



Technical note: the caRamel R package for Automatic Calibration by Evolutionary Multi Objective Algorithm

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Abstract. Environmental modelling is complex, and models often require the calibration of several parameters that are not directly evaluable from a physical quantity or a field measurement. The R package caRamel has been designed to easily implement a multi-objective optimizer in the R environment to calibrate these parameters. A multiobjective calibration allows to find a compromise between different goals by defining a set of optimal parameters. The algorithm is a hybrid of the Multiobjective Evolutionary Annealing Simplex method (MEAS) and the Nondominated Sorting Genetic Algorithm II (ϵ -NSGA-II algorithm). The optimizer was initially developed for the calibration of hydrological models but can be used for any environmental model. The main function of the package, caRamel(), requires to define a multi-objective calibration function as well as bounds on the variation of the underlying parameters to optimize.

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CaRamel is well adapted to complex modelling. As an example, caRamel converges quickly and has a stable solution after 5,000 model evaluations with robust results for a real study case of a hydrological problem with 8 parameters and 3 objectives of calibration. The comparison with another well-known optimizer (i.e. MCO, for Multiple Criteria Optimization) confirms the quality of the algorithm.

1 Introduction

20 Environmental modelling is complex, and models often require the prescription of many parameters that cannot be directly estimated from a physical quantity or a field measurement. Moreover, as models outputs exhibit errors whose statistical structure may be difficult to characterize precisely it is frequently necessary to use various objectives to evaluate the modelling performance. Put differently, it is often difficult to find a rigorous likelihood function or any sufficient statistic (Fisher, 1922) to be maximized/minimized: for example, it is well-know that errors in a simulated discharge time series are not normally distributed, and do not have constant variance and autocorrelation.

Multiobjective calibration allows to find a compromise between these different objectives by defining a set of optimal parameters. Evolutionary algorithms have become widely used to explore the Pareto-optimal front in multi-objective optimization problems that are too complex to be solved by descent methods. Not only because there are few alternatives for searching substantially large spaces for multiple Pareto-optimal solutions but also due to their inherent parallelism and their



capability to exploit similarities of solutions by recombination, they are able to approximate the Pareto-optimal front in a single optimization run (Zitzler et al., 2000). Many studies in environmental modeling (Oraei Zare et al., 2012; Ercan and Goodall, 2016; Smith et al., 2019) or land-use models (Gong et al., 2015; Newland et al., 2017) use the multi-objective approach.

5 The caRamel optimizer has been developed to meet the need of an automatic calibration procedure that delivers not only one but a family of parameters sets that are optimal regarding a multi-objective target.

CaRamel was initially developed and used for the calibration of hydrological models: Le Moine et al., 2015, Rothfuss et al., 2012, Magand et al., 2014, Monteil et al., 2015 (previously to the R-package release) or Rouhier et al. (2017, R version, calibration of a hydrologic model over the Loire basin, 35,707 km²). The interesting performances of caRamel algorithm led us to describe specifically the algorithm in that paper and to adapt it as an R-package, so that it can be used for any model in the R environment. The user has simply to define a vector-valued function (at least 2 objectives) for the model to calibrate and lower and upper bounds for the calibrated parameters.

This paper aims at describing the principles of caRamel algorithm and its use as an R-package. A comparison with another optimization package, "Multiple Criteria Optimization" (MCO, Mersmann et al., 2014), is also presented.

15 **2 CaRamel description**

The purpose of a multi-objective calibration is to find sets of parameters giving a compromise between several potentially conflicting objectives, for instance, flood objective and low flow objective in Hydrology. Multi-objective calibration is also a way to add some constraints to an underconstrained problem when many parameters have to be quantified. This can help to reduce the equifinality of parameters sets.

20 Equifinality may be caused by the model structure, when two sets of parameters give similar results. Another kind of equifinality is related to the calibration objectives, when two different model results give similar objective values. In this case, the use of additional objective may help to better constraint the calibration.

2.1 Principle of caRamel

CaRamel algorithm belongs to genetic algorithm family. The idea is to start from an ensemble of parameters sets (called "population") and to make this population evolve following some generation rules. At each generation, new sets are evaluated regarding the objectives and only the more "suitable" sets are kept to build the new population. CaRamel algorithm is largely inspired by:

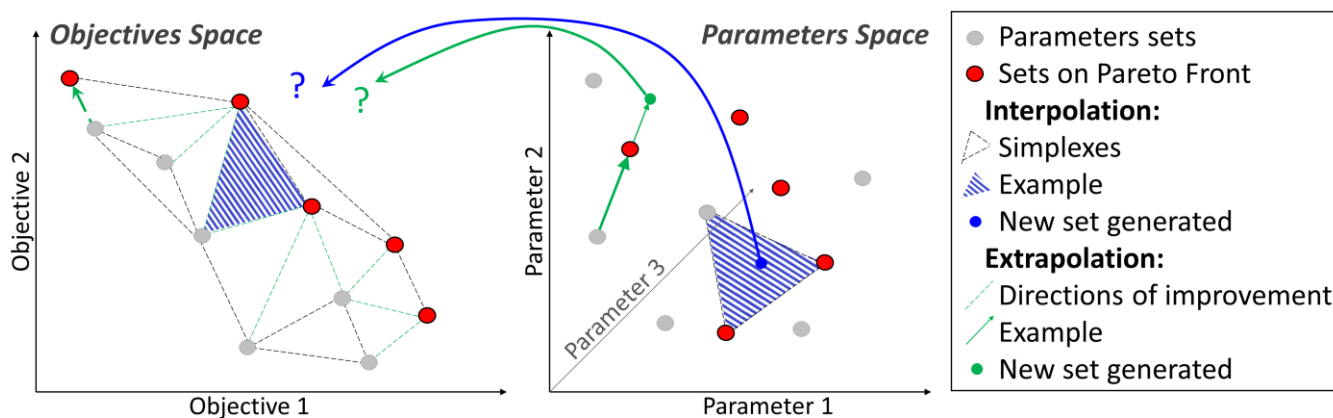
- 1) the Multiobjective Evolutionary Annealing Simplex method (MEAS, Efstratiadis and Koutsoyiannis, 2005), for the directional search method, based on the simplexes of the objectives space,
- 2) the Nondominated Sorting Genetic Algorithm II (ϵ -NSGA-II, Reed and Divireddy, 2004), for the classification of parameters vectors and the management of precision by ϵ -dominance.



2.1.1 Generation rules

The algorithm of caRamel has five rules for generating new solutions at each generation: (1) interpolation, (2) extrapolation, (3) independent sampling with a priori parameters variance, (4) sampling with respect of a correlation structure, and (5) recombination.

- 5 The first two rules (interpolation, extrapolation) are based on a N_P -dimensional Delaunay triangulation in the objectives space (N_P being the number of optimized parameters). They assume that two neighboring points in the objectives space have two adjacent points in the parameters space as antecedents, and therefore one can try to "guess" the directions of improvement in the parameters space from the improvement directions (in a Pareto sense) in the objective space, at least near the optimal zone (Fig. 1).



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Figure 1: Illustration of rules interpolation (1) and extrapolation (2) based on a N_P -dimensional Delaunay triangulation in the objectives space for a maximization problem (2 objectives, 3 parameters). Interpolation computes a new parameters vector for each simplex with a non-dominated vertex. Extrapolation derives a new vector for each direction of improvement.

The following two rules create new parameters sets by exploring the parameters space in a non-directional and less local way: either by independent variations in each parameter, or by multivariate sampling using the covariance structure of all parameters sets located near the estimated Pareto font at the current iteration.

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Finally, the recombination rule consists in creating new parameters sets using two partial subsets coming from a pair of previously evaluated parameters sets (inspired by Baluja and Caruana, 1995).

2.1.2 Population downsizing

- 20 At the end of each generation, population is kept under a maximum size (N_{MAX} sets). This stage uses the concept of ranking order of the Pareto front (according to nondomination) and it is adapted from ϵ -NSGA-II algorithm. The population downsizing is performed in 3 steps (Fig. 2):

- 1) sorting the sets according to ranking order of the Pareto level they belong to,
- 2) in the parameters space, keeping only one set by boxes defined by the defined precision (ϵ),
- 3) if the number of sets is still above N_{MAX} , keeping only the N_{MAX} sets of the smaller level.

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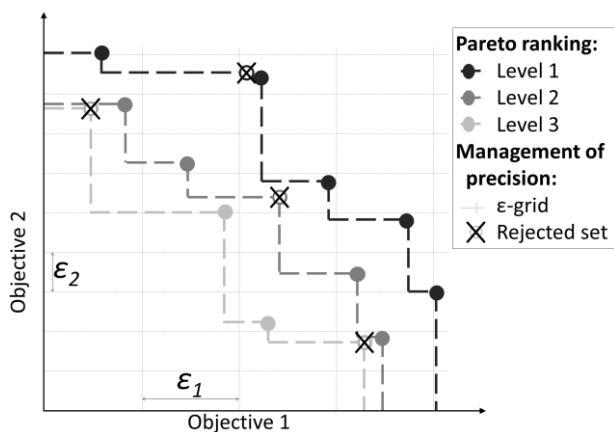


Figure 2. Method for population downsizing for a maximization problem with 2 objectives: Pareto ranking (Level 1 is the current approximated Pareto front) and management of precision by ϵ -dominance.

2.2 The caRamel R package

5 The caRamel package has been designed as an optimization tool for any environmental model, provided that it is possible to evaluate the objective functions in R. The main function, caRamel, is called with these syntax: caRamel (nobj, nvar, minmax, bounds, func, popsize, archsize, maxrun, prec). Arguments are detailed in Table 1.

The main argument of caRamel is the objective function that has to be defined by the user. This enables flexibility as the user gives all the necessary information: the number and the definition of all the objectives, the minimization or
 10 maximization goal for each objective function, the number of parameters to calibrate and their bounds, and other numerical parameters such as the maximum number of simulations allowed.

Additional optional arguments give the following possibilities:

- creation of blocks/subsets of parameters that should be jointly recombined (for example parameters of a same module),
- 15 • parallel or sequential computation,
- continuation of optimization starting from an existing population,
- saving of the population after each generation or only the final one,
- managing the number of parameters sets generated by generation.

As a result, the function returns a list of five elements:

- 20 • success: a logical, "TRUE" if the optimization process ran with no errors,
- parameters: matrix of parameters sets from the Pareto front (dimension [number of sets in the front, number of calibrated parameters]),
- objectives: matrix of associated objectives (dimension [number of sets in the front, number of objectives]),



- `save_crit`: matrix that describes the evolution of the optimization process: for each generation, first column is the number of model evaluations, and the following ones are the optimum of each objective taken separately (dimension [number of generation, (number of objectives + 1)]),
- `total_pop`: total population (dimension [number of parameters sets, (number of calibrated parameters + number of objectives)]).

The R package contains a R vignette which gives as example benchmark functions with 2 objectives and 1 or 3 parameters Schaffer (Schaffer, 1984) or Kursawe (Kursawe, 1991).

3. Optimization evaluation framework

To evaluate the optimizer performances, we chose metrics from the literature. Evaluating optimization techniques experimentally always involves the notion of performance. In the case of multiobjective optimization, the definition of quality is substantially more complex than for single-objective optimization problems, because the optimization goal itself consists of multiple objectives (Zitzler et al 2000). Riquelme et al. (2015) categorize the metrics to evaluate three main aspects:

- the accuracy which is the closeness of the solutions to the theoretical Pareto-front (if known) or relative closeness,
- the diversity which can be described with two aspects: the spread of the set (range of values covered by the solutions) and the distribution (relative distance among solutions in the set),
- the cardinality which qualifies the number of Pareto-optimal solutions in the set.

To quantify these aspects, we selected 3 different metrics:

- Generational Distance (GD) which is a distance based accuracy performance index (Van Veldhuizen, 1999),
- Generalized Spread (GS) evaluates the diversity of the set (Zhou et al., 2006),
- Hypervolume (HV) which is a volume based index that takes into account accuracy, diversity and cardinality (Zitzler and Thiele, 1999).

In addition, `caRamel` results are compared with results from another multi-objective optimizer available in the R environment: the `nsga2()` function of the R-package "Multiple Criteria Optimization" (MCO, Mersmann et al., 2014). This function is an implementation of NSGA-II algorithm. The arguments are the function to minimize, the input and output dimensions, the parameters bounds, the number of generations, the size of the population and the values for crossover and mutation probability and distribution index.

Evaluation of metrics GS and GD require to establish a reference front. It was built by evaluating the Pareto front over all the optimizations with the two optimizers in order to have the same reference for `caRamel` and MCO.



4. Examples of calibration

This section aims at giving examples of caRamel use, first with Kursawe test function (3 parameters, 2 objectives) then with an hydrological model (8 parameters, 3 objectives). We also compare caRamel results with results from an optimization with NSGA-II only (package MCO). In the next examples, population size has been set at 100 sets for both optimizers. As
5 caRamel and MCO algorithms use random functions, 40 optimizations of each test case have been run to get representative results.

4.1 Kursawe test function

The R script to run the Kursawe function optimization is available in Appendix A, or as a vignette in caRamel package. Figure 3 shows the results of 40 Kursawe test function optimizations. In the example of Pareto fronts (Fig 3a), the shape of
10 the final front is already reached after 1,000 model evaluations. GD and HV evolutions shows that CaRamel is converging quite rapidly for the accuracy, after about 1,000 model evaluations (Fig. 3b-c). The convergence for diversity (GS) is reached after 5,000 evaluations (Fig. 3d). Comparison with MCO (NSGA-II only) shows that the use of MEAS makes the optimization process converge more rapidly but with a lower diversity (Fig. 3d).

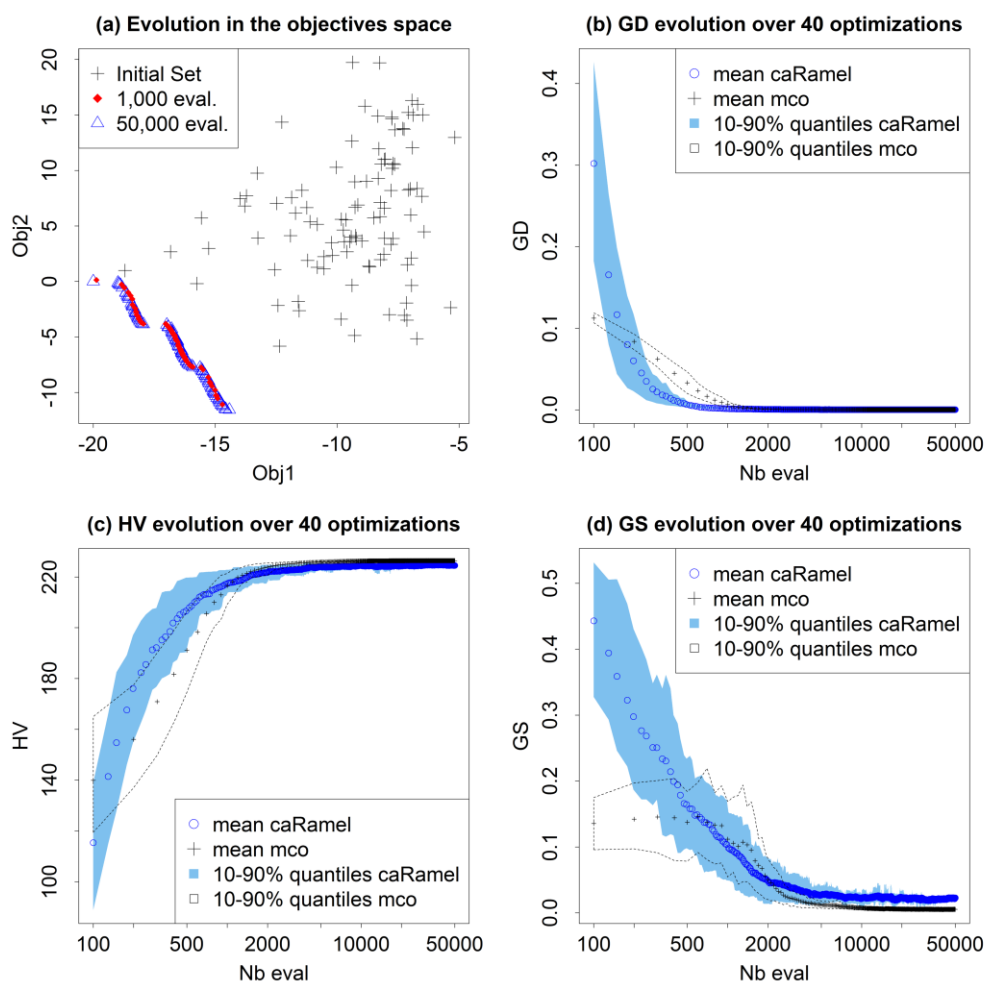


Figure 3: Characterization of Kursawe test function optimization: (a) distribution of initial population and Pareto front after 1,000 and 50,000 model evaluations (with caRamel), and mean and 10% 90% quantiles evolution of the metrics over 40 optimizations regarding the number of model evaluations with caRamel or MCO: (b) Hypervolume, (c) Generalized Spread, (d) Generational Distance.

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4.2 Hydrological modeling

For this example, we chose to calibrate MORDOR-SD hydrological model (Garavaglia et al., 2017). We first present the model and calibration conditions, then the comparison framework, and then some results. The main lines of the R script for the optimization with parallel computation are displayed in Appendix B.

10 4.2.1 Hydrological model

The rainfall-runoff model used for this study is the conceptual MORDOR-SD model. It is a semi-distributed hydrological model widely used for operational applications at Electricité de France (EDF, the French electric utility company).



This model was implemented at a daily time step for a French catchment, the Tarn catchment at Millau (Fig. 4), covering 2,335 km², and with middle altitude (350 to 1,600 m). The regime is pluvial, with almost no influence of snow.

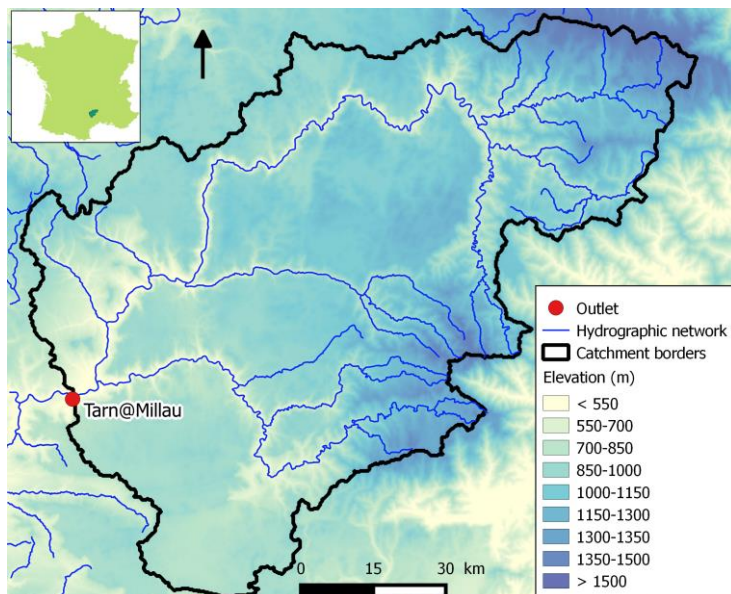


Figure 4: The Tarn catchment at Millau (2,335 km²)

- 5 Calibration is conducted over 10 years (1/01/2001–31/12/2010). Eight parameters are calibrated that describe the functioning of conceptual reservoirs, evapotranspiration correction and wave celerity (Table 2).

4.2.2 Calibration objectives

Calibration objectives are based on the KGE (Gupta et al., 2009) which is frequently used in Hydrology. Three objectives are estimated by computing KGE over three streamflow signatures: (1) the entire time-series (KGE daily runoff, "KGE"), which is the result of all the processes, (2) the inter-annual daily regime (KGE daily regime, "KGEr"), which reflects the interaction between water and energy availability as well as catchment storage, (3) the average of the monthly empirical cumulative distributions weighted by monthly runoff which focuses on floods produced by highly dynamic interactions ("KGEamd").

The calibration is then multiobjective. KGE optimal value is 1, the optimizer has to maximize the objectives and so the optimum is the point (1, 1, 1) in the objectives space.

15 4.2.3 Optimizers parameters

For the two optimizers caRamel and MCO, the size of initial population is 100 parameters sets. The end of one optimization is set to 15,000 model evaluations. To have representative results, we choose to run 40 optimizations of each test case and look at mean values and 10% -90% quantiles distribution.



Some previous calibration experiments have been conducted to determine the best parameters configuration for the each optimizer. In this case, caRamel has been set to generate 5 parameters sets for each rule by generation, meaning 25 parameters sets by generation, representing about 600 generations. MCO has been used with crossover probability set to 0.5 and mutation probability to 0.3. In MCO algorithm, the size of the generated population is the same of the size of initial population. The number of 15,000 model evaluations represents 150 generations.

4.2.4 Optimization results

3D Pareto front over 40 optimizations after 15,000 model evaluations are quite similar with caRamel or MCO (Fig. 5). CaRamel has a slightly better accuracy and MCO has a larger diversity with more sets with KGE under 0.85. This is also what show the final values of evaluation metrics which are quite the same for GD and HV and a lower GS with MCO (Fig.

10 6).

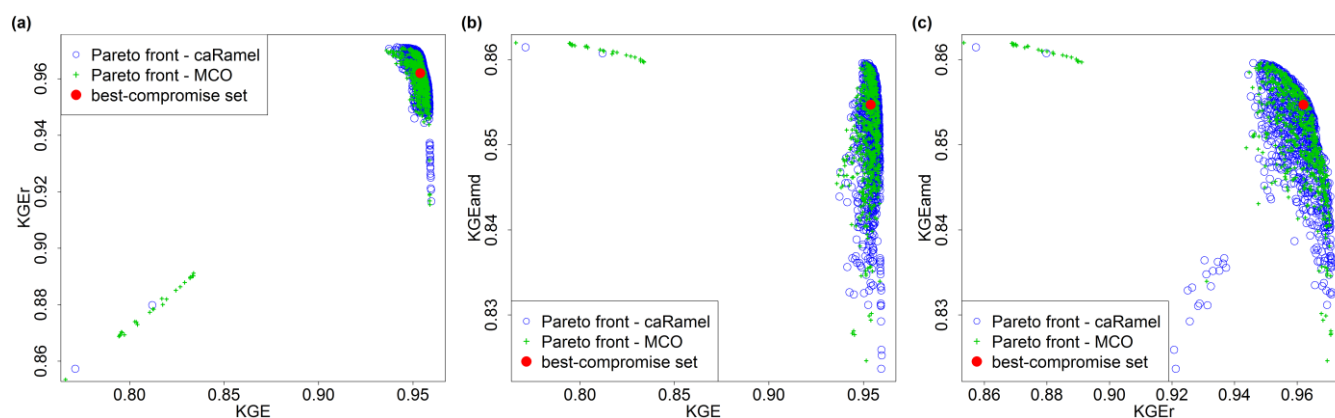


Figure 5: Pareto Front after 15,000 model evaluations and 40 optimizations of model MORDOR-SD over objectives KGE and KGE regime and KGE average of the monthly empirical cumulative distributions with caRamel or MCO. The red point represent a "best compromise" parameters set that is used to illustrate model results.

15 When comparing the evolution of the optimization, it appears that caRamel is converging more rapidly in accuracy with the final GD value reached after about 1,000 evaluations and the final HV value after 3,000 (Fig. 6a-b). GS metric is more variable, with a larger envelope for both optimizer. With caRamel, the envelope get thinner after 1,000 evaluations which means that the optimizer is more reproducible (Fig. 6c). GD indicates a larger diversity for MCO but the envelope is much larger meaning a lower reproducibility.

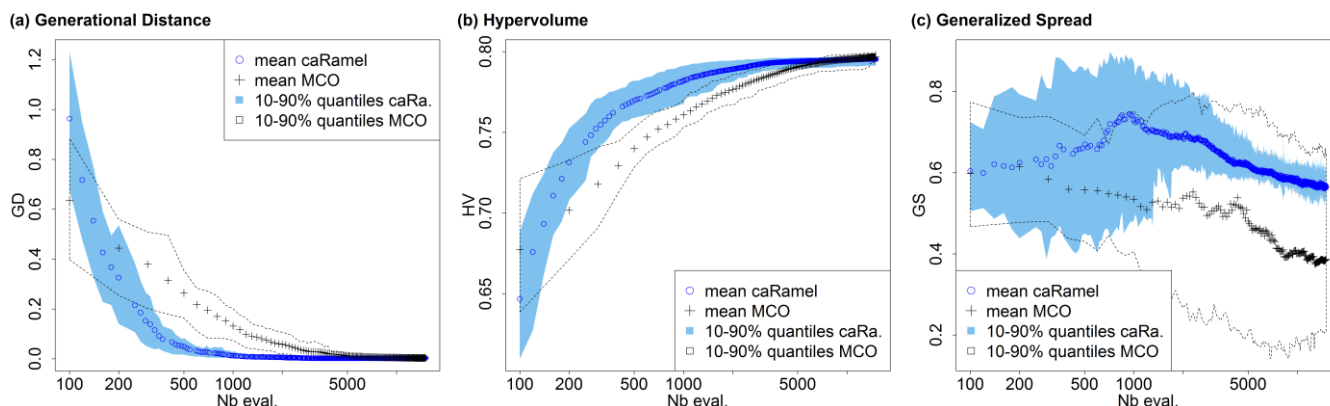


Figure 6: Metrics evolution over 40 optimizations of model MORDOR-SD with caRamel or MCO: mean evolution and 10-90% quantiles of the metrics regarding the number of model evaluations: (a) GD, (b) HV and (c) GS

In the parameters space, the two optimizers provides very similar results that explore the equifinality of the model, meaning 5 different parameters sets giving similar performances (Fig. 7). Some parameters (U_{max} , kr) may have optimized values on the whole range defined by the bounds while other parameters are better constrained (L_{max} , cel). These constitute a family of sets that are optimal regarding the chosen objectives.

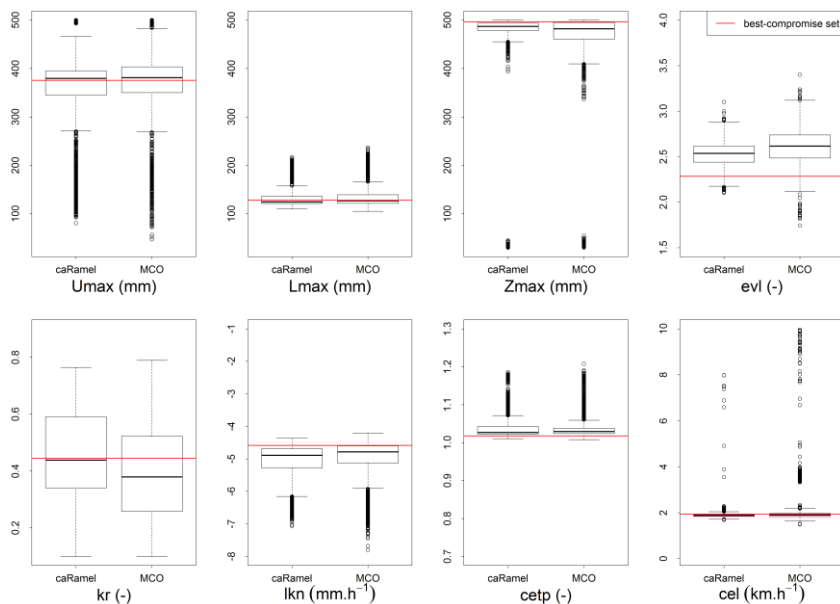


Figure 7: Calibrated parameters distribution for the sets on the Pareto front (y limits are the calibration bounds) with caRamel or MCO. Parameters values from the "best-compromise set" are displayed in red.

Consequences on the simulated streamflow are displayed on Fig. 8. The red line represents the simulated streamflow with the "best-compromise" set and it fits very well with the observed one (KGE 0.95). The gray area represents the envelope described by all simulated streamflow from all parameters sets on the Pareto front over the 40 optimizations, the envelope is quite narrow for the two optimizers.

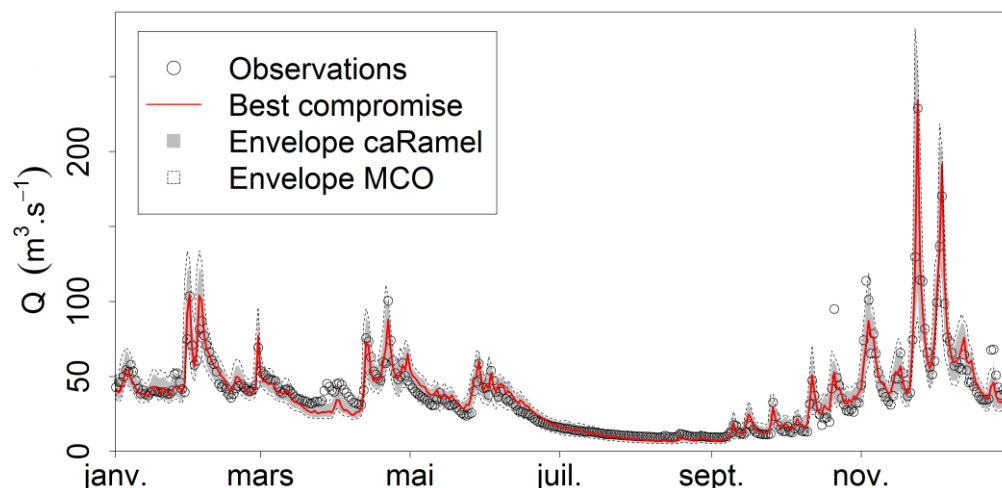


Figure 8: Daily runoff regime of Tarn River at Millau (2001–2010). "Observations": observed streamflow, "Best compromise": best-compromise simulated streamflow, "Envelope": simulated streamflow envelope using all parameters sets on the Pareto front (over 40 optimizations) with caRamel or MCO.

5 Conclusion

The R package caRamel has been designed to easily implement a multi-objective optimizer in the R environment. The algorithm is a hybrid of the Multiobjective Evolutionary Annealing Simplex (MEAS) algorithm (Efstratiadis and Koutsoyiannis, 2005) by using the directional search method based on the simplexes of the objective space and the ε -NGSA-II algorithm with the method of classification of the parameters vectors archiving management by ε -dominance (Reed and Devireddy, 2004). The main function of the package, caRamel(), requires a multiobjective function to be defined in a R script and bounds on the parameters involved in the calibration. In return, result of caRamel is a family of parameters sets that are Pareto optimal regarding the different objectives.

Two examples of optimization have been explained: Kursawe test function and a hydrological implementation. While comparing the results with nsga2 function from MCO R package (Mersmann et al., 2014), it appears that both optimizers give similar results after 15,000 model evaluations. However, caRamel is converging more rapidly and has a stable and more reproducible solution.

The optimizer was initially developed for the calibration of hydrological models, but it can be used for any environmental model, provided the model computation time is short enough to be run about 5,000 times for the calibration.

Code availability

The data analysis was performed with the open-source environment R (<https://www.r-project.org/>). The algorithm is provided as R package “caRamel”, which is available from GitHub at <https://github.com/fzao/caRamel>, or from CRAN: <https://cran.r-project.org/package=caRamel>.



Appendix A: Example of R script for Kursawe test function optimization

```
# Kursawe function definition
kursawe <- function(i) {
  Obj1 <- -10 * exp(-0.2 * sqrt(x[i,1]^2 + x[i,2]^2)) - 10 * exp(-0.2 * sqrt(x[i,2]^2 + x[i,3]^2))
5  Obj2 <- abs(x[i,1])^0.8 + 5 * sin(x[i,1]^3) + abs(x[i,2])^0.8 + 5 * sin(x[i,2]^3) + abs(x[i,3])^0.8 + 5 * sin(x[i,3]^3)
  return(c(Obj1, Obj2))
}

# Parameters definition and caRamel run
nobj <- 2 ; nvar <- 3 ; bounds <- matrix( c(rep(-5, nvar), rep(5, nvar)), ncol = 2 ) # range [-5, 5]
10 results <- caRamel (nobj = nobj , nvar = nvar , minmax = c(FALSE, FALSE) , bounds = bounds, func = kursawe, popsize =
  100 , archsize = 100, maxrun = 5000, prec = rep(1.e-3, nobj) )
```

Appendix B: Example of R script for MORDOR-SD optimization

```
# Initialization function for each node for parallel computation
InitMordor <- function(cl, numcores){
15  parLapply( cl, 1:numcores, function(xx){require('MordorPackage')})
  clusterExport(cl=cl, varlist=c("Qobs", "Data")) # Qobs and Data are global variables defined previously by the user
}

# Objectives evaluation function
EvalMordor <- function(i){
20  Q <- RunMordor(x[i,], Data) # x and i are caRamel global variables defined by caRamel
  Obj1 <- KGE(Qobs, Q) ; Obj2 <- KGEr(Qobs, Q) ; Obj3 <- KGEamd(Qobs, Q)
  return( c(Obj1, Obj2, Obj3) )
}

# Optimization
25 bounds <- cbind(c(0.7, 30, 30, 30, 1.5, 0.1, -8, 0.7, 0.1), c(1.3, 500, 500, 500, 4, 0.9, -1, 1.3, 10))
results <- caRamel (nobj = 3, nvar = 8, minmax = rep(TRUE, 3), bounds = bounds, func = EvalMordor, funcinit =
InitMordor, popsize = 100, archsize = 100, maxrun = 15000, prec = rep(1.e-4, 3) )

# Notations:
30 # MordorPackage: R package of the hydrological model (which is not open source)
# RunMordor: model run function (with 2 arguments: parameters vector, list of complementary data), result is the vector Q
of simulated discharges.
```



KGE, KGE_r, KGE_{amd}: evaluation functions for the 3 objectives.

Author contribution

NLM developed the algorithm in the Scilab platform. FH, FZ and CM adapted the algorithm as R package and performed various tests cases. CM prepared the manuscript with contributions from all co-authors.

5 Competing interest

The authors declare that they have no conflict of interest.

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Table 1: Arguments of caRamel() function. Optional arguments are printed in grey.

Name	Type	Description
nobj	integer, length = 1	number of objectives to optimize (at least 2)
nvar	integer, length = 1	number of variables
minmax	logical, length = nobj	indicates if each objective is either a maximization (TRUE) or a minimization (FALSE)
bounds	matrix, nrow = nvar, ncol = 2	lower and upper bounds for the variables
func	character, length = 1	name of the objective R function to optimize, with VecObj = func(i) where i is the tested set index in the population matrix (x), and VecObj is the vector of objectives for this set.
popsize	integer, length = 1	population size for the genetic algorithm
archsize	integer, length = 1	size of the Pareto front
maxrun	integer, length = 1	maximum number of model runs
prec	double, length = nobj	desired precision for the objectives (used for downsizing population)
repart_gene	integer, length = 4	number of new parameter sets for each rule and per generation
gpp	integer, length = 1	calling frequency for the rule (3)
blocks	list of vector integer	functional groups for parameters
pop	matrix, nrow = nset, ncol = nvar or nvar+nobj	initial population (used to restart an optimization)
objnames	character, length = nobj	name of the objectives
listsave	list of character	names of the listing files (NULL by default: no output)
write_gen	integer, length = 1	if = 1, save files 'pmt' and 'obj' at each generation (= 0 by default)
carallel	logical, length = 1	run parallel computations (TRUE by default)
numcores	integer, length = 1	number of cores for the parallel computations (all cores by default)
funcinit	character, length = 1	name of the initialization function applied on each node of cluster when parallel computation. Arguments must be cl and numcores.
graph	logical, length = 1	plot graphical output at each generation (TRUE by default)



Table 2: Parameters to calibrate for MORDOR-SD and bounds of variation

Parameter	Units	Prior range	Description
cetp	–	[0.7, 1.3]	PET correction factor
umax	mm	[30, 500]	Maximum capacity of the root zone
lmax	mm	[30, 500]	Maximum capacity of the hillslope zone
zmax	mm	[30, 500]	Maximum capacity of the capillarity storage
kr	–	[0.1, 0.9]	Runoff coefficient
evl	–	[1.5, 4]	Outflow exponent of storage L
lkn	mm.h ⁻¹	[-8, -1]	Outflow coefficient of storage N
cel	km.h ⁻¹	[0.1, 10]	Wave celerity