Evaluator object. In the example described here, the NOMAD::Evaluator object corresponds to an object of type My_Evaluator. A NULL pointer may also be used instead of the NOMAD::Evaluator object: in this case, the default evaluator will be used. Assuming that the parameter BB_EXE has been defined, this default evaluator consists in evaluating the objective function via a separated blackbox program and system calls. When an NOMAD::Evaluator object is used, parameters BB_EXE and SGTE_EXE are ignored. A more advanced NOMAD::Mads constructor with user-created caches is also available in \$NOMAD_HOME/src/Mads.hpp.

Once that the NOMAD::Mads object is declared, run the algorithm with NOMAD::Mads::run() (or NOMAD::Mads::multi_run() for multi-objective optimization). An example is shown in Figure 9.

It is also possible for the user to redefine the virtual method NOMAD::Evaluator::list_of_po-ints_preprocessing() to indicate a preprocessing strategy that will be applied by the algorithm before each series of evaluations is made. All points may then be modified according to this strategy. See \$NOMAD_HOME/src/Evaluator.hpp for the header of this method.

4.2.3 Access to the solution and to optimization data

In the example of \$NOMAD_HOME/examples/basic/library/single_obj, final information is displayed via a call to the operator << at the end of NOMAD::Mads::run(). More specialized access to solution and optimization data is allowed. To access the best feasible and infeasible points, use the methods NOMAD::Mads::get_best_infeasible(). To access optimization data or statistics, call the method NOMAD::Mads::get_stats() which returns access to a NOMAD::Stats object. Then, use the access methods defined in Stats.hpp. For example, to display the number of blackbox evaluations, write:

cout << "bb eval = " << mads.get_stats().get_bb_eval() << endl;</pre>

```
// display:
NOMAD::Display out ( std::cout );
// parameters creation:
NOMAD::Parameters p ( out );
p.set_DIMENSION (5);
                                // number of variables
// definition of output types:
vector<NOMAD::bb_output_type> bbot (3);
bbot[0] = NOMAD::OBJ;
bbot[1] = NOMAD::PB;
bbot[2] = NOMAD::EB;
p.set_BB_OUTPUT_TYPE ( bbot );
// starting point:
p.set_X0 ( NOMAD::Point ( 5 , 0.0 ) );
// lower bounds: all var. >= -6:
p.set_LOWER_BOUND ( NOMAD::Point ( 5 , -6.0 ) );
// upper bounds (x_4 and x_5 have no upper bounds):
NOMAD::Point ub ( 5 );
ub[0] = 5.0; // x_1 \le 5
ub[1] = 6.0; // x_2 <= 6
ub[2] = 7.0; // x_3 <= 7
p.set_UPPER_BOUND ( ub );
p.set_MAX_BB_EVAL (100);
                           // the algorithm terminates
                             // after 100 bb evaluations
// parameters validation:
p.check();
```

Figure 8: Example of parameters creation in library mode.

```
// custom evaluator creation:
My_Evaluator ev ( p );

// algorithm creation and execution:
NOMAD::Mads mads ( p , &ev , cout );
mads.run();
```

Figure 9: Evaluator and Mads objects usage.

4.3 Other functionalities of the library mode

4.3.1 Automatic calls to user-defined functions

Virtual methods are automatically invoked by NOMAD at some special events of the algorithm. These methods are left empty by default and you may redefine them so that your own code is automatically called. These virtual methods are defined in the NOMAD::Evaluator and NOMAD::Multi_Obj_Evaluator classes and are detailed below:

- NOMAD::Evaluator::list_of_points_preprocessing(): Called before the evaluation of a list of points (it allows the user to pre-process the points to be evaluated).
- NOMAD::Evaluator::update_iteration(): Invoked every time a MADS iteration is terminated.
- NOMAD::Evaluator::update_success(): Invoked when a new incumbent is found (single-objective) or when a new Pareto point is found (biobjective).
- NOMAD::Multi_Obj_Evaluator::update_mads_run(): For biobjective problems, this method is called every time a single MADS run is terminated.

It is possible to disable the automatic calls to these methods, with the functions NOMAD::Mads::enable_user_calls() and NOMAD::Mads::disable_user_calls(), or with the parameters USER_CALLS_ENABLED and EXTENDED_POLL_ENABLED. These parameters are automatically set to yes, except during the extended poll for categorical variables and during the VNS search.

4.3.2 Create groups of variables

This section gives some explanations about creating groups of variables in library mode. See Section 5.4.13 for defining such groups in batch mode. Groups of variable are created with the method NOMAD::Parameters::set_VARIABLE_GROUP() which has two different prototypes. The method must be called each time a new group is created. For both versions of the function, the user needs to give a list of the indexes of the variables composing the group. In NOMAD, a group of variable generates its own polling directions. The most complete prototype of set_VARIABLE_GROUP() allows to choose the types of these directions, for the primary and secondary polls. The detailed types of directions can be found in file defines.hpp and the enum type direction_type. The simplified prototype uses OrthoMads types of directions by default. In all cases a Halton seed must be provided, which is not considered if direction types do not correspond to OrthoMads. Otherwise, a value must be provided. This value should be larger than the nth prime number, and ideally be different for each group of variables. The method NOMAD::Directions::get_max_halton_seed() is available in order to get the highest Halton seed that has been used, and help determine such a value. It is also possible to use the method NOMAD::Directions::compute_halton_seed() which directly computes the Halton seed as the nth prime number.

Finally the function NOMAD::Parameters::reset_variable_groups() may be called to reset the groups of variables. Remember also that after a modification to a Parameters object is made, the method NOMAD::Parameters::check() needs to be called.

4.3.3 Multiple runs

The method NOMAD::Mads::run() may be invoked more than once, for multiple runs of the MADS algorithm.

A first solution for doing that is simply to declare the NOMAD::Mads object, as in Figure 10. But, in this case, the cache, containing all points from the first run, will be erased between the runs (since its it created and deleted with NOMAD::Mads objects).

```
{
  NOMAD::Mads mads ( p , &ev , cout );

  // run #1:
  mads.run();
}

// some changes...

{
  NOMAD::Mads mads ( p , &ev , cout );

  // run #2:
  mads.run();
}
```

Figure 10: Two runs of MADS with a NOMAD::Mads object at local scope. The cache is erased between the two runs.

A better solution consists in using the NOMAD::Mads::reset() method between the two runs and to keep the NOMAD::Mads object in a more global scope. The method takes two boolean arguments (set to false by default), keep_barriers and keep_stats, indicating if the barriers (true and surrogate) and statistics must be reseted between the two runs. An example is shown in Figure 11.

```
NOMAD::Mads mads ( p , &ev , cout );
// run #1:
mads.run();
// some changes...
mads.reset();
// run #2:
mads.run();
```

Figure 11: Two runs of MADS with a NOMAD::Mads object at a more global scope. The cache is kept between the two runs.

Two examples showing multiple MADS runs are described in the advanced examples directory.

5 Parameters description

Parameters described in this section correspond to those that can be entered in a parameters file that the batch mode will load. The same parameters description can be found by entering the command 'nomad -h', to see all the parameters, or 'nomad -h param_name' for a particular parameter.

In library mode, parameters are defined via a NOMAD::Parameters object and methods NOMAD::Parameters::set_PARAM_NAME(), where PARAM_NAME is the name used in this section. It is also possible to read a parameters file in library mode, with the method NOMAD::Parameters::read(). In batch mode, the problem directory is automatically determined by NOMAD. It can be defined in library mode with NOMAD::Parameters::set_PROBLEM_DIR().

All the entries of a line are ignored after the character '#'. Except for the file names, all strings and parameter names are case insensitive ('DIMENSION 2' is the same as 'Dimension 2'). File names refer to files in the problem directory. To indicate a file name containing spaces, use quotes ("name" or 'name'). These names may include directory information relatively to the problem directory. The problem directory will be added to the names, unless the '\$' character is used in front of the names. For example, if a blackbox executable is run by the command 'python script.py', define parameter BB_EXE with argument '\$python script.py'.

Some parameters require the entry of variable indexes. These indexes begin at 0 and may be entered directly or as index ranges with format 'i-j'. Character '*' may be used to replace '0-n-1' (where n is the number of variables). Other parameters require arguments of type bool: these values may be entered with the strings yes, no, y, n, 0, or 1. Finally, some parameters need vectors as arguments, use (v1 v2 ... vn) for those. Characters '-', 'inf', '-inf' or '+inf' are accepted to enter undefined real values (Nomad considers $\pm \infty$ as an undefined value). The following subsections show tables describing all Nomad parameters. Parameters are classified into different classes (problem, algorithm and output parameters). For each of these classes, basic and advanced parameters are described separately.

5.1 Parameters describing the problem

5.1.1 Basic

name	arguments	description	default
BB_EXE list of strings; see 5.4.1		blackbox executables (re-	none
		quired in batch mode)	
BB_INPUT_TYPE	see 5.4.2	blackbox input types	* R (all real)
BB_OUTPUT_TYPE	see 5.4.3	blackbox output types (re-	none
		quired)	
DIMENSION	integer	n the number of variables (re-	none
		quired)	
LOWER_BOUND	see 5.4.5	lower bounds	none
UPPER_BOUND	see 5.4.5	upper bounds	none

5.1.2 Advanced

name arguments		description	default
FIXED_VARIABLE see 5.4.8		fixed variables	none
PERIODIC_VARIABLE	index range	define variables in the range to	none
		be periodic (bounds required)	
SGTE_COST	integer c	the cost of c surrogate evalua-	∞
		tions is equivalent to the cost	
		of one blackbox evaluation	
SGTE_EVAL_SORT	bool	if surrogates are used to sort	yes
		list of trial points	
SGTE_EXE	list of strings; see 5.4.1	surrogate executables	none
VARIABLE_GROUP	index range	defines a group of variables;	none
		see 5.4.13	

Surrogates, or surrogate functions, are cheaper blackbox functions that are used, at least partially, instead of the true function f to minimize. The current version of Nomad uses only static surrogates which are not updated during the algorithm and which are provided by the user. If such functions are defined, Nomad will use them to drive its search. See [31] for a survey on surrogate optimization.

5.2 Algorithmic parameters

5.2.1 Basic

name arguments		description	default
DIRECTION_TYPE	DIRECTION_TYPE see 5.4.6		ORTHO
F_TARGET reals, f or (f1 f2)		NOMAD terminates if $f_i(x_k) \leq$ none fi for all objective functions	
HALTON_SEED integer		Halton seed for Ortho- MADS [6]	nth prime number
INITIAL_MESH_SIZE	see 5.4.9	$\Delta_0^m [18]$	r0.1 or 1.0
LH_SEARCH	2 integers: p0 and pi	LH (Latin-Hypercube) search (p0: initial, pi: iterative); see 6.2 for biobjective	
MAX_BB_EVAL	integer	maximum number of blackbox none evaluations; see 6.2 for biobjective	
MAX_TIME	integer	maximum wall-clock time (in seconds)	none
MULTI_NB_MADS_RUNS integer		number of Mads runs	see 6.2
MULTI_OVERALL_BB_EVAL	integer	max number of blackbox eval- uations for all MADS runs	see 6.2
se		opportunistic strategy; see 5.4.10	yes
OPPORTUNISTIC_LH bool		opportunistic strategy for LH search; see 6.2 for biobjective	see 5.4.10
SEED	integer or NONE	random seed; NONE or a negative integer to define a seed that will be different at each run	NONE
TMP_DIR	TMP_DIR string		problem directory
VNS_SEARCH	bool or real	VNS search; see 6.4	no
хо	see 5.4.14	starting point(s)	best point from a cache file or from an initial LH search

5.2.2 Advanced

name	arguments	description	default
ASYNCHRONOUS	bool	asynchronous strategy for the parallel version; see 6.5	yes
BB_INPUT_INCLUDE_SEED	bool	if the random seed is put as the first entry in blackbox in- put files	no
BB_INPUT_INCLUDE_TAG	bool	if the tag of a point is put as an entry in blackbox input files	no
BB_REDIRECTION	bool	if Nomad manages the creation of blackbox output files; see 5.4.4	yes
CACHE_SEARCH	bool	enable or disable the cache search (useful with extern caches)	no
EPSILON	real	precision on reals	1E-13
EXTENDED_POLL_ENABLED	bool	if no, the extended poll for categorical variables is dis- abled	yes
EXTENDED_POLL_TRIGGER	real	trigger for categorical variables; value may be relative; see 6.1	r0.1
H_MAX_O	real	initial value of h_{max} (will be eventually decreased throughout the algorithm)	1E+20
H_MIN	real v	x is feasible if $h(x) \ge v$	0.0
H_NORM	norm type in {L1, L2, Linf }	norm used to compute h	L2
HAS_SGTE	bool	indicates if the problem has a surrogate (only necessary in li- brary mode)	no or yes if SGTE_EXE is defined
INITIAL_MESH_INDEX	integer	initial mesh index ℓ_0 [6]	0
L_CURVE_TARGET	real	NOMAD terminates if it detects that the objective may not reach this value	none
MAX_CACHE_MEMORY	integer	NOMAD terminates if the cache reaches this memory limit expressed in MB	none
MAX EVAL	integer	max number of evaluations (includes cache hits and black- box evaluations, does not in- clude surrogate eval)	none
MAX_ITERATIONS	integer	max number of MADS iterations	none
MAX_MESH_INDEX	integer	max mesh index ℓ_{max} [6]	none
MAX_SGTE_EVAL	integer	max number of surrogate evaluations	none
MAX_SIM_BB_EVAL	integer	max number of simulated blackbox evaluations (includes initial cache hits)	none

name	arguments	description	default
MESH_COARSENING_EXPONENT	integer	$ w^+ [18] $	1
MESH_REFINING_EXPONENT	integer	$w^{-}[18]$	-1
MESH_UPDATE_BASIS	real	τ [18]	4.0
MIN_MESH_SIZE	see 5.4.9	Δ_{min}^m [18]	none
MIN_POLL_SIZE	see 5.4.9	$\Delta_{min}^{p} [18]$	none or 1 for int/bin variables
MULTI_F_BOUNDS	4 reals	see 6.2	none
MULTI_FORMULATION	string	see 6.2	PRODUCT or DIST_L2
MULTI_USE_DELTA_CRIT	bool	see 6.2	no
OPPORTUNISTIC_CACHE_SEARCH	bool	opportunistic strategy for cache search	no
OPPORTUNISTIC_LUCKY_EVAL	bool	see 5.4.10	none
OPPORTUNISTIC_MIN_EVAL	integer	see 5.4.10	none
OPPORTUNISTIC_MIN_F_IMPRVMT	real	see 5.4.10	none
OPPORTUNISTIC_MIN_NB_SUCCESS	integer	see 5.4.10	none
OPT_ONLY_SGTE	bool	minimize only with surrogates	no
RHO	real	ρ parameter of the progressive barrier	0.1
SCALING	see 5.4.11	scaling on the variables	none
SEC_POLL_DIR_TYPE	see 5.4.6	type of directions for the sec- ondary poll	see 5.4.6
SNAP_TO_BOUNDS	bool	snap to boundary trial points that are generated outside bounds	yes
SPECULATIVE_SEARCH	bool	Mads speculative search [18]	yes
STAT_SUM_TARGET	real	NOMAD terminates if STAT_SUM reaches this value	none
STOP_IF_FEASIBLE	bool	Nomad terminates if it generates a feasible solution	no
USER_CALLS_ENABLED	bool	if no, the automatic calls to user functions are disabled	yes

5.3 Output parameters

The displays have been simplified for the release of the version 3.4. Three different level of display can be set via the parameter DISPLAY_DEGREE, and these levels may be set differently for 4 different sections of the algorithm (general displays, search and poll displays and displays for each iteration data). The three different level can be entered with an integer in [0; 2], but also with the strings 'NO_DISPLAY', 'NORMAL_DISPLAY', or 'FULL_DISPLAY'. If the maximum level of display is set, then the algorithm informations are displayed within indented blocks. These blocks ease the interpretation of the algorithm logs when read from a text editor. The characters used to mark the beginning and the end of these blocks can be changed with the parameters OPEN_BRACE and CLOSED_BRACE.

From the implementation point of view, constants have been introduced for the display degrees: NOMAD::NO_DISPLAY, NOMAD::NORMAL_DISPLAY, and NOMAD::FULL_DISPLAY. In addition, a specific class is now responsible for the whole program displays. This class is named NOMAD::Display and is constructed from a std::ostream object such as std::cout. The use of a NOMAD::Display object is similar to the use of a std::ostream object, except that the outputs are organized within indented blocks. Compared to the previous versions of NOMAD, methods like NOMAD::Parameters::get_X_display_degree() have been removed and put inside the class NOMAD::Display. To access the NOMAD::Display object considered by the algorithm, call the method NOMAD::Parameters::out().

5.3.1 Basic

name	arguments	description	default
CACHE_FILE	string	cache file; if the file does not exist, it	none
		will be created	
DISPLAY_DEGREE	integer in [0;2] or a	0: no display; 2: full display	1
	string with four digits;		
	see 5.3.2		
DISPLAY_STATS	list of strings	what informations is displayed at	see 5.4.7
		each success; see 5.4.7	
HISTORY_FILE	string	file containing all trial points with	none
		format ($x1 x2 \dots xn$) on each	
		line; includes multiple evaluations	
SOLUTION_FILE	string	file to save the current best feasible	none
		point	
STATS_FILE	a string file_name plus a	the same as DISPLAY_STATS but for a	none
	list of strings	display into file file_name	

5.3.2 Advanced

name	arguments	description	default
ADD_SEED_TO_FILE_NAMES	bool	if the seed is added to the file names corresponding to parameters HISTORY_FILE, SOLUTION_FILE and STATS_FILE	yes
CACHE_SAVE_PERIOD	integer i	the cache files are saved every i iterations (disabled for biobjective)	25
CLOSED_BRACE	string	displayed at the end of indented blocks	'{'
DISPLAY_DEGREE	string with four digits, each in [0; 2]	1st digit: general display; 2nd digit: search display; 3rd digit: poll display; 4th digit: iterative display; example: DISPLAY_DEGREE 0010	1111
INF_STR	string	used to display infinity	'inf'
OPEN_BRACE	string	displayed at the beginning of indented blocks	'}'
POINT_DISPLAY_LIMIT	integer	maximum number of point coordinates that will be displayed at screen (-1 for no limit)	20
SGTE_CACHE_FILE	string	surrogate cache file (can not be the same as CACHE_FILE)	none
UNDEF_STR	string	used to display undefined values	,_,

5.4 Additional information for some parameters

5.4.1 Executable parameters BB_EXE and SGTE_EXE

In batch mode, BB_EXE indicates the names of the blackboxes executables. In library mode, it is optional as a custom NOMAD::Evaluator class may be written with its own eval_x() method. A single string may be given if a single blackbox is used and gives several outputs. It is also possible to indicate several blackbox executables. If the character '\$' is put at first position of a string, this string is considered as a global command or file and no path is added. We give the following examples:

```
BB_EXE
                                   # defines that 'bb.exe' is an
               bb.exe
BB_OUTPUT_TYPE OBJ EB EB
                                   # executable with 3 outputs
BB_EXE
                                   # defines two blackboxes
               bb1.exe bb2.exe
BB_OUTPUT_TYPE OBJ
                                   # 'bb1.exe' and 'bb2.exe'
                        EΒ
                                   # with one output each
BB_EXE "dir $with $spaces/bb.exe
                                   # use '$' to describe a
                                   # path with spaces
BB_EXE "$python bb.py"
                                   # the blackbox is a python
                                   # script: it is run with
                                   # command
                                   # 'python PROBLEM_DIR/bb.py'
BB_EXE "$nice bb.exe"
                                   # to run PROBLEM_DIR/bb.exe
                                   # in nice mode on X systems
```

The parameter SGTE_EXE associates surrogate executables with blackbox executables. It may be entered with two formats: 'SGTE_EXE bb_exe sgte_exe' to associate executables bb_exe and sgte_exe, or 'SGTE_EXE sgte_exe' when only one blackbox executable is used. Surrogates must display the same number of outputs as their associated blackboxes.

5.4.2 Blackbox input parameter BB_INPUT_TYPE

This parameter indicates the types of each variable. It may be defined once with a list of n input types with format (t1 t2 ... tn) or several times with index ranges and input types. Input types are values in $\{R, C, B, I\}$ or $\{Real, Cat, Bin, Int\}$. R is for real/continuous variables, C for categorical variable, B for binary variables, and I for integer variables. The default type is R.

5.4.3 Blackbox output parameter BB_OUTPUT_TYPE

This parameter defines the types of the values that the blackbox displays. The arguments are a list of m types, where m is the number of outputs of the blackbox. At least one of these values must correspond to the objective function that NOMAD minimizes. If two outputs are tagged as objectives, then the BIMADS algorithm will be executed. Other values typically are constraints of the form $c_i(x) \leq 0$, and the blackbox must display the left hand side of the constraint with this format. A certain terminology is used to describe the different types of constraints. This terminology can be consulted in [20]. EB constraints correspond to constraints that need to be always satisfied (unrelaxable constraints). The technique used to deal with those is the extreme barrier approach, consisting in simply rejecting the infeasible points. PB, PEB, and F constraints correspond to constraints that need to be satisfied only at the solution, and not necessarily at intermediate points (relaxable constraints). More precisely, F constraints are treated with the filter approach [17], and PB constraints are treated with the progressive barrier approach [20]. PEB constraints are treated first with the progressive barrier, and once satisfied, with the extreme barrier [22]. There may be another type of constraints, the hidden constraints, but these only appear inside the blackbox during an execution, and thus they cannot be indicated in advance to NOMAD (when such a constraint is violated, the evaluation simply fails and the point is not considered). If the user is not sure about

the nature of its constraints, we suggest using the keyword CSTR, which correspond by default to PB constraints.

There may be other types of outputs. All the types are:

```
Must be 0 or 1: count or not the blackbox evaluation
               (equivalent to the argument cnt_eval of NOMAD::Evaluator::eval_x()).
               Constraint treated with Extreme Barrier
               (infeasible points are ignored).
               Constraint treated with filter approach [17].
           F
NOTHING or -
               The output is ignored.
         OBJ
               Objective value to minimize.
  PB or CSTR Constraint treated with Progressive Barrier [20].
               Hybrid constraint PB/EB [22].
   STAT_AVG
               Average of this value will be computed for all blackbox calls
               (must be unique).
   STAT_SUM
               Sum of this value will be computed for all blackbox calls
               (must be unique).
```

Please note that F constraints are not compatible with CSTR, PB or PEB. However, EB can be combined with F, CSTR, PB or PEB.

5.4.4 Blackbox redirection parameter BB_REDIRECTION

If this parameter is set to yes (default), NOMAD manages the creation of the blackbox output file when the blackbox is executed via a system call (the redirection '>' is added to the system command). If no, then the blackbox must manage the creation of its output file named TMP_DIR/nomad.SEED.TAG.output. Values of SEED and TAG can be obtained in the blackbox input files created by NOMAD and given as first argument of the blackbox, only if parameters BB_INPUT_INCLUDE_SEED and BB_INPUT_INCLUDE_TAG are both set to yes. TMP_DIR is specified by the user. If no, TMP_DIR is the problem directory.

5.4.5 Bounds

Parameters LOWER_BOUND and UPPER_BOUND are used to define bounds on variables, and take similar arguments as parameter FIXED_VARIABLE (see 5.4.8). For example, with n = 7,

```
LOWER_BOUND 0-2 -5.0
LOWER_BOUND 3 0.0
LOWER_BOUND 5-6 -4.0
UPPER_BOUND 0-5 8.0
```

is equivalent to

```
LOWER_BOUND ( -5 -5 -5 0 - -4 -4 ) # '-' or '-inf' means that x_4 # has no lower bound UPPER_BOUND ( 8 8 8 8 8 8 inf ) # '-' or 'inf' or '+inf' means # that x_6 has no upper bound.
```

These two sequences define the following bounds
$$\begin{cases}
-5 \le x_1 \le 8 \\
-5 \le x_2 \le 8 \\
-5 \le x_3 \le 8 \\
0 \le x_4 \le 8 \\
x_5 \le 8 \\
-4 \le x_6 \le 8 \\
-4 \le x_7 .\end{cases}$$
5.4.6 Direction types

5.4.6 Direction types

The types of direction correspond to the arguments of parameters DIRECTION_TYPE and SEC_POLL_ DIR_TYPE. Up to 4 strings may be employed to describe one direction type. These 4 strings are s1 in $\{ORTHO,LT,GPS\}$, s2 in $\{\emptyset,1,2,N+1,2N\}$, s3 in $\{\emptyset,STATIC,RANDOM\}$, and s4 in $\{\emptyset,UNIFORM\}$. If only 1,2 or 3 strings are given, defaults are considered for the others. Combination of these strings may describe the following 14 direction types:

J			0	₽ 1	
	s1	s2	s3	s4	direction types
1	ORTHO	1			OrthoMads, 1.
2	ORTHO	2			OrthoMads, 2.
3	ORTHO				OrthoMads, 2n.
3	ORTHO	2N			OrthoMads, 2n.
4	LT	1			LT-Mads, 1.
5	LT	2			LT-Mads, 2.
6	LT	N+1			LT-MADS, $n+1$.
7	LT				LT-Mads, 2n.
7	LT	2N			LT-Mads, 2n.
8	GPS	BIN			GPS for binary variables.
9	GPS	N+1			GPS, n+1, static.
9	GPS	N+1	STATIC		GPS, n+1, static.
10	GPS	N+1	STATIC	UNIFORM	GPS, n+1, static, uniform angles.
11	GPS	N+1	RAND		GPS, n+1, random.
12	GPS	N+1	RAND	UNIFORM	GPS, n+1, random, uniform angles.
13	GPS				GPS, 2n, static.
13	GPS	2N			GPS, 2n, static.
13	GPS	2N	STATIC		GPS, 2n, static.
14	GPS	2N	RAND		GPS, 2n, random.

GPS directions correspond to the coordinate directions. LT and ORTHO directions correspond to the implementations LT-MADS [18] and ORTHOMADS [6] of MADS. The integer indicated after GPS, LT and ORTHO corresponds to the number of directions that are generated at each poll. The 14 different direction types may be chosen together by specifying DIRECTION_TYPE or SEC_POLL_DIR_TYPE several times. If nothing indicated, ORTHO is considered for the primary poll, and default direction types for the secondary poll are ORTHO 1 or 2, LT 1 or 2, and GPS N+1 STATIC depending on the value of DIRECTION_TYPE.

Output parameters DISPLAY_STATS and STATS_FILE

These parameters display information each time a new feasible incumbent is found. DISPLAY_STATS displays at the standard output and STATS_FILE writes a file. These parameters need a list of strings as argument, without any quotes. These strings may include the following keywords:

```
Blackbox evaluations.
        BBE
        BB0
              Blackbox outputs.
              Evaluations (includes cache hits).
       EVAL
              Mesh index \ell [6].
MESH_INDEX
              Mesh size parameter \Delta_k^m [18].
 MESH_SIZE
              Objective function value.
        OBJ
 POLL_SIZE
              Poll size parameter \Delta_k^p [18].
              Number of surrogate evaluations.
       SGTE
   SIM_BBE
              Simulated blackbox evaluations (includes initial cache hits).
        SOL
              Solution, with format iSOLj where i and j are two (optional)
              strings: i will be displayed before each coordinate, and j after
              each coordinate (except the last).
  STAT_AVG
              The AVG statistic (argument STAT_AVG of BB_OUTPUT_TYPE).
              The SUM statistic defined by argument STAT_SUM for parameter
  STAT_SUM
              BB_OUTPUT_TYPE.
       TIME
              Wall-clock time.
```

In addition, all outputs may be formatted using the C style. Possibilities and examples are shown in the following table:

Value of variable i. The index 0 corresponds to the first variable.

```
%e Scientific notation (mantise/exponent) using e character.
```

%E Scientific notation (mantise/exponent) using E character.

%f Decimal floating point.

%g Use the shorter of %e or %f.

%G Use the shorter of %E or %f.

%d or i Integer rounded value.

VARi

The number of columns (width) and the precision may also be indicated using also the C style as in the following examples:

format	width	precision
%f	auto	auto
%5.4f	5	4
%5f	5	auto
%.4f	auto	4
%.f	auto	0

For example, 'DISPLAY_STATS \$BBE\$ & (\$SOL,) & \$OBJ\$ \\' displays lines similar to '\$1\$ & (\$10.34\$, \$5.58\$) & \$-703.4734809\$ \\', which may be directed copied into LATEX tables. A similar example with formatting may be 'DISPLAY_STATS \$BBE\$ & (\$%5.1fSOL,) & \$%.2EOBJ\$ \\' which gives '\$1\$ & (\$ 10.3\$, \$ 5.6\$) & \$-7.03E+02\$ \\'. In case the user wants to explicitly display the '%' character, it must be entered using '\%'.

Default values are 'DISPLAY_STATS BBE OBJ' and 'DISPLAY_STATS OBJ' for single and biobjective optimization, respectively (there is no need to enter OBJ twice in order for the two objective values to be displayed).

To write these outputs into the file output.txt, simply add the file name as first argument of STAT_FILE: for example 'STATS_FILE output.txt BBE (SOL) OBJ'.

5.4.8 Fixed variables parameter FIXED_VARIABLE

This parameter is used to fix some variables to a value. This value is optional if at least one starting point is defined. The parameter may be entered with several types of arguments:

- A string indicating a text file containing n values. Variables will be fixed to the values that are not defined with the character '-'.
- A vector of n values with format (v0 v1 ... vn-1). Again, character '-' may be used for free variables.
- An index range if at least one starting point has been defined (see 5.4.14 for practical examples of index ranges).
- An index range and a real value, with format 'FIXED_VARIABLE i-j v': variables i to j will be fixed to the value v (i-j may be replaced by i).

5.4.9 Mesh and poll size parameters

The initial mesh size parameter Δ_0^m [18] is decided by INITIAL_MESH_SIZE. In order to achieve the scaling between variables, NOMAD considers the mesh size parameter as a vector of n elements. Note that a more explicit scaling method is available with the parameter SCALING (see Section 5.4.11). The same logic applies to the poll size parameter Δ_k^p . If d0 is a positive real value, INITIAL_MESH_SIZE may be entered with the following formats:

- INITIAL_MESH_SIZE d0: initial mesh size for all variables.
- INITIAL_MESH_SIZE (d0 d1 ... dn-1): for all variables ('-' may be used, and defaults will be considered).
- INITIAL_MESH_SIZE i dO: initial for variable i.
- INITIAL_MESH_SIZE i-j d0: initial for variables i to j.

The minimum mesh size Δ_{min}^m and the minimum poll size Δ_{min}^p (stopping criteria) may be defined the same way via parameters MIN_MESH_SIZE and MIN_POLL_SIZE. All values may also be preceded by 'r' to indicate a value relative to the bounds. For example, 'INITIAL_MESH_SIZE r0.1' means that $\Delta_0^m = (ub - lb)/10$ with $lb, ub \in \mathbb{R}^n$ and $lb \le x \le ub$ for all $x \in X$. Default is r0.1 for bounded variables and 1.0 otherwise.

5.4.10 Opportunistic strategy

The opportunistic strategy consists in terminating the evaluations of a list of trial points as soon as an improved value is found. This strategy is decided with the parameter OPPORTUNISTIC_EVAL and applies to both the poll and search steps. For the LH and Cache searches, the strategy may be chosen independently with OPPORTUNISTIC_LH and OPPORTUNISTIC_CACHE_SEARCH. If these parameters are not defined, the parameter OPPORTUNISTIC_EVAL applies to the LH and Cache searches. Other defaults are considered for biobjective optimization (see 6.2).

If the opportunistic strategy is enabled, some additional options may be defined via the following parameters:

• OPPORTUNISTIC_MIN_NB_SUCCESS i: do not terminate before i successes.

- OPPORTUNISTIC_MIN_EVAL i: do not terminate before i evaluations.
- OPPORTUNISTIC_MIN_F_IMPRVMT r: terminate only if f is reduced by r%.
- OPPORTUNISTIC_LUCKY_EVAL yes/no: perform an additional blackbox evaluation after an improvement.

5.4.11 Scaling parameter SCALING

Scaling in Nomado is automatically achieved via the mesh and poll size parameters which are vectors with one value per variable. However, this method relies on the existence of bounds. For the case when no bounds are available, or simply to give the user more control on the scaling, the parameter SCALING has been introduced in the version 3.4.

The parameter takes variable indexes and values as arguments. During the algorithm, variables are multiplied by their associated value before an evaluation and the call to NOMAD::Evaluator::eval_x(). The variables are unscaled after the evaluation.

All Nomad outputs (including files) display unscaled values. All variable-related parameters (bounds, starting points, fixed variables) must be specified without scaling. In a parameters file, the scaling is entered similarly to bounds or fixed variables. It is possible to specify a scaling for some variables and none for others. Enter the command nomad -h scaling for more details about the use of SCALING.

5.4.12 Temporary directory parameter TMP_DIR

If NOMAD is installed on a network, with the batch mode use, the cost of read/write files will be high if no local temporary directory is defined. On Linux/Unix/Mac OS X systems, the directory /tmp is local and we advise the user to define 'TMP_DIR /tmp'.

5.4.13 Group of variable parameter VARIABLE_GROUP

This parameter may be entered several times to define more than one group of variables. Variables in a group may be of different types (except for categorical variables). To define some particular types of directions or a particular Halton seed for this group, use the NOMAD library and NOMAD::Parameters::set_VARIABLE_GROUP(). In addition to the groups defined by parameters, NOMAD creates one group for all continuous, integer, and binary variables, and one group for categorical variables. If a group contains only binary variables, directions of type NOMAD::GPS_BINARY will be automatically used.

5.4.14 Starting point parameter X0

Parameter XO indicates the starting point of the algorithm. Several starting points may be proposed by entering this parameter several times. If no starting point is indicated, NOMAD considers the best evaluated point from an existing cache file (parameter CACHE_FILE) or from an initial Latin-Hypercube search (argument pO of LH_SEARCH). The XO parameter may take several types of arguments:

• A string indicating an existing cache file, containing several points (they can be already evaluated or not). This file may be the same as the one indicated with CACHE_FILE. If so, this file will be updated during the program execution, otherwise the file will not be modified.

- A string indicating a text file containing the coordinates of one or several points (values are separated by spaces or line breaks).
- n real values with format (v0 v1 ... vn-1).
- Two integers and one real:

```
- 'XO i v': (i+1)th coordinate set to v.
```

- 'XO i-j v': coordinates i to j set to v.
- 'XO * v': all coordinates set to v.
- One integer, another integer (or index range) and one real: the same as above except that the first integer k refers to the (k+1)th starting point.

The following example with n=3 corresponds to the two starting points (5 0 0) and (-5 1 1):

6 Special functionalities

6.1 Categorical variables

Categorical variables are discrete variables that can take a finite number of values. These are not integer or binary variables as there is no ordering property amongst the different values that can take the variables. To decide these values and to define a neighborhood structure, a user written procedure must be provided.

The algorithm used by NOMAD to treat such variables is defined in references [1, 8, 9, 15, 45] and works as follows.

6.1.1 Algorithm

At the end of an iteration, if no improvement has been made, a special step occurs, the *extended poll*. The extended poll first calls the user-provided procedure defining the neighborhood of categorical variables. The procedure returns a list of points that have been defined as neighbors of the current iterate. These points are called the *extended poll points*. The functions defining the problem are then evaluated at each of these points and the objective values are compared to the current best value.

If the difference between the objective value at the current iterate and at a extended poll point is less than a parameter called the *extended poll trigger*, this extended poll point is called an *extended poll center* and a new MADS run is performed from this point. This run is called an *extend poll descent* and occurs on meshes that cannot be reduced more than the mesh of the beginning of the extended poll. If the opportunistic strategy is active, then the different extended poll descents are stopped as soon as a new success is achieved.

If surrogates are available, they can be used to evaluate the neighbors and during the extended poll descent. The true functions will then be evaluated only on the most promising points. With surrogates, the extended poll costs at most the same number of true evaluations than the number of neighbors determined by the user-provided procedure.

6.1.2 Categorical variables with NOMAD

We suggest the reader to follow this section along with the reading of the example located in examples/advanced/categorical illustrating a simple mixed variable problem optimization. Dealing with such problems in Nomad implies the use of the library mode to define the categorical variables neighborhoods, although it is still possible to use a parameters file and separated blackbox executables.

Several steps are necessary. First the BB_INPUT_TYPE parameter must be defined with the value 'C' to identify categorical variables.

Then the library mode is needed to define the procedure for the categorical variable neighborhoods. This procedure corresponds to the virtual method NOMAD::Extended_Poll::construct_extended_points() and the user must design its own NOMAD::Extended_Poll subclass in which construct_extended_points() is coded. This method takes as argument a point (the current iterate) and constructs the list of extended poll points (the neighbors of the current iterate). These points are registered with the method NOMAD::Extended_Poll::add_extended_poll_point(). In its main function, the user gives its own NOMAD::Extended_Poll object to the NOMAD::Mads object used to optimize the problem. If no NOMAD::Extended_Poll is provided to the NOMAD::Mads object, the program will generate an error.

An important feature of Nomad about the handling of categorical variables is its ability to treat points with a variable number of variables. This behavior often happens in mixed variable problems, for example when a categorical variable indicates the number of continuous variables.

To deal with this, NOMAD uses the concept of *signature*, implemented in the NOMAD::Signature class. Each point in the algorithm possesses a signature, indicating the characteristics related to the variables. These characteristics are the number of variables, the types of the variables, their bounds, their scaling, fixed and periodic variables, and some information on the initial mesh size parameter for each variable.

In the user-provide NOMAD::Extended_Poll subclass, for each extended poll point, a signature must be provided. If the extended poll point have the same number of variables than the current iterate, the signature of the current iterate can be used. Otherwise, a new creature must be created and the user is responsible for dealing with the associated memory allocations and deallocations. See the NOMAD::Signature class for details about creating signatures.

The number of outputs of the evaluations must remain constant: if a problem has been defined with one objective and two constraints, even if the number of variables can change, each evaluation should return three values.

The parameter DIMENSION has still to be defined, and it corresponds to the number of variables of the provided starting points. For these starting points, the NOMAD::Parameters class will automatically create a standard signature. If no starting point is provided, the standard signature cannot be created, and a Latin-Hypercube search cannot be executed because it has no reference for defining values for categorical variables. So not providing starting points with mixed variable problems is not allowed.

The main parameter for mixed variable optimization is the extended poll trigger. Its value is indicated with the parameter EXTENDED_POLL_TRIGGER, and may be given as a relative value. The extended poll trigger is used to compare the objective values at an extended poll point y and at the current iterate x_k . If $f(y) < f(x_k)$ +trigger, then y becomes an extended poll center from which a MADS run is performed. The default trigger value is r0.2, meaning that an extended poll point will become an extended poll center if f(y) is less than $f(x_k) + f(x_k) \times 20\%$. See the function NOMAD::Extended_Poll::check_trigger() for the details of this test and for the cases where infeasible points or surrogate evaluations are considered.

Finally, note that the parameter EXTENDED_POLL_ENABLED can simply disable the extended poll. In this case, categorical variable are simply fixed.

6.2 Biobjective optimization

NOMAD performs biobjective optimization through the BIMADS algorithm described in [26]. Handling of more than two objective functions will be implemented in future versions.

The BIMADS algorithm solves biobjective problems of the form

$$\min_{x \in \Omega} F(x) = (f_1(x), f_2(x)). \tag{2}$$

The algorithm launches successive runs of MADS on single-objective reformulations of the problem. An approximation of the Pareto front, or the list of points that are dominant following the definition of [26], is constructed with the evaluations performed during these MADS runs.

Two considerations must be taken into account when generating Pareto fronts: the quality of approximation of the dominant points and the repartition of these points. The quality of approximation may be measured with the **surf** criterion that gives the ratio of the area under the graph of the front relatively to a box enclosing all points (small values indicate a good front).

The quality of the coverage of the Pareto front is measured by the δ criterion, which corresponds to the largest distance between two successive Pareto points.

To define that a problem has two objectives, two arguments of the parameter BB_OUTPUT_TYPE must be set to OBJ. Then, NOMAD will automatically run the BIMADS algorithm. Additional parameters are:

- MULTI_F_BOUNDS f1_min f1_max f2_min f2_max (real values): these 4 values are necessary to compute the surf criterion. If not entered or if not valid (for example if f1_min is too big), then surf is not computed.
- MULTI_FORMULATION (string): single-objective reformulation [27]. This is how Nomad computes one value from the two objective values. The argument must be in {NORMALIZED, PRODUCT, DIST_L1, DIST_L2, DIST_LINF} (DIST_LINF and NORMALIZED are equivalent). The default formulation is PRODUCT when VNS is not used, and DIST_L2 otherwise.
- MULTI_NB_MADS_RUNS (integer): the number of single-objective MADS runs.
- MULTI_OVERALL_BB_EVAL (integer): the maximum number of blackbox evaluations over all MADS runs.
- MULTI_USE_DELTA_CRIT (bool, default to no): use or not a stopping criterion based on the δ measure.

Default values are considered if these parameters are not entered. All other MADS parameters are considered and apply to single MADS runs, with some adaptations:

- The MAX_BB_EVAL parameter corresponds to the maximum number of blackbox evaluations for one MADS run.
- The F_TARGET parameter is adapted to biobjective: it must be given with the two values z_1 and z_2 . If a point x is generated such that $f_1(x) \leq z_1$ and $f_2(x) \leq z_2$, then the algorithm terminates.

- Latin-Hypercube (LH) search (LH_SEARCH p_0 p_1): in single-objective optimization, p_0 and p_1 correspond to the initial number of search points and to the number of search points at each iteration, respectively. In the biobjective context, p_0 is the number of initial search points generated in the first MADS run, and p_1 is the number of points for the second MADS run. If no LH search is defined by the user, and if only MULTI_OVERALL_BB_EVAL is defined, then a default LH search is performed. Moreover, this default LH search is non-opportunistic (OPPORTUNISTIC_LH set to no).
- The parameter SOLUTION_FILE is disabled.

The NOMAD solution represents an approximation of the Pareto front and is accessible via the DISPLAY_STATS or STATS_FILE parameters. If DISPLAY_DEGREE is greater than 1, then the two measures surf and δ are displayed.

For a given budget of blackbox evaluations (MULTI_OVERALL_BB_EVAL), if the quality of approximation is desired (small value for \mathtt{surf}), then single MADS optimizations must terminate after more severe criteria (for example a large number of blackbox evaluations, via MAX_BB_EVAL). If a better repartition of the points is desired (small value for δ), then the number of MADS runs should be larger, with less severe stopping criteria on single-objective optimizations.

6.3 Sensitivity analysis

Getting an optimizer is often insufficient for engineers. Two tools are available in the NOMAD package to perform sensitivity analyses for constraints, which is a useful tool to grasp more knowledge and see which constraints are important and which may be relaxed or tighten. What is generated by these tools is the data necessary to plot objective versus constraint graphs that help to understand the sensitivity. Details on the sensitivity analysis with blackboxes and some theoretical results on the smooth case may be consulted in reference [23].

The tools are available in directory \$NOMAD_HOME/tools/SENSITIVITY. The first program is called cache_inspect and performs the *simple analysis* which consists in inspecting the cache produced after the execution of NOMAD on a constrained problem (the CACHE_FILE parameter must be set). The necessary inputs of this tool are a cache file and two blackbox output indexes: one for the objective function, and one for the studied constraint. This last index may refer to a lower or an upper bound: in that case a file containing the bound values must be indicated. The program displays three columns with the values of the studied constraint $c_j(x)$ and of the objective f(x), and a 0/1 flag indicating whether or not the couple $(c_j(x), f(x))$ is nondominated in the sense of the dominance notion of [26]. An optional parameter allows to display only nondominated points. These values may be plotted for example with a MATLAB script (one is available in the cache_inspect directory).

The second program, called detailed_analysis, performs the detailed analysis. With this tool, the original problem with constraint $c_i(x) \leq 0$ is replaced with the biobjective problem

$$\min_{x \in \Omega_j} \quad (c_j(x), f(x))$$
s.t.
$$\underline{c}_j \le c_j(x) \le \overline{c}_j$$

where Ω_j is the feasible set Ω minus the constraint. The use of the BIMADS algorithm allows to focus explicitly on the studied constraint in order to obtain a more precise sensitivity. The program takes as inputs a parameters file, the constraint and objective indexes, and a cache file. The latter may be empty or not at the beginning of the execution, and it will be updated with the new evaluations. The updated cache file is in fact the output of the program and it may be

inspected with the cache_inspect tool in order to get the data for the sensitivity graphs. The \underline{c}_j and \overline{c}_j values used to bound the value of $c_j(x)$ may also be specified as input to the tool, as well as a maximum number of evaluations that bypasses the one inside the parameters file. Both programs may be executed without any input which result in the display of the required inputs description.

The typical way of using these tools is as follows: after a single run of MADS, the user uses the simple analysis in order to get a fast and free preview of the sensitivity. After that it is possible to get a more precise analysis on one or several constraints of interest using the detailed analysis, to the cost of additional evaluations.

6.4 Variable Neighborhood Search (VNS)

This search strategy is described in [12]. It is based on the Variable Neighborhood Search metaheuristic [49, 50] as a search strategy to escape local minima. VNS should only be used for problems with several such local optima. It will cost some additional evaluations, since each search performs another MADS run from a perturbed starting point. Though, it will be a lot cheaper if a surrogate is provided via parameter HAS_SGTE or SGTE_EXE. We advise the user not to use VNS with biobjective optimization, as the BIMADS algorithm already performs multiple MADS runs.

In order to use the VNS search, which is disabled by default, the user has to define the parameter VNS_SEARCH, with a boolean or a real. This expected real value is the *VNS trigger*, which corresponds to the maximum desired ratio of VNS blackbox evaluations over the total number of blackbox evaluations. For example, a value of 0.75 means that NOMAD will try to perform a maximum of 75% blackbox evaluations within the VNS search. If a boolean is given as value to VNS_SEARCH, then a default of 0.75 is taken for the VNS trigger.

From a technical point of view, VNS is coded as a NOMAD::Search sub-class, and it is a good example of how a user-search may be implemented. See files \$NOMAD_HOME/src/VNS_Search.*pp for details.

6.5 Parallel versions

Three parallel versions of the algorithm have been developed, namely P-MADS, COOP-MADS, and PSD-MADS. While P-MADS is directly implemented into NOMAD, the two others are programs using the NOMAD scalar library, and are located in the tools directory. These parallel versions are developed with MPI [52] under a master/slaves paradigm.

When creating blackbox problems it is important to keep in mind that the blackboxes will be called in parallel. So it is crucial that intermediary files possess different names: unique identifiers must be used. For that purpose, in library mode, in your custom eval_x() function, use the unique tag of the trial points with the method NOMAD::Eval_Point::get_tag(). It is also possible to use NOMAD::get_pid() to generate a unique identifier. In batch mode, NOMAD may communicate the seed and the tag of a point to the blackbox executable with the parameters BB_INPUT_INCLUDE_SEED and BB_INPUT_INCLUDE_TAG (see Section 5.2.2).

The user must be aware of the random aspect induced by the parallel versions. Even if deterministic directions such as ORTHOMADS are used, two parallel runs may not have the same outputs. Tests have suggested that P-MADS will give similar results than the scalar version, but much faster. The quality of the results may sometimes be less due to the fact that the usually efficient opportunistic strategy is not exploited as well as in the scalar version. However, the more evolved Coop-MADS strategy seems to give better results than the scalar version, and faster. The efficiency of the PSD-MADS algorithm is more noticeable on large problems (more than 20 and up to $\simeq 500$ variables) on which the other versions are not efficient.

A short description of the methods is given in the following sections, and for a more complete description as well as for numerical results, please consult [40].

6.5.1 The P-MADS method

P-Mads is the basic parallel version of the Mads algorithm where each list of trial points is simply evaluated in parallel. There are two versions of this method: first the **synchronous** version where an iteration is over only when all evaluations in progress are finished. With this strategy, some processes may be idle. The other version is the **asynchronous** method which consists in interrupting the iteration as soon a new success is made. If there are some evaluations in progress, these are not terminated. If these evaluations lead to successes after they terminate, then the algorithm will consider them and go back to these 'old' points. This version allows no process to be idle. The synchronous and asynchronous versions may be chosen via the parameter ASYNCHRONOUS whose default is yes.

The P-MADS executable is named nomad.MPI or nomad_MPI.exe depending on the operating system and is located in the bin directory. It can be executed with the mpirun or mpiexec commands with the following format under Linux:

where p is the number of processes and param.txt is a parameters file with the same format as for the scalar version. If you have a number c of processors, then it is suggested to choose np to be equal to c+1 (one master and c slaves). It may also be argued that np be proportional to the number of polling directions. For example, for a problem with n=3 variables and 2n polling directions, each poll is going to generate 6 trial points, and on a 8-processors machine, chosing np=7 may be a better choice than np=9.

6.5.2 The Coop-Mads method

The idea behind the COOP-MADS method is to run several MADS instances in parallel with different seeds so that no one has the same behavior.

A special process, called the cache server, replaces the usual master process. It implements a parallel version of the cache allowing each process to query if the evaluation at a given point has already been performed. This forbids any double evaluation. The cache server allows also the processes to perform the **cache search**, a special search consisting in retrieving, at each MADS iteration, the currently best known point.

The program given in the tools directory implements a simple version of the method where only one type of directions is used with different seeds: LT-Mads or OrthoMads, with a different random seed or a different Halton seed.

This program is not precompiled and the user must compile it as any other code using the NOMAD library. Makefiles for X systems and Windows are provided. Usage of the program is as follows:

as for P-MADS. Since the cache server is not demanding on computational time, the user can choose np to be the number of available processors plus one.

6.5.3 The PSD-MADS method

PSD-MADS corresponds to the parallel space decomposition of MADS described in [21]. The method aims at solving larger problems than the scalar version of NOMAD. While NOMAD is in general efficient on problems for problems up to $\simeq 20$ variables, PSD-MADS has solved problems up to 500 variables.

In PSD-MADS, each slave process has the responsibility for a small number of variables on which a MADS algorithm is performed. These subproblems are decided by the master process. In the program given in the NOMAD package, as in the original paper, these groups of variables are chosen randomly, without any specific strategy. Concerning other aspects, the program given here is a simplified version of the one used for the SIOPT article. A cache server is also used as in COOP-MADS to forbid double evaluations. A special slave, called the pollster, works on all the variables, but with a reduced number of directions. The pollster ensures the convergence of the algorithm.

PSD-MADS must be compiled exactly as COOP-MADS, with the available makefile, and it executes with the command:

```
mpirun -np p $NOMAD_HOME/tools/PSD-MADS/psdmads param.txt bbe ns
```

where bbe is the maximal number of evaluations performed by each slave and ns is the number of variables considered by the slaves. So far, tests suggested that small values for these two parameters lead to good performance. In [21] and [40], bbe=10 and ns=2 are considered. The suggested strategy for np consists in setting it to the number of processors plus two (master and cache server are not demanding).

Future research include the design of evolved strategies in order to choose smart groups of variables on which slaves focus.

7 Release notes

7.1 Version 3.4

This new version implements parallelism with the Message Passing Interface (MPI [52]). Three parallel versions are described in Section 6.5. Two minor revisions (3.4.1 and 3.4.2) have been released since the version 3.4.0 (see 7.1.3).

7.1.1 Major changes

- Parallelism: Three parallel algorithms are now available. See Section 6.5 for details.
- All Nomad types and classes are now included in the namespace NOMAD. Consequently enumeration types and constants have their names changed from _X_ to NOMAD::X.
- A documentation has been constructed in the HTML format with the doxygen documentation generator. It is available from the NOMAD website at www.gerad.ca/nomad/doxygen/html.
- Nomad is now distributed under the GNU Lesser General Public License (LGPL). The license can be found as a text file in the src directory or at www.gnu.org/licenses.

7.1.2 Minor changes

- The installation under Mac OS X has been modified. It is no more an installation program but rather a disk image (.dmg). The installation script for X systems has also been improved.
- The program displays have been simplified. See Section 5.3.
- A new parameter SCALING allowing the scaling of the variables. See Section 5.4.11.
- A new search based on the cache has been developed. This search is performed by the Coop-Mads method described in Section 6.5.2. The new associated parameters are CACHE_SEARCH and OPPORTUNISTIC_CACHE_SEARCH.
- A starting point file can now describe several starting points.
- The default value of the parameter SEED has been modified from 0 to NONE.
- In library mode, calls to the user-defined function eval_x() are now included into a try block. See Section 4.1 for precisions.
- Prototype for the user-defined function NOMAD::Evaluator::update_iteration() has been modified and now allows the user to stop the algorithm.
- The examples directory has been reorganized and the tools directory has been added.
- Most of the examples may be executed in parallel.
- Compatibility with the AMPL [41] format. See Section 2.4.

7.1.3 Specific changes for versions 3.4.1 and 3.4.2

- Tool for sensitivity analysis (see Section 6.3).
- Output display formats of real values (see Section 5.4.7).
- Better behavior with integer variables.
- New parameters UNDEF_STR and INF_STR (characters for undefined values and infinity, see Section 5.3.2).
- Bug corrections.

7.1.4 List of modified classes or methods

- New classes NOMAD::Slave and NOMAD::Display.
- New method for computing Halton seeds: NOMAD::Directions::compute_halton_seed().
- New convenient way of computing mesh and poll sizes with NOMAD::Mesh::get_delta_m() and NOMAD::Mesh::get_delta_p().
- Prototypes of methods add_eval_point() and eval_list_of_points() from the class NOMAD
 ::Evaluator_Control have changed.

- New functions NOMAD::begin() and NOMAD::end() that must be called at the beginning and at the end of programs using the NOMAD library. The new NOMAD::Slave::stop_slaves() method must also be called at the end of a program calling the parallel NOMAD library.
- NOMAD::Search objects no longer need a NOMAD::Evaluator_Control object during their construction. Instead, use mads.get_evaluator_control() with the mads argument given to NOMAD::Search::search().
- NOMAD::Evaluator::get_p() has been removed and replaced by the protected member NOMAD ::Evaluator::_p().

7.1.5 List of main changes for programs using the Nomad library

This list summarizes the main changes for a program linking with the previous versions of the NOMAD library to work with the new version. Some other minor changes may also be necessary. For example, some prototypes of the functions described in Section 4.3.1 may have changed. We refer the user to the numerous examples illustrating these changes in the examples directory.

- Add the statement 'using namespace NOMAD;' or use 'NOMAD::' in front of all the NOMAD types. Change the constants or enumeration types from '_X_' to 'NOMAD::X'. For example, if you described the objective output with '_OBJ_', then change it to 'NOMAD::OBJ' or to 'OBJ' if you added 'using namespace NOMAD;'.
- Declare a NOMAD::Display object for the displays. This object is provided only to the NOMAD::Parameters constructor, and no more to the other NOMAD main classes such as NOMAD::Mads, NOMAD::Evaluator, or NOMAD::Search.
- Change the main function prototype from 'int main (void)' to 'int main (int argc, char** argv)'.
- Add the NOMAD::begin() and NOMAD::end() functions. Add also NOMAD::Slaves::stop_slaves() at the end of the program if it uses the parallel library.

7.2 Previous versions

7.2.1 Version 3.3

• Handling of categorical variables for mixed variable problems (MVP). See Section 6.1.

7.2.2 Version 3.2

- Variable Neighborhood Search (VNS) described in Section 6.4.
- **Installers** for X systems.
- Help on parameters included in the executable: the command 'nomad -h keyword' displays help on the parameters related to keyword. Typing only 'nomad -h' or 'nomad -help' displays all the available help: a complete description of all parameters. Also, 'nomad -i' or 'nomad -info' displays information on the current release, and 'nomad -v' displays the current version.

7.2.3 Version 3.1

- Biobjective optimization: see Section 6.2.
- Periodic variables: if some variable are periodic, this may be indicated via parameter PERIODIC_VARIABLE. Bounds must be defined for these variables. The MADS algorithm adapted to periodic variables is described in [24].
- Groups of variables can be defined with the parameter VARIABLE_GROUP. At every MADS poll, different directions will be generated for each group. For example, for a location problem, if groups correspond to spatial objects, these will be moved one at a time.

7.3 Future versions

Future algorithm developments include:

- Adaptive surrogates and use of the surrogate management framework [31].
- Multi-Mads: multi-objective variant of Mads [26], with 3 and more objective functions.
- Use of simplex gradients [34, 35].

Acknowledgments

The developers of Nomad wish to thank Florian Chambon, Mohamed Sylla and Quentin Reynaud, all from ISIMA, for their contribution to the project during Summer internships, and to Anthony Guillou and Dominique Orban for their help with configure and AMPL, and their suggestions. Thanks also to Annie Angers, Maud Bay, Eve Bélisle, Vincent Garnier, Michal Kvasnicka, Alexander Lutz, Rosa-Maria Torres-Calderon, Christophe Tribes, and an anonymous user for their tests, feedback, and various help. Finally, many thanks to the TOMS anonymous referees for their useful comments which helped a lot to improve the code and the text of [38].

Related publications

- [1] M. A. Abramson. Mixed variable optimization of a load-bearing thermal insulation system using a filter pattern search algorithm. *Optimization and Engineering*, 5(2):157–177, 2004.
- [2] M. A. Abramson. Second-order behavior of pattern search. SIAM Journal on Optimization, 16(2):315–330, 2005.
- [3] M. A. Abramson and C. Audet. Convergence of mesh adaptive direct search to second-order stationary points. SIAM Journal on Optimization, 17(2):606-619, 2006.
- [4] M. A. Abramson, C. Audet, G. Couture, J. E. Dennis, Jr., and S. Le Digabel. The NOMAD project. Software available at http://www.gerad.ca/nomad.
- [5] M. A. Abramson, C. Audet, and J. E. Dennis, Jr. Generalized pattern searches with derivative information. *Mathematical Programming*, Series B, 100:3–25, 2004.
- [6] M. A. Abramson, C. Audet, J. E. Dennis, Jr., and S. Le Digabel. OrthoMADS: A deterministic MADS instance with orthogonal directions. SIAM Journal on Optimization, 20(2):948–966, 2009.

- [7] M. A. Abramson, O. A. Brezhneva, J. E. Dennis Jr., and R. L. Pingel. Pattern search in the presence of degenerate linear constraints. *Optimization Methods and Software*, 23(3):297–319, 2008.
- [8] M.A. Abramson, C. Audet, J.W. Chrissis, and J.G. Walston. Mesh adaptive direct search algorithms for mixed variable optimization. *Optimization Letters*, 3(1):35–47, January 2009.
- [9] M.A. Abramson, C. Audet, and J. E. Dennis, Jr. Filter pattern search algorithms for mixed variable constrained optimization problems. *Pacific Journal on Optimization*, 3(3):477–500, 2007.
- [10] C. Audet. Convergence Results for Pattern Search Algorithms are Tight. Optimization and Engineering, 5(2):101–122, 2004.
- [11] C. Audet, V. Béchard, and J. Chaouki. Spent potliner treatment process optimization using a MADS algorithm. *Optimization and Engineering*, 9(2):143–160, 2007.
- [12] C. Audet, V. Béchard, and S. Le Digabel. Nonsmooth optimization through mesh adaptive direct search and variable neighborhood search. *Journal of Global Optimization*, 41(2):299–318, June 2008.
- [13] C. Audet, A. J. Booker, J. E. Dennis, Jr., P. D. Frank, and D. W. Moore. A surrogate-model-based method for constrained optimization. Presented at the 8th AIAA/ISSMO Symposium on Multidisciplinary Analysis and Optimization, 2000.
- [14] C. Audet, A. L. Custódio, and J. E. Dennis, Jr. Erratum: Mesh adaptive direct search algorithms for constrained optimization. SIAM Journal on Optimization, 18(4):1501–1503, 2008.
- [15] C. Audet and J. E. Dennis, Jr. Pattern search algorithms for mixed variable programming. SIAM Journal on Optimization, 11(3):573–594, 2000.
- [16] C. Audet and J. E. Dennis, Jr. Analysis of generalized pattern searches. SIAM Journal on Optimization, 13(3):889–903, 2003.
- [17] C. Audet and J. E. Dennis, Jr. A pattern Search Filter Method for Nonlinear Programming without Derivatives. SIAM Journal on Optimization, 14(4):980–1010, 2004.
- [18] C. Audet and J. E. Dennis, Jr. Mesh adaptive direct search algorithms for constrained optimization. SIAM Journal on Optimization, 17(1):188–217, 2006.
- [19] C. Audet and J. E. Dennis, Jr. Nonlinear programming by mesh adaptive direct searches. SIAG/Optimization Views-and-News, 17(1):2–11, 2006.
- [20] C. Audet and J. E. Dennis, Jr. A Progressive Barrier for Derivative-Free Nonlinear Programming. SIAM Journal on Optimization, 20(4):445–472, 2009.
- [21] C. Audet, J. E. Dennis, Jr., and S. Le Digabel. Parallel space decomposition of the mesh adaptive direct search algorithm. *SIAM Journal on Optimization*, 19(3):1150–1170, 2008.
- [22] C. Audet, J. E. Dennis, Jr., and S. Le Digabel. Globalization strategies for mesh adaptive direct search. *Computational Optimization and Applications*, 46(2):193–215, June 2010.
- [23] C. Audet, J. E. Dennis, Jr., and S. Le Digabel. Sensitivity to constraints in blackbox optimization. Technical Report G-2010-NA, Les cahiers du GERAD, 2010.

- [24] C. Audet and S. Le Digabel. The mesh adaptive direct search algorithm for periodic variables. Technical Report G-2009-23, Les cahiers du GERAD, 2009.
- [25] C. Audet and D. Orban. Finding optimal algorithmic parameters using derivative-free optimization. SIAM Journal on Optimization, 17(3):642–664, 2006.
- [26] C. Audet, G. Savard, and W. Zghal. Multiobjective optimization through a series of single-objective formulations. SIAM Journal on Optimization, 19(1):188–210, 2008.
- [27] C. Audet, G. Savard, and W. Zghal. A mesh adaptive direct search algorithm for multiobjective optimization. *European Journal of Operational Research*, 204(3):545–556, 2010.
- [28] A. J. Booker, E. J. Cramer, P. D. Frank, J. M. Gablonsky, and J. E. Dennis, Jr. Movars: Multidisciplinary optimization via adaptive response surfaces. AIAA Paper 2007–1927, Presented at the 48th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, Honolulu, 2007.
- [29] A. J. Booker, J. E. Dennis, Jr., P. D. Frank, D. W. Moore, and D. B. Serafini. Managing surrogate objectives to optimize a helicopter rotor design – further experiments. AIAA Paper 1998–4717, Presented at the 8th AIAA/ISSMO Symposium on Multidisciplinary Analysis and Optimization, St. Louis, 1998.
- [30] A. J. Booker, J. E. Dennis, Jr., P. D. Frank, D. B. Serafini, and V. Torczon. Optimization using surrogate objectives on a helicopter test example. In J. Borggaard, J. Burns, E. Cliff, and S. Schreck, editors, *Optimal Design and Control*, Progress in Systems and Control Theory, pages 49–58, Cambridge, Massachusetts, 1998. Birkhäuser.
- [31] A. J. Booker, J. E. Dennis, Jr., P. D. Frank, D. B. Serafini, V. Torczon, and M. W. Trosset. A rigorous framework for optimization of expensive functions by surrogates. *Structural Optimization*, 17(1):1–13, February 1999.
- [32] A. Brooke, D. Kendrick, and A. Meeraus. *GAMS: A Users' Guide*. The Scientific Press, Danvers, Massachusetts, 1988.
- [33] E. J. Cramer, J. E. Dennis, Jr., P. D. Frank, R. M. Lewis, and G. R. Shubin. Problem formulation for multidisciplinary optimization. In AIAA Symposium on Multidisciplinary Design Optimization, September 1993.
- [34] A. L. Custódio, J. E. Dennis, Jr., and L. N. Vicente. Using simplex gradients of nonsmooth functions in direct search methods. *IMA Journal of Numerical Analysis*, 28(4):770–784, 2008.
- [35] A. L. Custódio and L. N. Vicente. Using sampling and simplex derivatives in pattern search methods. SIAM Journal on Optimization, 18(2):537–555, May 2007.
- [36] J. E. Dennis, Jr., C. J. Price, and I. D. Coope. Direct search methods for nonlinearly constrained optimization using filters and frames. *Optimization and Engineering*, 5(2):123–144, June 2004.
- [37] J. E. Dennis, Jr. and V. Torczon. Direct search methods on parallel machines. SIAM Journal on Optimization, 1(4):448–474, November 1991.
- [38] S. Le Digabel. NOMAD: Nonlinear optimization with the MADS algorithm. Technical Report G-2009-39, Les cahiers du GERAD, 2009.

- [39] S. Le Digabel. NOMAD user guide. Technical Report G-2009-37, Les cahiers du GERAD, 2009.
- [40] S. Le Digabel, M.A. Abramson, C. Audet, and J. E. Dennis, Jr. Parallel versions of the MADS algorithm for black-box optimization. In *Optimization days*, Montreal, May 2010. Slides available at www.gerad.ca/Sebastien.Le.Digabel/talks/2010_JOPT_25mins.pdf.
- [41] R. Fourer, D. M. Gay, and B. W. Kernighan. *AMPL: A Modeling Language for Mathematical Programming*. Thomson/Brooks/Cole, Pacific Grove, California, second edition, 2003.
- [42] K.R. Fowler, J.P. Reese, C.E. Kees, J.E. Dennis Jr., C.T. Kelley, C.T. Miller, C. Audet, A.J. Booker, G. Couture, R.W. Darwin, M.W. Farthing, D.E. Finkel, J.M. Gablonsky, G. Gray, and T.G. Kolda. Comparison of derivative-free optimization methods for groundwater supply and hydraulic capture community problems. Advances in Water Resources, 31(5):743–757, May 2008.
- [43] N. I. M. Gould, D. Orban, and Ph. L. Toint. CUTEr (and SifDec): a constrained and unconstrained testing environment, revisited. ACM Transactions on Mathematical Software, 29(4):373–394, 2003.
- [44] R. E. Hayes, F. H. Bertrand, C. Audet, and S. T. Kolaczkowski. Catalytic combustion kinetics: Using a direct search algorithm to evaluate kinetic parameters from light-off curves. *The Canadian Journal of Chemical Engineering*, 81(6):1192–1199, 2003.
- [45] M. Kokkolaras, C. Audet, and J. E. Dennis, Jr. Mixed variable optimization of the number and composition of heat intercepts in a thermal insulation system. *Optimization and Engineering*, 2(1):5–29, 2001.
- [46] A. L. Marsden, M. Wang, J. E. Dennis, Jr., and P. Moin. Optimal aeroacoustic shape design using the surrogate management framework. *Optimization and Engineering*, 5(2):235–262, 2004.
- [47] A. L. Marsden, M. Wang, J. E. Dennis, Jr., and P. Moin. Suppression of airfoil vortex-shedding noise via derivative-free optimization. *Physics of Fluids*, 16(10):L83–L86, 2004.
- [48] A. L. Marsden, M. Wang, J. E. Dennis, Jr., and P. Moin. Trailing-edge noise reduction using derivative-free optimization and large-eddy simulation. *Journal of Fluid Mechanics*, 572:13–36, February 2007.
- [49] N. Mladenović and P. Hansen. Variable neighborhood search. Computers and Operations Research, 24(11):1097–1100, 1997.
- [50] P. Hansen N. Mladenović. Variable neighborhood search: principles and applications. *European Journal of Operational Research*, 130(3):449–467, 2001.
- [51] M. S. Ouali, H. Aoudjit, and C. Audet. Optimisation des stratégies de maintenance. *Journal Européen des Systèmes Automatisés*, 37(5):587–605, 2003.
- [52] M. Snir, S. W. Otto, S. Huss-Lederman, D. W. Walker, and J. Dongarra. MPI: The Complete Reference. The MIT Press, Cambridge, Massachusetts, 1995.
- [53] T. A. Sriver, J. W. Chrissis, and M. A. Abramson. Pattern search ranking and selection algorithms for mixed variable stochastic optimization, 2004. Preprint.