Environmental Modelling and Software 158 (2022) 105561

Contents lists available at ScienceDirect

Environmental Modelling and Software

journal homepage: www.elsevier.com/locate/envsoft

Cyber-enabled autocalibration of hydrologic models to support Open Science

Adnan Rajib [a,1], I Luk Kim [b,1], Mehmet B. Ercan [c], Venkatesh Merwade [d,*], Lan Zhao [b], Carol Song [b], Kuan-Hung Lin [d]

[a] Hydrology & Hydroinformatics Innovation Lab, Department of Environmental Engineering, Texas A&M University, Kingsville, Texas, USA
[b] Rosen Center for Advanced Computing, Purdue University, West Lafayette, Indiana, USA
[c] Department of Engineering Systems and Environment, University of Virginia, Charlottesville, Virginia, USA
[d] Lyles School of Civil Engineering, Purdue University, West Lafayette, Indiana, USA

A R T I C L E I N F O

Keywords:
Calibration
High performance computing
Hydrology
SWAT model
SWATShare

A B S T R A C T

Automatic calibration (autocalibration) of models is a standard practice in hydrologic sciences. However, hydrologic modelers, while performing autocalibrations, spend considerable amount of time in data pre-processing, coding, and running simulations rather than focusing on science questions. Such inefficiency, as this paper outlines, stems from: (i) platform dependence, (ii) limited computational resource, (iii) limited programming literacy, (iv) limited model structure and source code literacy, and (v) lack of data-model interoperability in the so-called autocalibration process. By expanding and enhancing an existing web-based modeling platform SWATShare, developed for the Soil and Water Assessment Tool (SWAT) hydrologic model, this paper demonstrates a generalizable pathway to making autocalibration efficient via cyberinfrastructure (CI) solutions. SWATShare is a collaborative platform for sharing and visualization of SWAT models, model results, and metadata online. This paper describes the front and back end architectures of SWATShare for enabling efficient SWAT model autocalibration on the web. In addition, this paper also demonstrates three implementation case studies to validate the autocalibration workflow and results. Results from these implementations show that SWATShare autocalibration can produce streamflow hydrograph and parameters that are comparable with commonly used offline SWATCUP calibration outputs. In some instances, the parameter values from SWATShare calibration are more physically relevant than those from SWATCUP. Although the discussion in this paper is in the context of SWAT and SWATShare, the conceptual and technical design presented here can be used as an Open Science blueprint for similar CI-enabled developments in other hydrologic models, and more importantly, in other domains of Earth system sciences.

Software availability

- **Name**: SWATShare 2.0
- **Type**: Web-based platform
- **Year of first version release**: 2016
- **Year of second version release**: 2022
- **Availability**: Openly available at https://mygeohub.org/groups/water-hub/swatshare
- **Cyberinfrastructure used for deployment**: myGeoHub (https://mygeohub.org) via HUBzero platform, Purdue University
- **Software/web services/programming languages used**: Adobe Flash, PHP, JavaScript, JAVA, REST API, Redhat Linux, MySQL, LAMP (Linux-Apache-MySQL-PHP) software stack, Tomcat web services, python (gdal, fiona), R (dataRetrieval, hydroGOF), Network File System (NSF), Non-Sorting Genetic Algorithm-II
- **High Performance Computing Resources used:** A Purdue campus cluster and the Extreme Science and Engineering Discovery Environment (XSEDE) Comet Cluster
- **Developers**: I Luk Kim, Adnan Rajib, Lan Zhao, Venkatesh Merwade, Carol Song

* Corresponding author.
E-mail address: vmerwade@purdue.edu (V. Merwade).
[1] shared lead authorship.

https://doi.org/10.1016/j.envsoft.2022.105561
Received 12 September 2022; Received in revised form 18 October 2022; Accepted 19 October 2022
Available online 22 October 2022

1.0. Introduction

The predictability of a hydrologic model largely depends on how well its parameters are calibrated. Because numerous manual iterations to search representative parameter values can be time-consuming (Dawdy and O'Donnell, 1965), hydrologic modelers use an automated iterative process using complex algorithms (hereafter, autocalibration) (Duan et al., 2006; Gupta et al., 1999; Samadi et al., 2020; Wu et al., 2021). Over time, this autocalibration has become a standard practice in hydrologic model applications, leading to the widespread development of open-source tools that can link calibration algorithms with respective model source-codes (e.g., Abbaspour, 2015; Wi et al., 2017; Wu and Liu, 2012). These autocalibration tools, when provided with adequate reference datasets, produce hydrologic simulations with reasonably high accuracy. Yet, it will not be an overstatement to refer the term "autocalibration" as a misnomer because many data- and model-integration tasks required to set up and run the contemporary autocalibration tools heavily rely on modelers' manual interventions. As a result, despite the notable recent improvements in calibration algorithms and open-source tools (e.g., Baracchini et al., 2020; Chlumsky et al., 2021; Femeena et al., 2020; Sadler et al., 2019; Wang and Brubaker, 2015; Zhang et al., 2013), hydrologic modelers spend considerable time in data pre-processing, coding, and running simulations rather than focusing on science questions. Therefore, having a guided step-by-step workflow and/or an intuitive graphical user interface do not necessarily lead to an *efficient* autocalibration procedure. Addressing the root cause(s) of inefficiency in hydrologic model autocalibration still remains a challenge. Below we identify five root causes of inefficiency in autocalibration tools and then we compare some of the contemporary hydrologic models according to the efficiency of their respective autocalibration tools (Table 1).

(1) *Platform dependence*: Most of the autocalibration tools recognized across the hydrologic modeling community are developed as offline, desktop-based *black box* software (e.g., SWAT-CUP for the Soil and Water Assessment Tool (SWAT), VIC-ASSIST for the Variable Infiltration Capacity (VIC) model, HSPEXP/HSPEXP+ for the Hydrologic Simulation Program–Fortran (HSPF)) (Abbaspour, 2015; EPA, 2015; Wi et al., 2017). These tools rely on a particular computer operating system (i.e., Windows or Linux), dependencies (e.g., specific program libraries, packages, and their versions), and licensing requirements. Correspondingly, a major issue associated with such platform dependence is maintenance and updating of functions (Yu et al., 2019). Over time, some autocalibration tools (e.g., HSPEXP; EPA, 2015) have become obsolete due to incompatibility with current computer operating systems.

(2) *Limited computing resource*: Commonly used desktop-based autocalibration tools often conduct one calibration job at a time on a single desktop computer. The computing resource in a desktop computer may be adequate to run small-scale calibrations involving small watershed areas and short simulation periods. However, such small-scale calibrations become computationally intensive when the models undergo multi-objective calibrations with spatially distributed data and involves a large parameter set (e.g., Kunnath-Poovakka et al., 2016; Rajib et al., 2018a). Obviously, calibrations involving large watersheds and long simulation periods (e.g., Du et al., 2018), high spatial resolution (e.g., Lin et al., 2018), and complex spatial discretization schemes (e.g., Evenson et al., 2018) demand more computing resources than an average desktop computer alone can provide. In any case, modelers commonly run multiple instances of the same calibration setup as trial runs to gather priori knowledge of sensitive parameters, suitable parameter values, and characteristic model bias (Kuzmin et al., 2008) which make the overall computational footprint and run-time unmanageable. Against these needs, efficiency of commonly used desktop-based autocalibration tools remains limited by the processing power and available storage space in modelers' personal computers. Some of the recent autocalibration tools allow model calibration to be remotely executed in High Performance Computing (HPC) clusters (e.g., LCC-SWAT and gSWAT-BASHYT for the SWAT model (Bacu et al., 2011; Cau et al., 2013; Zamani et al., 2021); the model independent cloud-based Parameter ESTimation (PEST) tool (Fienen et al., 2011)). There are also efforts to speed-up calibration tools using Graphics Processing Units (GPU)-aided parallel computing

Table 1
Comparison of contemporary hydrologic models according to the efficiency of their respective autocalibration tools: × means inefficient and √ means efficient. For a particular tool, × or √ is a relative indicator of its efficiency compared to all other tools/models presented in the table.

Model	Calibration tool	Reference	Platform independence	Access to HPC resources	Reduced need for programming literacy	Reduced need for model structural literacy	Data-model interoperability
GSSHA	PEST	Skahill et al. (2012)	×	×	×	×	×
SWMM	OSTRICH-SWMM#	Behrouz et al. (2020); Macro et al. (2019)	✓	×	×	×	×
SWMM	DREAM-SWMM#	Gao et al. (2020)	✓	×	×	×	×
SWAT	R-SWAT-FME#	Wu and Liu (2012), 2014	✓	×	×	×	×
WRF-Hydro	PyWrfHydroCalib#	NCAR (2019)	✓	×	×	×	×
HSPF	HSPEXP/ HSPEXP+	EPA (2015)	×	×	✓	×	×
VIC¶	VIC-ASSIST*	Wi et al. (2017)	×	×	✓	×	×
SWAT	SWAT-CUP*	Abbaspour (2015)	×	×	✓	×	×
SWAT	SWATShare 1.0	Rajib et al. (2016)	×	✓	✓	×	×
SWAT	LCC-SWAT	Zamani et al. (2021)	×	✓	✓	×	×
SWAT	gSWAT-BASHYT†	Bacu et al. (2011); Cau et al. (2013)	✓	✓	✓	×	×
SWAT	SWATShare 2.0	This paper	✓	✓	✓	✓	✓

#OSTRICH-SWMM, DREAM-SWMM, R-SWAT-FME, and PyWrfHydroCalib are coded in platform independent language. Therefore, these tools have potential to access HPC resources via a web interface, but the existing literature mostly shows desktop-based applications.
¶Recent VIC modeling architectures to support web-based model applications and reproducibility (e.g., Hamman et al., 2018) are not yet fully developed to address autocalibration inefficiencies.
*Some functionalities in VIC-ASSIST and SWAT-CUP are designed to reduce model structural literacy.
†To the best of authors' knowledge, gSWAT-BASHYT is no longer in use.

(Ercan et al., 2014; Freitas et al., 2022; Kan et al., 2019). Yet, it is widely acknowledged that running autocalibration tools using HPC and/or parallel computing also requires a client-server interface and standard web services for job management, resource monitoring, messaging, user verification, data transfer, encrypting, and various notification mechanisms (Hokkanen et al., 2021; Zhu et al., 2016), which may be challenging to sustain unless the tool is part of a large, holistic modeling platform.

(3) *Programming literacy*: Some of the autocalibration tools do not have a graphical user interface. In such cases, running the tool requires substantial literacy on programming languages, syntax, and execution. For example, use of pyWrfHydroCalib for the WRF-Hydro model (Lin et al., 2018; NCAR, 2019), R-SWAT-FME for the SWAT model (e.g., Wu and Liu, 2012, 2014), and OSTRICH for the Storm Water Management Model (SWMM) (Behrouz et al., 2020; Macro et al., 2019) require medium-to high-level skills in python and R codes. Similarly, without knowing how to write in Command-Line Interface, modelers cannot run the PEST tool for the Gridded Surface Subsurface Hydrologic Analysis (GSSHA) model (Skahill et al., 2009, 2012). In short, it is challenging to run some of the existing autocalibration tools without programming skills, which limits their wider acceptability within the hydrologic modeling community.

(4) *Model structural literacy*: Besides the knowledge of hydrologic processes and steps to setup and calibrate a model, it is necessary for a modeler to clearly understand the model's internal structure including the model's geodatabase, source-code, and parameter definitions. Because the existing autocalibration tools are not fully coupled with the model structure, modelers running these tools with limited model structural literacy need to follow a steep learning curve. For example, while using pyWrfHydroCalib and HSPEXP/HSPEXP+, modelers need to manually decide on the spatial scale at which the tool will iterate a parameter (at individual subbasin-scale or entire basin-scale) or the nodes the tool will use as calibration sites (specific subbasin or river IDs) (EPA, 2015; NCAR, 2019; also see the scaling problem discussed by Nijzink et al., 2018; Tsai et al., 2021; Xu et al., 2014; Zhang et al., 2017). Some tools do not offer a function to automatically fit the most optimal parameter combinations back into the model source-code after completing a batch of iterations (e.g., SWAT-CUP and LCC-SWAT; Ozdemir and Leloglu, 2019; Zamani et al., 2021). Nonetheless, the reduced need for model structural literacy is the most desired service that an autocalibration tool can offer to educators who often want to avoid the steep learning curve. The intuitive graphical user interface in tools like SWAT-CUP and VIC-ASSIST is helpful yet inadequately detailed to substantially reduce the need for model structural literacy.

(5) *Data-model interoperability*: Use of multiple sources/types of reference datasets in model calibration requires a meaningful *linking* of the data with the model structure, which should handle the space-time-variable continuum without misleading the parameter search procedure (Dembélé et al., 2020; Gardner et al., 2018; Jadidoleslam et al., 2020). While there are advances in developing web-based platforms to perform spatio-temporal query across a region and bulk-download available in-situ and remotely sensed Earth observation datasets (Ames et al., 2012; CSISS, 2021; GEE, 2022), none of the existing autocalibration tools can automatically do the data post-processing and model-linking tasks. Therefore, for a large-scale model calibration involving many in-situ measurements (e.g., Abbaspour, 2015; Du et al., 2018; Lin et al., 2018; Rajib et al., 2020a,b) or for a small watershed-scale model calibration involving spatially distributed remotely sensed estimates (Rajib et al., 2018a), it may be easy to download required datasets through web-based platforms, but it remains an excruciatingly labor-intensive task for a modeler to process the data let alone link each of those datasets explicitly with the corresponding calibration sites in the model (e.g., river IDs). Unfortunately, all the existing calibration tools are designed with an assumption that downloading, pre-processing, and making the reference datasets ready for the calibration tool are auxiliary tasks conducted outside the tool's graphical/coding interface.

Scientific cyberinfrastructures (CIs) can address all five root causes of inefficiency in hydrologic model autocalibration through a Findable, Accessible, Interoperable, and Reusable (FAIR) Open Science platform (Bandaragoda et al., 2019; Chen et al., 2020; Govindaraju et al., 2009; Kalyanam et al., 2019, 2020; Maidment, 2008; Voinov and Costanza, 1999; Wilkinson et al., 2016). The *FAIRness* or *Openness* of CIs is due to their building blocks which generally include HPC resources, containerized models, code wrappers, automated workflows, geospatial data analysis, GIS interface, and other tools needed for their interoperability and reproducibility – all through an open, web-based environment (e.g., Essawy et al., 2020; Le et al., 2015; Wu et al., 2013; Zhang et al., 2019). Considering these benefits, many contemporary developments in Earth system sciences reflect a trend of CI solutions. For example, recently developed web-based GIS environments allow running a hydrologic model using HPC resources without having to possess in-depth programming and model development skills (e.g., Liu et al., 2014; Lyu et al., 2019). Similarly, inclusion and removal of modules and codes in a simple drag-and-drop plug-and-play fashion, and thereby enabling the total platform independence of a modeling workflow is becoming increasingly feasible (Dunlap et al., 2013; Lodhi et al., 2020; Peckham and Goodall, 2013; Zeng et al., 2020). What has further widened the scope of hydrologic modeling in a CI platform is the ability to link multiple CIs that allows greater utilization of available data repositories, computational environments, and model Application Programming Interfaces (APIs) (Castronova et al., 2013; Essawy et al., 2018; Choi et al., 2021). Correspondingly, modelers are now developing interoperability engines (Zhang et al., 2021) to resolve the heterogeneity in model and data types (e.g., Chen et al., 2020; Gregersen et al., 2007; Hutton et al., 2020; Peckham et al., 2013).

In line with the above efforts, SWATShare (Rajib et al., 2016; referred here as SWATShare 1.0; https://mygeohub.org/groups/water-hub/swatshare) was developed as a unique SWAT modeling platform leveraging the CI capabilities of myGeoHub (Kalyanam et al., 2019, 2020; https://mygeohub.org). Besides the collaborative platform for model and metadata sharing, and interoperability with other collaborative CIs like HydroShare (Morsy et al., 2017; Tarboton et al., 2018), SWATShare 1.0 offered basic autocalibration functionalities unable to address all five root causes of calibration inefficiency identified earlier (see Table 1). Thus, SWATShare 1.0 has been substantially modified in SWATShare 2.0 by incorporating a new, highly efficient autocalibration tool that addresses all root causes of calibration inefficiency by harnessing CI capabilities.

The overall goal of this paper is to introduce the new SWAT model autocalibration tool in SWATShare 2.0. The specific objectives of this paper are to (i) describe the CI-enabled functionalities in SWATShare that make the new autocalibration tool efficient compared to the previous version (Rajib et al., 2016) as well as a widely used desktop-based tool called SWAT-CUP, (ii) describe the software architecture and simulation workflow of the new tool, and (iii) present three implementation case studies to validate the tool's design concepts as well as physical consistency in terms of hydrologic processes and parameters. Although the discussion presented in this paper is in the context of SWAT and SWATShare, the conceptual and technical design can be used as a blueprint to reproduce similar functionalities in other hydrologic model autocalibration tools.

2.0. SWAT model autocalibration in SWATShare

2.1. The genetic algorithm

The Non-Sorting Genetic Algorithm-II (NSGA-II) (Deb et al., 2002) is incorporated into SWATShare 2.0 for SWAT parameter optimization, replacing the Shuffled Complex Evolution Algorithm (SCE-UA; Duan et al., 1992; Van Griensven and Bauwens, 2003; Van Liew et al., 2005) previously used in SWATShare 1.0 (Rajib et al., 2016). NSGA-II has proven to be effective for multi-objective hydrologic model calibrations and complex watershed management decisions (e.g., Alam et al., 2018; Bekele and Nicklow, 2007; Dai et al., 2017; Ercan et al., 2020; Monteil et al., 2020). Besides genetic algorithms' ability to mimic natural selection in the physical world using the principles of genetics, and thereby produce physically meaningful solutions to parameter optimization problems (Haupt and Haupt, 2003; Gregory, 2009), there are three key factors that make NSGA-II a better fit than SCE-UA for hydrologic modeling CIs. These factors include: (i) ease of use in a web interface due to minimal user inputs, (ii) rapid convergence to optimal solution, and (iii) adaptability with a parallel computing environment (Jeon et al., 2014; Tang et al., 2006; Zhang et al., 2012, 2013). A preliminary version of SWATShare's NSGA-II algorithm written in python programming language has been evaluated by Ercan and Goodall (2016). A brief description of this algorithm is provided below.

The NSGA-II in SWATShare uses Latin Hypercube Sampling (LHS) method to create the initial parent population (Ercan and Goodall, 2016), thus reducing the number of generations significantly to reach the Pareto front much quicker than starting with a random parent population (Ercan and Goodall, 2016; Bekele and Nicklow, 2007). Initial parent population size must be at least twice the population size. Once the initial parent population objective functions are evaluated within the SWAT model, the non-dominated sorting method ranks solutions in groups. The best performing groups are selected to create the mate population which has a predetermined constant size (population size). The crowding distance method is used to select members within the same ranking to reach the exact population size. Then, the mate population goes through crossover and mutation, an essential part of the searching process, to create a child population. Once the objective functions through SWAT runs are calculated for the child population, the mate and child populations are combined to create the next generation parent population. This process repeats for each generation until the termination criteria are met. Ercan and Goodall (2016) explained these procedures in detail. Before incorporating into SWATShare, the original NSGA-II source-code (Ercan and Goodall, 2016) has been modified to facilitate new functionalities and make them compatible with SWATShare's workflow within myGeoHub.

2.2. CI-enabled autocalibration functionalities

Fig. 1 summarizes the new autocalibration functionalities in SWATShare, showing how each of these functionalities is driven by and/or benefited from CI in terms of the efficiency matrix introduced in Table 1 – platform independence, access to HPC, reduced need for programming literacy, reduced need for model structural literacy, and data-model interoperability. Additionally, Fig. 1 categorically explains whether and to what extent SWATShare's current version leverages CI benefits and improves autocalibration efficiency compared to its predecessor (Rajib et al., 2016) and a contemporary, widely used desktop-based tool called SWAT-CUP.

2.2.1. Web-based interface with hierarchical progression

SWATShare is equipped with a web-based interface to facilitate platform independent calibration of SWAT models. Various functions of the interface associated with model calibration are grouped under four

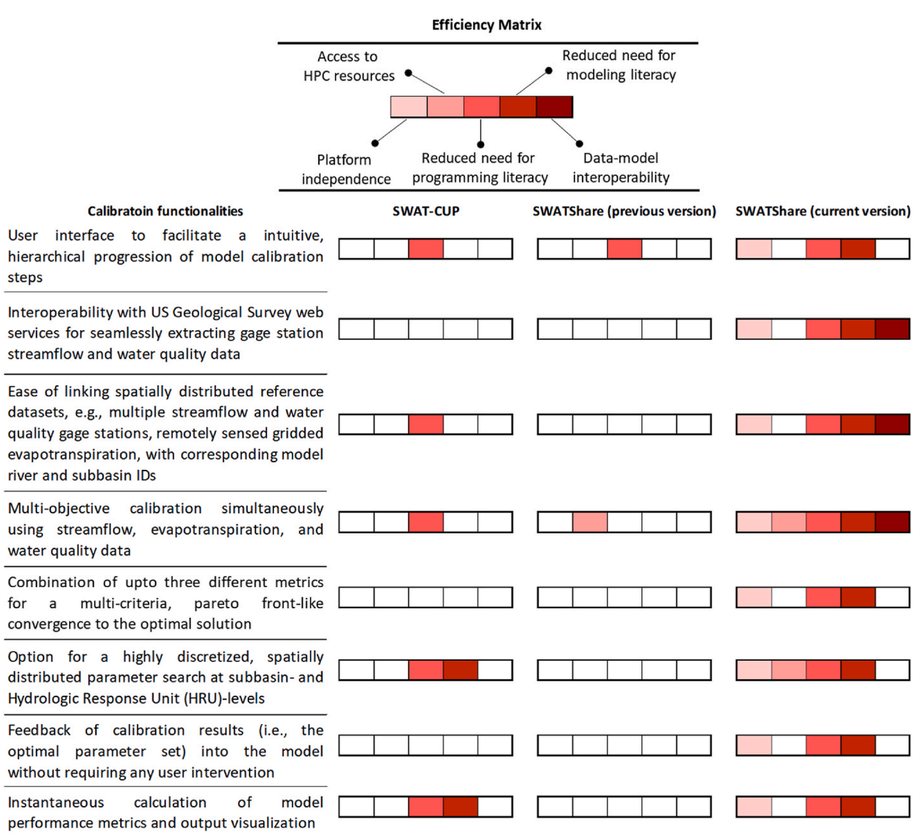


Fig. 1. An efficiency matrix comparing model autocalibration functionalities across the current and previous versions of SWATShare and a widely used desktop-based tool called SWAT-CUP.

graphical control elements (or tabs): *Discovery*, *My Models*, *Simulation*, and *Visualization*. The *Discovery* tab provides an interactive GIS environment to search and download existing models previously uploaded and calibrated in SWATShare, including the models' metadata and geographical extent (Fig. 2a). The *My Models* tab enables users to initiate calibration by first uploading the model input files from their personal computers or seamlessly importing them from an external resource in HydroShare. Upon uploading a new model, SWATShare automatically maps the watershed on the interface and extracts key metadata (e.g., number of subbasins and HRUs in the model, watershed drainage area, simulation time step and duration) following an extended Dublin Core metadata framework in HydroShare (Morsy et al., 2017) (Fig. 2b). Finally, SWATShare creates a dedicated web link for the model which allows modelers to directly view the model metadata and watershed map via a web browser without having to login to SWATShare. The *Simulation* tab allows modelers to set up the calibration protocol, including the number of iterations, objective function, objective variables, reference datasets, and a list of parameters along with their minimum-maximum ranges (Figs. 3–4). In its current design, the *Simulation* interface lets modelers undergo an intuitive, hierarchical progression across different tasks and in a specific sequence – a critical element of interface design (Carrillo et al., 2006) that reduces (or eliminates in some cases) the need for both programming and model structural literacy. SWATShare's previous version had a web-based *Simulation* interface as well, yet the interface only allowed uploading a pre-processed zip file so that modelers had to set up the calibration offline; such an interface reduced programming literacy to some extent (by running the calibration online) but it was implicitly platform dependent with high model structural literacy needs (due to the offline setup in modelers' local computers). The SWAT-CUP interface, on the other hand, is user-friendly but not particularly intuitive as the modelers have to manually intervene at critical steps such as defining specific subbasins or rivers as calibration nodes, linking the corresponding reference data with the model nodes, and feeding the optimized parameters back into the model, among others (further discussed in the following sections).

2.2.2. Interoperability for seamless extraction of reference data from the source

SWATShare offers interoperability so that it can seamlessly and instantaneously extract streamflow and water quality datasets through the United States Geological Survey web services (USGS, 2022). While modelers have the option to upload pre-processed reference datasets in CSV (Comma Separated Values) format (configurable size limit; currently set at 10 GB), they can activate the interoperability functionality by simply uploading a CSV file with a list of USGS gage stations that they want to be included as reference nodes/model constraints (Fig. 3). Such a high level of automation in data-model interoperability correspondingly reduces modelers' need for both modeling and programming literacy. To the best of authors' knowledge, a similar data-model interoperability functionality is not available in any other contemporary hydrologic model autocalibration tools. Currently designed for US watersheds (limited by the availability of a USGS web service), the interoperability function in SWATShare can be easily extended to other regions of the world once suitable web services become available. Nonetheless, the current implementation reveals the potential for future development to make SWATShare interoperable with emerging remote sensing Earth Observation platforms.

2.2.3. Ease of linking spatially distributed reference datasets with the model

SWATShare lets modelers upload multiple reference datasets in CSV file format, with each CSV file representing a specific variable (i.e.,

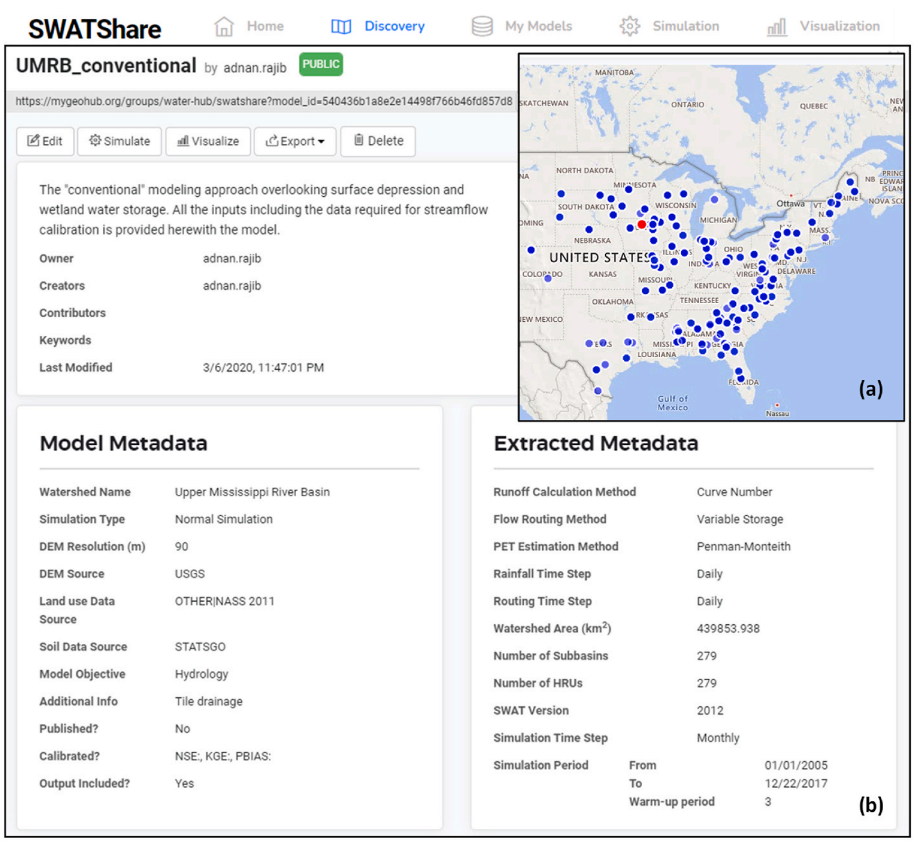


Fig. 2. SWATShare interface: Sharing SWAT model and metadata before setting up the calibration. (a) A modeler can also access models that are developed and shared by other modelers. (b) For a given model, SWATShare automatically extracts metadata such as number of subbasins, simulation time-step and duration, warmup period etc. without having to manually search such information amidst numerous input/output files.

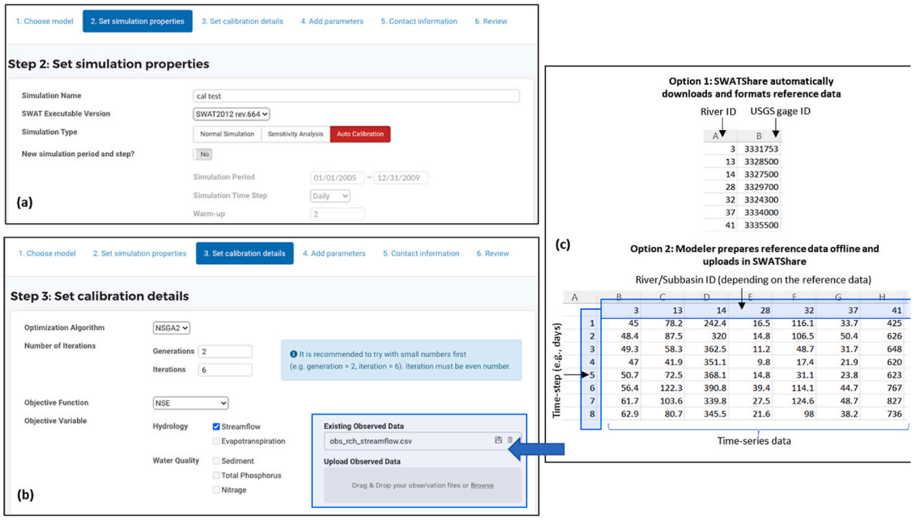


Fig. 3. Setting up autocalibration in SWATShare: (a–b) multi-objective calibration with the option of simultaneously calibrating streamflow, evapotranspiration, sediment, phosphorus, and nitrate, and multi-criteria convergence to optimal solution with the option of using a combination of up to three performance metrics (objective functions), (c) two different options to define reference datasets, i.e., (1) extracting reference data directly from the source without requiring any offline data-preprocessing tasks (the current version of SWATShare offers this functionality only for US watersheds through interoperability with USGS web services), and (2) enabling the ease of linking a user-defined reference dataset with the corresponding calibration nodes without requiring any manual intervention or coding.

streamflow, evapotranspiration). Regardless of the CSV file(s) with pre-processed reference data or the CSV file(s) with location list for seamlessly extracting reference data from the source (section 2.2.2), SWATShare uses the same CSV file(s) to recognize and link relevant model subbasin and/or river IDs with corresponding datasets (Fig. 3c). There was no such functionality in the previous version of SWATShare as it required preparing the calibration setup offline and simply provided a web interface to submit the calibration job to HPC. In case of SWAT-CUP, the graphical interface eases the inclusion of reference datasets, but modelers not well-versed with SWAT input/output files may still find it challenging to manually link reference datasets with the corresponding subbasin and/or river IDs. The current version of SWATShare, as noted above, offers a parsimonious yet highly efficient way so that modelers can link large, spatially distributed datasets with the model in *a single step*, without having to deal with coding to prepare the data in a specific format or being well-versed about the model's file structure and nomenclature.

2.2.4. *Multi-objective calibration*

SWATShare can calibrate various internal dynamics and signatures across the watershed in addition to calibrating streamflow only at the watershed outlet (Kunnath-Poovakka et al., 2016; Nijzink et al., 2018; Rajib et al., 2018a). Specifically, SWATShare offers the option of calibrating up to five hydrology and water quality variables, simultaneously and across different spatial scales, including streamflow (river reach), evapotranspiration (subbasin), sediment (river reach), phosphorus (river reach), and nitrate (river reach). More variables can be added in the future with minimal changes in the overall workflow. However, the data- and computation-intensive nature of multi-objective calibration is a deterring factor (Asgari et al., 2022) which drives modelers towards the traditional streamflow-only calibration and produces right answers for wrong reasons (Rajib et al., 2018a). Besides the interoperability with data platforms and the ease of linking data with model structure (sections 2.2.2-2.2.3), the free access to HPC in SWATShare reduces data and computational burden at the modelers' end and encourages the use of multi-objective calibration to obtain accurate understanding of hydrologic processes. Executing multi-objective calibrations remains challenging in many contemporary autocalibration tools (e.g., high model structural literacy requirements to enable multi-objective calibration in PyWrfHydroCalib and SWAT-CUP; no multi-objective option in PEST-GSSHA), but SWATShare users can activate multi-objective calibration simply by clicking a few check-boxes on the interface (Fig. 3a–b).

2.2.5. *Multi-criteria convergence to the optimal solution*

Model performance criteria measure calibration performance by expressing the agreement between simulation and reference data. Commonly used criteria, e.g., Percent Bias (PBIAS), Correlation (r), Nash Sutcliffe Efficiency (NSE), Kling Gupta Efficiency (KGE) (Knoben et al., 2019; Krause et al., 2005; Legates and McCabe, 1999) are not equally representative benchmarks for different hydrologic regimes (Knoben et al., 2019), and also the choice of criteria during model calibration is often arbitrary (see Moriasi et al., 2007). Therefore, the so-called best parameter set (the optimal solution) based on a single criterion is hardly the best for all criteria simultaneously. Considering multiple criteria simultaneously may produce a trade-off solution, generally known as *Pareto optimal solutions* or non-dominated solutions. These solutions are optimal in the sense that no other solutions in the parameter space are better than them or can dominate them when all the criteria are considered (Ercan and Goodall, 2016). While many existing tools (e.g., SWAT-CUP and PyWrfHydro) use a single criterion to search optimality, SWATShare lets modelers select a combination of up to three criteria to search Pareto optimality (Fig. 3b).

2.2.6. *Spatially distributed parameter search*

Employing spatially distributed reference data in multi-objective calibrations (e.g., evapotranspiration from satellites, streamflow and water quality from multiple gage stations across the watershed) does not automatically guarantee spatially distributed parameter search. For example, despite being fed with spatially distributed data, autocalibration tools often let parameters undergo the same degree of change across the entire watershed during the iteration process (e.g., Rajib et al., 2016). Because such an approach overlooks the relative locations of calibration nodes and the space-time-variable continuum of the data (Dembélé et al., 2020; Gardner et al., 2018; Jadidoleslam et al., 2020), it can mislead the parameter search to an equifinal solution. As a remedial solution, the new SWATShare interface provides an option similar to SWAT-CUP so that modelers can divide a watershed into multiple zones according to the spatial distribution/proximity of the calibration nodes (and also the knowledge of watershed properties), and correspondingly apply different degrees of change to the same parameter across these zones (Fig. 4a). The increased computational need for such a highly discretized, spatially distributed parameter search is supported by SWATShare's HPC resource.

2.2.7. *Feedback of optimal parameters into the model*

As noted above, choice of performance criteria in traditional hydrologic model calibration practices is largely arbitrary. As such, developers of autocalibration tools often automate the iterative parameter

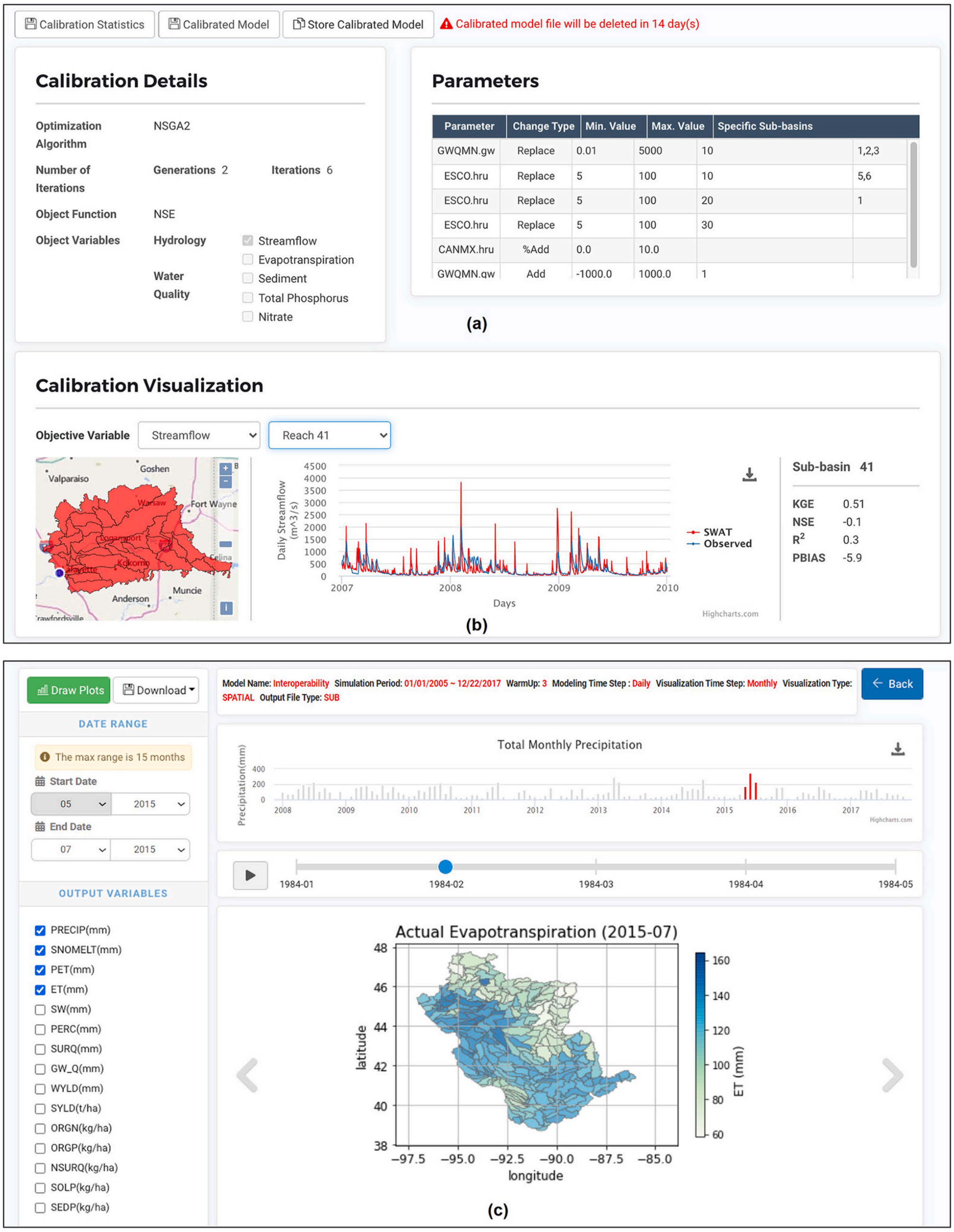


Fig. 4. (a) Spatially distributed parameter search in SWATShare where modelers have the option to set a parameter with multiple possible initial ranges across the model's spatial units, i.e., subbasins and Hydrologic Response Units (HRUs). (b) Visualization of calibration performance: time-series comparison and performance metrics. This visualization page also displays metadata related to the calibration setup and allows downloading the calibrated model. It also lets modelers check an auto-generated simulation log for debugging purposes. (c) Additional visualization services that allow spatial mapping and time-series plotting of all simulated water balance components in the calibrated model to have a more in-depth understanding of the model's physical consistency.

search process but decouple the final step from the calibration workflow where the best parameter values are fed into the model source code to produce the optimal model. This is to let modelers check which performance criteria shows the best performance, select the corresponding best parameter set, and do manual parameter adjustments if necessary (e.g., Mengistu et al., 2019). The contemporary SWAT autocalibration tools, e.g., SWAT-CUP and R-SWAT-FME, invariably use this approach. Although such an approach gives modelers some flexibility to evaluate the physical consistency of the calibration results outside the autocalibration workflow (Abbaspour, 2015), it is subjective and highly susceptible to equifinality, not to mention the cumbersome tasks of handling model parameters manually and chances of errors therein. SWATShare, on the other hand, applies a feedback loop to automatically insert the best parameter set into the model after finishing a batch of iterations. The underlying idea here is to trade-off the aforesaid flexibility for other opportunities, such as use of spatially distributed data, multi-criteria optimization, and in-depth visualization of model outputs (elaborated in section 2.2.8), which can ultimately reduce subjectivity and equifinality in model calibration and may in fact produce a more robust calibrated model.

2.2.8. *Instantaneous visualization and evaluation of calibration performance*

When a calibration job is completed, SWATShare sends an email notification to the modeler thus providing more flexibility in SWATShare's remote work environment. Through an interactive interface similar to SWAT-CUP, modelers can evaluate calibration performance by visualizing the time series of simulated and reference data along with the performance metrics. SWATShare allows users to make explainable adjustments to the prior calibration protocol and subsequently re-run the calibration as necessary. SWATShare enables this by displaying the corresponding calibration nodes (i.e., subbasin, river) in a dynamic map so that the modelers can visually interpret the variation of model performance at different spatial scales (e.g., upstream-to-downstream gradient) and geophysical properties across the watershed (e.g., topography, land use, climate) (Fig. 4b).

Further, SWATShare lets modelers instantaneously create time-series and spatial maps for all the simulated hydrologic processes corresponding to the most optimal parameter set. Especially, for the spatial maps (Fig. 4c), SWATShare shows a precipitation time-series so that modelers can correlate the spatial patterns of water balance components with climatic drivers and sense inconsistencies in their choice of calibration protocol. Such an instantaneous yet comprehensive evaluation of calibration performance through multiple layers of visualization aids is a feature unique to SWATShare currently absent in the contemporary autocalibration tools. Additionally, calibration statistics (e.g., optimal parameter values, performance metrics) and the calibrated model can be downloaded from SWATShare to facilitate offline experiments and/or published through SWATShare (Fig. 2) for broader community consumption.

2.3. The software architecture and simulation workflow

SWATShare architecture, as shown in Fig. 5, consists of three main structural components: front end web interface, back end services, and external resources. Although the three main structural components remain the same as in the previous SWATShare version (Rajib et al., 2016), the associated software architecture has been modified to better fit the sustainability model and the common geospatial data management and analysis infrastructure myGeoHub provides to the other hosted projects (Kalyanam et al., 2019).

2.3.1. Front end interface

The front end of SWATShare is an interactive web application deployed through myGeoHub (Kalyanam et al., 2019, 2020; https://mygeohub.org) – a geospatial science gateway in the HUBzero CI. HUBzero is a CI to create and host interactive web portals for scientific research, education, and outreach activities (McLennan and Kennell, 2010). It provides out-of-the-box data management tools for users such as group, project, publication, ticket tracking, wiki, forum, and an automated process to contribute contents and publish online

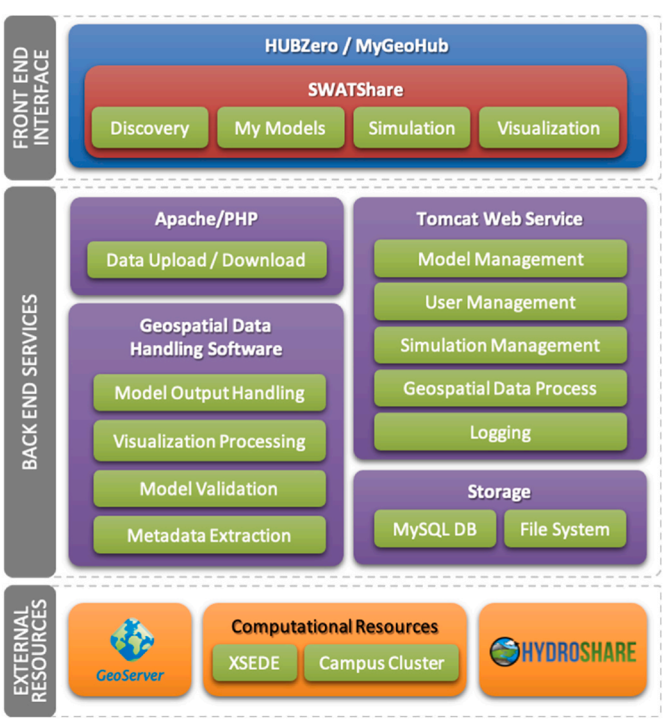


Fig. 5. SWATShare software architecture.

tools. The access control for SWATShare is integrated with the HUBzero authentication system. It enables private model and simulation management for each modeler as well as resource usage monitoring and data sharing. The earlier version of the SWATShare's graphical user interface was implemented using Adobe Flash. Since Adobe no longer supports Flash Player after year 2020, a new version of SWATShare as a HUBzero component is implemented using PHP and JavaScript, which are the main programming languages for web application development on the HUBzero platform. Specifically, it is a single-page application (SPA) providing dynamic content by actively communicating with myGeoHub web server eliminating the need to refresh the entire web page. This enables a faster transition, and thus a better user experience as if they were using a native application.

2.3.2. Back end services

The back end of the SWATShare system is built on Redhat Linux distribution. It consists of a set of services that are responsible for handling modelers' requests through the web interface. In particular, the Apache/PHP services provide data upload and download functions via HTTP messages. The Tomcat web services are written in JAVA and support REpresentational State Transfer (REST) web APIs for managing models, users, and simulations. They also perform geospatial data processing functions including model output transformation, data visualization, model validation, and metadata extraction, using open source python and R software, such as gdal (Warmerdam et al., 2022), fiona (Gillies, 2020), dataRetrieval (De Cicco et al., 2022), and hydroGOF (Zambrano-Bigiarini, 2020). The metadata for users, simulations, and models are stored securely in a MySQL database. This Linux-Apache-MySQL-PHP (LAMP) software stack is a widely used web development platform having an open-source ecosystem, and providing cost efficiency (Lawton, 2005). The uncalibrated models uploaded by different modelers and their corresponding calibrated models/outputs are stored in a high-performance file system.

2.3.3. External resources

SWATShare utilizes and interoperates with several external resources. A GeoServer is used for rendering interactive maps that allows users to search models by geographic location and metadata. GeoServer is a standard-conforming, community-based tool that has proved stable and efficient in GIS application developments (Parker et al., 2015). SWAT model autocalibration usually require a large amount of computational resources. For instance, one calibration job for a SWAT model normally includes more than 500 iterative simulations. In order to get better performance and scalability, SWATShare connects to the HPC resources at the Extreme Science and Engineering Discovery Environment (XSEDE) Comet cluster and a Purdue campus cluster. This enables users to get simulation results much sooner than using their desktop environments. Moreover, they can run multiple simulations at the same time without performance degradation. SWATShare also connects to HydroShare (Tarboton et al., 2018), a collaborative CI aiming at enabling the hydrologic user community to share their data, models, and analysis. Users from either system can easily access data and tools across the networks without the need to create new accounts or manually import or export models.

2.3.4. Simulation workflow

SWATShare runs calibration as well as normal simulations remotely on HPC resources via secure shell (ssh). The overview of the simulation workflow is described in Fig. 6. When the modeler submits a job, the web front end collects the user input and creates a simulation specification file that describes the input, simulation name, simulation period, and SWAT executable version (see, e.g., Fig. 3a). It then invokes the SWATShare job submission web service with the simulation specification. Additional calibration details are collected and passed to the web service, such as the optimization algorithm to use, the number of iterations, and parameter information, and reference data files (see, e.g.,

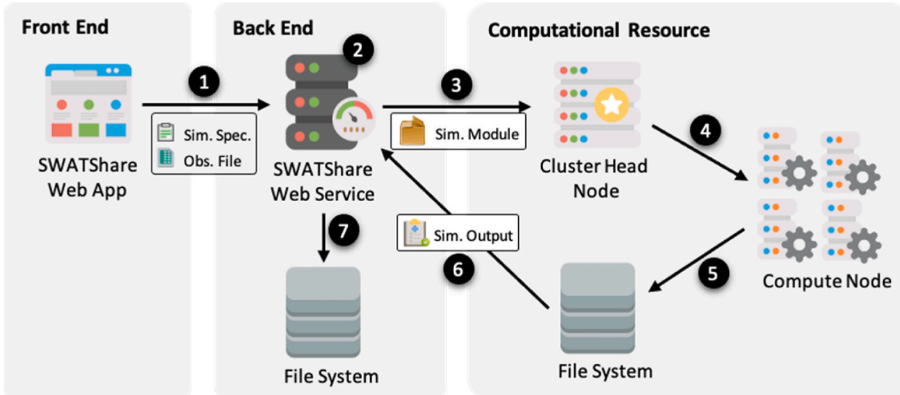


Fig. 6. Overview of the SWATShare simulation workflow.

Fig. 3b–c, 4a).

When the SWATShare web service receives the request, it prepares a job submission module to be submitted to the HPC resources. In particular, it parses the specification and creates a simulation module containing the SWAT model input file, a definition file including calibration information, and the reference data file(s). Along with the input files, the module also includes a simulation execution engine consisting of several automation scripts and a SWAT executable. Next, the web service sends a job request with the module to the Slurm workload manager on the head node of the remote cluster via ssh. The job will enter a waiting queue until a suitable compute node is available. When a compute node is assigned, the automation scripts in the simulation module are executed and the simulation is run iteratively. The SWATShare job monitoring web service keeps track of the job status. When the job completes, it fetches the simulation output from the file system of the computational resource and stores it to a Network File System (NSF) mounted to the back-end server. Finally, it checks for successful run of a simulation and updates the MySQL database accordingly.

3.0. Implementation case studies

In our previous study, we conducted modeling experiments to introduce SWATShare's model sharing, high performance computation, and visualization capabilities in a real-time multi-user environment (Rajib et al., 2016). In the present study, we conducted experiments to demonstrate (i) how the new CI capabilities of SWATShare calibration facilitate data-model interoperability, (ii) how SWATShare allows spatially distributed parameter search as opposed to a conventional approach, and (iii) whether the SWATShare calibration results are consistent with those from a widely used desktop-based SWAT calibration tool SWAT-CUP.

3.1. Data-model interoperability

SWATShare's data-model interoperability is demonstrated in Fig. 7 using a SWAT model originally developed by Rajib et al. (2018b) for the Upper Wabash River watershed in central Indiana, United States. This watershed has 7 streamflow gage stations that satisfies the data availability criteria and are considered as calibration nodes. To activate data-model interoperability, a CSV file listing the gage and the corresponding river IDs is uploaded. SWATShare retrieves other key inputs from the prior steps, including the simulation period, time-step, and objective variable (see Fig. 3a–b) and feeds this information into the dataRetreival software (De Cicco et al., 2022) to seamlessly fetch the

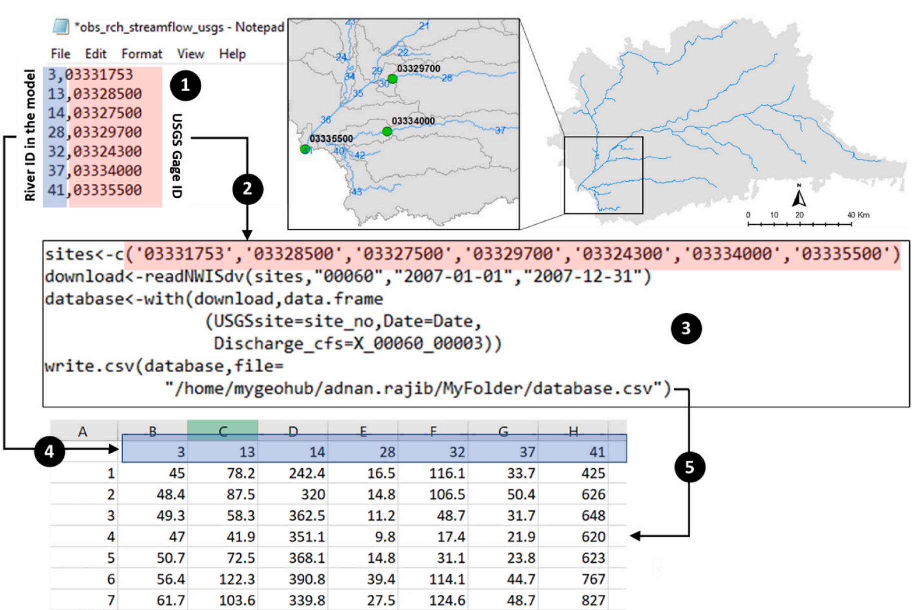


Fig. 7. The steps SWATShare would follow to enable data-model interoperability for calibrating a SWAT model of the Upper Wabash watershed, United States. The information in (1) are the only user inputs; the rest of the steps including the R code in (3) are automatically executed by SWATShare.

required time-series data from USGS. Next, SWATShare uses a python post-processor to transform the downloaded time-series in a specified format while linking them with the corresponding river IDs. In addition to the Wabash watershed test presented here, this functionality has been tested using different watersheds with varying density of gage stations, simulation period, and objective variables (e.g., water quality). For the Upper Wabash test case, a modeler with moderate SWAT modeling, GIS, and programming experience could save one working day (about 8 h) in data processing tasks when using SWATShare's data-model interoperability functionality as opposed to the manual data search, download, and processing for 7 gaging stations.

3.2. Spatially distributed parameter search

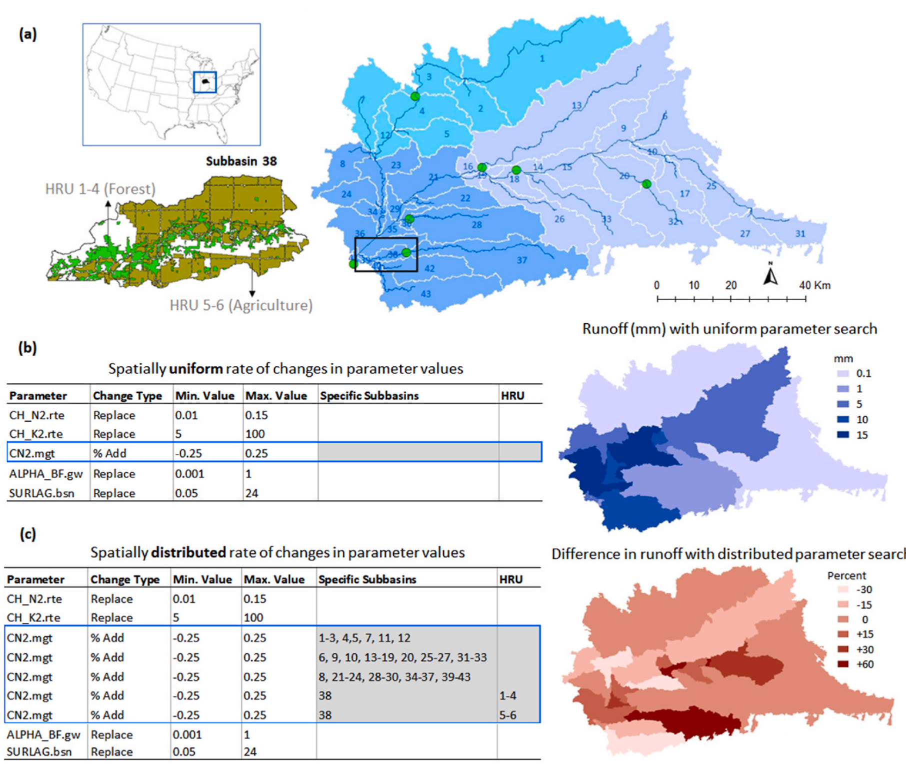
Fig. 8 shows SWATShare's capability to perform spatially distributed parameter search using the same model setup for the Upper Wabash watershed demonstrated earlier. The 7 streamflow gage stations used in the model's calibration are somewhat uniformly distributed across 43 subbasins and numerous Hydrologic Response Units (HRUs) within the subbasins (Fig. 8a).

By making a ±25% change in the default curve number (CN2) or replacing the default channel roughness (CH_N2) with a new value between 0.01 and 0.15 irrespective of subbasins and river reaches (Fig. 8b), these parameters are allowed to undergo the same degree of change across the entire watershed without considering the relative locations of calibration nodes (i.e., gage station locations). On one hand, this *spatially uniform* optimization limits the ability of a parameter to represent watershed features (e.g., land use and topography). On the other hand, such an approach makes a distributed model function like a lumped model, thus underutilizing the data, labor, and computational cost of highly resolved process-based simulations. Yang et al. (2019) conceptualized this as the *Calibration Density and Consistency* problem while Xie et al. (2021) linked this to a dimensionality problem. Creating a model with high spatial resolutions (Fenicia et al., 2016; Kuppel et al., 2018; Marcé et al., 2008) or using spatially distributed reference data in model calibrations (Rajib et al., 2018a) alone does not address this problem.

As a remedial solution, the new calibration interface in SWATShare uses an approach suggested by Abbaspour (2015) to explicitly relate reference data with the corresponding model subbasins and/or HRUs. This functionality is demonstrated in Fig. 8c that shows how the same parameter (e.g., Curver Number (CN2)) can undergo different degrees of optimization across three different watershed zones. Briefly, the sub-basins are grouped in three zones according to their proximity to gage stations in an upstream-to-downstream gradient. The parameter optimization is further distributed at HRU-level in one of the subbasins according to different land use types (see Fig. 8a and c). The resulting calibrated model with spatially distributed parameter search option produced notable changes in model outputs. For example, subbasin-level surface runoff after a particular storm event is −30% to +60% different in the spatially distributed option compared to that in the spatially uniform option. Although this demonstration is based on point observations at a limited number of gage stations, the spatially distributed parameter search option shown here makes SWATShare a user-friendly, futuristic tool for calibrating large-scale high-resolution hydrologic models with increasingly available gridded Earth observation datasets.

3.3. Consistency across SWATShare and SWAT-CUP calibration results

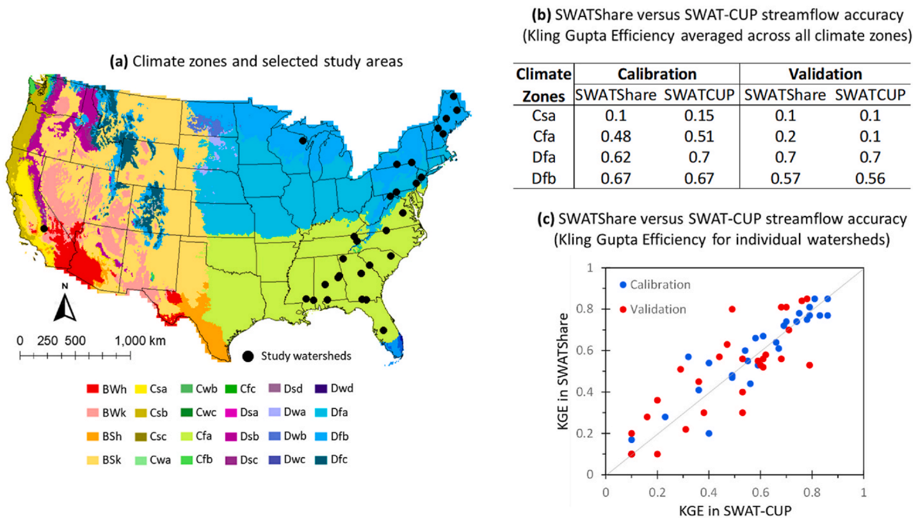
In this experiment, separate SWATShare and SWAT-CUP calibrations of 30 SWAT models across four different climate zones in the United States (see Fig. 9a) are conducted. This is the first calibration experiment at such an extensive scale because prior studies often considered a single watershed to evaluate alternative calibration tools (e.g., Paul and Negahban-Azar, 2018; Yang et al., 2008). This extensive calibration experiment facilitates a conclusive understanding of whether and to what extent SWATShare and SWAT-CUP results are consistent. The metadata corresponding to each of these test models can be accessed through the *Discovery* function of SWATShare (Fig. 2) using the



Parameter	Change Type	Min. Value	Max. Value	Specific Subbasins	HRU
CH_N2.rte	Replace	0.01	0.15		
CH_K2.rte	Replace	5	100		
CN2.mgt	% Add	-0.25	0.25		
ALPHA_BF.gw	Replace	0.001	1		
SURLAG.bsn	Replace	0.05	24		

Parameter	Change Type	Min. Value	Max. Value	Specific Subbasins	HRU
CH_N2.rte	Replace	0.01	0.15		
CH_K2.rte	Replace	5	100		
CN2.mgt	% Add	-0.25	0.25	1-3, 4,5, 7, 11, 12	
CN2.mgt	% Add	-0.25	0.25	6, 9, 10, 13-19, 20, 25-27, 31-33	
CN2.mgt	% Add	-0.25	0.25	8, 21-24, 28-30, 34-37, 39-43	
CN2.mgt	% Add	-0.25	0.25	38	1-4
CN2.mgt	% Add	-0.25	0.25	38	5-6
ALPHA_BF.gw	Replace	0.001	1		
SURLAG.bsn	Replace	0.05	24		

Fig. 8. Effect of spatially distributed parameter search approach in SWATShare as opposed to the commonly used spatially uniform approach (demonstrated using the Curve Number parameter as an example). The model used in this example is adapted from Rajib et al. (2018b).



Climate Zones	Calibration		Validation	
	SWATShare	SWATCUP	SWATShare	SWATCUP
Csa	0.1	0.15	0.1	0.1
Cfa	0.48	0.51	0.2	0.1
Dfa	0.62	0.7	0.7	0.7
Dfb	0.67	0.67	0.57	0.56

Fig. 9. Comparison of SWATShare and SWAT-CUP calibration performance. The map shows 30 watersheds across four different climates zones used for this comparison (also see supplementary information S1). The climate zones are based on a global climate classification map (Beck et al., 2018) where Cfa = humid subtropical, Csa = Mediterranean hot summer, Dfa = hot summer continental, Dfb = warm summer continental.

supplementary information in S1.

All 30 models are simulated at a daily time-step with a 2-year period of initialization (2001–2002), followed by a 5-year calibration (2003–2007) and a 3-year validation (2008–2010) using gage station streamflow data as reference. Identical set of calibration parameters (N = 18) and their respective initial ranges are selected across all 60 setups (see supplementary information S1). The models are calibrated with the NSGA-II algorithm in SWATShare and the Sequential Uncertainty Fitting-versions 2 (SUFI-2) algorithm in SWAT-CUP. SUFI-2 in SWAT-CUP is used because of its well-documented applications in the literature. Models in SWATShare are set with 20 generations and 100 iterations, whereas models in SWAT-CUP are set with 1000 iterations each across two successive batches of iterations. This is a measure to ensure an equivalent number of total simulations although such a distribution of generation, iteration, and batch numbers may not translate the same meaning across two conceptually different calibration tools.

The results indicate that SWATShare and SWAT-CUP yield nearly consistent calibration performance in terms of streamflow Kling Gupta Efficiency (KGE) (Knoben et al., 2019) values averaged separately for calibration and validation, and across all the watersheds located within a climate zone (Fig. 9b). These averaged estimates of calibration performance are also supported by individual watershed-KGE values (Fig. 9c; note the adherence of KGE values around the SWATShare - SWAT-CUP 1:1 line). Despite such consistency in overall calibration performance, optimal parameter values in SWATShare may be inconsistent with those in SWAT-CUP. As a result, the most optimal parameter values in SWATShare, with a few exceptions, showed low correlation with the corresponding parameter values in SWAT-CUP (Fig. 10a). Importantly, a *behavioral change* is observed revealing how some of these parameters represented hydrologic processes in the two calibration tools. For example, the optimal value for parameter ESCO in SWATShare is greater than EPCO across all four climate zones – a pattern completely opposite compared to SWAT-CUP (Fig. 10b). Because ESCO and EPCO are the key parameters controlling SWAT's soil moisture accounting and evapotranspiration mechanisms (Neitsch et al., 2011; Rajib et al., 2016), their opposite behavior shown in Fig. 10b indicates two potentially different states of water balance in the same model regardless of similar calibration performances. Although it is hard to disentangle the underlying factors for such behavioral change in parameters' responses, these findings add new insights into how the choice of calibration tool can cause equifinality.

4. Conclusions and future directions

Data for streamflow, climate, hydrography, topography, land use, and soil over the internet date back to early 2000s. Naturally, development and use of Cyberinfrastructure (CI) for hydrology, or water resources in general, had long been focused on instantaneous access to data, standardizations of data publication and integration, and platforms for data storage and sharing. Therefore, CIs and Open Science platforms geared towards hydrologic modeling needs had been limited. SWATShare 1.0 (https://mygeohub.org/groups/water-hub/swatshare) partially filled this gap by providing a collaborative platform for sharing, simulation, and visualization of SWAT models (Rajib et al., 2016). This

(a) Correlation between SWATShare and SWAT-CUP parameter values

Parameters	R^2 value
ALPHA_BF	0.68
CH_N2	0.57
ESCO	0.56
GWQMN	0.46
SMTMP	0.43
CH_K2	0.36
EPCO	0.36
GW_DELAY	0.29
SURLAG	0.00

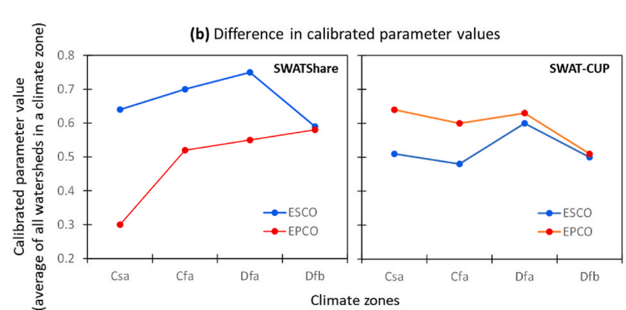


Fig. 10. Comparison of the most optimal parameter values for SWAT models calibrated separately with SWATShare and SWAT-CUP. SWATShare and SWAT-CUP in this model intercomparison experiment used NSGA-II and SUFI-2 optimization algorithms respectively.

paper introduces SWATShare 2.0 – a substantially improved version incorporating a new autocalibration tool and demonstrating how CI capabilities can be harnessed to solve five root causes of inefficiency in traditional hydrologic model calibration practices, including (i) platform dependence, (ii) limited computing resource, (iii) lack of programming literacy, (iv) lack of model structural literacy, and (v) no data-model interoperability. The online interface of SWATShare ensures platform independence by letting modelers perform complex calibration tasks in a web browser without requiring any specific computer operating system, software packages, and their versions and licenses. The free access to High Performance Computing (HPC) resource allows SWATShare to lower the computational burden, and thereby offer multi-objective calibration options involving up to five hydrology and water quality variables and a highly discretized parameter search option involving spatially distributed datasets. SWATShare's data-model interoperability, by seamlessly and instantaneously extracting streamflow and water quality datasets through the USGS web services and automatically recognizing and linking those datasets with corresponding model subbasin and/or river IDs, show a unique example of CI capabilities currently absent in any other hydrologic model autocalibration tools. Searching the optimal solution using a combination of up to three performance criteria, direct feedback of optimal parameters into the model, and instantaneous visualization and evaluation of calibration performance are the additional functionalities that further increase the efficiency of the autocalibration process in SWATShare without the need for excessive pre- and post-processing tasks. SWATShare's online interface serves as the one-stop platform to let modelers perform all the above calibration steps through an intuitive, hierarchical progression, thus minimizing the need for a modeler to have high programming and model-structural literacy. Finally, and more importantly, results from SWATShare autocalibration show that its streamflow prediction is comparable with that from the commonly used offline calibration platform SWATCUP, but for some of the study areas, parameters estimated from SWATShare may be more meaningful to the physical processes.

While SWATShare demonstrates an example application using the SWAT model, except the model, most of the workflow is generic and can be adopted for any model. For example, the SWAT model itself is evolving and is currently being modified as SWAT+. SWAT+ can be brought under SWATShare via simple code modifications to incorporate the model's new file naming conventions and data structures, without having to change SWATShare's overall workflow. Plan to do this is already underway.

No doubt the above developments of SWATShare addressed a critical need of the hydrologic modeling community. Yet, future developments and re-developments of SWATShare harnessing newer and better CI and Open Science capabilities to address broader community needs are imminent. There is a push and also broader consensus within the scientific community, including hydrology, for reproducibility. Reproducibility cannot be accomplished without the ability to run complete scientific workflows which may, and in most cases they do, demand a more extensive architecture for interoperability and computing. For example, currently SWATShare cannot create a SWAT model directly from input datasets; it relies on modelers to upload their existing models, meaning modelers cannot run complete scientific workflows – from model creation to model calibration – within SWATShare interface. Fortunately, besides access to XSEDE distributed HPC (https://www.xsede.org), SWATShare's current capabilities to interoperate across multiple CIs including myGeoHub (https://mygeohub.org), HydroShare (https://www.hydroshare.org), and USGS′ National Water Information System (https://waterdata.usgs.gov/nwis) have already created the building blocks to achieve that *reproducibility* goal. Efforts to link models and enable model interoperability is also booming. The generalizable software pieces developed for SWATShare can further excel these interoperability efforts by brining other models and myriad open access autocalibration codes under one platform. In essence, with calls for adopting FAIR or Open Science principles and increasing need for convergent approaches to address societal problems involving water and climate, platforms like SWATShare can serve as a blueprint for new CI-enabled developments in hydrology, and beyond hydrology in other disciplinary domains of Earth system sciences.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

See the software availability section in the manuscript

Acknowledgment

This work was funded by the U.S. National Science Foundation (NSF) grants # 1835822 and # 1829764. A.R.'s contribution was partially funded by the National Aeronautics and Space Administration (NASA) grant # 80NSSC22K1661. The views expressed in this article are those of the authors and do not necessarily represent the views or the policies of the funding agencies.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envsoft.2022.105561.

References

Abbaspour, K.C., 2015. SWAT-CUP 2012: SWAT Calibration and Uncertainty Programs — A User Manual. Available online at: http://swat.tamu.edu/media/114860/usermanual_swatcup.pdf. (Accessed 9 June 2022).

Alam, M.J., Ercan, M.B., Zahura, F.T., Goodall, J.L., 2018. Using geospatial analysis and hydrologic modeling to estimate climate change impacts on nitrogen export: case study for a forest and pasture dominated watershed in North Carolina. ISPRS Int. J. Geo-Inf. 7 https://doi.org/10.3390/ijgi7070280.

Ames, D.P., Horsburgh, J., Cao, Y., Kadlec, J., Whiteaker, T., Valentine, D., 2012. HydroDesktop: Web Services-Based Software for Hydrologic Data Discovery, Download, Visualization, and Analysis, vol. 37. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2012.03.013.

Asgari, M., Yang, W., Lindsay, J., Tolson, B., Dehnavi, M., 2022. A review of parallel computing applications in calibrating watershed hydrologic models. Environ. Model. Software 151. https://doi.org/10.1016/j.envsoft.2022.105370.

Bacu, V., Mihon, D., Rodila, D., Stefanut, T., Gorgan, D., 2011. Grid based architectural components for SWAT model calibration. In: HPCS 2011 International Conference on High Performance Computing and Simulation, pp. 193–199. https://doi.org/10.1109/HPCSim.2011.5999824.

Bandaragoda, C., Castronova, A., Istanbulluoglu, E., Strauch, R., Nudurupati, S.S., et al., 2019. Enabling Collaborative Numerical Modeling in Earth Sciences Using Knowledge Infrastructure, vol. 120. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2019.03.020.

Baracchini, T., Hummel, S., Verlaan, M., Cimatoribus, A., Wüest, A., 2020. An automated calibration framework and open source tools for 3D lake hydrodynamic models. Environ. Model. Software 134. https://doi.org/10.1016/j.envsoft.2020.104787.

Beck, H., Zimmermann, N., McVicar, T., et al., 2018. Present and future Köppen-Geiger climate classification maps at 1-km resolution. Nature Scientific Data 5. https://doi.org/10.1038/sdata.2018.214.

Bekele, E., Nicklow, J., 2007. Multi-objective automatic calibration of SWAT using NSGA-II. J. Hydrol. 341 https://doi.org/10.1016/j.jhydrol.2007.05.014.

Behrouz, M., Zhu, Z., Matott, L.S., Rabideau, A.J., 2020. A new tool for automatic calibration of the Storm Water Management Model (SWMM). J. Hydrol. 581 https://doi.org/10.1016/j.jhydrol.2019.124436.

Carrillo, A., Falgueras, J., Guevara, A., 2006. Gdit - tool for the design, specification and generation of goals driven user interfaces. In: Proceedings of the Eighth International Conference on Enterprise Information Systems - HCI. https://doi.org/10.5220/0002496601350138, 135-13.

Castronova, A., Goodall, J., Ercan, M., 2013. Integrated Modeling within a Hydrologic Information System: an OpenMI Based Approach, vol. 39. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2012.02.011.

Cau, P., Bacu, V., Manca, S., Lehman, A., Muroni, D., Gorgan, D., 2013. An interoperable GIS oriented information and support system for water resources management. Int. J. Adv. Comput. Sci. Appl. https://doi.org/10.14569/SpecialIssue.2013.030309.

Chen, M., Voinov, A., Ames, D.P., Kettner, A., Goodall, J., et al., 2020. Position paper: open web-distributed integrated geographic modelling and simulation to enable broader participation and applications. Earth Sci. Rev. 207 https://doi.org/10.1016/j.earscirev.2020.103223.

Chlumsky, R., Mai, J., Craig, J., Tolson, B., 2021. Simultaneous calibration of hydrologic model structure and parameters using a blended model. Water Resour. Res. 57 (5) https://doi.org/10.1029/2020WR029229.

Choi, Y.-D., Goodall, J., Sadler, J., Castronova, A., Bennett, A., et al., 2021. Toward Open and Reproducible Environmental Modeling by Integrating Online Data Repositories, Computational Environments, and Model Application Programming Interfaces, vol. 135. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2020.104888.

CSISS, 2021. Geospatial Web Service for U.S. Crop Condition and Soil Moisture Data Analysis. Center for Spatial Information Science and Systems (CSISS), George Mason University. Available online at: https://nassgeo.csiss.gmu.edu/Crop-CASMA-Developer. (Accessed 17 April 2022).

Dai, L., Zhang, P., Wang, Y., Jiang, D., Dai, H., et al., 2017. Multi-objective optimization of cascade reservoirs using NSGA-II: a case study of the Three Gorges-Gezhouba cascade reservoirs in the middle Yangtze River, China. Hum. Ecol. Risk Assess. 23 (4) https://doi.org/10.1080/10807039.2017.1285692.

Dawdy, D.R., O'Donnell, T., 1965. Mathematical models of catchment behavior. ASCE Journal of the Hydraulics Division 91 (4). https://doi.org/10.1061/JYCEAJ.0001271.

De Cicco, L.A., Lorenz, D., Hirsch, R.M., Watkins, W., Johnson, M., 2022. dataRetrieval: R Packages for Discovering and Retrieving Water Data Available from U.S. Federal Hydrologic Web Services. https://code.usgs.gov/water/dataRetrieval. (Accessed 18 July 2022).

Deb, K., Pratap, A., Agarwal, S., Meyarivan, T., 2002. A fast and elitist multiobjective genetic algorithm: NSGA-II. IEEE Trans. Evol. Comput. 6 (2) https://doi.org/10.1109/4235.996017.

Dembélé, M., Hrachowitz, M., Savenije, H., Mariéthoz, G., Schaefli, B., 2020. Improving the predictive skill of a distributed hydrological model by calibration on spatial patterns with multiple satellite data sets. Water Resour. Res. 56 (1) https://doi.org/10.1029/2019WR026085.

Du, L., Rajib, A., Merwade, V., 2018. Large scale spatially explicit modeling of blue and green water dynamics in a temperate mid-latitude basin. J. Hydrol. 562 https://doi.org/10.1016/j.jhydrol.2018.02.071.

Duan, Q., Schaake, J., Andréassian, V., Franks, S., Gotetie, G., Gupta, H.V., et al., 2006. Model Parameter Estimation Experiment (MOPEX): an overview of science strategy and major results from the second and third workshops. J. Hydrol. 320 (1–2) https://doi.org/10.1016/j.jhydrol.2005.07.031.

Duan, Q., Sorooshian, S., Gupta, V., 1992. Effective and efficient global optimization for conceptual rainfall-runoff models. Water Resour. Res. 28 (4) https://doi.org/10.1029/91WR02985.

Dunlap, R., Rugaber, S., Mark, L., 2013. A feature model of coupling technologies for Earth System Models. Comput. Geosci. 53 https://doi.org/10.1016/j.cageo.2011.10.002.

EPA, 2015. BASINS Tutorials and Training, US Environmental Protection Agency. Available online at: https://www.epa.gov/ceam/basins-tutorials-and-training. (Accessed 10 July 2022).

Ercan, M., Goodall, J., Castronova, A., et al., 2014. Calibration of SWAT Models Using the Cloud. Environmen. Model. Software 62. https://doi.org/10.1016/j.envsoft.2014.09.002.

Ercan, M., Goodall, J., 2016. Design and implementation of a general software library for using NSGA-II with SWAT for multi-objective model calibration. Environ. Model. Software 84. https://doi.org/10.1016/j.envsoft.2016.06.017.

Ercan, M., Maghami, I., Bowes, B., Morsy, M., Goodall, J., 2020. Estimating potential climate change effects on the upper neuse watershed water balance using the SWAT model. J. Am. Water Resour. Assoc. 56 https://doi.org/10.1111/1752-1688.12813.

Essawy, B., Goodall, J., Zell, W., Voce, D., Morsy, M., et al., 2018. Integrating Scientific Cyberinfrastructures to Improve Reproducibility in Computational Hydrology: Example for HydroShare and GeoTrust, vol. 105. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2018.03.025.

Essawy, B., Goodall, J., Voce, D., Morsy, M., Sadler, J., et al., 2020. A Taxonomy for Reproducible and Replicable Research in Environmental Modelling, vol. 134. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2020.104753.

Evenson, G., Golden, H., Lane, C., McLaughlin, D., D'Amico, E., 2018. Depressional wetlands affect watershed hydrological, biogeochemical, and ecological functions. Ecol. Appl. 28 (4) https://doi.org/10.1002/eap.1701.

Femeena, P.V., Chaubey, I., Aubeneau, A., McMillan, S.K., Wagner, P., Fohrer, N., 2020. Developing an improved user interface for a physically-based stream solute transport model. Environ. Model. Software 129. https://doi.org/10.1016/j.envsoft.2020.104715.

Fenicia, F., Kavetski, D., Savenije, H., Pfister, L., 2016. From spatially variable streamflow to distributed hydrological models: analysis of key modeling decisions. Water Resour. Res. 52 (2) https://doi.org/10.1002/2015WR017398.

Fienen, M.N., Kunicki, T.C., Kester, D.E., 2011. cloudPEST — A python Module for Cloud-Computing Deployment of PEST, a Program for Parameter Estimation: U.S. Geological Survey Open-File Report 2011–1062, p. 22. Available online at: https://pubs.usgs.gov/of/2011/1062. (Accessed 15 July 2022).

Freitas, H., Mendes, C., Ilic, A., 2022. Performance Optimization of the MGB Hydrological Model for Multi-Core and GPU Architectures, vol. 148. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2021.105271.

Gardner, M., Morton, C., Huntington, J., Niswonger, R., Henson, W., 2018. Input Data Processing Tools for the Integrated Hydrologic Model GSFLOW, vol. 109. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2018.07.020.

Gao, X., Yang, Z., Han, D., Huang, G., Zhu, Q., 2020. A framework for automatic calibration of SWMM considering input uncertainty, hydrol. Earth Syst. Sci. Data. https://doi.org/10.5194/hess-2020-367.

Gee, 2022. Google Earth Engine Data Catalog. Available online at: https://developers.google.com/earth-engine/datasets/catalog. (Accessed 15 July 2022).

Gillies, 2020. The Fiona User Manual. Available online at: https://fiona.readthedocs.io/en/latest/manual.html. (Accessed 18 July 2022).

Gregory, T.R., 2009. Understanding natural selection: essential concepts and common misconceptions. Evo Edu Outreach 2. https://doi.org/10.1007/s12052-009-0128-1.

Govindaraju, R.S., Engel, B., Ebert, D., Fossum, B., Huber, M., et al., 2009. Vision of cyberinfrastructure for end-to-end environmental explorations (C4E4). ASCE Journal of Hydrologic Engineering 14 (1). https://doi.org/10.1061/(ASCE)1084-0699(2009)14:1(53).

Gregersen, J., Gijsbers, P.J.A., Westen, S.J.P., 2007. OpenMI: open modelling interface. J. Hydroinf. 9 (3) https://doi.org/10.2166/hydro.2007.023.

Gupta, H., Sorooshian, S., Yapo, P., 1999. Status of automatic calibration for hydrologic models: comparison with multilevel expert calibration. ASCE Journal of Hydrologic Engineering 4 (2). https://doi.org/10.1061/(ASCE)1084-0699(1999)4:2(135).

Hamman, J., Nijssen, B., Bohn, T., et al., 2018. The Variable Infiltration Capacity model version 5 (VIC-5): infrastructure improvements for new applications and reproducibility. Geosci. Model Dev. (GMD) 11. https://doi.org/10.5194/gmd-11-3481-2018.

Haupt, R., Haupt, S., 2003. Practical Genetic Algorithms, second ed. John Wiley & Sons, Inc. https://doi.org/10.1002/0471671746.

Hokkanen, J., Kollet, S., Kraus, J., et al., 2021. Leveraging HPC accelerator architectures with modern techniques — hydrologic modeling on GPUs with ParFlow. Comput. Geosci. 25 https://doi.org/10.1007/s10596-021-10051-4.

Hutton, E., Piper, M., Tucker, G., 2020. The Basic Model Interface 2.0: a standard interface for coupling numerical models in the geosciences. Journal of Open Source Software 5 (51). https://doi.org/10.21105/joss.02317.

Jadidoleslam, N., Goska, R., Mantilla, R., Krajewski, W., 2020. Hydrovise: A Non-proprietary Open-Source Software for Hydrologic Model and Data Visualization and Evaluation, vol. 134. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2020.104853.

Jeon, J.-H., Park, C.-G., Engel, B.A., 2014. Comparison of performance between genetic algorithm and SCE-UA for calibration of SCS-CN surface runoff simulation. Water 6. https://doi.org/10.3390/w6113433.

Kalyanam, R., Zhao, L., Song, C., Merwade, V., Jin, J., Baldos, U., Smith, J., 2020. GeoEDF: an extensible geospatial data framework for FAIR science. Proceedings of PEARC '20. Practice and Experience in Advanced Research Computing 207–214. https://doi.org/10.1145/3311790.3396631.

Kalyanam, R., Zhao, L., Song, C., Biehl, L., Kearney, D., et al., 2019. MyGeoHub—a sustainable and evolving geospatial science gateway. Future Generat. Comput. Syst. 94 https://doi.org/10.1016/j.future.2018.02.005.

Kan, G., He, X., Li, J., et al., 2019. Computer aided numerical methods for hydrological model calibration: an overview and recent development. Arch. Comput. Methods Eng. 26 https://doi.org/10.1007/s11831-017-9224-5.

Kuppel, S., Tetzlaff, D., Maneta, M., Soulsby, C., 2018. What can we learn from multi-data calibration of a process-based ecohydrological model? Environ. Model. Software 101. https://doi.org/10.1016/j.envsoft.2018.01.001.

Knoben, W.J.M., Freer, J.E., Woods, R.A., 2019. Technical note: inherent benchmark or not? Comparing nash–sutcliffe and kling–gupta efficiency scores. Hydrol. Earth Syst. Sci. 23 https://doi.org/10.5194/hess-23-4323-2019.

Krause, P., Boyle, D.P., Bäse, F., 2005. Comparison of different efficiency criteria for hydrological model assessment. Adv. Geosci. 5 https://doi.org/10.5194/adgeo-5-89-2005.

Kunnath-Poovakka, A., Ryu, D., Renzullo, L.J., George, B., 2016. The efficacy of calibrating hydrologic model using remotely sensed evapotranspiration and soil moisture for streamflow prediction. J. Hydrol. 535 https://doi.org/10.1016/j.jhydrol.2016.02.018.

Kuzmin, V., Seo, D.-J., Koren, V., 2008. Fast and efficient optimization of hydrologic model parameters using a priori estimates and stepwise line search. J. Hydrol. 353 https://doi.org/10.1016/j.jhydrol.2008.02.001.

Lawton, G., 2005. LAMP lights enterprise development efforts. Computer 38 (9). https://doi.org/10.1109/MC.2005.304.

Le, P., Kumar, P., Valocchi, A.J., Dang, H.-V., 2015. GPU-based high-performance computing for integrated surface–sub-surface flow modeling. Environ. Model. Software 73. https://doi.org/10.1016/j.envsoft.2015.07.015.

Legates, D., McCabe, G., 1999. Evaluating the use of "goodness-of-fit" Measures in hydrologic and hydroclimatic model validation. Water Resour. Res. 35 (1) https://doi.org/10.1029/1998WR900018.

Lin, P., Rajib, A., Yang, Z.-L., Somos-Valenzuela, M., Merwade, V., 2018. Spatiotemporal evaluation of simulated evapotranspiration and streamflow over Texas using the WRF-hydro-RAPID modeling framework. J. Am. Water Resour. Assoc. 54 (1) https://doi.org/10.1111/1752-1688.12585.

Liu, Y., Padmanabhan, A., Wang, S., 2014. CyberGIS Gateway for enabling data-rich geospatial research and education. Concurrency Comput. Pract. Ex. 27 (2) https://doi.org/10.1002/cpe.3256.

Lodhi, A., Godrej, A., Sen, D., Baran, A., 2020. URUNME: a generic software for integrated environmental modeling. Environ. Model. Software 134. https://doi.org/10.1016/j.envsoft.2020.104737.

Lyu, F., Yin, D., Padmanabhan, A., Choi, Y., Goodall, J., et al., 2019. Reproducible hydrological modeling with CyberGIS-jupyter: a case study on summa. In: Proceedings of PEARC '19: Proceedings of the Practice and Experience in Advanced

Research Computing on Rise of the Machines (Learning). https://doi.org/10.1145/3332186.3333052 article no. 21.
Macro, K., Matott, L., Rabideau, A., Ghodsi, S.M., Zhu, Z., 2019. OSTRICH-SWMM: A New Multi-Objective Optimization Tool for Green Infrastructure Planning with SWMM, vol. 113. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2018.12.004.
Maidment, D., 2008. Bringing water data together. ASCE Journal of Water Resources Planning and Management 134 (2). https://doi.org/10.1061/(ASCE)0733-9496(2008)134:2(95).
Marcé, R., Ruiz, C., Armengol, J., 2008. Using spatially distributed parameters and multi-response objective functions to solve parameterization of complex applications of semi-distributed hydrological models. Water Resour. Res. 44 (2) https://doi.org/10.1029/2006WR005785.
McLennan, M., Kennell, R., 2010. HUBzero: a platform for dissemination and collaboration in computational science and engineering. Comput. Sci. Eng. 12 (2) https://doi.org/10.1109/MCSE.2010.41.
Mengistu, A., van Rensburg, L., Woyessa, Y., 2019. Techniques for calibration and validation of SWAT model in data scarce arid and semi-arid catchments in South Africa. J. Hydrol.: Reg. Stud. 25 https://doi.org/10.1016/j.ejrh.2019.100621.
Monteil, C., Zaoui, F., Le Moine, N., Hendrickx, F., 2020. Multi-objective calibration by combination of stochastic and gradient-like parameter generation rules – the caRamel algorithm. Hydrol. Earth Syst. Sci. 24 https://doi.org/10.5194/hess-24-3189-2020.
Moriasi, D., 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. Transactions of the ASABE 50 (3). https://doi.org/10.13031/2013.23153.
Morsy, M., Goodall, J., Castronova, A., Dash, P., Merwade, V., Sadler, J., Rajib, A., Horsburgh, J., Tarboton, D., 2017. Design of a metadata framework for environmental models with an example hydrologic application in HydroShare. Environ. Model. Software 93. https://doi.org/10.1016/j.envsoft.2017.02.028.
NCAR, 2019. Overview of National Water Model Calibration General Strategy & Optimization. National Center for Atmospheric Research, United States. Available online at: https://ral.ucar.edu/sites/default/files/public/9_RafieeiNasab_CalibOverview_CUAHSI_Fall019_0.pdf. (Accessed 12 July 2022).
Nijzink, R., Almeida, S., Pechlivanidis, I.G., Capell, R., Gustafssons, D., et al., 2018. Constraining conceptual hydrological models with multiple information sources. Water Resour. Res. 54 (10) https://doi.org/10.1029/2017WR021895.
Ozdemir, A., Leloglu, U., 2019. A fast and automated hydrologic calibration tool for SWAT. Water Environ. J. 33 (4) https://doi.org/10.1111/wej.12419.
Parker, J., Donnellan, A., Glasscoe, M., Fox, G., Wang, J., Pierce, M., Ma, Y., 2015. Advantages to geoscience and disaster response from QuakeSim implementation of interferometric radar maps in a GIS database system. Pure Appl. Geophys. 172 (8) https://doi.org/10.1007/s00024-014-0886-8.
Paul, M., Negahban-Azar, M., 2018. Sensitivity and uncertainty analysis for streamflow prediction using multiple optimization algorithms and objective functions: san Joaquin Watershed, California. Model. Earth Syst. Environ. 4 https://doi.org/10.1007/s40808-018-0483-4.
Peckham, S., Hutton, E., Norris, B., 2013. A component-based approach to integrated modeling in the geosciences: the design of CSDMS. Comput. Geosci. 53 https://doi.org/10.1016/j.cageo.2012.04.002.
Peckham, S., Goodall, J., 2013. Driving plug-and-play models with data from web services: a demonstration of interoperability between CSDMS and CUAHSI-HIS. Comput. Geosci. 53 https://doi.org/10.1016/j.cageo.2012.04.019.
Rajib, A., Liu, Z., Merwade, V., Tavakoly, A., Follum, M., 2020a. Towards a large-scale locally relevant flood inundation modeling framework using SWAT and LISFLOOD-FP. J. Hydrol. 581 https://doi.org/10.1016/j.jhydrol.2019.124406.
Rajib, A., Golden, H., Lane, C., 2020b. Surface depression and wetland water storage improves major river basin hydrologic predictions. Water Resour. Res. 56 (7) https://doi.org/10.1029/2019WR026561.
Rajib, A., Evenson, G.R., Golden, H.E., Lane, C.R., 2018a. Hydrologic model predictability improves with spatially explicit calibration using remotely sensed evapotranspiration and biophysical parameters. J. Hydrol. 567 https://doi.org/10.1016/j.jhydrol.2018.10.024.
Rajib, A., Merwade, V., Zhiqiang, Yu, 2018b. Rationale and efficacy of assimilating remotely sensed potential evapotranspiration for reduced uncertainty of hydrologic models. Water Resour. Res. 54 https://doi.org/10.1029/2017WR021147.
Rajib, A., Merwade, V., Kim, I.L., Zhao, L., Song, C., Zhe, S., 2016. SWATShare – A Web Platform for Collaborative Research and Education through Online Sharing, Simulation and Visualization of SWAT Models, vol. 75. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2015.10.032.
Sadler, J., Goodall, J., Behl, M., Morsy, M., Culver, T., Bowes, B., 2019. Leveraging open source software and parallel computing for model predictive control of urban drainage systems using EPA-SWMM5. Environ. Model. Software 120. https://doi.org/10.1016/j.envsoft.2019.07.009.
Samadi, S., Pourreza-Bilondi, M., Wilson, C.A.M.E., Hitchcock, B.D., 2020. Bayesian model averaging with fixed and flexible priors: theory, concepts, and calibration experiments for rainfall-runoff modeling. AGU Journal of Advances in Modeling Earth Systems 12. https://doi.org/10.1029/2019MS001924.
Skahill, B., Downer, C., Baggett, J., 2012. A Practical Guide to Calibration of a GSSHA Hydrologic Model Using ERDC Automated Model Calibration Software -efficient Local Search. US Army Corps of Engineers. ERDC/CHL TR-12-3.
Skahill, B., Baggett, J., Frankenstein, S., Downer, C., 2009. More efficient PEST compatible model independent model calibration. Environ. Model. Software 24. https://doi.org/10.1016/j.envsoft.2008.09.011.
Tarboton, D., Idaszak, R., Horsburgh, J.S., Ames, D., Goodall, J., 2018. HydroShare: A Platform for Collaborative Data and Model Sharing in Hydrology. HydroShare. http://www.hydroshare.org/resource/1785fd9bb6714b29846c7dac4911f3b8.
Tang, Y., Reed, P., Wagener, T., 2006. How effective and efficient are multiobjective evolutionary algorithms at hydrologic model calibration? Hydrol. Earth Syst. Sci. 10 https://doi.org/10.5194/hess-10-289-2006.
Tsai, W.-P., Feng, D., Pan, M., Beck, H., Lawson, K., et al., 2021. From calibration to parameter learning: harnessing the scaling effects of big data in geoscientific modeling. Nat. Commun. 5988 https://doi.org/10.1038/s41467-021-26107-z.
USGS, 2022. US Geological Survey REST. Available online at: https://waterservices.usgs.gov/rest. (Accessed 14 July 2022).
van Griensven, A., Bauwens, W., 2003. Multiobjective autocalibration for semidistributed water quality models. Water Resour. Res. 39 (2) https://doi.org/10.1029/2003WR002284.
Van Liew, M., Arnold, J.G., Bosch, D.D., 2005. Problems and potential of autocalibrating a hydrologic model. Transactions of the ASAE 48 (3). https://doi.org/10.13031/2013.18514.
Voinov, A., Costanza, R., 1999. Watershed management and the web. J. Environ. Manag. 56 (4) https://doi.org/10.1006/jema.1999.0281.
Wang, Y., Brubaker, K., 2015. Multi-objective Model Auto-Calibration and Reduced Parameterization: Exploiting Gradient-Based Optimization Tool for a Hydrologic Model, vol. 70. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2015.04.001.
Warmerdam, F., Rouault, E., et al., 2022. GDAL Documentation. Code available at. https://doi.org/10.5281/zenodo.6352176. Available online at. https://gdal.org/gdal.pdf (Accessed 18 July 2022).
Wi, S., Ray, P., Demaria, E., Steinschneider, S., Brown, C., 2017. A user-friendly software package for VIC hydrologic model development. Environ. Model. Software 98. https://doi.org/10.1016/j.envsoft.2017.09.006.
Wilkinson, M., Dumontier, M., Aalbersberg, I., et al., 2016. The FAIR Guiding Principles for scientific data management and stewardship. Nature Scientific Data 3. https://doi.org/10.1038/sdata.2016.18.
Wu, H., Chen, B., Ye, X., et al., 2021. An improved calibration and uncertainty analysis approach using a multicriteria sequential algorithm for hydrological modeling. Nature Scientific Report 11, 16954. https://doi.org/10.1038/s41598-021-96250-6.
Wu, Y., Li, T., Sun, L., Chen, J., 2013. Parallelization of a hydrological model using the message passing interface. Environ. Model. Software 43. https://doi.org/10.1016/j.envsoft.2013.02.002.
Wu, Y., Liu, S., 2014. Improvement of the R-SWAT-FME framework to support multiple variables and multi-objective functions. Sci. Total Environ. 466–467. https://doi.org/10.1016/j.scitotenv.2013.07.048.
Wu, Y., Liu, S., 2012. Automating Calibration, Sensitivity and Uncertainty Analysis of Complex Models Using the R Package Flexible Modeling Environment (FME): SWAT as an Example, vol. 31. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2011.11.013.
Xie, K., Liu, P., Zhang, J., Wang, G., Zhang, X., Zhou, L., 2021. Identification of spatially distributed parameters of hydrological models using the dimension-adaptive key grid calibration strategy. J. Hydrol. 598 https://doi.org/10.1016/j.jhydrol.2020.125772.
Xu, X., Li, J., Tolson, B., 2014. Progress in integrating remote sensing data and hydrologic modeling. Prog. Phys. Geogr.: Earth Environ. 38 (4) https://doi.org/10.1177/0309133314536583.
Yang, Y., Pan, M., Beck, H., Fisher, C., Beighley, R.E., Kao, S.-C., Hong, Y., Wood, E., 2019. In quest of calibration density and consistency in hydrologic modeling: distributed parameter calibration against streamflow characteristics. Water Resour. Res. 55 (9) https://doi.org/10.1029/2018WR024178.
Yang, J., Reichert, P., Abbaspour, K., Xia, J., Yang, H., 2008. Comparing uncertainty analysis techniques for a SWAT application to the Chaohe Basin in China. J. Hydrol. 358 https://doi.org/10.1016/j.jhydrol.2008.05.012.
Yu, Q.-Y., Bagas, L., Yang, P.-H., Zhang, D., 2019. GeoPyTool: a cross-platform software solution for common geological calculations and plots. Geosci. Front. 10 (4) https://doi.org/10.1016/j.gsf.2018.08.001.
Zamani, M., Shrestha, N., Akhtar, T., Boston, T., Daggupati, P., 2021. Advancing model calibration and uncertainty analysis of SWAT models using cloud computing infrastructure: LCC-SWAT. J. Hydroinf. 23 (1) https://doi.org/10.2166/hydro.2020.066.
Zambrano-Bigiarini, 2020. Goodness-of-Fit Functions for Comparison of Simulated and Observed Hydrological Time Series. Code available at: https://github.com/hzambran/hydroGOF. (Accessed 18 July 2022).
Zeng, S., Du, H., Xia, J., 2020. Development of an interface-oriented add-in modeling framework for integrated water system simulation and its application. Environ. Model. Software 134. https://doi.org/10.1016/j.envsoft.2020.104840.
Zhang, F., Chen, M., Kettner, A., Ames, D.P., Harpham, Q., et al., 2021. Interoperability Engine Design for Model Sharing and Reuse Among OpenMI, BMI and OpenGMS-IS Model Standards, vol. 144. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2021.105164.
Zhang, F., Chen, M., Ames, D.P., Shen, C., et al., 2019. Design and Development of a Service-Oriented Wrapper System for Sharing and Reusing Distributed Geoanalysis Models on the Web, vol. 111. Environmental Modelling & Software. https://doi.org/10.1016/j.envsoft.2018.11.002.
Zhang, Y., Hou, J., Gu, J., Huang, C., Li, X., 2017. SWAT-based hydrological data assimilation system (SWAT-HDAS): description and case application to river basin-scale hydrological predictions. Water Resour. Res. 9 (8) https://doi.org/10.1002/2017MS001144.
Zhang, X., Beeson, P., Link, R., Manowitz, D., Izaurralde, R., et al., 2013. Efficient multi-objective calibration of a computationally intensive hydrologic model with parallel

computing software in Python. Environ. Model. Software 46. https://doi.org/10.1016/j.envsoft.2013.03.013.
Zhang, X., Izaurralde, R.C., Zong, Z., Zhao, K., Thomson, A., 2012. Evaluating the efficiency of a multi-core aware multi-objective optimization tool for calibrating the SWAT model. Transactions of the ASABE 55 (5). https://doi.org/10.13031/2013.42363.
Zhu, D., Echendu, S., Xuan, Y., Webster, M., Cluckie, I., 2016. Coupled hydro-meteorological modelling on a HPC platform for high-resolution extreme weather impact study, Hydrol. Earth Syst. Sci. 20 https://doi.org/10.5194/hess-20-4707-2016.