1 Design and Implementation of a General Software Library for using NSGA-II

2 with SWAT for Multi-Objective Model Calibration

- 3
- 4 Mehmet B. Ercan
- 5 Water Resources Engineer, Arcadis, Indianapolis, IN
- 6 Previously
- 7 Research Assistant, Department of Civil and Environmental Engineering, University of South
- 8 Carolina, Columbia, SC, USA.
- 9
- 10 Jonathan L. Goodall, Associate Professor, Department of Civil and Environmental Engineering,
- 11 University of Virginia, Charlottesville, VA, USA.
- 12 And
- 13 Adjunct Professor, Department of Civil and Environmental Engineering, University of South
- 14 Carolina, Columbia, SC, USA.
- 15
- 16 Corresponding Author: Jonathan L. Goodall, goodall@virginia.edu, PO Box 400742,
- 17 Charlottesville, Virginia 22904, (434) 243-5019
- 18
- 19
- 20

21 Highlights

- We present an open-source software library for calibration of SWAT models
- The library implements the NSGA-II multi-objective genetic algorithm
- The library is used to calibrate a SWAT model of the Upper Neuse Watershed, NC
- The library can be used within SWAT-CUP for data visualization

26 Abstract

27	Calibrating watershed-scale hydrologic models remains a critical but challenging step in the
28	modeling process. The Soil and Water Assessment Tool (SWAT) is one example of a widely
29	used watershed-scale hydrologic model that requires calibration. The calibration algorithms
30	currently available to SWAT modelers through freely available and open source software,
31	however, are limited and do not include many multi-objective genetic algorithms (MOGAs). The
32	Non-Dominated Sorting Genetic Algorithm II (NSGA-II) has been shown to be an effective and
33	efficient MOGA calibration algorithm for a wide variety of applications including for SWAT
34	model calibration. Therefore, the objective of this study was to create an open source software
35	library for multi-objective calibration of SWAT models using NSGA-II. The design and
36	implementation of the library are presented, followed by a demonstration of the library through a
37	test case for the Upper Neuse Watershed in North Carolina, USA using six objective functions in
38	the model calibration.
39	
40	Keywords: Multi-Objective Calibration; Genetic Algorithms; Watershed Modeling; SWAT;
41	NSGA-II
42	
43	Software availability: The software is available free and open source on Github:

44 <u>https://github.com/mehmetbercan/NSGA-II_Python_for_SWAT_model</u>.

45 **1. Introduction**

46 The Soil and Water Assessment Tool (SWAT) is a widely used watershed model with 47 numerous applications around the world for water quantity and quality simulations (e.g., Cools et 48 al., 2011; Gassman et al., 2007; Liu et al., 2013). It can be classified as a semi-distributed 49 conceptual watershed model that is capable of running on a daily or sub-daily time step over long 50 time periods. SWAT is able to simulate large watersheds with different management scenarios 51 where the impact on water supply and non-point source pollution can be assessed (Arnold et al., 52 1998). For SWAT and other similar watershed models, there are often hundreds of modeling 53 units in a model for a single watershed and dozens of model parameters used to describe 54 properties within the model. One of the modeler's most important and difficult tasks is to 55 calibrate these model parameters so that the model's output matches observational data such as 56 streamflow observations collected within the watershed. 57 Many algorithms and tools have been developed and applied for calibrating SWAT models. SWAT-CUP represents one widely used tool in the SWAT community for applying calibration 58 59 algorithms to SWAT models. SWAT-CUP includes different calibration algorithms, as well as 60 routines for sensitivity analysis, validation, and uncertainty analysis of SWAT models 61 (Abbaspour et al., 2007). There are other procedures and algorithms developed in the scientific 62 community for calibration that have not yet been included in SWAT-CUP, but that would benefit 63 SWAT modelers. For example, SWAT-CUP does not include multi-objective calibration 64 approaches, nor does it include genetic algorithm calibration approaches (Abbaspour, 2013).

65 SWAT modelers, however, could benefit from these calibration procedures, especially for large

66 watersheds where multiple streamflow observations are available (Arnold et al., 1999; Bekele

and Nicklow, 2007; Kirsch et al., 2002; Santhi et al., 2001; White and Chaubey, 2005).

68	Genetic Algorithms (GAs) offer the ability to effectively solve highly non-linear
69	optimization problems and have been used for a variety of water resources challenges. Being an
70	evolutionary algorithm, GAs use principles of genetics and natural selection for optimization
71	(Haupt and Haupt, 2004). They are well suited for hydrologic models, which usually cannot be
72	adequately calibrated by gradient-based calibration algorithms. The objective function for each
73	solution in a GA can be evaluated in parallel computations, which provide computational
74	advantages (Zhang et al., 2013, 2012a). The heuristic search procedure of GAs, relying on
75	stochastic search rules, increases the probability of finding non-unique solutions. Previous
76	studies have shown that these properties of GAs allow them to converge to optimal solutions for
77	a variety of problems (Winston et al., 2003) including the challenge of calibrating watershed-
78	scale hydrologic models (Arabi et al., 2006; Nicklow and Muleta, 2001).
79	Multi-objective calibration algorithms have been shown to increase model performance for
80	hydrologic models of large watersheds (Andersen et al., 2001). In contrast to the more widely
81	used single-objective calibration algorithms available to SWAT users now in tools like SWAT-
82	CUP, multiple-objective calibration better constrains the calibration process, resulting in a
83	calibrated model that better matches the physical conditions within the watershed (Niraula et al.,
84	2012). Watershed models may use multiple objective functions in a calibration procedure to
85	account for potentially competing objectives, even for cases when only a single streamflow
86	station is available for calibration (e.g., two objectives might be to match peak flows and
87	maintain annual water volume balance between the model and observations). They can also
88	allow modelers to take advantage of multiple observational time series (e.g., streamflow at two
89	or more locations in the watershed or streamflow and soil moisture observations at two or more
90	locations in the watershed).

91 There is a class of calibration routines that combine the benefits of both multi-objective and 92 genetic algorithm calibration approaches: the so called multi-objective genetic algorithms 93 (MOGAs). One of the most popular MOGAs is the Non-Dominated Sorting Genetic Algorithm 94 II (NSGA-II). NSGA-II is a fast and efficient population-based optimization technique that can 95 be parallelized. The algorithm has been shown to be superior to other MOGAs (Deb et al., 2002; Zitzler et al., 2000) and it has the potential to reduce calibration time through efficiency in the 96 97 algorithm itself and its ability to easily be mapped to parallel computing resources (Deb et al., 98 2002; Tang et al., 2006; Zitzler et al., 2000). The algorithm has significant improvements over 99 the original NSGA (Srinivas and Deb, 1994) including adding elitism, reducing the complexity 100 of the non-dominated sorting procedure, and replacing a sharing function with a crowded-101 comparison function. The NSGA-II algorithm has also been shown to be an effective tool for 102 watershed model calibration (Bekele and Nicklow, 2007; Confesor and Whittaker, 2007; Hejazi 103 et al., 2008; Kayastha et al., 2011; Khu and Madsen, 2005; Lu et al., 2014; Shafii and Smedt, 104 2009; Zhang et al., 2012b).

105 While NSGA-II has been used for calibrating watershed models, there is no known software 106 implementation of NSGA-II for calibrating SWAT models that is freely available to the 107 community. One study did report creating a multi-objective calibration tool for SWAT models 108 using NSGA-II (Bekele and Nicklow, 2007). However, based on personal communication with 109 the authors, the source code for this implementation is no longer available. The goal of this work, 110 therefore, is to create an open source and freely-available NSGA-II software library for SWAT 111 model calibration. We designed the tool to be library that can be used alone or incorporated into 112 other software tools. We specifically designed the software to be easily integrated into SWAT-113 CUP given the popularity of this tool with the SWAT community. We chose to implement the

library using the Python programming language because of its growing popularity in thescientific computing community.

116 In the remaining sections of this paper, we first describe the algorithm for using NSGA-II

117 with SWAT for model calibration, then describe the design and implementation of the NSGA-

- 118 II/SWAT library including compatibility with SWAT-CUP, and finally present a test case
- application of the library for calibrating a SWAT model of the Upper Neuse watershed in North

120 Carolina. As part of this test case application, we compare the results of the NSGA-II calibration

121 to results from a single-objective calibration to show the improvement obtained by using the

122 multi-objective NSGA-II algorithm. We have provided the source code for the NSGA-II/SWAT

123 library as an open source and freely available repository through GitHub:

124 <u>https://github.com/mehmetbercan/NSGA-II_Python_for_SWAT_model</u>.

125

126 **2. The NSGA-II Algorithm and its Integration with SWAT**

127 2.1 Overall Process Flow

In this section we explain the NSGA-II algorithm and how we integrated SWAT calibration into the algorithm when designing the NSGA-II/SWAT library. Our approach follows the example of past work using NSGA-II for SWAT calibration (e.g., Bekele and Nicklow, 2007; Kayastha et al., 2011; Lu et al., 2014), but extends this past work to create a general and reusable software tool. For further detail on the NSGA-II algorithm itself, readers are referred to Deb et al. (2002). For convenience, we provide a mapping between NSGA-II and SWAT calibration terminology in Table 1.

NSGA-II Term	Description for Application to SWAT Calibration
Solution	An individual of a population that includes a SWAT calibration parameter set and NSGA-II processing data for the parameter set
Gene	The SWAT calibration parameter set that exists in a solution
Chromosome	An individual of a gene that represents a single SWAT calibration parameter
Binary Value	Binary representation of chromosome in a user defined number of bits

137

A standard NSGA-II process typically begins with a random parent population P_i (Deb et al., 2002). However, here we start with a Latin Hypercube Sampling (LHS) (See Step 1 in Figure 1) because better results have been achieved for SWAT models using this approach (Bekele and Nicklow, 2007). The LHS operator is executed first to create an initial combined population (R_{i=0}). We use the subscription "i" to represent a generation (iteration) number. The initial combined population must be at least twice as large the population size for reasons that will become clearer in forthcoming steps of the algorithm.





148

146

149 Each solution in the initial combined population $(R_{i=0})$ is considered to be a SWAT 150 calibration parameter set. The SWAT input files are edited to include this solution, the model is 151 executed, and the objective functions are evaluated using observational data and the SWAT 152 model output data (See Steps 2-4 in Figure 1). These model runs can be performed in parallel for 153 each solution within the population. Once this process has been completed, the solutions within the population (R_i) are ranked using the results of the objective function evaluation process and a 154 155 non-dominating sorting approach (See Step 5 in Figure 1). Details of this non-dominating sorting 156 approach are provided in Section 2.2.1.

157 The best performing solutions from R_i as determined by the non-dominating sorting 158 approach are used to form the parent population (P_i). The number of solutions in the parent 159 population is determined by the user defined population size. In the case of ties where multiple 160 solutions exist with the exact same ranking at the cut-off point for creating P_i, a crowded distance 161 sorting operator is used to break the tie (See Step 6 in Figure 1). This operator is explained in 162 Section 2.2.2. In short, the solutions with the larger crowding distance value, which acts as a 163 dummy fitness in the sorting operator, are chosen to fill the remaining spots in P_i . Using the 164 parent population, a new child population ($C_{i+=1}$) is determined through a selection, crossover 165 and mutation operator (See Step 7 in Figure 1), which is explained in Section 2.2.3. This entire 166 procedure is repeated until the termination criteria are met.

167

168 2.2 NSGA-II Operators

We provide in this section details for the specific operators used in the NSGA-II algorithmthat are mentioned in the previous section.

171 2.2.1 Non-Dominated Sorting

The non-dominated sorting operator is a process of ranking solutions that exist in the combined population (R_i) (Deb et al., 2002; Srinivas and Deb, 1994). In this operator, the objective functions are evaluated for given solutions to determine domination. Domination is established when the objective function evaluations of a solution outperform all other solutions with the same rank. The process terminates when all members of the combined population (R_i) have been assigned a rank.

178 2.2.2 Crowding Distance Sorting

Crowding distance sorting is used to break ties for solutions with the same rank at the cut off point for being included in the parent population (P_i) (Deb et al., 2002). First, the solutions in that rank are sorted based on the value of an objective function. Then, a solution is selected and the distance between that solution and each of the adjacent solutions is calculated. These distances are normalized by dividing by the distance between the maximum and minimum value of the objective function for all solutions. Finally, crowding distance for the solution is calculated as the sum of the normalized distance for the adjacent solutions.

This process is repeated for all objective functions and the final crowding distance value for a solution is the summation of crowding distances calculated for all objective functions. It is then repeated for all solutions within the parent population. One exception is the maximum and minimum solutions in a rank. Because they do not have adjacent solutions on both sides, they are typically assigned an arbitrarily large distance value. When breaking ties, the preference is to select solutions with a large crowding distance value, which means the solution has more distant neighbors and selecting this solution helps to protect the diversity of the population.

193 2.2.3 Selection, Crossover, and Mutation

194 Selection is a process that chooses solutions from a parent population (P_{i+1}) that go into a 195 child population (C_{i+=1}) based on non-dominated and crowding distance sorting values. It starts 196 by randomly selecting two solutions from P_{i+1} . Then, it selects the solution that has the smaller 197 rank. If two solutions have the same rank from non-dominated sorting, it selects the solution that 198 has the greater crowding distance value. This process continues until all spots in C_{i+1} are filled. 199 After completion of the selection process, the crossover process begins. There are two 200 techniques for the crossover operation: regular crossover and uniform crossover. In regular 201 crossover, each pair of adjacent solutions from C_{i+1} are progressively chosen. Then, a random 202 number is generated and compared to a crossover probability. If the random number is smaller 203 than the crossover probability, crossover occurs where chromosomes between the two solutions 204 flip for a randomly generated number of chromosomes.

205 Uniform crossover is different from regular crossover in that the crossover happens at a 206 binary level instead of at a solution level. The uniform crossover goes through all binary values 207 (0 or 1) (of chromosomes) for every evenly indexed C_{i+1} solution. Uniform crossover happens if 208 a random number is smaller than the crossover probability. In this case, the binary value is replaced with the binary value from the corresponding next (oddly indexed) $C_{i+=1}$ solution. 209 210 Finally, mutation happens through C_{i+1} solutions at a binary level similar to uniform 211 crossover. The mutation process simply flips the binary value (from 1 to 0, or vice versa) if a 212 random number is smaller than the mutation probability.

213

214 **3. Design and Implementation of the NSGA-II/SWAT Calibration Library**

215 The NSGA-II/SWAT calibration library implements the algorithm summarized in the prior 216 section where NSGA-II was used for SWAT model calibration. The library was designed as a 217 general, object-oriented application programming interface (API) library and implemented in the 218 Python programing language because it is open source and widely used in scientific 219 communities. The library was tested against an established NSGA-II implementation written in 220 the C programing language (Deb et al., 2002) to ensure that it is able to reproduce the same 221 results. The library was designed to be compatible with SWAT-CUP (Abbaspour, 2013; 222 Abbaspour et al., 2007), which is a widely used tool for calibration of SWAT models, as 223 described later in this section. 224 3.1 Class Diagram 225 The NSGA-II/SWAT calibration library includes one main class called nsga2 and two utility 226 classes for lower level NSGA-II and SWAT operations (Figure 2). The nsga2 class is heart of

227 NSGA-II algorithm and includes operations such as creating child and parent populations.

228 During the initialization phase, the nsga2 class stores inputs such as population size, genes, 229 chromosomes, and objective functions provided by the user. The nsga2 class offers two options 230 for creating an initial combined population ($R_{i=0}$): (i) using the Latin Hypercube Sampling (LHS) 231 method and (ii) reading the last generation from a previous calibration. The LHS method is 232 included because, as stated earlier, it creates a better initial solutions for SWAT models (Bekele 233 and Nicklow, 2007). On the other hand, reading the last generation from the previous calibration 234 allows users to continue from previous but ultimately unsuccessful calibrations (for example, if a 235 calibration fails to complete midway through the calibration process).



236

237 Figure 2: The NSGA-II/SWAT calibration library design.

238

239 The utility classes supplement the calibration process by providing lower-level functionality

240 specific to the NSGA-II algorithm and for communication with SWAT. The nsga2 class uses

241 nsga2 utilities to complete methods such as Crossover() or Unicross() required when creating

child populations based on the user's choice along with *Selection()* and *Mutation()* methods.

Similarly, creating a parent population requires methods like *NonDominatedSorting()* and *CrowdingDistance()*, which are also implemented in the nsga2 utility class. SWAT utilities are
used for objective function calculations using methods like *Nash-Sutcliffe()* and *PercentBias()*.
By separating the SWAT-specific functionality into its own class, our design goal was to provide
a pattern that could be repeated when expanding the library to support other hydrologic models.

248

249 3.2 Application for SWAT Calibration

250 To obtain SWAT model parameter values (genes), the binary values of chromosomes from 251 solutions of C_i go through a decoding process (*decode()*). Then, the SWAT model input files are 252 ready to be edited and executed to calculate objective functions using the SWAT utility class 253 method, *CalculateObjectiveFunctions()*. This method first creates a *model.in* file containing genes. Then, it executes a batch file called *nsga2_mid.cmd* that creates the *model.out* file by 254 255 using the *model.in* file and the SWAT model engine. Finally, the *CalculateObjectiveFunctions()* 256 method uses the model.out file and calculates the objective function values by using other SWAT 257 utility functions such as *Nash-Sutcliffe()*. This process continues until each solution of C_i is 258 assigned objective function values.

259 The *nsga2_mid.cmd* file is a batch file that executes a series of commands for SWAT
260 calibration. It uses SWAT executable (*swat.exe*) and two Python scripts

261 (SWAT_ParameterEdit.py and Extract_rch.py) in order to create the model.out file. It first runs

262 SWAT_ParameterEdit.py to change SWAT model parameters based on information in model.in

263 file. Then, it executes *swat.exe* to execute the SWAT model using the parameter values included

- in the *model.in* file. Finally, it runs *Extract_rch.py* to extract SWAT model outputs into
- 265 *model.out* file. The *nsga2_mid.cmd* file gives flexibility to edit the SWAT side of the calibration

procedure. To illustrate, inorganic nitrogen flux is the sum of nitrite (NO2) and nitrate (NO3),
which SWAT prints separately. Thus, an intermediate script could be inserted in *nsga2_mid.cmd*file to sum these two nitrogen flux terms in *model.out* file for use in later calibration steps.

269

270 3.3 Compatibility with SWAT-CUP

271 The NSGA-II/SWAT calibration library was designed so that it can be integrated into 272 SWAT-CUP. First, we included a *Backup* folder as a reference to default parameter values as 273 done in SWAT-CUP. The input/output file and folder names were created following the SWAT-274 CUP pattern. For example, the SWATtxtInOut folder contains the NSGA-II input and output 275 folders named NSGA2.IN and NSGA2.OUT. We further followed SWAT-CUP patterns by 276 creating files with the same structure. The calibration parameter definition file (*nsga2_par.def*) is 277 named with the calibration method and followed with _par.def. The structure of nsga2_par.def 278 file is defined as "X_parameter.ext min max" where the X defines the parameter editing method, 279 the *parameter* defines the SWAT parameter, the *ext* defines the extension of SWAT files, and the 280 *min* and *max* define the minimum and the maximum parameter limits. 281 In addition to the structure and naming conventions, internal parts of the NSGA-II/SWAT 282 library also follow the SWAT-CUP pattern. The SWAT_ParameterEdit.py script is equivalent to

283 SWAT_edit.exe of SWAT-CUP. Both scripts edit SWAT files based on the model.in file created

by the calibration algorithm. Also, the *Extract_rch.py* script is equivalent to SWAT-CUP's

285 extracting script, *Extract_rch.exe*, which extracts SWAT outputs into *model.out* file in the

- equivalent format. The batch file (*nsga2_mid.cmd*) mentioned in a prior section (which also
- 287 exists in SWAT-CUP) can be used to run extensive SWAT-CUP editing and extracting

288 executable files, rather than our parameter editing and extracting scripts. All these properties 289 were intentionally included to ease the integration of our software library into SWAT-CUP. Instructions for running NSGA-II through SWAT-CUP are provided on the software's 290 291 GitHub site. The basic procedure is to override the GLUE method and replace it with the NSGA-292 II method. This is not a long-term solution, but rather a proof-of-concept solution that does not 293 require altering the SWAT-CUP code-base. Later work can easily extend this proof-of-concept 294 by allowing SWAT-CUP to include both the NSGA-II method along side the existing methods. 295 The output generated by NSGA-II conforms to a structure expected by SWAT-CUP, allowing 296 users to visualize the calibration results like any other calibration routine currently within 297 SWAT-CUP (Figure 3).

298



299

300 Figure 3: Example visualizations of NSGA-II calibration results through SWAT-CUP Graphical

301 User Interface (GUI).

302

303	This proof-of-concept could be formalized by modifying SWAT-CUP so that new
304	calibration routines can be plugged-in without the need to recompile the core SWAT-CUP code.
305	This plug-in architecture would allow third-party developers to create calibration routines to be
306	added to the software system more easily. Given the existing capabilities of SWAT-CUP for data
307	management and visualization, a plug-in architecture could be very powerful for incorporating
308	the latest calibration methods and providing them to SWAT modelers in a convenient and
309	familiar. It would save the work of recoding the visualization capabilities already available
310	through SWAT-CUP and provide a consistent UI experience for end users. Libraries like the
311	NSGA-II/SWAT library created in this study could be easily structured to follow a standard
312	required for integrated into SWAT-CUP as a plug-in.

313

314 **4. Test Case**

315 The NSGA-II/SWAT library is demonstrated for a test case application using a SWAT 316 model of the Upper Neuse Watershed in North Carolina. The library is used to calibrate this 317 model to match streamflow records at three observation sites using two fitness criteria. In the 318 following subsections, we first briefly discuss how we created a SWAT model for Upper Neuse 319 watershed, second show how we used our NSGA II library to calibrate the SWAT model, and 320 third present the results of the calibration. The primary goal of this section is to illustrate how the 321 library would work for end users interested in applying the library to calibrate a SWAT model. A 322 secondary goal is to explore how the model calibration resulting from using the NSGA-II/SWAT 323 library compares to the widely used single-objective calibration strategy.

324 4.1 Study Area and Model Preparation

The Upper Neuse watershed (Figure 4) is a level-8 watershed that includes the Flat, Little, and Eno River watersheds defined by the United States Geological Survey (USGS) codes 02085500, 0208521324 and 02085070, respectively. The study area has a mild climate and gently rolling topography. The soil type of the watershed is dominated by silty clay and loam, and the land cover of the watershed is dominated by forest and cultivated crops.

330



332 Figure 4: Study area: the Upper Neuse Watershed in North Carolina, USA.

333

331

Terrain and land cover data were obtained from the United States Geological Survey
(USGS) National Elevation Dataset (NED) and the 2006 version of the National Land Cover
Database (NLCD). Soil data were obtained from the State Soil Geographic (STATSGO) dataset
provided by the United States Department of Agriculture (USDA). Air temperature, wind speed,
and humidity were obtained from the National Climatic Data Center (NCDC). Precipitation data
was obtained from National Weather Service (NWS) for Nexrad-derived rainfall estimates and

from NCDC for gauge observed rainfall estimates. These two precipitation estimates were
combined using the approach described by Ercan and Goodall (2012) to create a composite
rainfall dataset for the watershed area. Lastly, daily average streamflow data from the USGS
National Water Information System (NWIS) were downloaded using the Consortium of
Universities for the Advancement of Hydrologic Science, Inc. (CUAHSI) Hydrologic
Information System (HIS) (Tarboton et al., 2009).

346 We divided the watershed into subbasins based on the USGS streamflow station locations 347 and homogeneity of land characteristics. We used threshold values of 10% for soil, slope, and 348 land cover to reduce variability within the subbasins. The result was a total of 837 Hydrologic 349 Response Units (HRUs) for the 93 subbasins in the watershed, which is within the 350 HRU/subbasin ratio range recommended in SWAT documentation. The commonly used settings 351 were chosen to configure the model that include the Natural Resources Conservation Service 352 (NRCS) Curve Number (CN) surface runoff method, the Penman-Monteith potential 353 evapotranspiration method, and the variable storage channel routing method. The ArcSWAT 354 software program was used for much of the data preprocessing steps required to create the 355 model.

356 4.2 Model Calibration

Streamflow observations at the Flat, Little, and Eno watershed outlets were used in the
calibration. For each outlet, the Nash-Sutcliffe (E) and Percent Bias (PB) statistics were used as
measures of the goodness of fit. Therefore, the calibration used six objective functions (3 sites x
2 fitness). We ran Generalized Likelihood Uncertainty Estimation (GLUE) (Beven and Binley,
1992) available in SWAT-CUP to find the sensitivity of the flow parameters on streamflow

362 prediction. The six most sensitive parameters were chosen for model calibration with the

acceptable ranges and replacement operations shown in Table 2.

364

365 Table 2: Model parameters, their calibrated values, acceptable ranges, and replacement

366 operations

Parameter	Value	Range	Operation	
Alpha_Bf	0.99	0.01-1.00	Replaced	
Cn2	0.07	±0.25	% Relative	
Ch_K2	30.59	0.01-150.00	Replaced	
Canmx	9.53	0.01-10.00	Replaced	
Esco	0.94	0.01-1.00	Replaced	
Sol_Aw c	-0.06	±0.25	% Relative	

367

We used the following settings for calibrating the Upper Neuse watershed model with NSGA-II. The LHS size was set to 1000 and crossover probability was set to 0.5 using uniform crossover. The mutation probability and the seed for the random number generation were set to 0.5. Population size and generation number were set to 80. Since our parameters do not have a wide range, we used 8 bits for binary crossover and mutations. Figure 5 provides the pseudo code for the NSGA-II calibration to briefly illustrate how it

374 was used in the case study. The first line initializes the nsga2 class, which reads in the inputs

375 from the SWATtxtInOut folder such as PopulationSize, GenerationNumber and Observations.

376 Then the initial combined population is created followed by the generation loop. In the

377 generation loop, the code first creates the parent population from the combined population.

378 Second, it creates the child population using the parent population. Then the child population is

379 used to run the SWAT model and the model's output is used to evaluate the objective functions.

380 Finally, the parent and child populations are used to create the new combined population for the

381 next generation. As seen in Figure 4, this library can easily be adapted to other watershed

382 simulation models by modifying the initialization method of the nsga2 class and the

383 *CalculateObjectiveFunctions()* process that exists in the SWAT utility class.

384

```
NSGAII = Nsga2.nsga2(SWATtxtInOut)
R<sub>i=0</sub> = NSGAII.CreateInitialPopulation()
R<sub>i=0</sub> = SWATUtilities.CalculateObjectiveFunctions(R<sub>i=0</sub>)
FOR i = 0 to NSGAII.GenerationNumber
P<sub>i</sub> = NSGAII.CreateParentPopulation(R<sub>i</sub>)
C<sub>i</sub> = NSGAII.CreateChildPopulation(P<sub>i</sub>)
C<sub>i</sub> = SWATUtilities.CalculateObjectiveFunctions(C<sub>i</sub>)
R<sub>i+1</sub> = P<sub>i</sub> + C<sub>i</sub>
END FOR
```

Figure 5: The pseudo code for applying the NSGAII/SWAT library for calibrating the test caseSWAT model.

388

385

```
389 4.3 Calibration Results
```

390 The Pareto front solutions for the case study example are shown in Figure 5. There are six 391 objective functions for 80 solutions. The objective functions are percent bias (PB) and one minus 392 Nash-Sutcliffe (1-E) for the stations at the outlets of the Flat, Little and Eno watersheds. The 393 number of solutions is defined by the population size because all solutions in the final generation 394 are in the first front (ranking). A zero value on the figure indicates an optimal result while higher 395 values indicate worse model efficiency. The figure shows the range in performance of the three 396 watersheds in terms of PB and 1-E values. The values ranged between 0.00 and 0.39 for PB and 397 between 0.23 and 0.88 for E across the three observation sites.

398 We highlighted the tradeoffs in Figure 6. The thick black line shows the solution selected 399 with an equal weight for all objective functions, defining the best possible solutions considering 400 all three objective functions equally. When we put a large weight on the 1-E objectives, we get 401 the thick dashed grey line that slightly improves on 1-E values, but is worse for PB values. In the 402 last case with the thick grey line, we selected the lowest 1-E value (best E) for the Eno watershed 403 ignoring all other criteria. In this case, which represents calibration using a single objective 404 function, the E value improves for the Eno watershed as expected, but the other objective 405 functions, including PB for the Eno watershed, are worse compared to the equally weighted 406 multi-objective case.



408 Figure 6: Six dimensional NSGA-II Pareto front.

409

410

411

412

413

414

415

416

417

418

419

420

421

422

423

424

a 0.40 ь 0.40 Flat Average 0.35 0.35 Little 0.30 0.30 Eno 0.25 0.25 ₩0.20 **원** 0.20 0.15 0.15 0.10 0.10 0.05 0.05 Ø 0.00 0.00 0.9 0.9 0.2 0.3 0.40.5 0.6 0.7 0.80.2 0.3 0.4 0.5 0.6 0.7 0.81-E 1-E

For visualization of tradeoffs, we displayed the same Pareto front in Figure 6 using two

dimensional graphs. Because of difficulties of showing all six objective functions on a single

graph, we averaged fitness values over the Flat, Little and Eno watershed outlets in Figure 7b.

Significant tradeoffs are illustrated between E and PB objective functions for the three outlets

(Figure 7a) as was also shown by Bekele and Nicklow (2007). This illustrates the utility of a

multi-objective calibration of SWAT models by attempting to balance multiple competing

The equally weighted objective functions are also highlighted in Figure 7. Better PB and 1-E

values exist on Figure 7a. However, these values are connected to other objective functions that

responses between the three watersheds, but a more significant relationship between the Flat and

are much worse (e.g. the grey dashed and solid lines in Figure 6). Figure 7a indicates similar

Little watersheds. This is expected as all the watersheds are in the same region and the Eno

watershed is partially urbanized whereas the Flat and Little are not.

objectives when selecting optimal parameter sets.

425 Figure 7: (a) NSGA-II Pareto front with (b) results averaged across the three watersheds.

426

427	Table 2 shows the parameter set values for the chosen solution (objective functions are
428	equally weighted). We ran the SWAT model based on this solution and prepared the model
429	statistics against observations (Table 3). The daily and monthly statistics showed good
430	agreement between simulated and observed streamflows for each site. PB values are considered
431	to be "very good" for both the calibration and validation periods except for the Flat River
432	watershed during the validation period, which is considered to be "good" (Moriasi et al., 2007).
433	Monthly E values, on the other hand, were considered to be "good" for the calibration period and
434	"very good" for the validation period (Moriasi et al., 2007). Lastly, daily statistics showed very
435	good accuracy compared to previous SWAT studies (Gassman et al., 2007), indicating the
436	strength of the calibration method.

437

Table 3: Results of the fitness values during the calibration and evaluation time periods for theFlat, Little, and Eno watersheds.

2005-2008 ^a				2009-2012 ^b						
Watershed	E	E ^c	R^2	R ^{2c}	PB	E	E ^c	R^2	R ^{2c}	PB
Flat	0.74	0.73	0.75	0.74	0.04	0.62	0.8	0.62	0.82	-0.13
Little	0.75	0.72	0.76	0.73	0.08	0.61	0.8	0.61	0.81	-0.09
Eno	0.65	0.65	0.73	0.7	0.02	0.59	0.77	0.64	0.82	-0.11

a Calibration period

b Evalutation period

c Daily predicted and observed values aggregated to monthly

440

441 The solution with the equally weighted objective functions within the Pareto front is also
442 illustrated in Figure 8. Similar to Table 3, the Little and Flat watersheds are slightly better at

443 matching high flows (better E value) compared to the Eno watershed. All of the watersheds tend

to underestimate streamflow for the calibration period and overestimate streamflow for the
evaluation period. In general, the monthly accumulated streamflow values support the accuracy
of the model as both the calibration and evaluation periods generally fit well to observed
streamflow for all three sites.

448



450 Figure 8: Comparison of monthly simulated and observed streamflow.

451

Finally, we examined the solution with the best E value for Eno watershed (highlighted with the thick grey line in Figure 6). This case is equivalent to single-objective calibration as we selected a solution with regard to only one objective function and ignored all other objective functions. When using this parameter set, the E value for the Eno watershed improved by 0.06 and 0.02 for calibration and validation periods, respectively, compared to the results when using 457 the parameter set from the equally weighted multi-objective solution. However, all other 458 statistics for the calibration and validation period for the three watersheds decreased when using 459 the parameter set from the single objective optimization. The magnitude of decrease in fitness 460 values was often similar to the gain in E for the Eno watershed. However, the PB values deteriorated into an unacceptable model range (Moriasi et al., 2007) where PB values ranged 461 462 from 0.31 to 0.38 and 0.15 to 0.16 for calibration and validation periods, respectively, for the 463 three watersheds. This provides evidence to support the claim that multi-objective calibration 464 increases confidence in the model's predictive capabilities compared to using a single-objective 465 calibration routine.

466

467 **5. Conclusion**

468 The powerful Non-Dominated Sorting Genetic Algorithm II (NSGA-II) is a popular multi-469 objective optimization genetic algorithm (MOGA) that has been shown to be effective for 470 calibrating watershed models including SWAT. Because there is no known open source and 471 freely-available software for linking NSGA-II with SWAT for model calibration, we created an 472 open source NSGA-II/SWAT library using the Python programming language. We designed the 473 library to be used either as a standalone tool for those experienced with Python, or as a library 474 that can be incorporated by developers into existing third-party Graphical User Interface (GUI) 475 software tools. In particular, a design goal was to allow for easy integration of the NSGA-476 II/SWAT library with the widely used SWAT-CUP program that includes many algorithms for 477 calibrating SWAT models, but currently does not include the NSGA-II algorithm. 478 We demonstrated how the NSGA-II/SWAT library could be used through a test case 479 application for calibrating a SWAT model of the Upper Neuse Watershed in North Carolina. The

480 test case considered six objective functions: maximize Nash-Sutcliffe (E) and minimize Percent 481 Bias (PB) as the fitness coefficients for three streamflow stations located in the watershed. Six 482 model parameters were used in the calibration based on results obtained from using the GLUE 483 sensitivity analysis procedure. Results from applying the NSGA-II/SWAT library to this test 484 case showed large tradeoffs between fitness coefficients in the study watershed as illustrated in 485 the Pareto front. In general, the Eno watershed had lower E values compare to the other two 486 watersheds, and we suspect that this is due to urbanization within the Eno watershed that is not 487 present in the other two watersheds.

488 We chose the optimal parameter set from the Pareto front when weighting all objective 489 functions equally and used this parameter set to create the calibrated SWAT model. Results from 490 running the calibrated SWAT model during the time period used to calibrate the model were E 491 values ranging between 0.65 and 0.75 and PB values ranging between 0.02 and 0.08 for the three 492 streamflow stations used for calibration. The results from running the model during an 493 independent evaluation period not used for calibrating the model showed E values ranging 494 between 0.59 and 0.62 and PB values ranging between -0.13 and -0.09. All results for the 495 calibration and evaluation periods were considered to have satisfactory performance (Moriasi et 496 al., 2007) and improved results obtained from executing the SWAT model using an optimal 497 parameter set generated when considering only one of the six objective functions. Therefore, the 498 model calibration resulting from using the NSGA-II/SWAT library resulted in a well-calibrated 499 SWAT model that increases our confidence in the model's predictive capabilities compared to 500 the more common approach of using a single objective function.

The NSGA-II/SWAT tool was written to allow for easy expansion to include other
 calibration algorithms and interfaces for other hydrological and environmental models that might

503	require multi-objective calibration. By having the source code in a public repository, the code
504	can be easily obtained and extended by others to include these enhancements. Furthermore, the
505	software was designed in a way so that it can be easily incorporated into front-end Graphical
506	User Interface (GUI) software tools, most notably SWAT-CUP. A proof-of-concept for
507	incorporating the library into SWAT-CUP was shown that leverages the existing data
508	visualization capabilities already available through SWAT-CUP and provides a new and
509	powerful calibration routine to SWAT-CUP users. Future work could formalize the proof-of-
510	concept by extending SWAT-CUP to accept 3 rd party calibration routines as plug-ins. This would
511	encourage adoption of new calibration algorithms more quickly and easily into the community-
512	supported and widely used SWAT-CUP.
513	
514	Acknowledgments
515	This work was funded in part by the US National Science Foundation under the award
516	CBET:0846244 and by the National Oceanic and Atmospheric Administration (NOAA) Global
517	Interoperability Program and the NOAA Environmental Software Infrastructure and
518	Interoperability Group.
519	
520	References
521 522	Abbaspour, K.C., 2013. SWAT-CUP 2012: SWAT calibration and uncertainty programs-A user manual, in: Swiss Federal Institute of Aquatic Science and Technology, Eawag.
523 524 525	Abbaspour, K.C., Vejdani, M., Haghighat, S., 2007. SWAT-CUP calibration and uncertainty programs for SWAT, in: MODSIM 2007 International Congress on Modelling and Simulation, Modelling and Simulation Society of Australia and New Zealand.
526 527	Andersen, J., Refsgaard, J.C., Jensen, K.H., 2001. Distributed hydrological modelling of the Senegal River Basinmodel construction and validation. J. Hydrol. 247. 200–214.
528 529	Arabi, M., Govindaraju, R.S., Hantush, M.M., 2006. Cost-effective allocation of watershed management practices using a genetic algorithm. Water Resour. Res. 42.

- Arnold, J.G., Srinivasan, R., Muttiah, R.S., Williams, J.R., 1998. Large area hydrologic
 modeling and assessment part I: Model development1. JAWRA J. Am. Water Resour.
 Assoc. 34, 73–89.
- Arnold, J.G., Srinivasan, R., Ramanarayanan, T.S., DiLuzio, M., 1999. Water resources of the
 Texas gulf basin. Water Sci. Technol. 39, 121–133.
- Bekele, E.G., Nicklow, J.W., 2007. Multi-objective automatic calibration of SWAT using
 NSGA-II. J. Hydrol. 341, 165–176.
- Beven, K., Binley, A., 1992. The future of distributed models: model calibration and uncertainty
 prediction. Hydrol. Process. 6, 279–298.
- Confesor, R.B., Whittaker, G.W., 2007. Automatic Calibration of Hydrologic Models With
 Multi-Objective Evolutionary Algorithm and Pareto Optimization. JAWRA J. Am. Water
 Resour. Assoc. 43, 981–989.
- 542 Cools, J., Broekx, S., Vandenberghe, V., Sels, H., Meynaerts, E., Vercaemst, P., Seuntjens, P.,
 543 Van Hulle, S., Wustenberghs, H., Bauwens, W., others, 2011. Coupling a hydrological
 544 water quality model and an economic optimization model to set up a cost-effective emission
 545 reduction scenario for nitrogen. Environ. Model. Softw. 26, 44–51.
- 546 Deb, K., Pratap, A., Agarwal, S., Meyarivan, T., 2002. A fast and elitist multiobjective genetic
 547 algorithm: NSGA-II. Evol. Comput. IEEE Trans. 6, 182–197.
- 548 Ercan, M.B., Goodall, J.L., 2012. Estimating Watershed-Scale Precipitation by Combining
 549 Gauge and Radar Derived Observations. J. Hydrol. Eng. 120807052807006.
 550 doi:10.1061/(ASCE)HE.1943-5584.0000687
- Gassman, P.W., Reyes, M.R., Green, C.H., Arnold, J.G., 2007. The soil and water assessment
 tool: Historical development, applications, and future research directions. Trans. ASABE
 50, 1211–1250.
- Haupt, R.L., Haupt, S.E., 2004. Practical genetic algorithms. John Wiley & Sons.
- Hejazi, M., Cai, X., Borah, D., 2008. Calibrating a watershed simulation model involving human
 interference: an application of multi-objective genetic algorithms. J. Hydroinformatics 10,
 97–111.
- Kayastha, N., Shenlang, L., Betrie, G.D., Zakayo, Z., Griensven, A. van, Solomatine, D.P., 2011.
 Dynamic linking of the watershed model SWAT to the multi-objective optimization tool
 NSGAX, in: 8th IWA Symposium on Systems Analysis and Integrated Assessment, June
 20-22, San Sebastian, Spain.
- Khu, S.T., Madsen, H., 2005. Multiobjective calibration with Pareto preference ordering: An
 application to rainfall-runoff model calibration. Water Resour. Res. 41.
- Kirsch, K., Kirsch, A., Arnold, J.G., 2002. Predicting sediment and phosphorus loads in the Rock
 River basin using SWAT. Forest 971, 10.
- Liu, R., Zhang, P., Wang, X., Chen, Y., Shen, Z., 2013. Assessment of effects of best
 management practices on agricultural non-point source pollution in Xiangxi River
 watershed. Agric. Water Manag. 117, 9–18.
- Lu, S., Kayastha, N., Thodsen, H., van Griensven, A., Andersen, H.E., 2014. Multiobjective
 calibration for comparing channel sediment routing models in the soil and water assessment

- 571 tool. J. Environ. Qual. 43, 110–20. doi:10.2134/jeq2011.0364
- Moriasi, D.N., Arnold, J.G., Van Liew, M.W., Bingner, R.L., Harmel, R.D., Veith, T.L., 2007.
 Model evaluation guidelines for systematic quantification of accuracy in watershed
 simulations. Trans. ASABE 50, 885–900.
- Nicklow, J.W., Muleta, M.K., 2001. Watershed management technique to control sediment yield
 in agriculturally dominated areas. Water Int. 26, 435–443.
- 577 Niraula, R., Norman, L.M., Meixner, T., Callegary, J.B., 2012. Multi-gauge Calibration for
 578 modeling the Semi-Arid Santa Cruz Watershed in Arizona-Mexico Border Area Using
 579 SWAT. Air, Soil Water Res.
- Santhi, C., Arnold, J.G., Williams, J.R., Hauck, L.M., Dugas, W.A., 2001. Application of a
 watershed model to evaluate management effects on point and nonpoint source pollution.
 Trans. ASAE 44, 1559–1570.
- Shafii, M., Smedt, F. De, 2009. Multi-objective calibration of a distributed hydrological model
 (WetSpa) using a genetic algorithm. Hydrol. Earth Syst. Sci. 13, 2137–2149.
- 585 Srinivas, N., Deb, K., 1994. Muiltiobjective optimization using nondominated sorting in genetic
 586 algorithms. Evol. Comput. 2, 221–248.
- Tang, Y., Reed, P., Wagener, T., others, 2006. How effective and efficient are multiobjective
 evolutionary algorithms at hydrologic model calibration? Hydrol. Earth Syst. Sci. Discuss.
 10, 289–307.
- Tarboton, D.G., Horsburgh, J.S., Maidment, D.R., Whiteaker, T., Zaslavsky, I., Piasecki, M.,
 Goodall, J., Valentine, D., Whitenack, T., 2009. Development of a community hydrologic
 information system, in: 18th World IMACS Congress and MODSIM09 International
 Congress on Modelling and Simulation, Ed. RS Anderssen, RD Braddock and LTH
 Newham, Modelling and Simulation Society of Australia and New Zealand and
- 595 International Association for Mathematics and Comput. pp. 988–994.
- White, K.L., Chaubey, I., 2005. Sensitivity analysis, calibration, and validations for a multisite
 and multivariable swat model1. JAWRA J. Am. Water Resour. Assoc. 41, 1077–1089.
- Winston, W.L., Venkataramanan, M., Goldberg, J.B., 2003. Introduction to mathematical
 programming. Thomson/Brooks/Cole.
- Zhang, X., Beeson, P., Link, R., Manowitz, D., Izaurralde, R.C., Sadeghi, A., Thomson, A.M.,
 Sahajpal, R., Srinivasan, R., Arnold, J.G., 2013. Efficient multi-objective calibration of a
 computationally intensive hydrologic model with parallel computing software in Python.
 Environ. Model. Softw. 46, 208–218. doi:10.1016/j.envsoft.2013.03.013
- 604 Zhang, X., Izaurralde, R.C., Zong, Z., Zhao, K., Thomson, A.M., 2012a. EVALUATING THE
 605 EFFICIENCY OF A MULTI-CORE AWARE MULTI-OBJECTIVE OPTIMIZATION
 606 TOOL FOR CALIBRATING THE SWAT MODEL. Trans. ASABE, 55(5)1723-1731.
- 607 Zhang, X., Izaurralde, R.C., Zong, Z., Zhao, K., Thomson, A.M., 2012b. EVALUATING THE
 608 EFFICIENCY OF A MULTI-CORE AWARE MULTI-OBJECTIVE OPTIMIZATION
 609 TOOL FOR CALIBRATING THE SWAT MODEL. Trans. ASABE, 55(5)1723-1731.
- 610 Zitzler, E., Deb, K., Thiele, L., 2000. Comparison of multiobjective evolutionary algorithms:
 611 Empirical results. Evol. Comput. 8, 173–195.