

QUICS: Quantifying Uncertainty in Integrated Catchment Studies

D1.4 Tools for SWAT model uncertainty

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Acronyms and Abbreviations

MPI	Message Passing Interface	
QUICS	Quantifying Uncertainty in Integrated Catchment Studies	
SPOTPY	SPOTting model parameters using a ready-made PYthon package	
SWAT	Soil Water Assessment Tool	

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Executive Summary

This report describes the new SPOTPY package. SPOTPY is an open source project that contains a number of functionalities relevant for model parametrization, calibration and validation as well as sensitivity and uncertainty analysis. The tool allows fitting models with a number of different algorithms and a range of likelihood as well as objective functions. Apart from simulating discharge, SPOTPY also can make use of addition hydrological signatures. It further has a number of built-in parameter distribution functions. SPOTPY is platform and model independent and can therefore be applied to almost any kind of (environmental) model. Due to its MPI support, it can make use of fast parallel computing. In the frame of the QUICS project, SPOTPY has primarily been applied in combination with the Soil Water Assessment Tool (SWAT) to case studies in Luxembourg and Germany.

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1 Background

As part of the deliverables in the QUICS project, the project partner from Justus Liebig University Giessen (JLU) developed a software package to estimate the uncertainty of various components of the SWAT model. In addition, the tool is able to run sensitivity analyses as well as calibration routines.

Instead of hard coding a software package into the SWAT code, JLU decided to set up an independent framework that can be used outside of any model code to ensure flexibility and code sharing. The resulting SPOTPY package developed is a Python tool that enables the use of computational optimization techniques for calibration, uncertainty and sensitivity analysis techniques of almost every (environmental-) model.

As SPOTPY is an ongoing, open source project, documentation, recommendations for installation and use as well as code development is organized via GitHub. Hence, we primarily refer the reader to a number of websites where the latest code development stages are featured. In the following, we shortly summarize the main features of the tool, its components and the ongoing work related to the QUICS project where SPOTPY is used.

2 Features of SPOTPY

Complex formal Bayesian, informal Bayesian and non-Bayesian algorithms bring complex tasks to link them with a given model. SPOTPY makes this task as easy as possible. Some features you can use with the SPOTPY package are:

- Fitting models to evaluation data with different algorithms. Available algorithms are Monte Carlo (MC), Markov-Chain Monte-Carlo (MCMC), Maximum Likelihood Estimation (MLE), Latin-Hypercube Sampling (LHS), Simulated Annealing (SA), Shuffled Complex Evolution Algorithm (SCE-UA), DiffeRential Evolution Adaptive Metropolis Algorithm (Dream), RObust Parameter Estimation (ROPE), Artificial Bee Colony (ABC), Fitness Scaled Chaotic Artificial Bee Colony (FSCABC) and Fourier Amplitude Sensitivity Test (FAST).
- Wide range of objective functions, likelihood functions and hydrological signatures to validate the sampled results. Available objective functions are: Bias, Nash-Sutcliff (NSE), log Nash-Sutcliff (logNSE), Logarithmic probability (logp), Correlation Coefficient (r), Coefficient of Determination (r²), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), Relative Root Mean Squared Error (RRMSE), Agreement Index (AI), Covariance, Decomposed MSE (dMSE) and Kling-Gupta Efficiency (KGE).
- Wide range of **likelihood functions** to validate the sampled results: logLikelihood, Gaussian Likelihood to account for Measurement Errors, Gaussian Likelihood to

account for Heteroscedasticity, Likelihood to account for Autocorrelation, Generalized Likelihood Function, Lapacian Likelihood, Skewed Student Likelihood assuming homoscedasticity, Skewed Student Likelihood assuming heteroscedasticity, Skewed Student Likelihood assuming heteroscedasticity and Autocorrelation, Noisy ABC Gaussian Likelihood, ABC Boxcar Likelihood, Limits Of Acceptability, Inverse Error Variance, Shaping Factor, Nash Sutcliffe Efficiency Shaping Factor, Exponential Transform Shaping Factor, Sum of Absolute Error Residuals.

- Wide range of hydrological signature functions to validate the sampled results: Slope, Flooding/Drought events, Flood/Drought frequency, Flood/Drought duration, Flood/Drought, variance, Mean flow, Median flow, Skewness, compare percentiles of discharge
- Prebuild parameter distribution functions: Uniform, Normal, lognormal, Chisquare, Exponential, Gamma, Wald, Weilbull
- SPOTPY is platform independent and due to MPI support it can make use of fast parallel computing

3 Documentation and Installation

The SPOTPY package has been published in the open source journal PLoS One (Houska et al., 2015). It is hosted on GitHub, a public available, internet-based service to host software code that is under ongoing development. SPOTPY <u>https://github.com/thouska/spotpy</u>. Access to SPOTPY is granted through the Python package website at <u>https://pypi.org/project/spotpy/</u>. Documentation is available at <u>http://fb09-pasig.umwelt.uni-giessen.de/spotpy</u>.

Installing SPOTPY is easy. Just use: pip install spotpy. Or, after downloading the source code and making sure python is in your path: python setup.py install. Further information can be found on the aformentioned websites and GitHub. For getting started, have a look at https://github.com/thouska/spotpy/tree/master/spotpy/examples and https://github.com/thouska/spotpy/tree/master/spotpy/examples and https://github.com/thouska/spotpy/tree/master/spotpy/examples and https://github.com/thouska/spotpy/tree/master/spotpy/examples and https://github.com/thouska/spotpy/tree/master/spotpy/examples and https://github.com/thouska/spotpy/Tutorial/2-Rosenbrock/

4 Referenced work of SPOTPY

SPOTPY is on the verge to become a widely used tool. Despite that published work using SPOTPY is currently more or less restricted to our working group (e.g. Houska et al., 2017b, 2017a; Kellner et al., 2017; Maier et al., 2017), we are aware of many further researchers interested in using SPOTPY in their work to be published. For updated information, see the following Google Scholar website: <u>https://scholar.google.de/scholar?cites=</u> 17155001516727704728&as_sdt=2005&sciodt=0,5&hl=de

5 Ongoing work in QUICS

The SPOTPY package has been used to calibrate and assess the uncertainty of the SWAT model applied to the Luxembourg catchment of the Wiltz river as part of the QUICS project (Camargos et al., 2018). In this application, the effects of input data uncertainty resulting from the digital elevation model (DEM), soil information and land use/land cover on water flux components are investigated.

In an ongoing follow up simulation study, we make use of a number of various SPOTPY features to compare the effect of different parameter optimization strategies and objective functions on model performance and uncertainty. For this, we set up SWAT for the Schwingbach catchment (Lauer et al., 2013; Orlowski et al., 2014, 2016), a catchment-scale field laboratory in the vicinity of Giessen, Germany. The Schwingbach catchment is characterized by a mix of forest, cropland and grassland in a low mountainous cultivated landscape, typical for many in mid-Europe. Due to several projects in the past, a large number of data is available for the catchment, making it a suitable test case for the SWAT – SPOTPY experiment.

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