2023 CESM Workshop
Land Model Working Group

Improving the hydrological performance of CTSM through parameter optimization and large-sample watershed modeling

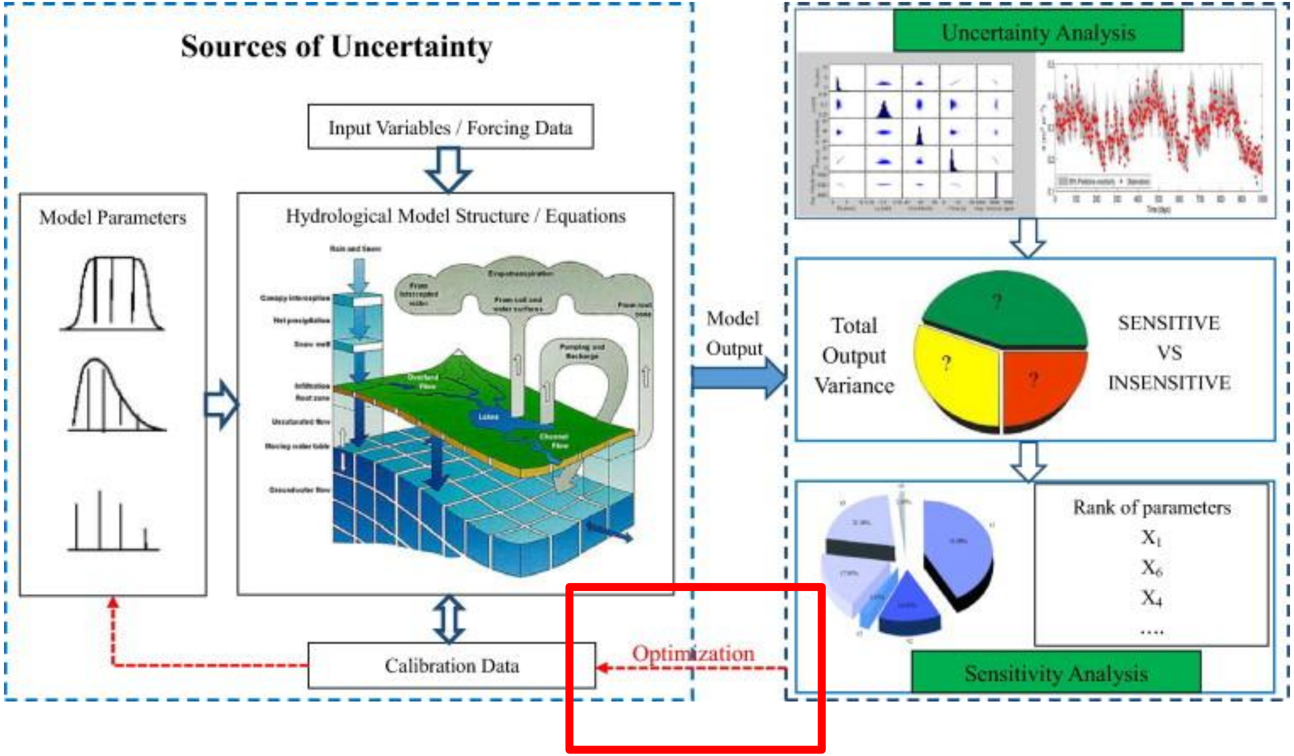
Guoqiang Tang, Andy Wood, Sean Swenson
CGD/TSS, NCAR

NCAR

June 12, 2023

Using a model to represent real-world hydrology

- Model representations require choices of model structure and physics (parameterizations) and depend on specification of inputs: forcings and parameter values.
- These modeling choices and input specifications are inherently uncertain … *a long-standing challenge*



Song et al, 2015

Different communities approach this challenge differently

The **earth system modeling** community advances model *fidelity* through:

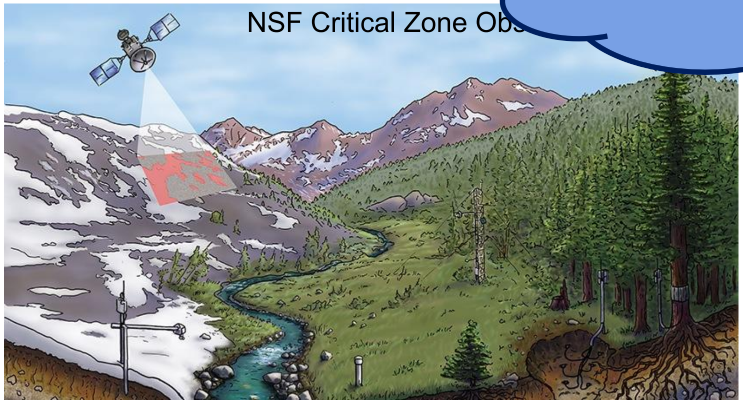
- improving observational analyses to better estimate inputs (forcings, parameters, structure)
- using observational studies to refine parameterizations (physics)
- increasing complexity of process representation
- **philosophy**: *we can eventually re[...] everything through better obser[...] improvement*

The **applied hydrological modeling** community advances model *performance* through:

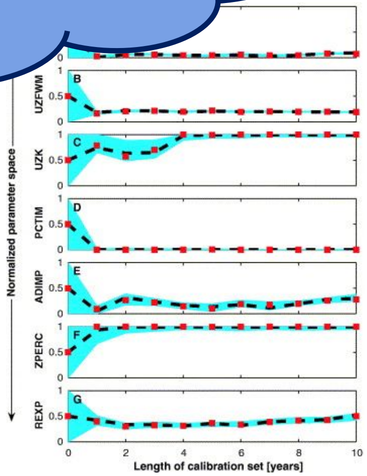
- improving observational analyses to better estimate inputs (forcings, parameters)
- optimization of model parameters and structure given the existing parameterizations
- [...]rovement of physics -- but only as needed
- [...] *we will never represent everything but [...]timize what we don't know*

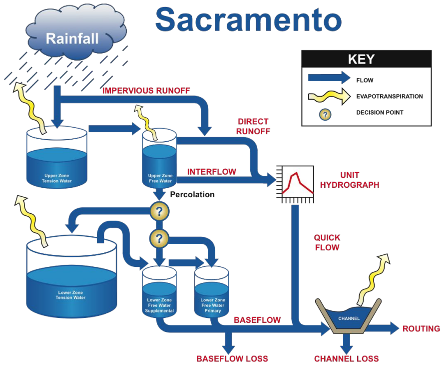
This project brings an applied hydrology mindset to the ESM development context

NSF Critical Zone Obs[...]



https://www.nsf.gov/news/newsmedia/ENV-discoveries/CZO-discovery-series.jsp





Applied ESM-based modeling seeks both realism and hydrologic performance

A number of new water security related projects are exploring the use of CTSM as a process/physics advance over more common or traditional ‘applied hydrology’ models

- climate change studies – land modeling uncertainty is a key component (Lehner et al., 2019)
- flood, drought, and hydrologic prediction applications – supporting water management agency missions

This presentation describes initial work supporting a climate change project sponsored by USACE*

Overarching goal

- develop land models that can represent current hydrology (performance) as well as climate change impacts on hydrology (fidelity) in both coupled and offline context

Immediate goal

- develop CTSM configurations and parameter sets that perform well for hydrology – and with robust climate-hydrology sensitivities

First steps

- use common parameter estimation approaches from applied hydrological modeling for CTSM
- develop a large-sample small-watershed CTSM implementation *testbed* for investigating parameter estimation and configuration strategies (US-focused, for now)

SPONSOR: US Army Corps of Engineers (USACE) – Climate Preparedness and Resilience Program

Hydrologic model parameter estimation

- A decades-old practice in applied hydrology with many algorithms and much theory (geo-informatics)
- Multiple available multi-method packages for parameter sensitivity assessment and optimization exist

Mathematical and statistical methods to help scientists and engineers assess and improve the accuracy of computational models

DAKOTA

Explore and predict with confidence

https://dakota.sandia.gov/

v17

OSTRICH - Optimization Software Toolkit

OSTRICH, developed by L. Shawn Matott, is a model-independent multi-algorithm paralell-friendly optimization and parameter estimation tool that implements numerous model-independent optmization and calibration (parameter estimation) algorithms,

http://www.civil.uwaterloo.ca/envmodelling/Ostrich.html

MO-ASMO

Water Resources Research

Research Article | Open Access

Multiobjective adaptive surrogate modeling-based optimization for parameter estimation of large, complex geophysical models

Wei Gong, Qingyun Duan, Jianduo Li, Chen Wang, Zhenhua Di, Aizhong Ye, Chiyuan Miao, Yongjiu Dai

https://agupubs.onlinelibrary.wiley.com/doi/full/10.1002/2015WR018230

Welcome to SPOTPY SPOTPY

A Statistical Parameter Optimization Tool for Python

https://spotpy.readthedocs.io/en/latest/

PEST

Model Independent Parameter Estimation & Uncertainty Analysis

https://pesthomepage.org/

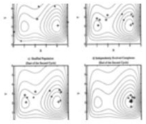
e.g., MCMC

Review | Open Access | Published: 29 May 2020

A survey of Monte Carlo methods for parameter estimation

David Luengo, Luca Martino, Mónica Bugallo, Víctor Elvira & Simo Särkkä

EURASIP Journal on Advances in Signal Processing **2020**, Article number: 25 (2020) | Cite this article



Shuffled Complex Evolution (SCE-UA) Method

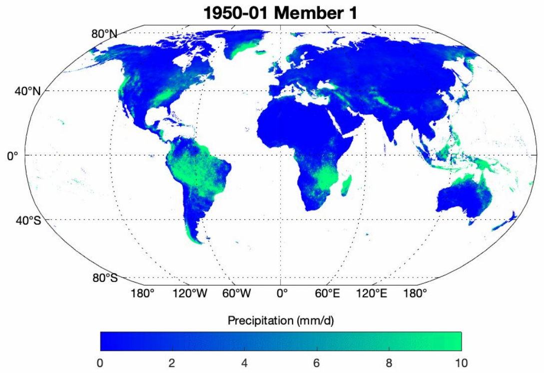
Version 1.0.0.0 (420 KB) by Qingyun Duan

An efficient and robuse global optimization method.

Duan et al, WRR, 1992

An example of large-sample watershed hydrological modeling

EM-Earth ensemble meteorological dataset



Three types of datasets

A. deterministic_raw_daily

B. deterministic_hourly

C. probabilistic_daily (25 members)

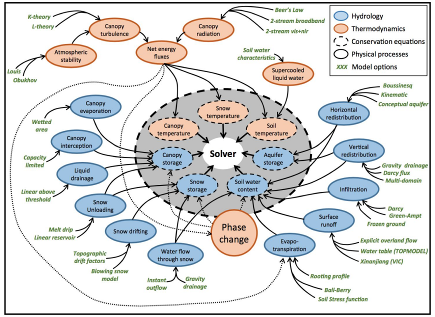
Tang et al., 2022, BAMS

***Dataset**:*

https://doi.org/10.20383/102.0547

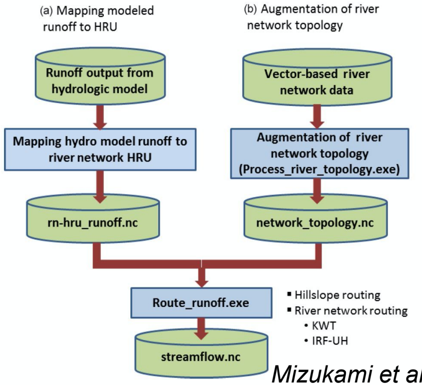
+

SUMMA hydrological model



A schematic of SUMMA's framework, often referred to as the horrendogram by SUMMA's developers, illustrates how SUMMA supports multiple options for a range of physical processes integrated with a common numerical solver, see [Clark et al. 2015a,b] for details.

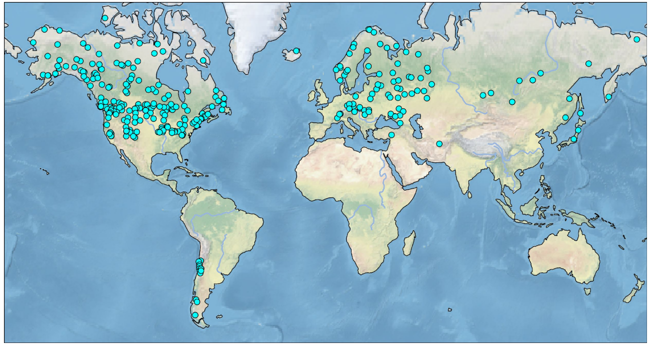
mizuRoute routing model



Mizukami et al., 2016

+

289 representative cryosphere basins



Basins are selected from a global database of ~19,000 basins:

- Basin clustering
  - ✔ k-means clustering
- Define basic basin requirements
  - ✔ Area
  - ✔ Period
  - ✔ Human impact
  - ✔ Snow
- Basin selection:
  - ✔ Space window-based selection

Tang et al., 2023

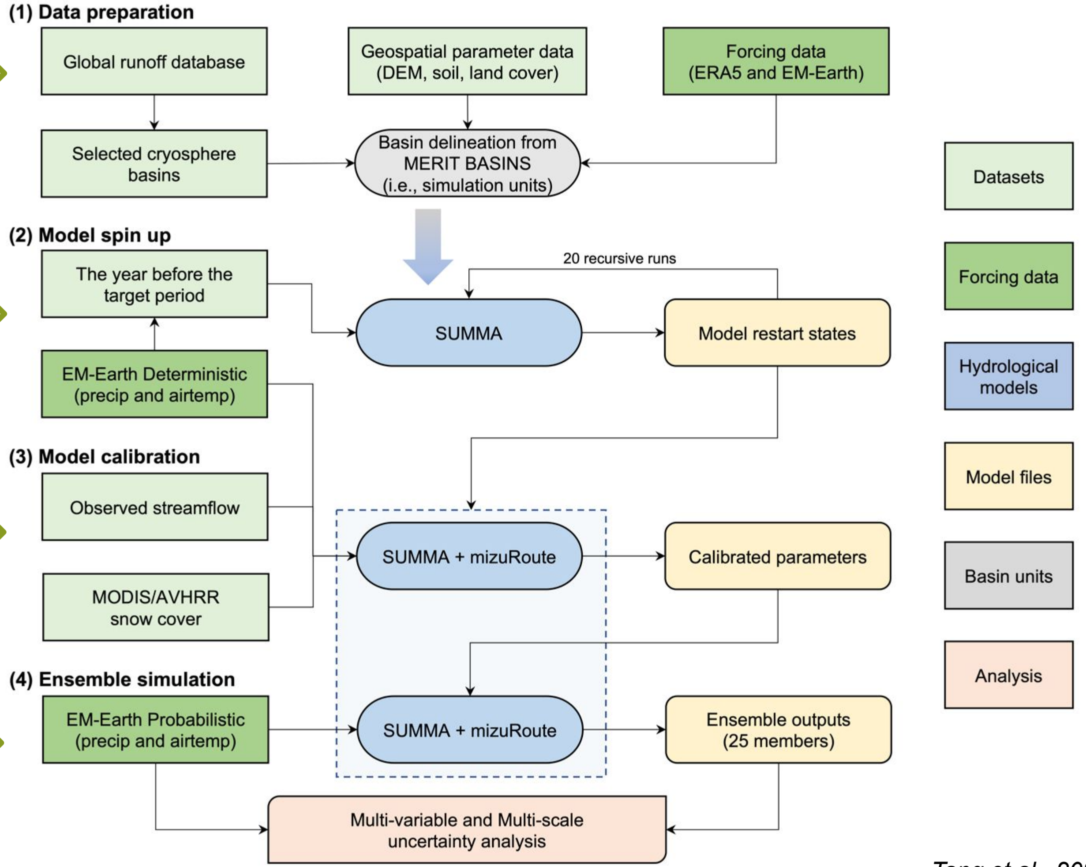
An example of large-sample watershed hydrological modeling

(1) Data preparation
- Streamflow data, geospatial parameter data, forcing data, MODIS/AVRHRR snow cover data.

(2) Spin up
- SUMMA is recursively run 20 times using forcing in the year before the calibration period.

(3) Calibration
- SUMMA/mizuRoute is calibrated using streamflow and MODIS/AVHRR snow cover data.

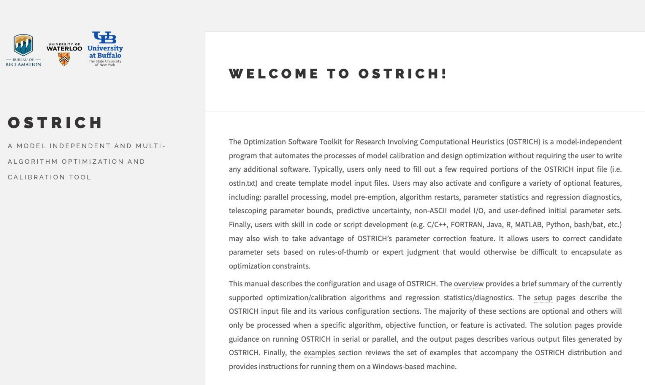
(4) Ensemble simulation
- EM-Earth probabilistic estimates from 25 members are used to drive SUMMA/mizuRoute during the validation period.



Tang et al., 2023

An example of large-sample watershed hydrological modeling

Ostrich calibration tool


WELCOME TO OSTRICH!

OSTRICH

A MODEL INDEPENDENT AND MULTI-ALGORITHM OPTIMIZATION AND CALIBRATION TOOL

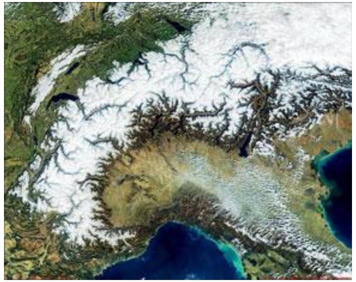
The Optimization Software Toolkit for Research Involving Computational Heuristics (OSTRICH) is a model-independent program that automates the processes of model calibration and design optimization without requiring the user to write any additional software. Typically, users only need to fill out a few required portions of the OSTRICH input file (i.e. ostIn.txt) and create template model input files. Users may also activate and configure a variety of optional features, including: parallel processing, model pre-emption, algorithm restarts, parameter statistics and regression diagnostics, telescoping parameter bounds, predictive uncertainty, non-ASCII model I/O, and user-defined initial parameter sets. Finally, users with skill in code or script development (e.g. C/C++, FORTRAN, Java, R, MATLAB, Python, bash/bat, etc.) may also wish to take advantage of OSTRICH's parameter correction feature. It allows users to correct candidate parameter sets based on rules-of-thumb or expert judgment that would otherwise be difficult to encapsulate as optimization constraints.

This manual describes the configuration and usage of OSTRICH. The overview provides a brief summary of the currently supported optimization/calibration algorithms and regression statistics/diagnostics. The setup pages describe the OSTRICH input file and its various configuration sections. The majority of these sections are optional and others will only be processed when a specific algorithm, objective function, or feature is activated. The solution pages provide guidance on running OSTRICH in serial or parallel, and the output pages describes various output files generated by OSTRICH. Finally, the examples section reviews the set of examples that accompany the OSTRICH distribution and provides instructions for running them on a Windows-based machine.

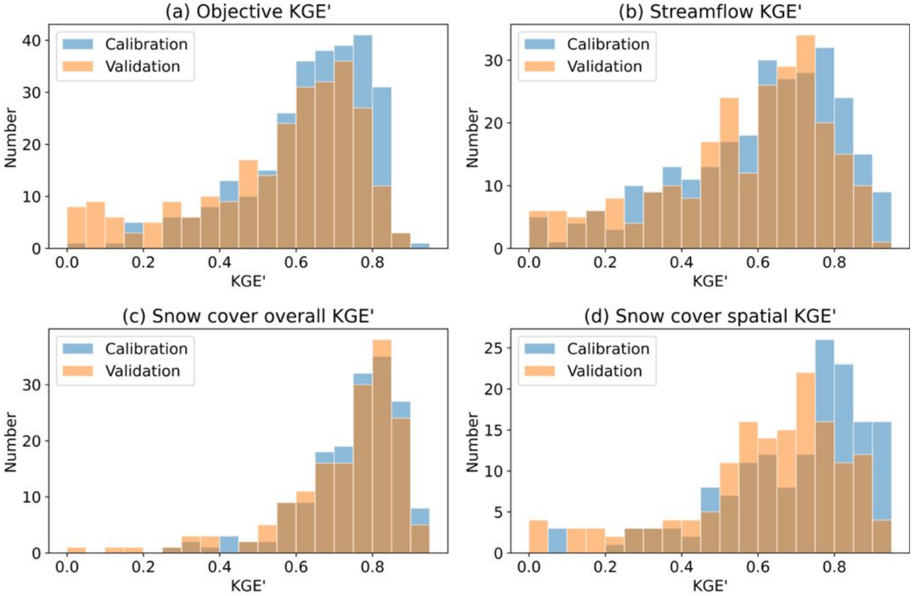
https://usbr.github.io/ostrich

Streamflow measurement

Remote sensing snow cover

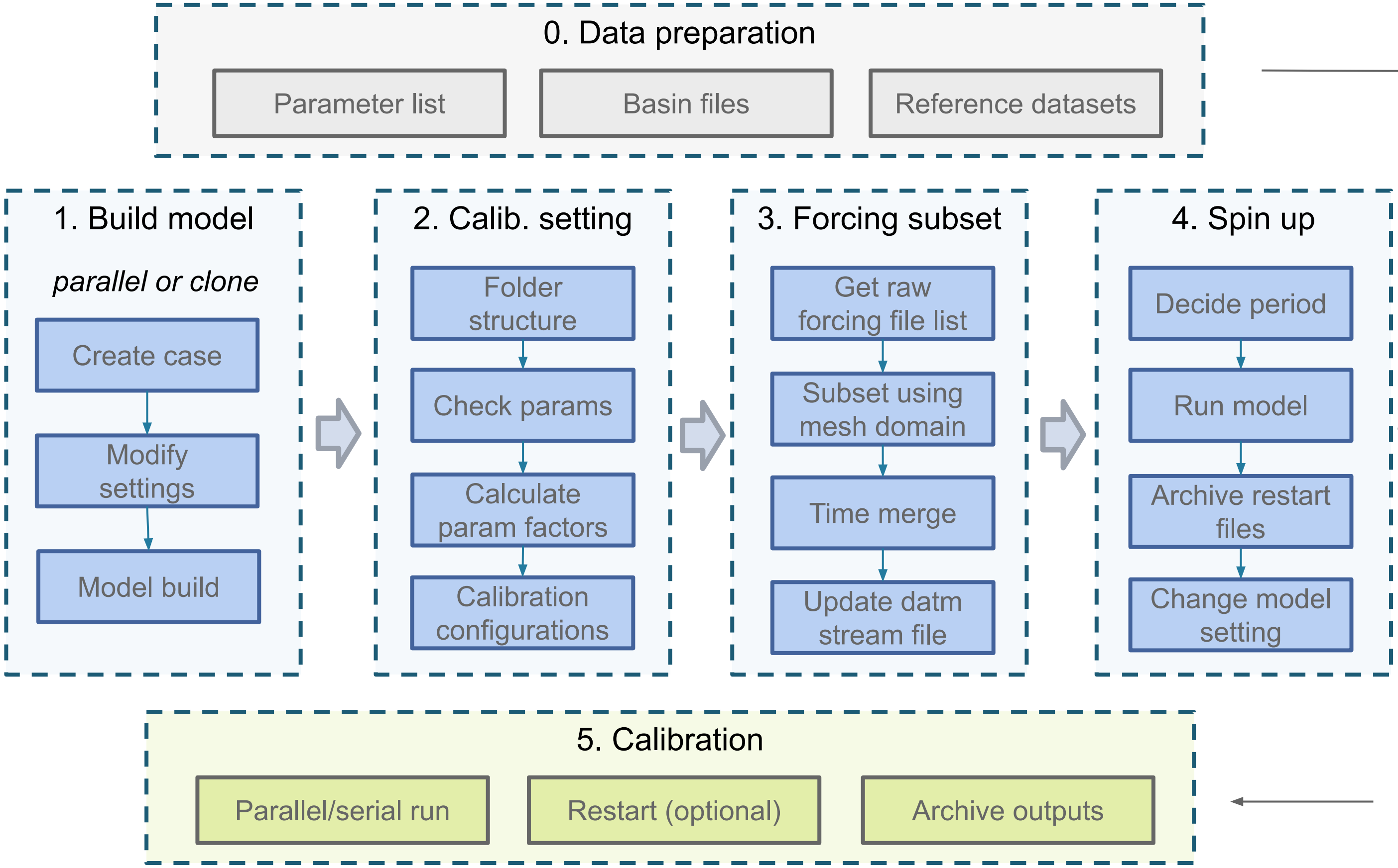


The calibration design is to preliminarily constrain the a-priori parameters and approach the behavioral parameter space rather than achieve optimal parameter estimation. But we still obtain substantial performance improvement after the limited calibration. The median objective KGE' values are 0.66 and 0.60 in the calibration and validation periods, respectively.



Tang et al., 2023

A CTSM Parameter Optimization Workflow



- Dataset dependent

- Python
- Configuration file
- Automatic workflow

All data and settings can be generated by submitting one job.

Tools:
*** Ostrich**
* MO-ASMO (new)
* ML/DL (next)

A CTSM Parameter Optimization Workflow

0. Data preparation

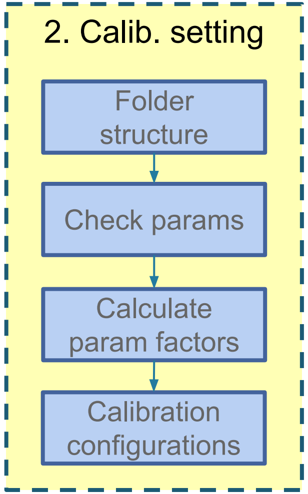
Parameter list | Basin files | Reference datasets

The parameters are selected based on expert identification of key hydrological processes/controls, with added perspective/confirmation from the PPE results.

1	Parameter	Default	Lower	Upper	Source	Method	Type	Binding
2	vcmaxha	72000	20000	250000	Param	Multiplicative	Hydrology	None
3	om_frac_sf	1	0.25	2	Param	Multiplicative	Hydrology	None
4	slopebeta	-3	-10	-0.5	Param	Multiplicative	Hydrology	None
5	fff	0.5	0.01	10	Param	Multiplicative	Hydrology	None
6	e_ice	6	1	8	Param	Multiplicative	Hydrology	None
7	liq_canopy_storage_scalar	0.1	0.025	4	Param	Multiplicative	Hydrology	None
8	baseflow_scalar	Default	0.0005	0.1	Namelist	Multiplicative	Hydrology	None
9	FMAX	Default	0.2	0.8	Surfdata	Multiplicative	Hydrology	None
10	hksat_sf	Default	0.9	9	Param	Multiplicative	Hydrology	None
11	krmax	1.22E-09	5.83E-11	6.90E-09	Param	Multiplicative	Plant hydrau	None
12	d_max	15	5	100	Param	Multiplicative	Stomatal resi	None
13	frac_sat_soil_dsl_init	0.8	0.25	2	Param	Multiplicative	Stomatal resi	None
14	cv	0.01	0.0025	0.04	Param	Multiplicative	Stomatal resi	None
15	a_coef	0.13	0.05	0.15	Param	Multiplicative	Stomatal resi	None
16	upplim_destruct_metamorph	175	10	500	Namelist	Multiplicative	Snow Proces	None
17	n_melt_coef	200	25	600	Param	Multiplicative	Snow Proces	None
18	medlynintercept	100	1	20000	Param	Multiplicative	Stomatal resi	None
19	precip_repartition_nonglc_all_rain_t	2	0	4	Namelist	Additive	Hydrology	precip_repart

- Parameters in parameter netcdf, surface data netcdf, and namelist text files are supported
- Multiplicative and additive factors are supported
- Binding parameters will use the same factors.
- Default and Type are optional.

A CTSM Parameter Optimization Workflow



The Optimization Software Toolkit for Research Involving Computational Heuristics (**OSTRICH**) is a model-independent program that automates the processes of model calibration and design optimization without requiring the user to write any additional software.

Global search algorithms implemented within OSTRICH

Acronym	Algorithm	# Objectives	Serial?*	Parallel?	Warm Start?	Pre-Emption?	Parameter Correction?	List of Initial Parameters?	Math and Stats?	Line Search?	Reference or Contact Information
APPSO	Asynchronous Parallel Particle Swarm Optimization	1		■	■	■	■	■			(Venter and Sobieszczanski-Sobieski, 2006)
BEERS	Balanced Exploration-Exploitation Random Search	1	■		■						lsmatott@buffalo.edu
BGA	Binary-coded Genetic Algorithm	1	■	■	■		■	■			(Yoon and Shoemaker, 1999)
CSA	Combinatorial Simulated Annealing	1	■		■						(Kirkpatrick *et al.*, 1983)
DDDS	Discrete DDS	1	■		■	■					(Tolson *et al.*, 2009)
DDS	Dynamically Dimensioned Search	1	■		■	■	■				(Tolson and Shoemaker, 2007)
PDDS	Asynchronous Parallel DDS	1		■	■	■	■	■			(Tolson *et al.*, 2014)
PSO	Particle Swarm Optimization	1	■	■	■	■	■	■			(Beielstein *et al.*, 2002; Kennedy *et al.*, 2001; Kennedy and Eberhart, 1995)
RGA	Real-coded Genetic Algorithm	1	■	■	■		■	■			(Yoon and Shoemaker, 2001)
SA	Simulated Annealing	1	■	■	■		■				(Dougherty and Marryott, 1991; Marryott *et al.*, 1993)
SCE	Shuffled Complex Evolution	1	■		■		■				(Duan *et al.*, 1993; Duan *et al.*, 1992)
SMPLR	Sampling Algorithm (Big Bang - Big Crunch)	1	■		■			■			(Erol and Eksin, 2006)
VSA	Vanderbilt-Louie Simulated Annealing	1	■	■	■		■				(Vanderbilt and Louie, 1984)

https://usbr.github.io/ostrich Matott et al., 2011, 2012

A CTSM Parameter Optimization Workflow

3. Forcing subset

- Get raw forcing file list
- Subset using mesh domain
- Time merge
- Update datm stream file

ctsmforc.NLDAS2.0.125d.v1.Prec.1980-01.nc
ctsmforc.NLDAS2.0.125d.v1.Prec.1980-02.nc
ctsmforc.NLDAS2.0.125d.v1.Prec.1980-03.nc
…
ctsmforc.NLDAS2.0.125d.v1.Prec.2018-12.nc

Raw forcing

subset_ctsmforc.NLDAS2.0.125d.v1.Prec.1980-01.nc
subset_ctsmforc.NLDAS2.0.125d.v1.Prec.1980-02.nc
subset_ctsmforc.NLDAS2.0.125d.v1.Prec.1980-03.nc
…
subset_ctsmforc.NLDAS2.0.125d.v1.Prec.2018-12.nc

Subsetting
- Effectively reduce time cost for regional studies

subset_ctsmforc.NLDAS2.0.125d.v1.Prec.1980-1984.nc
subset_ctsmforc.NLDAS2.0.125d.v1.Prec.1985-1989.nc
subset_ctsmforc.NLDAS2.0.125d.v1.Prec.1990-1994.nc
…
subset_ctsmforc.NLDAS2.0.125d.v1.Prec.2015-2018.nc

Time merging (month to X-years)
- Easier file management
- Avoid excess file numbers in some systems

Using large-sample watershed modeling to support learning and development

Benefits of large-sample watershed modeling

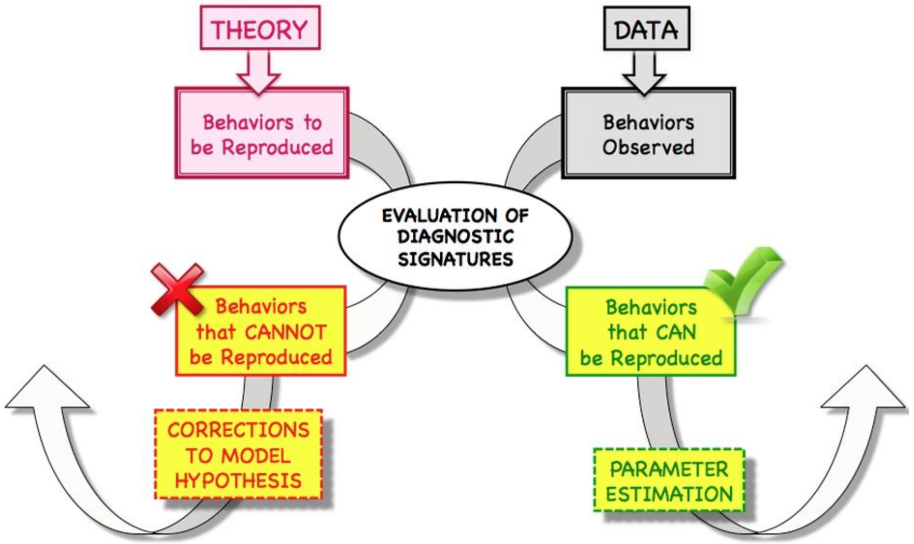
- **Improved accuracy**: Broad understanding of the model's performance, limitations and variability

- **Statistical robustness**: Increase the statistical robustness of the simulation and calibration results

- **Regional variations**: To identify and account for regional variations in model parameters and to test the generalizability of the model across different basins.

- **Improved understanding**: Reveal important relationships and dependencies between the model parameters, leading to a deeper understanding of the underlying hydrological processes.

- **Better representation**: A better representation of the diversity and variability of natural systems, enabling the assessment of the impacts of changes in a more comprehensive manner.

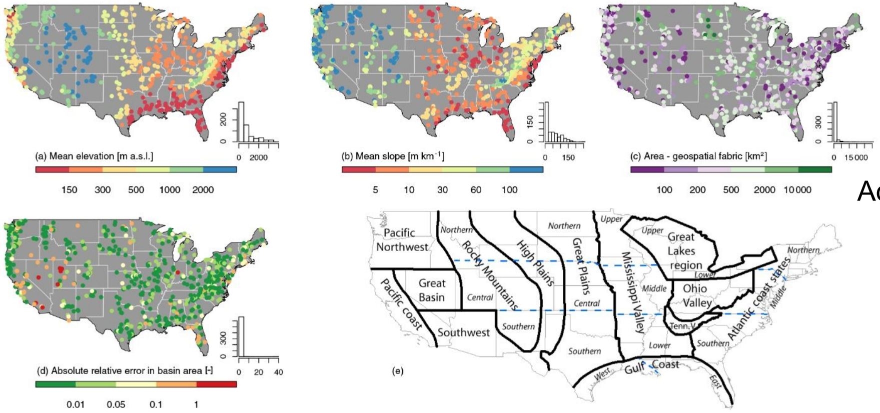


Gupta et al., Large-sample hydrology: a need to balance depth with breadth. HESS. 2014

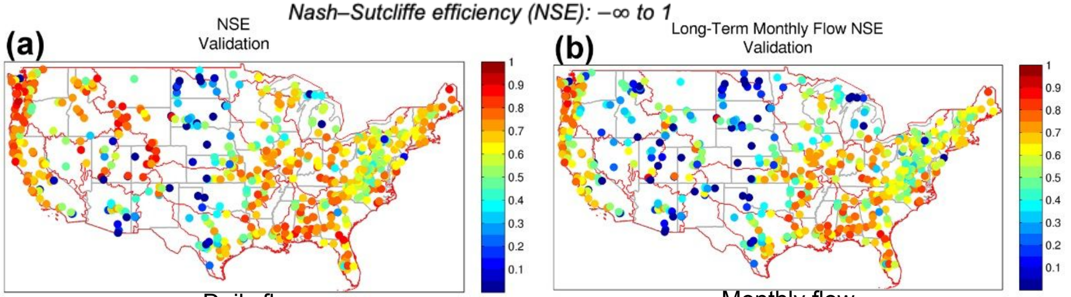
Large-sample watershed modeling using CTSM and CAMELS

CAMELS (Catchment Attributes and Meteorology for Large-sample Studies)

- A comprehensive set of catchment attributes, meteorological variables, streamflow observations, and model results for 671 US catchments
- Widely used in hydrology research to develop and evaluate hydrological models, variability and predictability
- Has been a central dataset in the global rise of machine learning in hydrology
- Has been extended in many countries by independent efforts
- Was originally developed in **NCAR RAL** to study streamflow predictability and model complexity



Addor et al., 2017

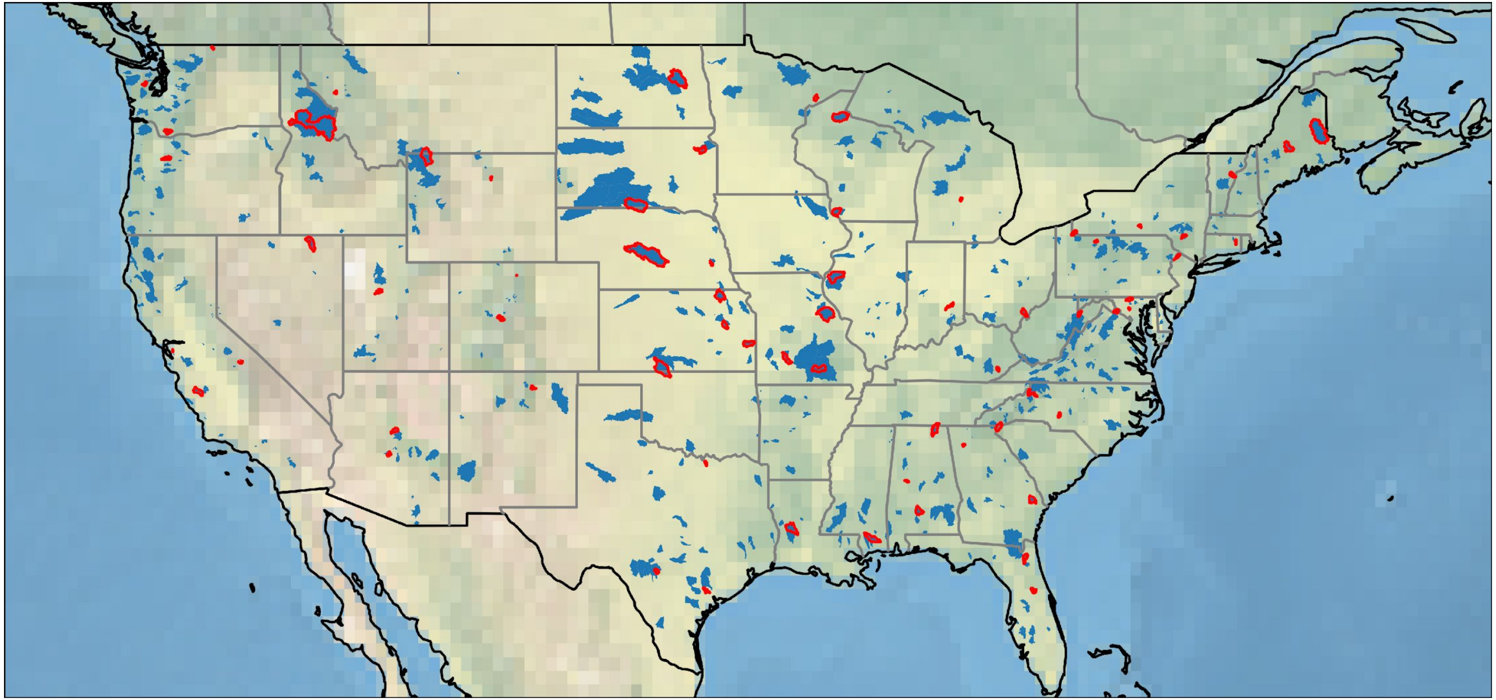


Daily flow

Monthly flow

Newman et al., 2015

Large-sample watershed modeling using CTSM and CAMELS



Blue: 671 CAMELS basins

Red: 10% randomly selected basins for this presentation.

- Each basin is simplified as a mesh grid to facilitate large-sample modeling.
- For nested basins (i.e., upstream VS downstream), the split strategy is adopted to subtract upstream basins from downstream basins because mesh grids cannot overlap.
- All the 671 basins of CAMELS will be used in the subsequent experiments.

Large-sample watershed modeling using CTSM and CAMELS

Modified Kling-Gupta Efficiency (KGE')
$-\infty$ *(worst) to 1* (best)

$$KGE' = 1 - \sqrt{(r-1)^2 + (\beta-1)^2 + (\gamma-1)^2}$$

Correlation coefficient | Bias ratio | Variability ratio

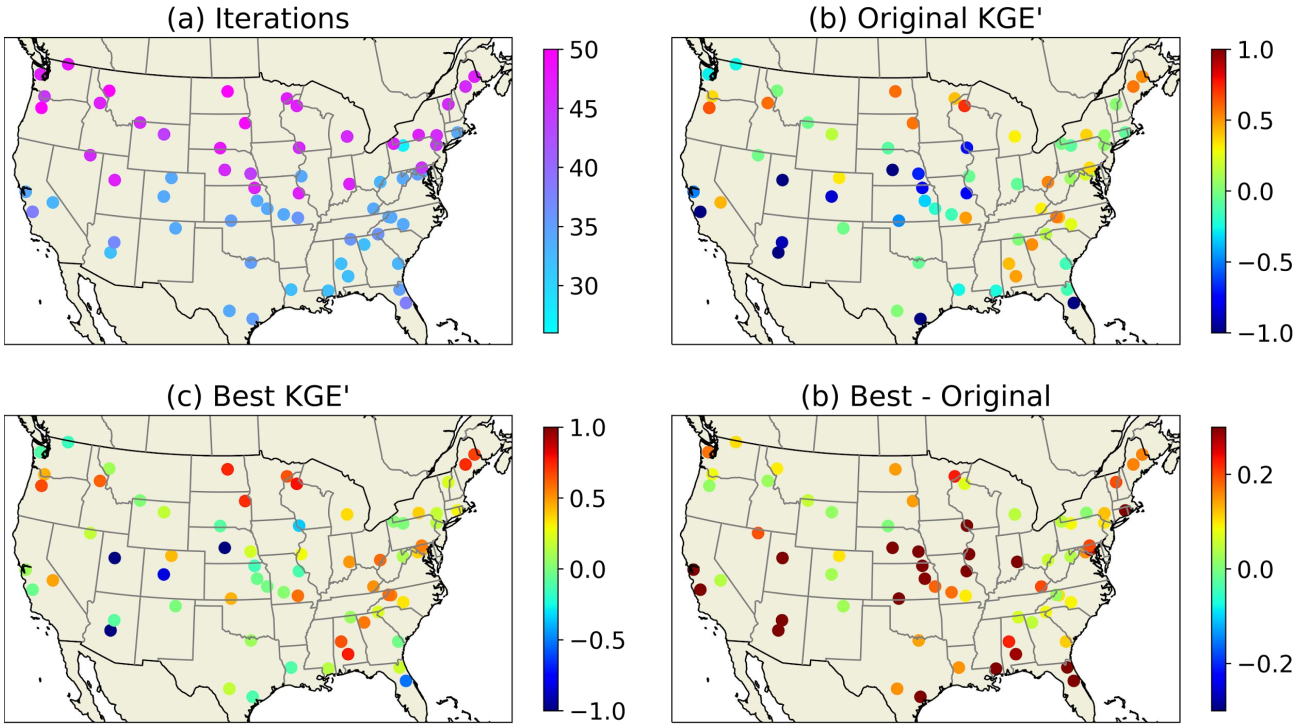
For the calibration period:

Computation

- 1 CPU and12 hours are allocated to each basin
- ~40 trials per basin, while normally hundreds of trials are needed to achieve ideal calibration

Results

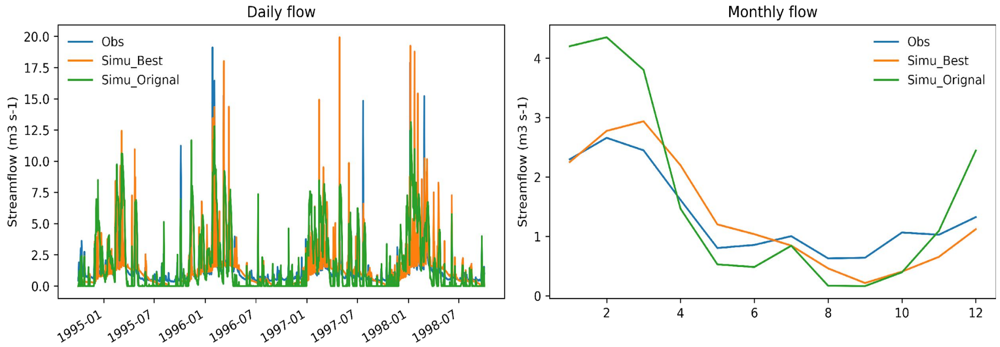
- KGE' increases in 66 out of 67 basins after calibration.
- The median KGE' increases from -0.01 to 0.17 after calibration.
- The median/mean of "Best - Original" KGE' is 0.15/0.53.



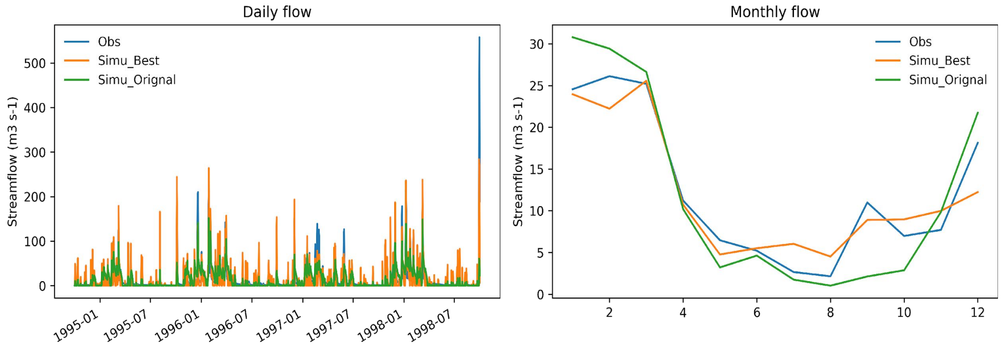
Prelim. testing on 10% of CAMELS basins

Large-sample watershed modeling using CTSM and CAMELS

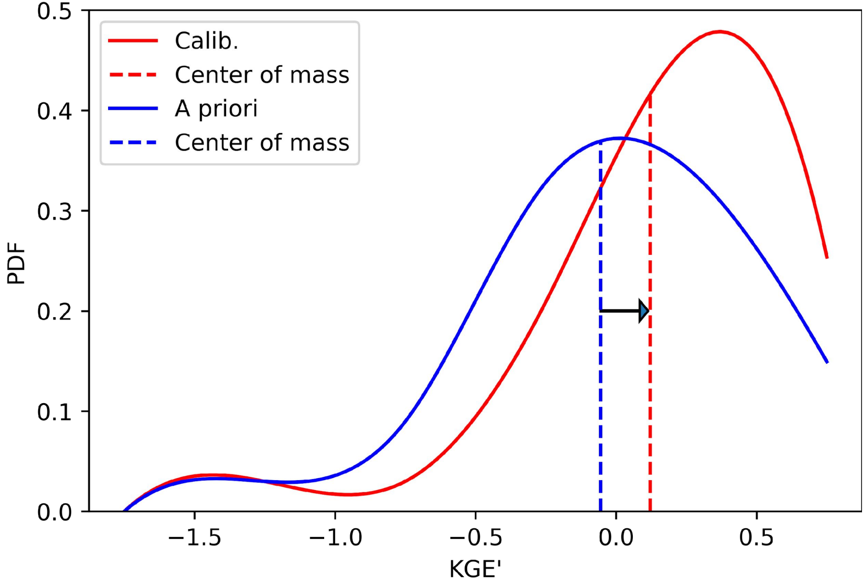
Example-1: 02465493 KGE’: 0.43 -> 0.64



Example-2: 02427250 KGE’: 0.48 -> 0.76

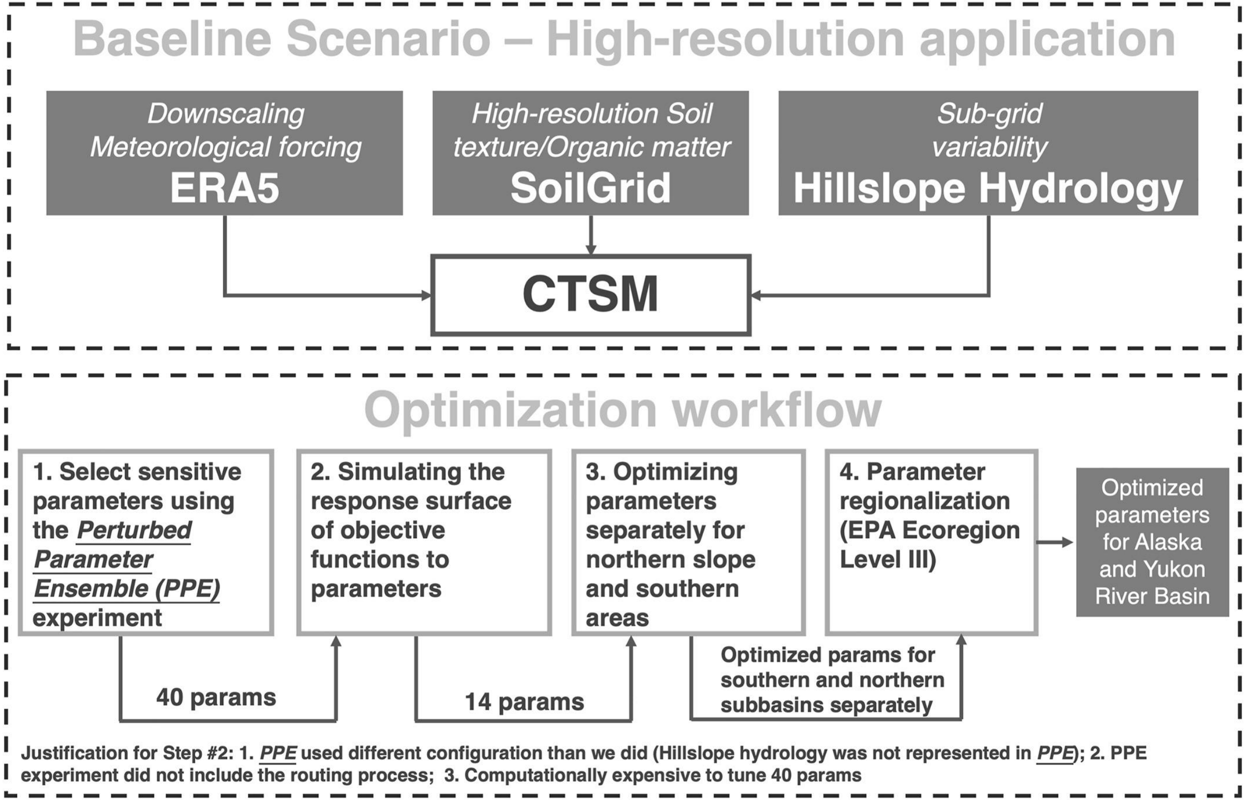


KGE’ PDF shift after calibration



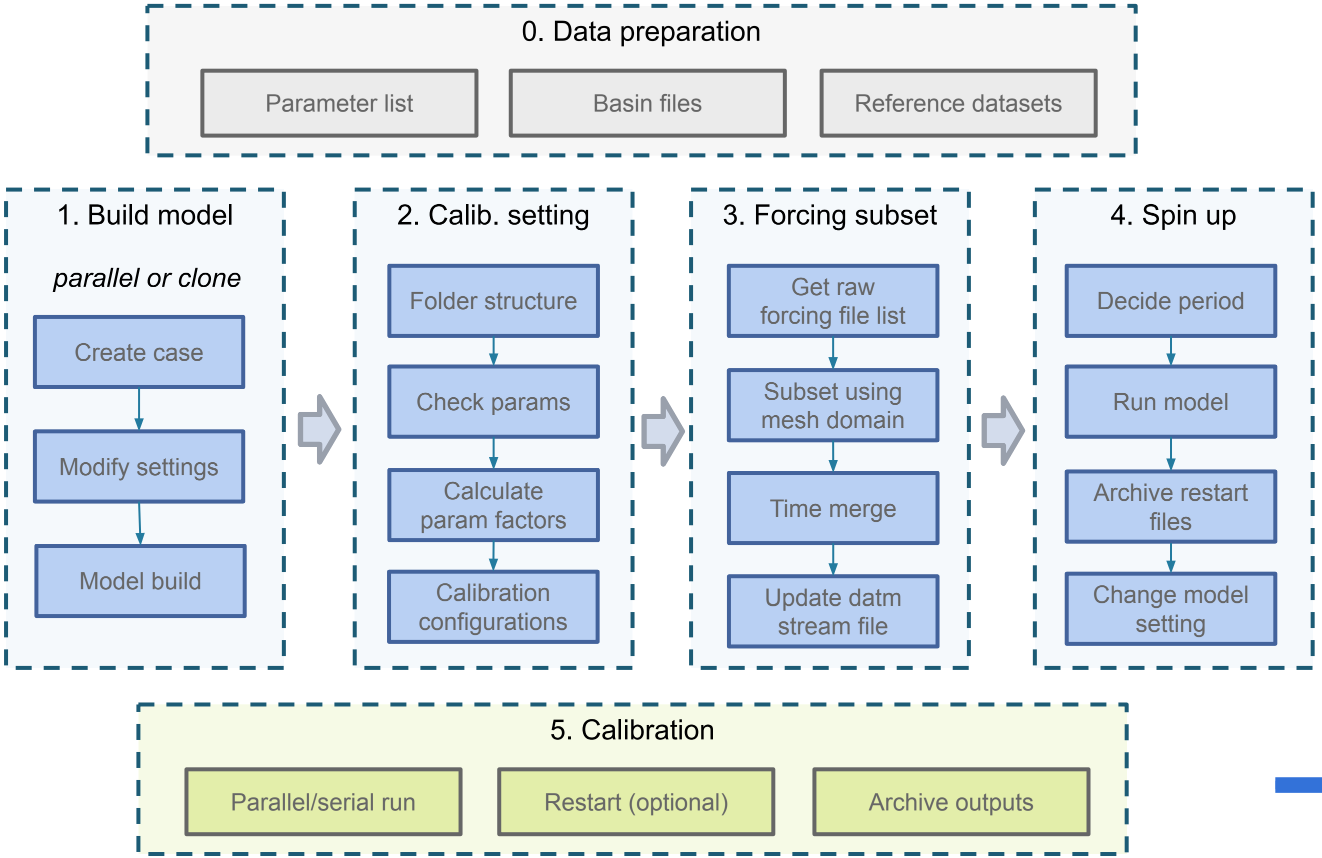
Moving toward multi-objective emulation-based optimization of CTSM

- Calibration of the CTSM model in Alaska and the Yukon River Basins
- Used MO-ASMO algorithm (surrogate modeling)
- The mean Kling-Gupta Efficiency (KGE) score of daily streamflow increased from 0.43 to 0.63

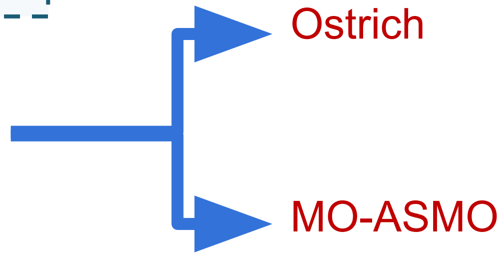


Cheng et al., 2023

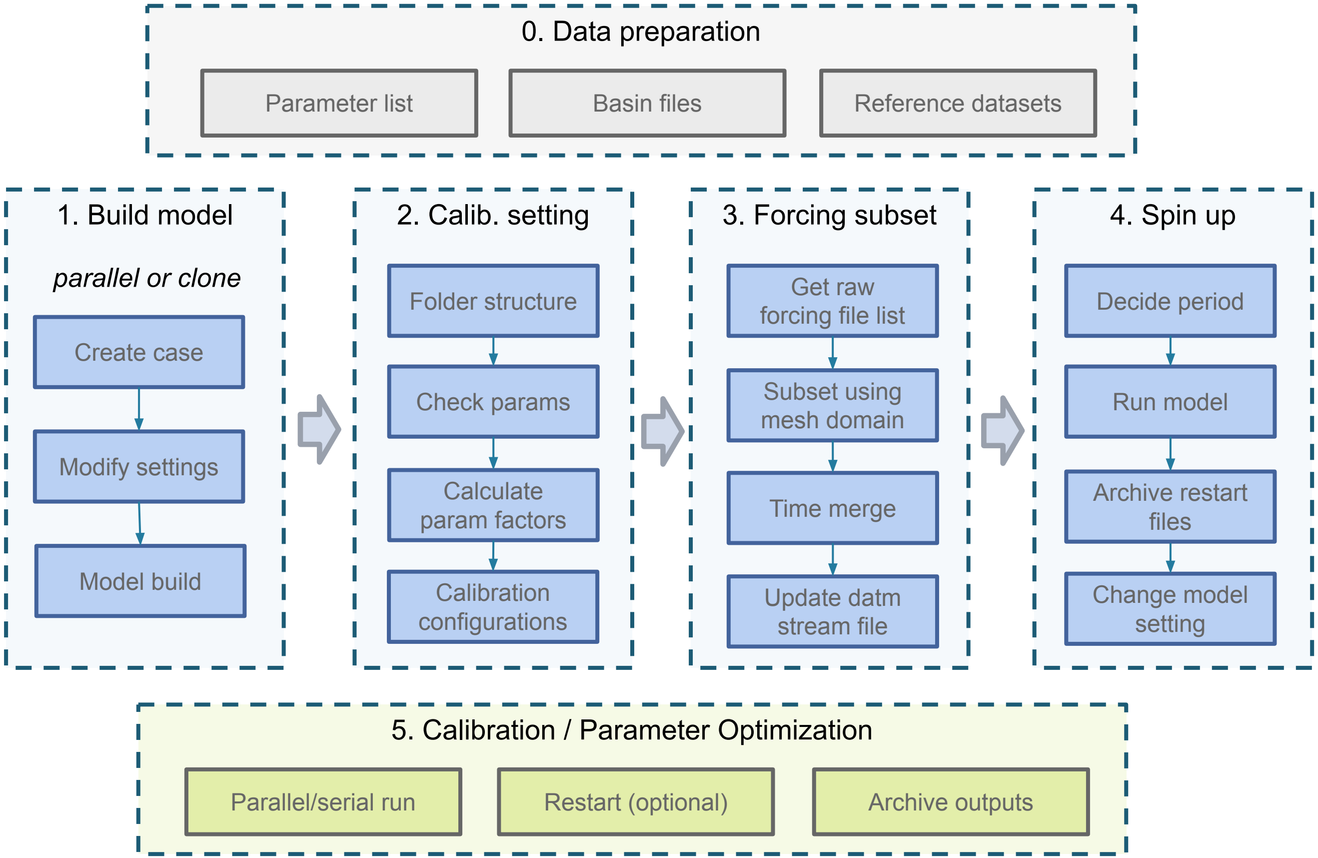
Moving toward multi-objective emulation-based optimization of CTSM



We are extending the CTSM parameter optimization workflow to include the MO-ASMO algorithm because of its multi-objective and parallelization functionality.



Moving toward multi-objective emulation-based optimization of CTSM

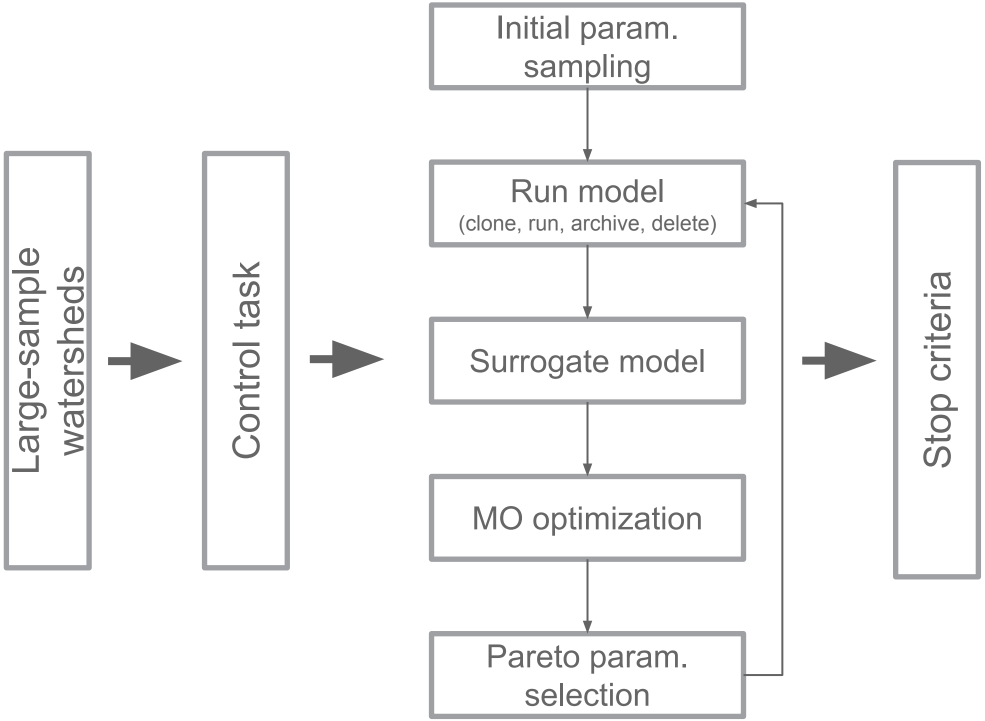


Optimization tools:

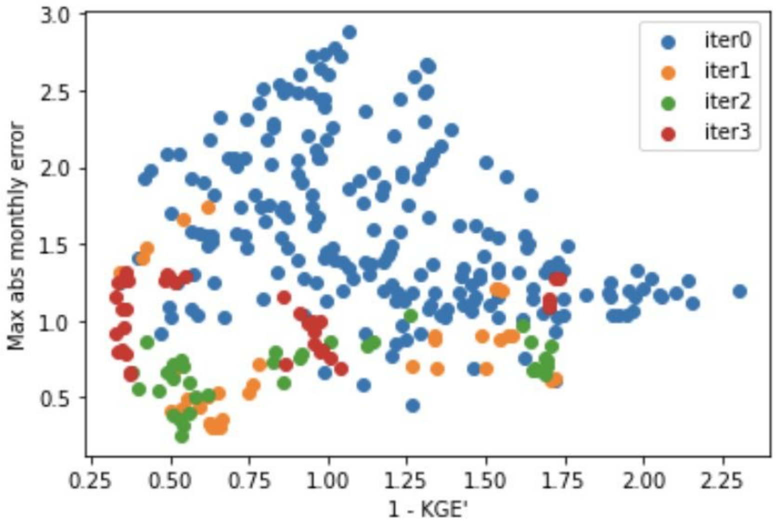
- Ostrich (initial)
  - Mattott et al (2017)
- MO-ASMO (*new*)
  - surrogate modeling
  - Gong et al (2016)
  - Cheng et al (2021)
- ‘differentiable learning’ (next)
  - ie, ML/DL emulators
  - Feng et al, WRR, 2022

Moving toward multi-objective optimization of CTSM

MO-ASMO workflow for large-sample watersheds



A test example of the workflow output using random forest as the surrogate model



We aim to streamline hands-on model setup and calibration effort

Summary and Next Steps

We developed a streamlined CTSM calibration workflow and hydrology 'testbed':

- This new CTSM calibration capability development supports a larger project to assess the robustness of different hydrological model configurations for projecting forced responses to climate change.
- The CAMELS-CTSM implementation offers a useful and efficient testbed for evaluating alternative CTSM model configurations and development choices.
- The parameter estimation workflow will enhance the local performance of the CTSM hydrology component and yield insights into regional to continental parameter estimation strategies.

Next steps:

- Future calibration development efforts include:
  - improving parallel computation
  - further parameter refinement
  - incorporating full ML/DL emulation approaches for 'differentiable learning' (Feng et al, WRR, 2022)
  - **assessing alternative CTSM configuration choices (including the hillslope parameterization)**
  - distributed domains
  - the use of river routing
  - regionalization to uncalibrated basins, and eventually to the global domain

Thank you!

guoqiang@ucar.edu