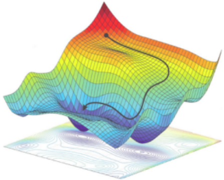
A new multi-objective calibration R package for SWAT and SWAT+ models

International SWAT Conference (Aarhus, Denmark)

June 29th, 2023



Rodrigo Marinao Rivas[1,2], Mauricio Zambrano-Bigiarini[3,2]

[1] MSc(c) in Engineering Sciences, Universidad de La Frontera, Temuco, Chile.
[2] Center for Climate and Resilience Research (CR2), Santiago, Chile.
[3] Department of Civil Engineering, Universidad de La Frontera, Temuco, Chile.

Why do we need multi-objective optimisation?

Limitations of single-objective calibration

- The application of single-objective algorithms leads to equifinality (Beven, 1993), where multiple parameter sets can produce equally good model outputs.
- No single-objective function is able to capture all the interactions between model output variables and its observed counterparts (Yapo et al., 1998; Wagener, 2003).

Advantages of multi-objective calibration

- Multi-objective calibration is able to exploit all of the information about the physical system contained in the observed time series (Yapo et al., 1998) (e.g., Q, SM, ET, GPP, NO_3).
- Using several model outputs reduces parametric and model output uncertainties → more reliable model predictions (Efstratiadis and Koutsoyiannis, 2010).

Why do we need a new MO calibration software?

- Most of the publicly available calibration software still relies on single-objective (SO) optimisation algorithms (SCE_UA, SA, DE, PSO).
- There are several multi-objective optimisation algorithms available, including MOSCEM, NSGA-II, MOPSO, MEAS, SPEA (Efstratiadis and Koutsoyiannis, 2010).
- Publicly available multi-objective optimisation software are not designed to calibrate hydrological models, e.g., `pymoo` (Blank and Deb, 2020), `rmoo` (Benitez and Pinto-Roa, 2022).
- To the best of our knowledge the only model-oriented software publicly available is `caRamel` (Monteil et al., 2020), which is not model-independent.

∴ There is a lack of flexible multi-objective optimisation software that can be easily coupled with a user-defined hydrological model (e.g., SWAT+).

hydroMOPSO - General description

- Is a new R package for multi-objective calibration of environmental/hydrological models, specifically designed to calibrate real-world models.
- Is inspired and closely follows the philosophy of the single objective `hydroPSO` R package (Zambrano-Bigiarini and Rojas, 2013), which has been applied to a wide variety of models.
- Is based on the NMPSO algorithm (Lin et al., 2016, 2015), which combines two search mechanisms (PSO and genetic operators) to maintain the population's diversity and accelerate its convergence towards the Pareto-optimal set.

hydroMOPSO - Main features:

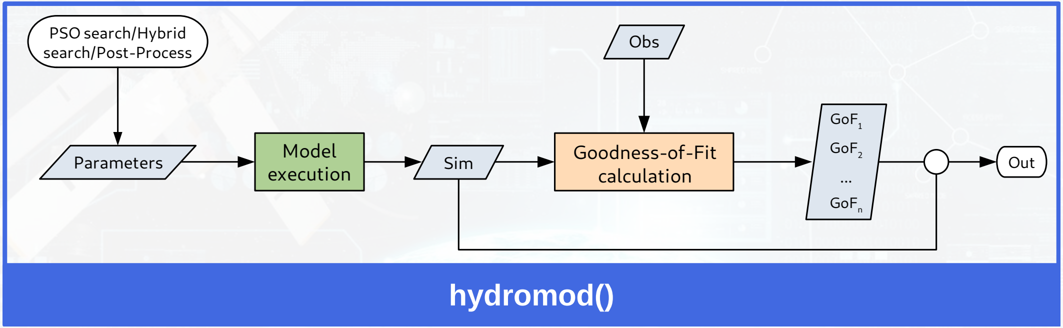
- Model-independent: can be used to calibrate **R-based models** (e.g., TUWmodel, GR-models) and **R-external models** (e.g., SWAT+, SWAT, Raven, WEAP, MODFLOW).
- Platform-independent: It can be run in **GNU/Linux**, **MacOS** and **Windows** machines.
- Computationally efficient: It takes advantage of **multi-core machines** and **network clusters** → important reduction of execution time.
- Highly configurable: It has several **fine-tuning options** and an effective default configuration. (Marinao-Rivas and Zambrano-Bigiarini, 2021).

The package is already available on CRAN (`https://cran.r-project.org/package=hydroMOPSO`)

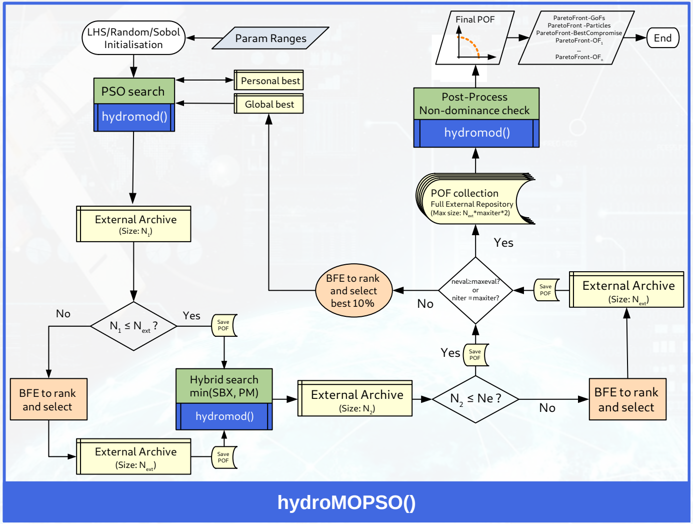
hydroMOPSO: Main functions

- hydromod: Runs the model to be calibrated using its **executable file** (e.g., SWATplus_rev60.5.4.exe) and a **single parameter set**.
  For SWAT and SWAT+, it requires the definition of two additional files: ParameterRanges.txt, and ParameterFiles.txt,
- hydroMOPSO: Runs the multi-objective calibration of the user-defined model (e.g., SWAT+)
- ReadResults: Reads all the output files created by hydroMOPSO (e.g., POF, GoFs, Best Compromise Solution)
- PlotResults: Plots the results of the multi-objective calibration (POF, dotty plots, observations1 vs simulations1, etc).

hydromod function - flowchart



hydroMOPSO function - flowchart



Addional files required for SWAT/SWAT+:

To make parameter changes in SWAT/SWT+, the user needs to prepare two files:

- ParamRanges.txt: Indicates the **physical ranges** used to calibrate each parameter.
- ParamFiles.txt: Indicates the **name of the input files that stores the parameters** being calibrated and the type of change (abs, rel, add).

ParamFiles.txt

ParameterNmbr	ParameterName	Filename	Row.Number	Col.Start	Col.End	DecimalPlaces	TypeChange	RefValue	MinValue	MaxValue
1	par_1	file_1	x_1	y_1	z_1	dec_1	typ_1	ref_1	min_1	max_1
2	par_2	file_2	x_2	y_2	z_2	dec_2	typ_2	ref_2	min_2	max_2
3	par_3	file_3	x_3	y_3	z_3	dec_3	typ_3	ref_3	min_3	max_3
4	par_4	file_4	x_4	y_4	z_4	dec_4	typ_4	ref_4	min_4	max_4
.	.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.
n	par_n	file_m	x_n	y_n	z_n	dec_n	typ_n	ref_n	min_n	max_n

ParamRanges.txt

ParameterNmbr	ParameterName	MinValue	MaxValue
1	par_1	minval_1	maxval_1
2	par_2	minval_2	maxval_2
3	par_3	minval_3	maxval_3
4	par_4	minval_4	maxval_4
.	.	.	.
.	.	.	.
.	.	.	.
n	par_n	minval_n	maxval_n

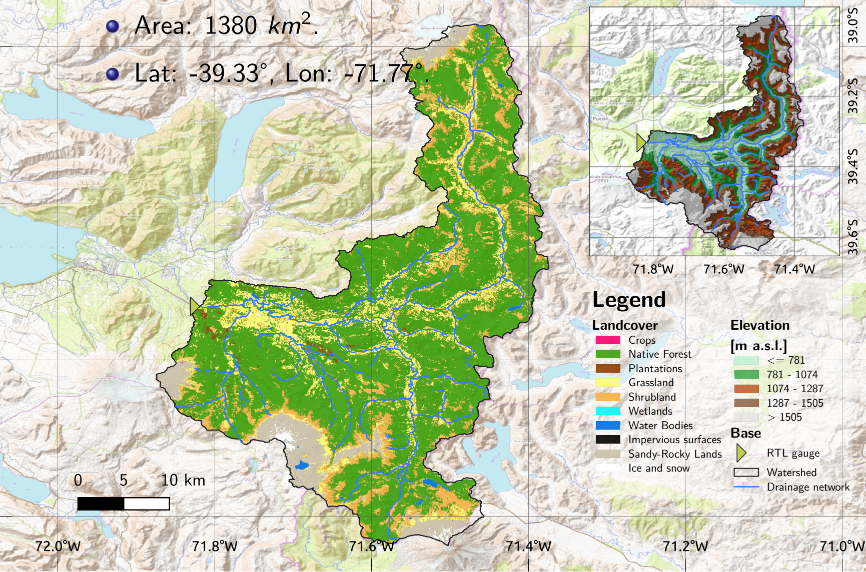
Wrapper function to run SWAT/SWAT+:

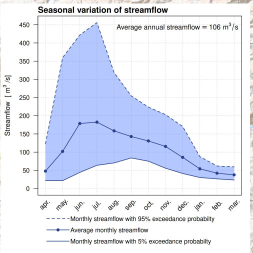
A minimal example of the wrapper function to run SWAT/SWAT+:

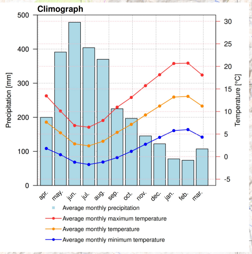
```
Wrapper4SWATplus <- function(param.values, obs, ...){
  # Runing SWAT+
  sim <- hydromod(param.values = param.values,
                              exe.fname="./SWATplus_rev60.5.4.sh", ...)

  # Getting simulated variables
  sim.var1 <- sim[[1]] # simulated variable 1
  sim.var2 <- sim[[2]] # simulated variable 2

  # Getting observations (from user-defined input files)
  obs.var1 <- obs[[1]] # observed variable 1
  obs.var1 <- obs[[2]] # observed variable 2

  # Calculating 2 goodness-of-fit measures:
  gof1 <- KGE(sim = sim.var1, obs = obs.var1) # GoF for variable 1
  gof2 <- NSE(sim = sim.var2, obs = obs.var2) # GoF for variable 2

  # Outputs to be returned to hydroMOPSO
  out[[1]]<- list(gofs = c(gof1, gof2),
                          sims = list(sim.var1, sim.var2))
  return(out)
}
```

Trancura antes de Llafenco

- Andean sub-basin with a pluvio-nival regime.
- Area: 1380 km^2.
- Lat: -39.33°, Lon: -71.77°.

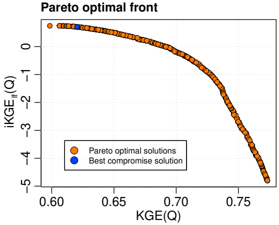


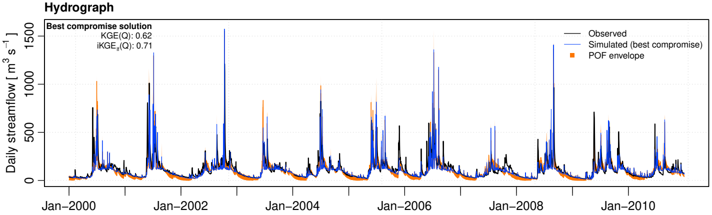




Example 1: Two different objective functions (OF)

- **OF 1**: Daily high-medium flows using $KGE(Q)$.
- **OF 2**: Daily low flows using $KGE_{lf}(Q)$, a specific metric proposed by Garcia et al. (2017) .

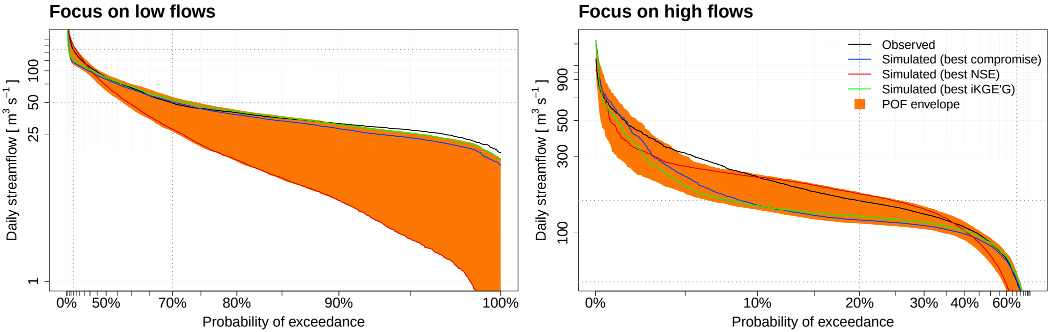




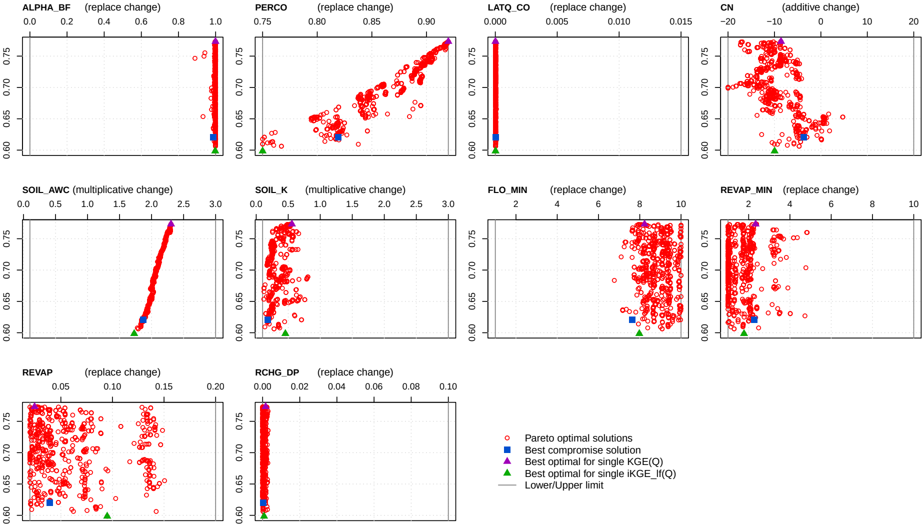
Legend in graph:

- **Observed**: observed daily discharges.
- **Simulated (best compromise)**: discharges obtained in SWAT+ with a single point of the POF, whcih balances the two OF.
- **POF envelope**: Uncertainty bands encompassing all simulations derived from the POF.

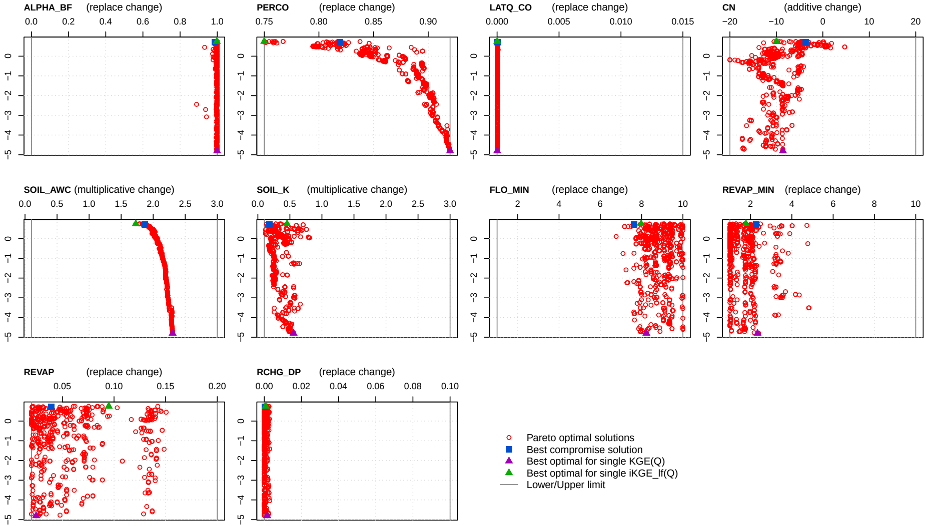
Example 1: Flow duration curves



Example 1: Dottyplots for $KGE(Q)$

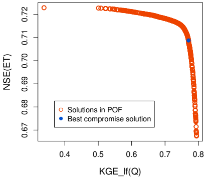


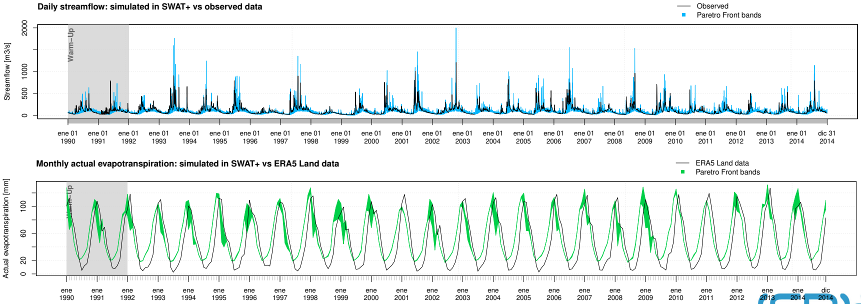
Example 1: Dottyplots for $KGE_{lf}(Q)$



Example 2: Multi-variable calibration

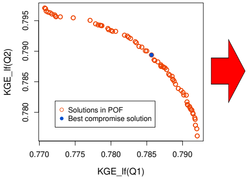
- **OF 1**: Daily low flows using $KGE_{lf}(Q)$.
- **OF 2**: Monthly actual evapotranspiration using Nash-Sutcliffe efficiency (NSE).

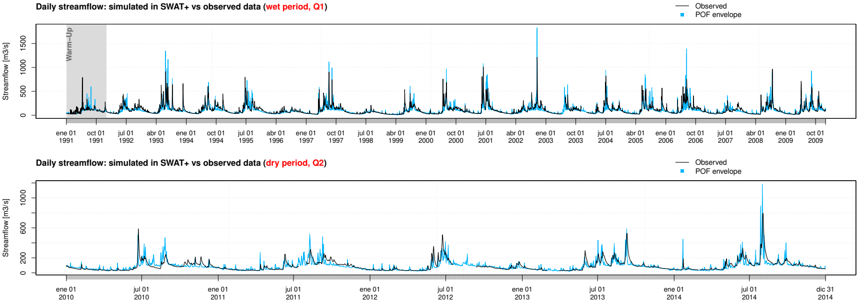




Example 3: Multi-period calibration

- **OF 1**: Daily low flows using $KGE_{lf}(Q)$ for a wet period (1992-2009).
- **OF 2**: Daily low flows using $KGE_{lf}(Q)$ for a dry period (2010-2014).





Conclusions

- hydroMOPSO is a new and flexible R package designed for reproducible multi-objective optimisation of any real-world environmental/hydrological model.
- hydroMOPSO can be easily coupled with any environmental/hydrological model.
- Three case studies with SWAT+ demonstrated its versatility to take advantaje of different types of information contained in the input data.
- Can be easily run in parallel (without modifying the SWAT source code) → important time saving !.
- The package's documentation and a series of tutorials are avilable at https://cran.r-project.org/package=hydroMOPSO.
- We invite to the SWAT and SWAT+ community to explore the potential of hydroMOPSO for analysing the **parametric and predictive uncertainty** of complext MOO problems.

< mauricio.zambrano [at] ufrontera.cl >

References I

Benitez, F., Pinto-Roa, D.P., 2022. rmoo: Multi-Objective Optimization in R. URL: https://CRAN.R-project.org/package=rmoo/. r package version 0.2.2.

Beven, K., 1993. Prophecy, reality and uncertainty in distributed hydrological modelling. Advances in Water Resources 16, 41–51. doi:10.1016/0309-1708(93)90028-E.

Blank, J., Deb, K., 2020. Pymoo: Multi-objective optimization in python. IEEE Access 8, 89497–89509. doi:10.1109/ACCESS.2020.2990567.

Deb, K., Thiele, L., Laumanns, M., Zitzler, E., 2005. Scalable Test Problems for Evolutionary Multiobjective Optimization. Springer London, London. pp. 105–145. doi:10.1007/1-84628-137-7_6.

Efstratiadis, A., Koutsoyiannis, D., 2010. One decade of multi-objective calibration approaches in hydrological modelling: a review. https://doi.org/10.1080/02626660903526292 55, 58–78. URL: https://www.tandfonline.com/doi/abs/10.1080/02626660903526292, doi:10.1080/02626660903526292.

Garcia, F., Folton, N., Oudin, L., 2017. Which objective function to calibrate rainfall–runoff models for low-flow index simulations? Hydrological Sciences Journal 62, 1149–1166. doi:10.1080/02626667.2017.1308511.

Kursawe, F., 1991. A variant of evolution strategies for vector optimization. Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics) 496 LNCS, 193–197. doi:10.1007/BFB0029752/COVER.

References II

Lin, Q., Li, J., Du, Z., Chen, J., Ming, Z., 2015. A novel multi-objective particle swarm optimization with multiple search strategies. European Journal of Operational Research 247, 732–744. doi:10.1016/J.EJOR.2015.06.071.

Lin, Q., Liu, S., Zhu, Q., Tang, C., Song, R., Chen, J., Coello, C.A.C., Wong, K.C., Zhang, J., 2016. Particle swarm optimization with a balanceable fitness estimation for many-objective optimization problems. IEEE Transactions on Evolutionary Computation 22, 32–46. doi:10.1109/TEVC.2016.2631279.

Marinao-Rivas, R., Zambrano-Bigiarini, M., 2021. Towards best default configuration settings for nmpso in multi-objective optimization. 2021 IEEE Latin American Conference on Computational Intelligence, LA-CCI 2021 doi:10.1109/LA-CCI48322.2021.9769844.

Monteil, C., Zaoui, F., Moine, N.L., Hendrickx, F., 2020. Multi-objective calibration by combination of stochastic and gradient-like parameter generation rules - the caramel algorithm. Hydrology and Earth System Sciences 24, 3189–3209. doi:10.5194/HESS-24-3189-2020.

Parajka, J., Merz, R., Blöschl, G., 2007. Uncertainty and multiple objective calibration in regional water balance modelling: case study in 320 austrian catchments. Hydrological Processes 21, 435–446. doi:10.1002/HYP.6253.

Perrin, C., Michel, C., Andréassian, V., 2003. Improvement of a parsimonious model for streamflow simulation. Journal of Hydrology 279, 275–289. doi:10.1016/S0022-1694(03)00225-7.

References III

Wagener, T., 2003. Evaluation of catchment models. Hydrological Processes 17, 3375–3378. doi:10.1002/HYP.5158.

Yapo, P.O., Gupta, H.V., Sorooshian, S., 1998. Multi-objective global optimization for hydrologic models. Journal of Hydrology 204, 83–97. doi:10.1016/S0022-1694(97)00107-8.

Zambrano-Bigiarini, M., Rojas, R., 2013. A model-independent particle swarm optimisation software for model calibration. Environmental Modelling & Software 43, 5–25. URL: https://doi.org/10.1016/j.envsoft.2013.01.004, doi:10.1016/j.envsoft.2013.01.004.

Zitzler, E., Thiele, L., 1999. Multiobjective evolutionary algorithms: A comparative case study and the strength pareto approach. IEEE Transactions on Evolutionary Computation 3, 257–271. doi:10.1109/4235.797969.

hydroMOPSO performance evaluation

Benchmark functions

- Three well-known DTLZ problems: DTLZ1, DTLZ2 and DTLZ3 (Deb et al., 2005), each one with three objectives.
- Kursawe function: with two objectives (Kursawe, 1991).

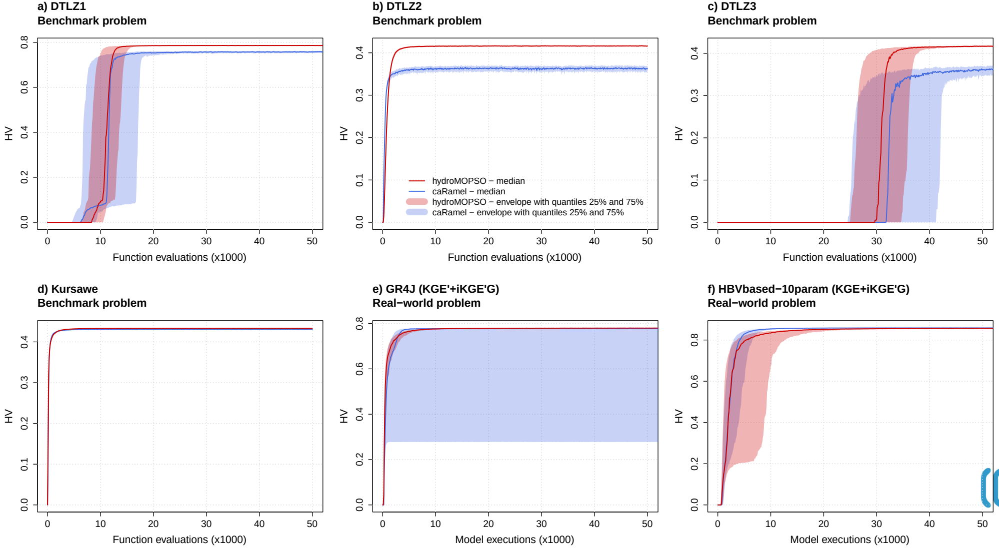
Calibration problems (study zone required)

- GR4J calibration: MOO calibration of `GR4J` (Perrin et al., 2003) hydrological model, with two objectives.
- TUWmodel calibration: MOO calibration of HBV-based `TUWmodel` (Parajka et al., 2007), with two objectives.

Basic details:

- Identify the Pareto Optimal Front (**POF**)
- Use the hypervolume (HV) (Zitzler and Thiele, 1999) to assess the **accuracy** and **diversity** of the POF.
- Use the generational distance (GD) (Zitzler and Thiele, 1999) to assess the **diversity** of the POF.
- Evaluate the number of model runs required to achieve the POF $\rightarrow$ **efficiency**.

Performance evaluation



Performance evaluation