Land Model / Biogeochemistry Working Group Meeting 2024

Evaluating hydrological parameter sensitivities in CTSM using large-sample watershed modeling in CONUS

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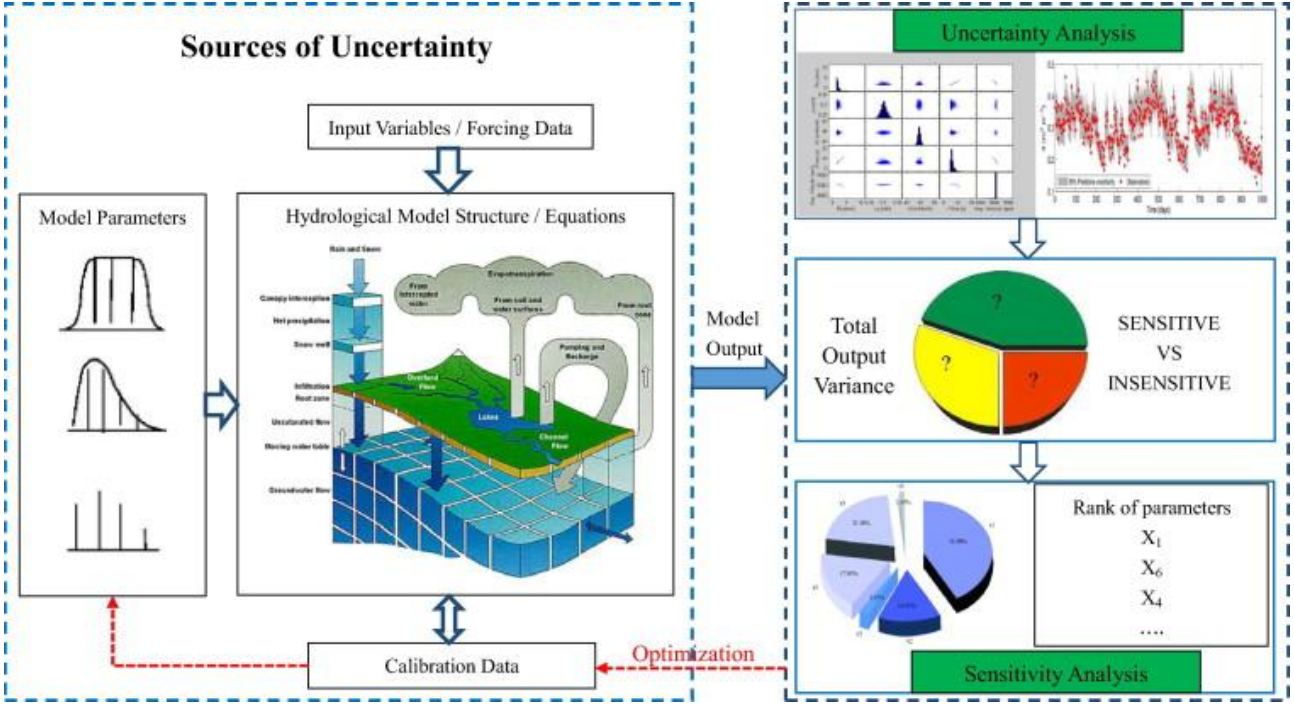
Using a model to represent real-world hydrology

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



Song et al, 2015

Applied ESM-based modeling seeks both realism *AND* performance

Several current water security related projects are exploring the use of CTSM as a process/physics advance over more common '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

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

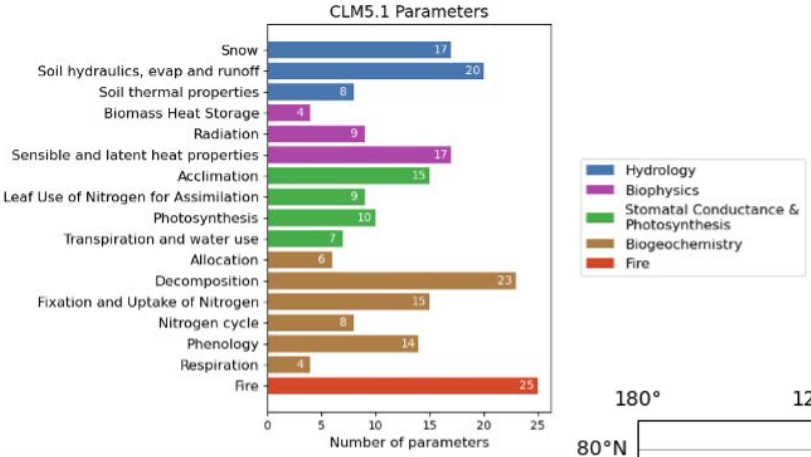
- develop CTSM configurations and parameter sets that perform well for hydrology – and with robust climate-hydrology sensitivities

First steps

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

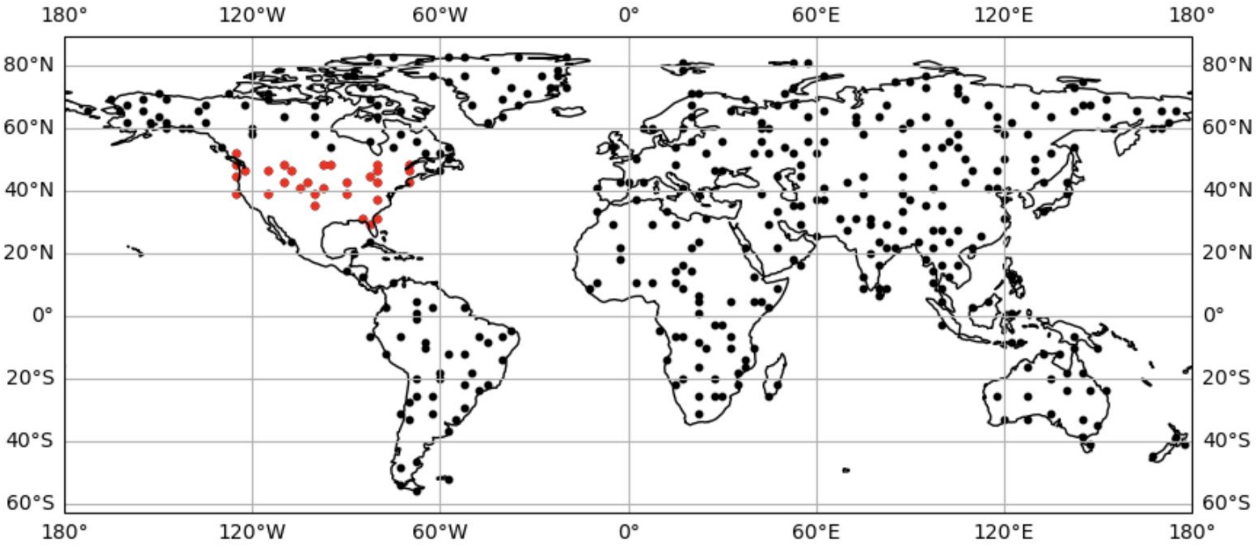
Sponsor: US Army Corps of Engineers (USACE) – Climate Preparedness and Resilience Program

Identify sensitive runoff parameters based on CLM PPE



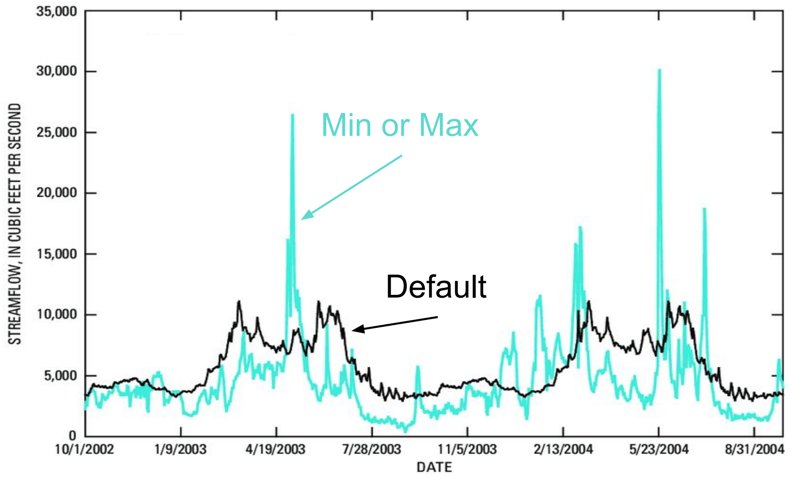
CLM PPE performs one-at-a-time parameter perturbations experiments for ~200 CLM parameters. This can be used a good start point for selecting runoff sensitive parameters.

Among the 400 CLM PPE global sparse grids, we select the 30 grids within NLDAS extent. CLM SP simulations are used.



Identify sensitive runoff parameters based on CLM PPE

Alterations in parameter values can influence runoff variability, indicating parameter sensitivity. Nonetheless, the choice of metrics can yield varying assessments of runoff changes.



In this study, we assess the variations in runoff by comparing the daily QRUNOFF outputs derived from default parameters and min/max parameters. We employ the modified Kling-Gupta Efficiency (KGE') metric.

$$KGE' = 1 - \sqrt{\underbrace{(r-1)^2}_{\text{correlation}} + \underbrace{(\beta-1)^2}_{\text{relative bias}} + \underbrace{(\gamma-1)^2}_{\text{variability}}}$$

$$\beta = \frac{\mu_s}{\mu_o}$$

$$\gamma = \frac{CV_s}{CV_o} = \frac{\sigma_s/\mu_s}{\sigma_o/\mu_o}$$

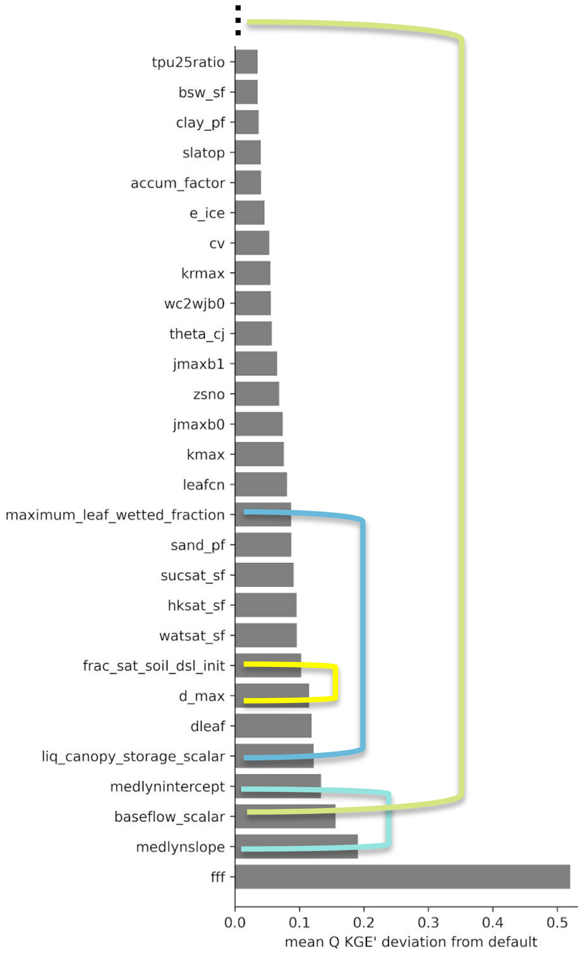
Kling et al., 2012

KGE-based indicators of sensitivity

- *KGE'_min* is the KGE' difference between min and default parameters.
- *KGE'_max* is the KGE' difference between max and default parameters.
- *KGE'_deviation* = 1 - (KGE'_min + KGE'_max) / 2

Larger *KGE'_deviation* indicates larger parameter sensitivity

Identify sensitive runoff parameters based on CLM PPE

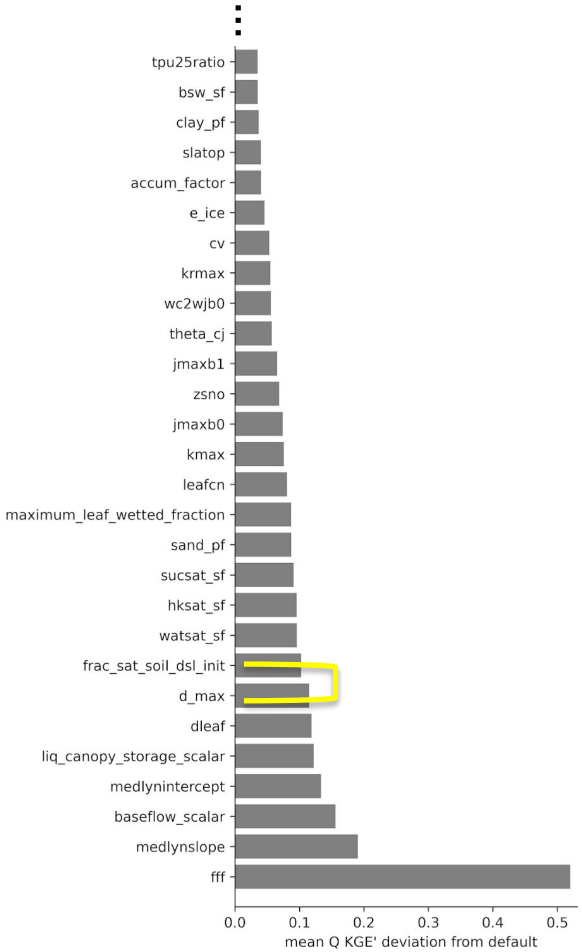


For a parameter, higher KGE' deviation means stronger QRUNOFF sensitivity.

Parameter	Description
fff	decay factor for fractional saturated area

Parameters affecting same processes

Identify sensitive runoff parameters based on CLM PPE



The thickness of the dry surface layer is given by

$$DSL = \begin{cases} D_{max} \frac{(\theta_{init} - \theta_1)}{(\theta_{init} - \theta_{air})} & \theta_1 < \theta_{init} \\ 0 & \theta_1 \geq \theta_{init} \end{cases} \tag{2.5.77}$$

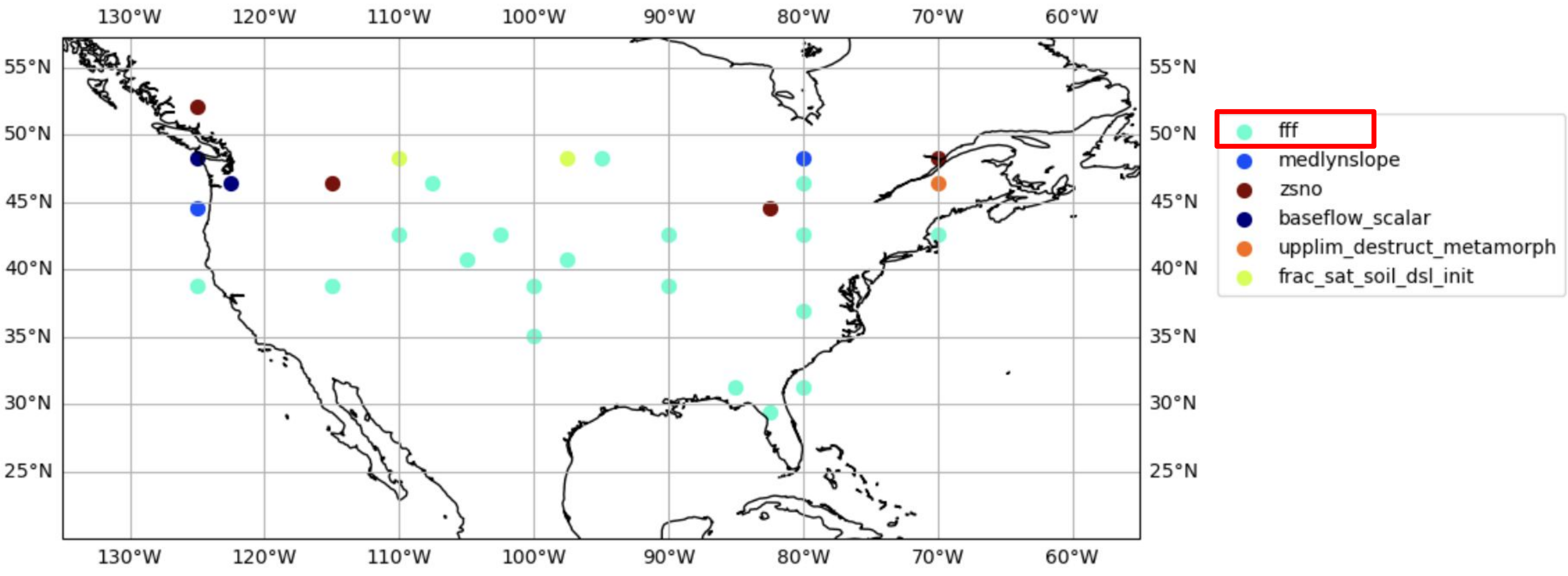
dsl(c) = ***d_max*** ** max(0.001, (****frac_sat_soil_dsl_init*** ** eff_por_top - vwc_liq)) / max(0.001, (****frac_sat_soil_dsl_init*** ** watsat(c,1) - aird))*

d_max and **frac_sat_soil_dsl_init** parameters control the calculation of **dsl** (dry surface layer thickness). Both parameters are quite sensitive but including them in the sensitivity analysis or parameter calibration is not ideal because it is hard to disentangle their interactive effects in both sensitivity analysis and parameter optimization with limited model runs.

Therefore, we exclude parameters from the same or similar processes.

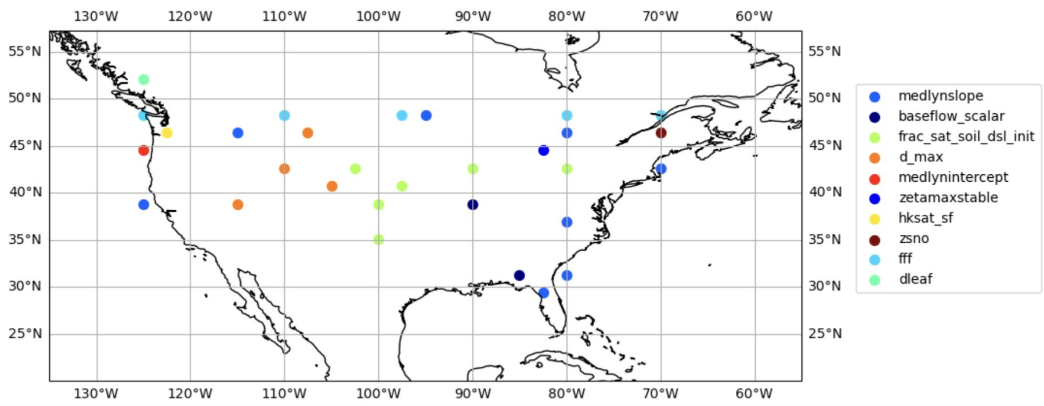
Identify sensitive runoff parameters based on CLM PPE

Most sensitive parameters for each grid



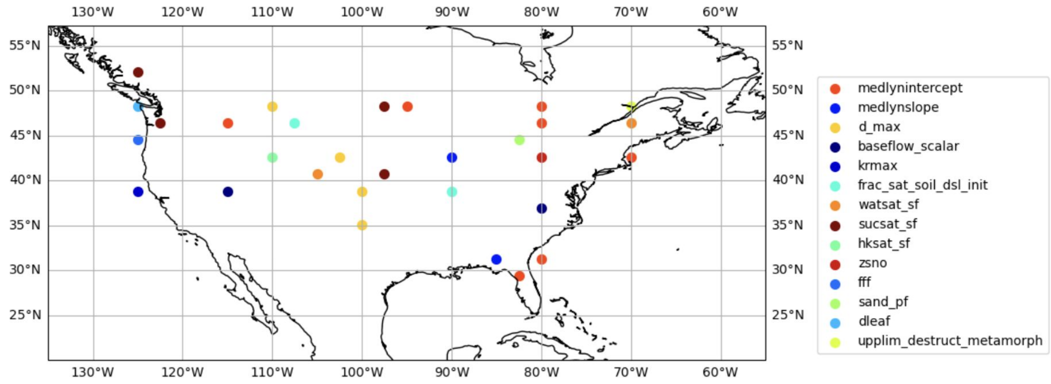
Identify sensitive runoff parameters based on CLM PPE

The 2nd most sensitive parameter



The spatial patterns of parameter sensitivity become less coherent as we look at parameters with lower sensitivity

The 3nd most sensitive parameter



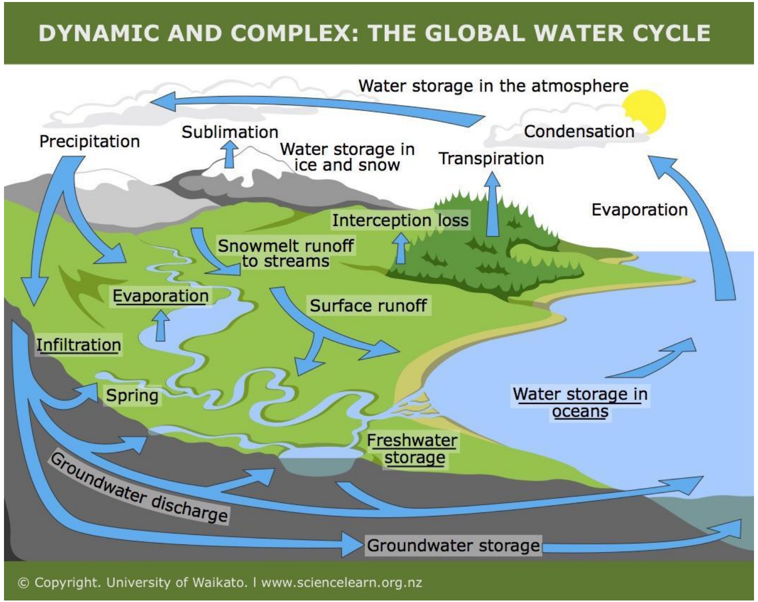
Balancing PPE sensitivity and hydrologic process importance

The CLM PPE information is useful, but the ultimate selection of parameters for calibration is also guided by a process-based strategy for influencing hydrology, leveraging prior knowledge.

- **Process importance**
  - For example, **n_melt_coef** is insensitive for runoff according to PPE but we include it due to its control on snow melting and expand its parameter range.
  - We added parameters not used in PPE, such as including **FMAX** (maximum fractional saturated area) and **precip_repartition_nonglc_all_rain_t** (rain and snow classification).

Some key hydrological processes

- infiltration
- soil drainage rate in all layers (transmission of water through soil)
- soil storage capacity (porosity, wilting point, layer thickness, etc)
- aquifer or groundwater recharge
- aquifer or groundwater storage capacity
- canopy interception
- sublimation
- transpiration
- bare-soil evaporation
- snow accumulation
- snow melt
- catchment runoff routing (e.g., hillslope routing function, GIUH)
- channel routing (celerity, attenuation)



Balancing PPE sensitivity and hydrologic process importance

In addition to the sensitive parameters identified from CLM PPE, we also utilize prior knowledge to help screen parameters.

- **Process importance**
  - For example, **n_melt_coef** is insensitive according to PPE but we include it due to its control on snow melting and expand its parameter range.
  - We added two parameters not used in PPE: including **FMAX** (maximum fractional saturated area) and **precip_repartition_nonglc_all_rain_t** (rain and snow classification).

- **Direct hydrology relevance**
  - For example, more than 10 stomatal resistance and photosynthesis parameters have notable impact on runoff, while hydrological models would use simplified parameterizations to represent the impact of vegetation on direct hydrological processes like ET. So, we only use three of them.
  - photosynthetic rate (**jmaxb0**), stomatal conductance (**medlynslope**), and hydraulic conductivity (**kmax**)

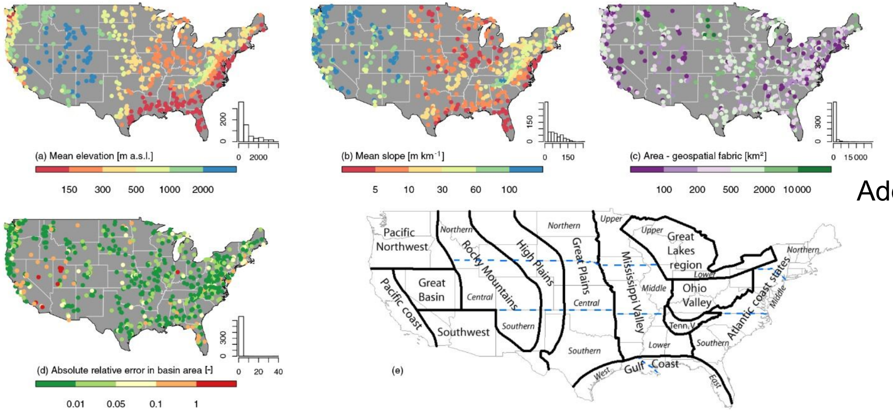
In the end, we select **27 parameters** for further runoff sensitivity analysis.

Establishing a large-sample testbed for hydrologic assessment with CTSM

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

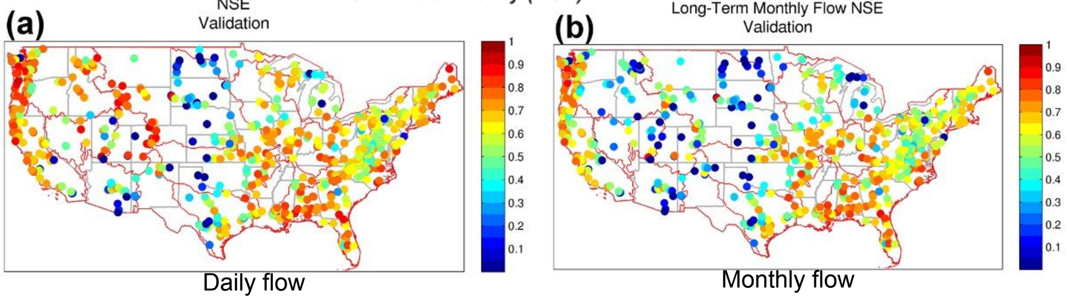
- A comprehensive set of catchment attributes, meteorological variables, streamflow observations, and model results for 671 US catchments
- Widely used in hydrology research to develop and evaluate hydrological models, variability and predictability
- Has been a central dataset in the global rise of 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

We created a simulation workflow for CTSM over these catchments.



Addor et al., 2017

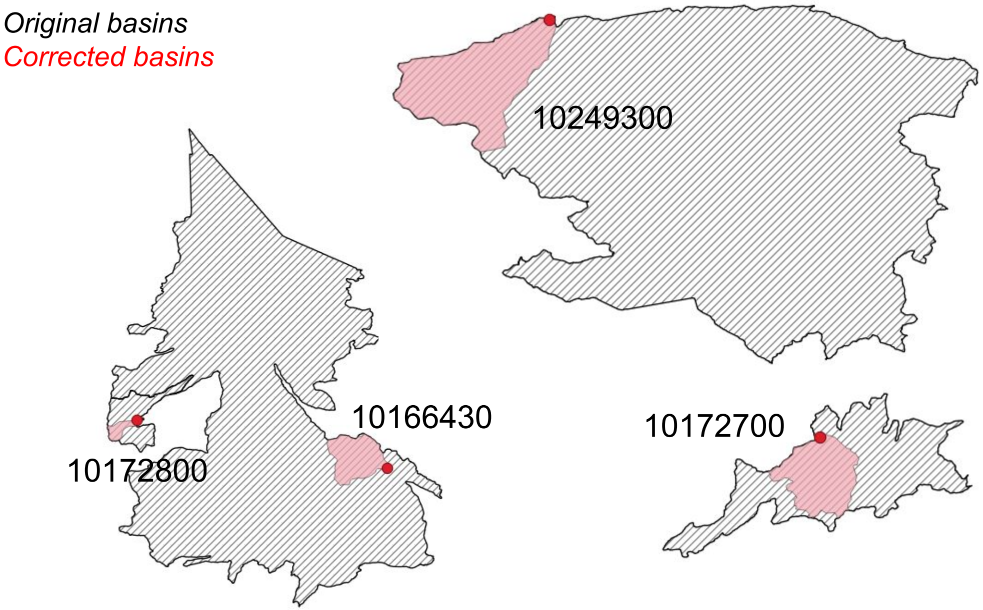
Nash–Sutcliffe efficiency (NSE): −∞ to 1



Newman et al., 2015

Quality control of the CAMELS basin dataset

The CAMELS basin shapefiles contained area biases caused by inaccurate streamflow gauge positions and imperfect boundary delineation. In some prior work, e.g., Yan et al. (2023), significant portions were discarded (207 out of the 671 basins) that had basin area errors greater than 2%.



We tried corrected the CAMELS basin delineations by merging information from multiple sources:

- original CAMELS
- TDX-Hydro catchments
- MERIT-Hydro
- USGS HUC12 boundaries
- re-derived boundaries from TDX-Hydro 12m DEM derivatives
- HydroSHEDS

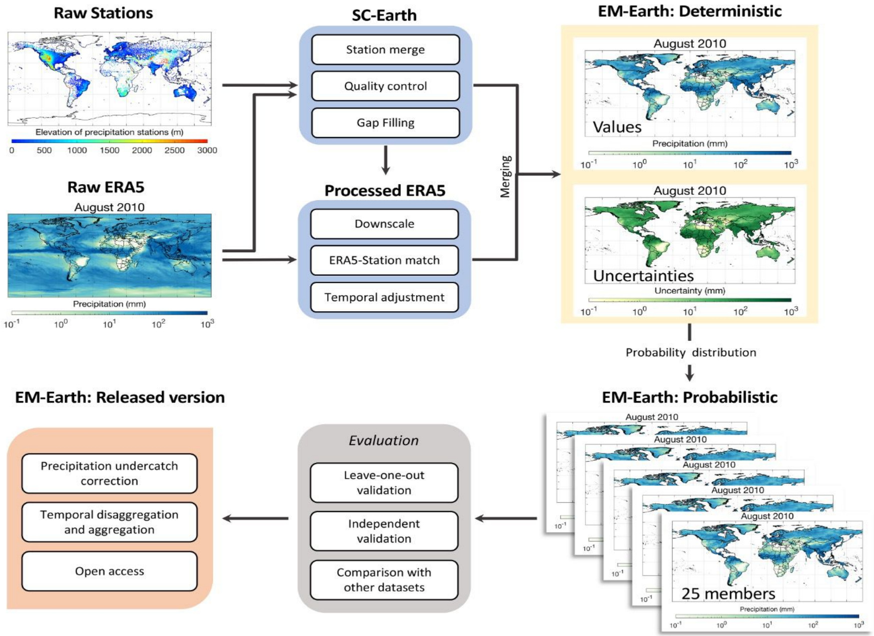
In end, we used the USGS Gages-II shapefiles which were unbiased.

We now use 627 headwater-only (non-nested) basins.

Meteorological forcing for CONUS modeling

We generate a long-term high-resolution forcing to support watershed CTSM modeling in CONUS.

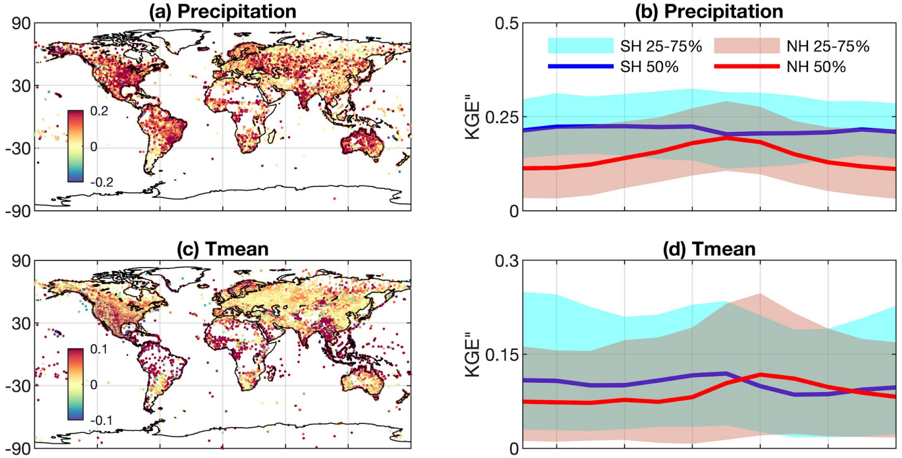
- 1950 to 2019
- Hourly, 0.1° resolution
- Precipitation and air temperature are from EM-Earth
- Other forcing variables are from ERA5-Land



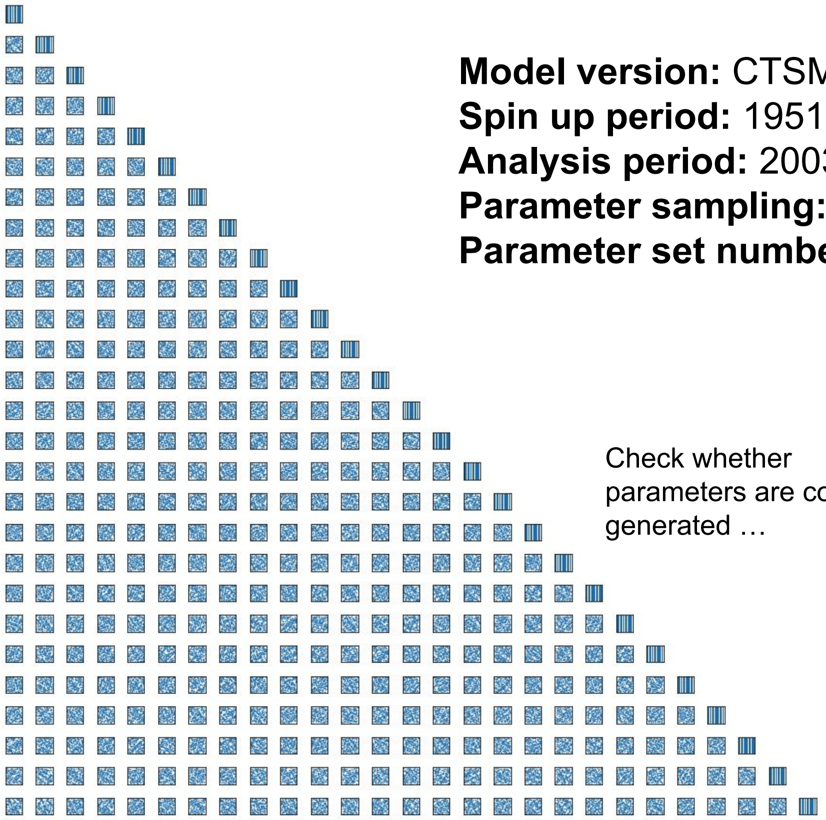
Tang et al., 2022 BAMS

EM-Earth is an ensemble meteorological dataset which merges data from dense ground stations and ERA5 reanalysis.

KGE": EM-Earth minus ERA5



Model set up



Model version: CTSM hillslope hydrology from Sean Swenson
Spin up period: 1951-01 to 2003-9
Analysis period: 2003-10 to 2009-9 (ignoring the first year for each simulation)
Parameter sampling: Latin hypercube
Parameter set number: 200

Check whether parameters are correctly generated …

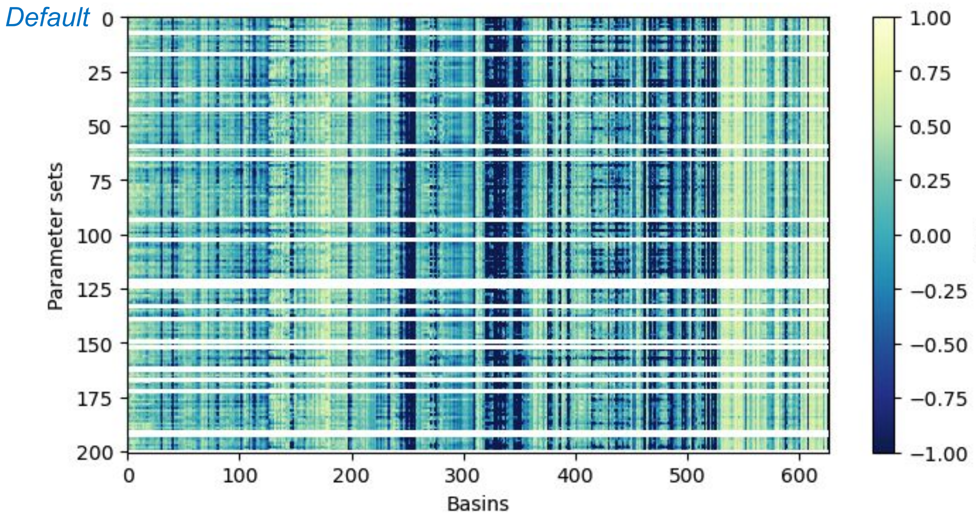
Scatter plots between each pair of parameters
Histograms (on the diagonal line) of each parameter

CTSM runoff performance

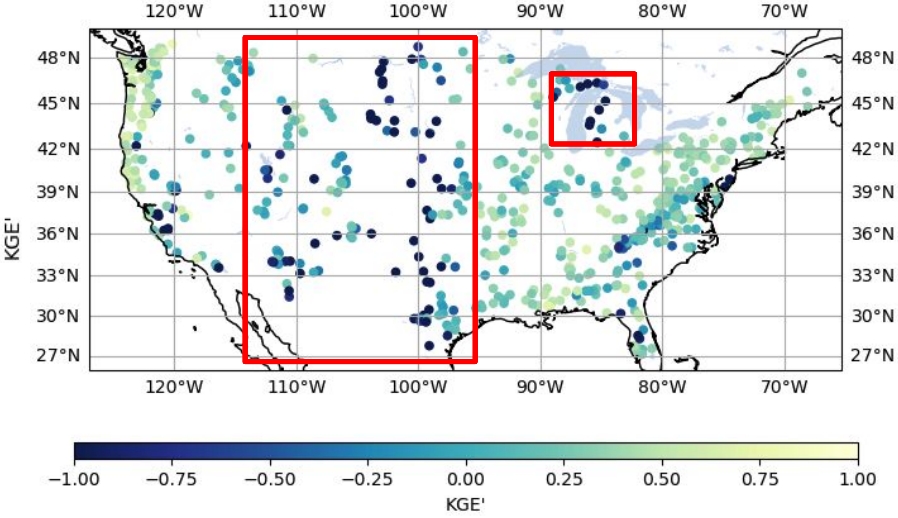
Observed streamflow is used to evaluate CLM runoff outputs.

- For default parameters, the median KGE' is 0.22, while the mean KGE' is -0.29 due to the impact of a few basins. The highest median KGE' of all parameter sets is 0.31.
- The hillslope version achieves better performance than the CLM standard version using default parameters.

The KGE' of all basins and parameter sets

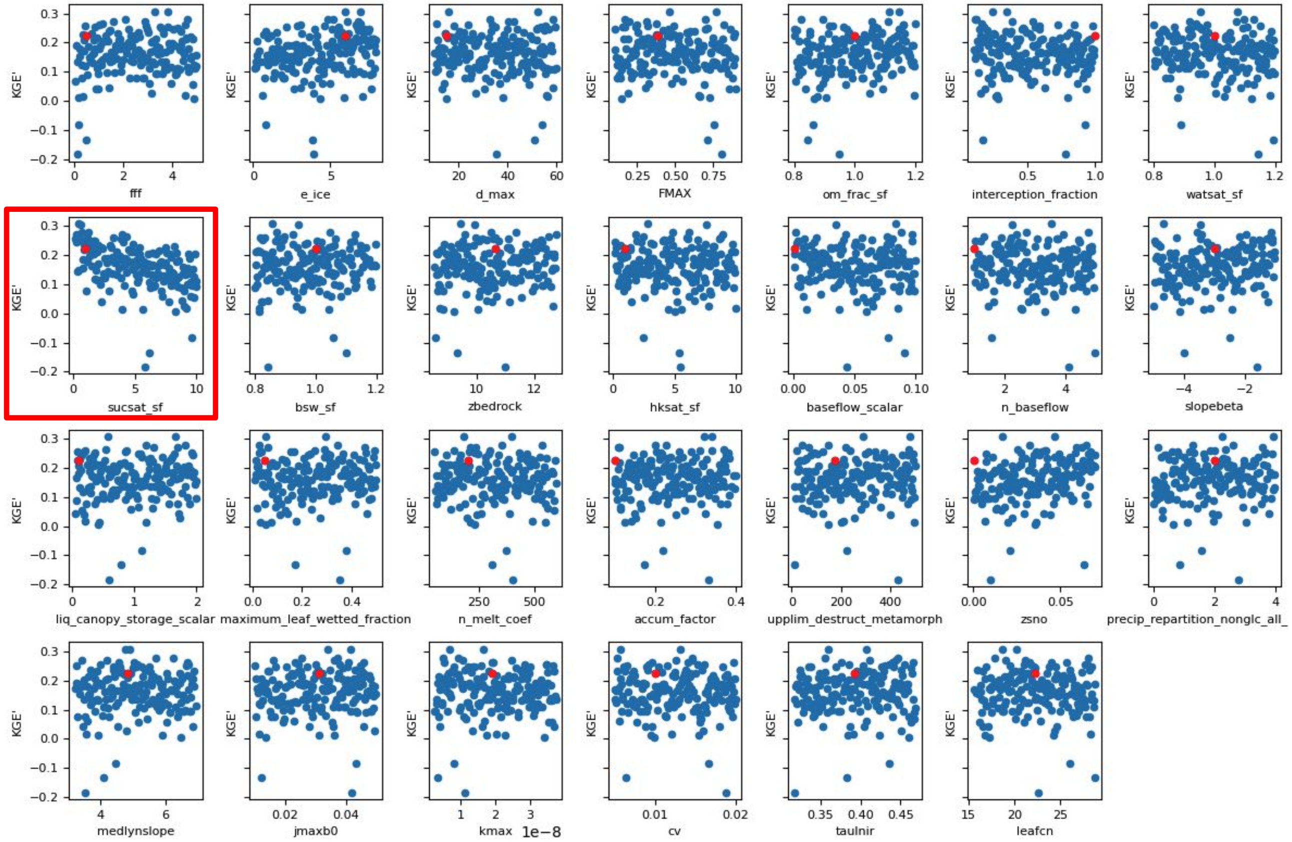


Spatial distribution of KGE' based on default parameters



CTSM runoff performance

Comparison between default parameters and LHS parameters

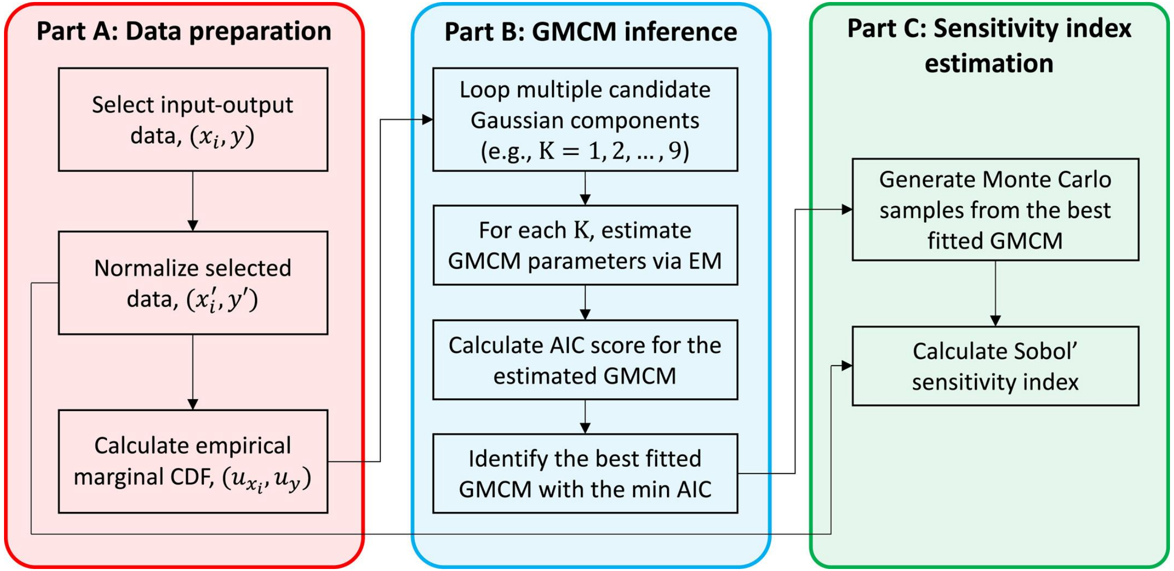


sucsat (soil matric potential) refers to the tension with which water is held in the soil at saturation.

Higher sucsat_sf means the soil can hold more water before it becomes saturated. This could lead to reduced runoff and increased soil moisture availability for evapotranspiration.

Sensitivity analysis method and tool

Varlance-based Sensitivity analysis using COpulaS (VISCOUS) first uses a **Gaussian Mixture Copula Model (GMCM)** to approximate the joint probability distribution between the input (e.g., the perturbations in the model parameters) and output data (e.g., the model responses given parameter perturbations); and then approximates the first- and total-order Sobol' sensitivity indices based on the fitted GMCM.



Sobol' sensitivity indices

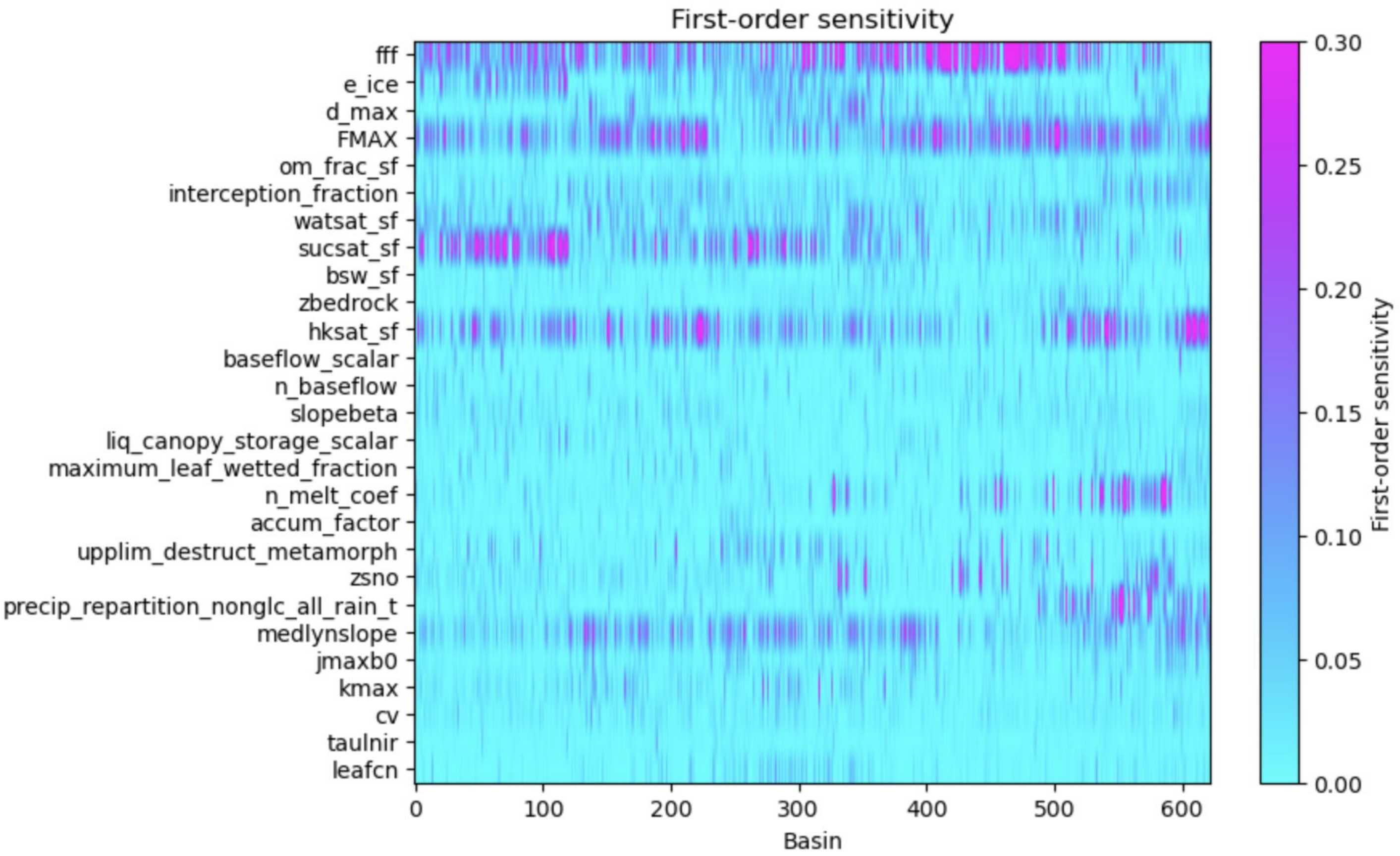
First-order sensitivity index: the direct impact of each input on its own

Total-order sensitivity index: the overall impact, including all interactions with other inputs

Liu et al., 2024; Sheikholeslami et al., 2022

pyviscous: https://github.com/CH-Earth/pyviscous

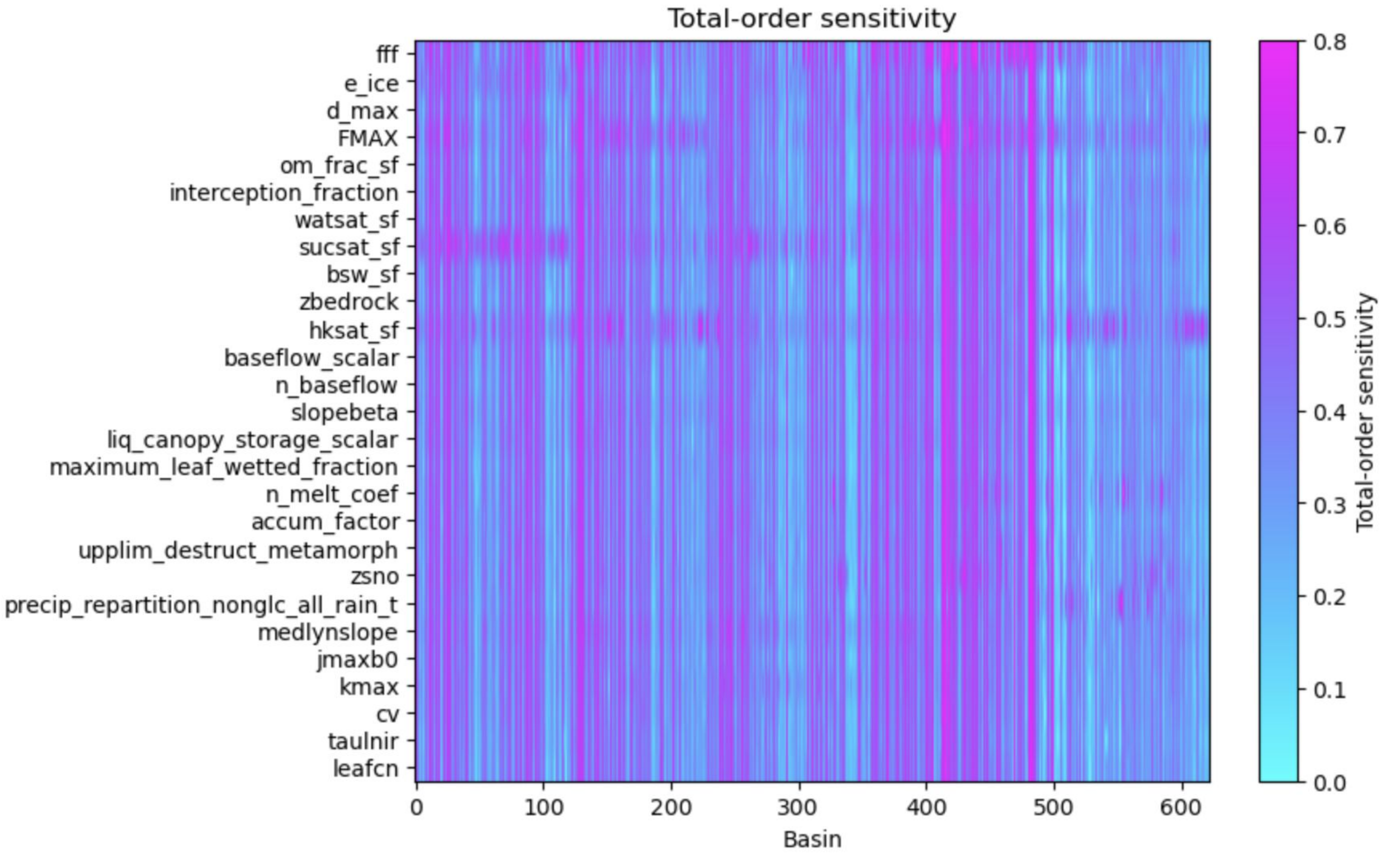
First-order runoff sensitivity



Several parameters such as fff, FMAX, sucsat_sf, hksat_sf, and medlynslope, show high sensitivities in many basins.

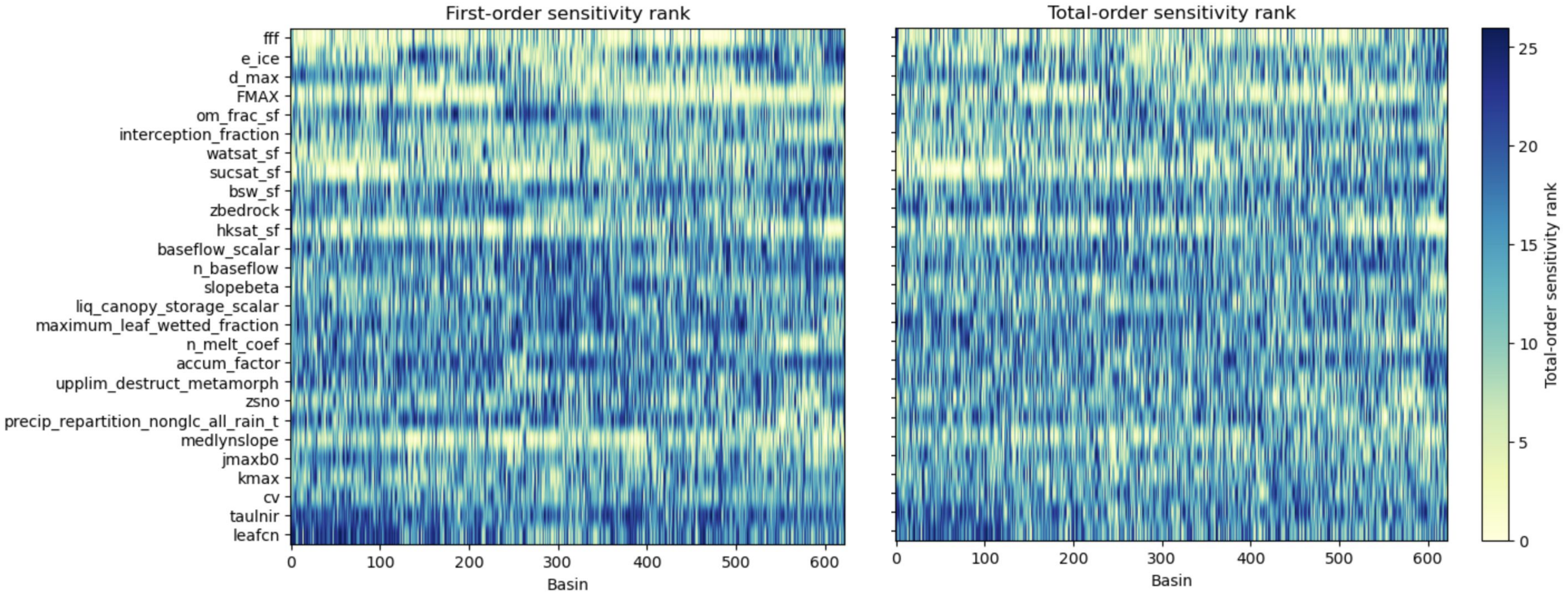
Notable variability exists concerning the sensitivities.

Total-order runoff sensitivity



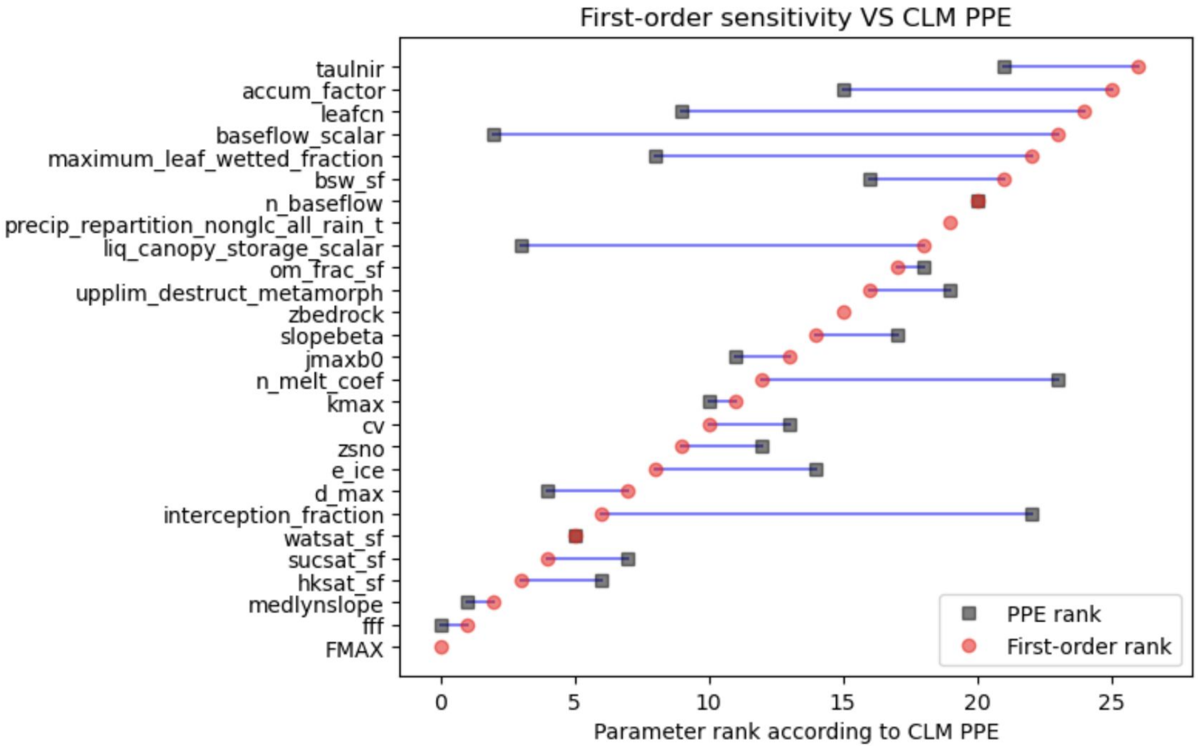
Because of the large number of input parameters (27) and small number of simulations (200), total-order sensitivity values are less reliable. However, parameter ranks are still reliable.

Parameter rank based on runoff sensitivity



A lower rank means the parameter is more sensitive. Ranks based on first-order sensitivity values and total-order sensitivity values are generally similar, despite differences for some basins and parameters.

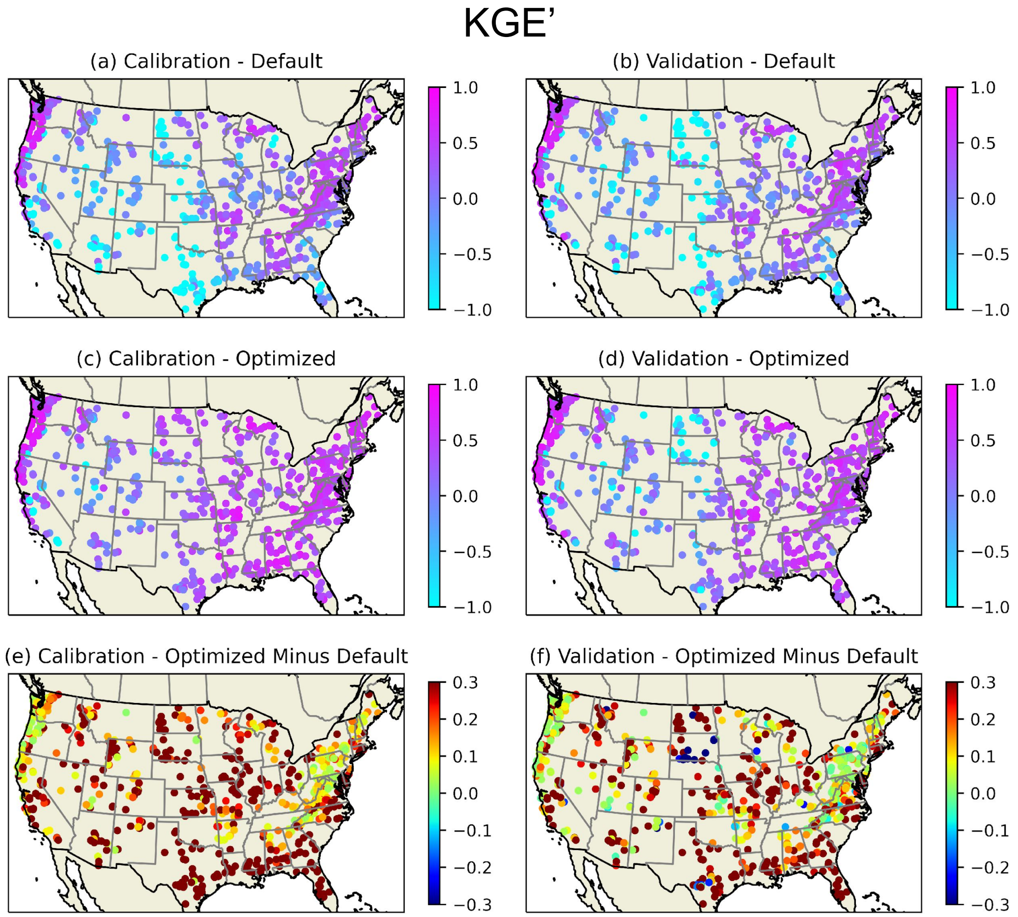
Comparison between CLM PPE and runoff sensitivity analysis



The first-order sensitivity is compared to CLM PPE one-at-a-time results. Some parameters show big differences.

Parameter	PPE	SA
FMAX	N/A	0
interception_fraction	22	6
e_ice	14	7
n_melt_coef	23	12
liq_canopy_storage_scalar	3	18
maximum_leaf_wetted_fraction	8	22
baseflow_scalar	2	23

Parameter optimization: single objective



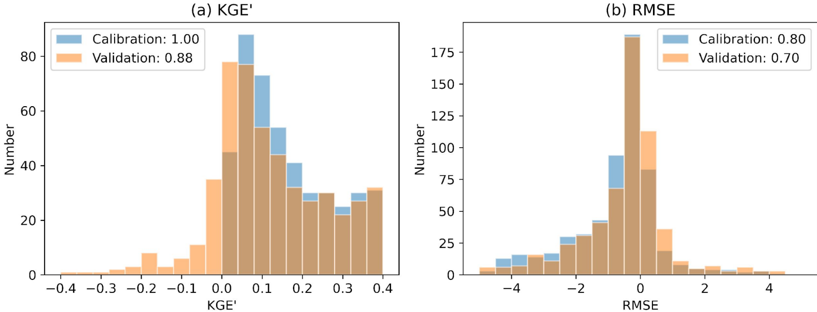
Calibration was initially performed for individual basins using the DDS algorithm within the Ostrich optimization package.

After calibration, the KGE' is improved for most basins. For median KGE:

- calibration: 0.15 to 0.46
- validation: 0.15 to 0.40

A few basins show worse KGE' in the validation periods after the calibration. Further analysis is needed.

The difference between optimized and a priori parameters during calibration and validation periods

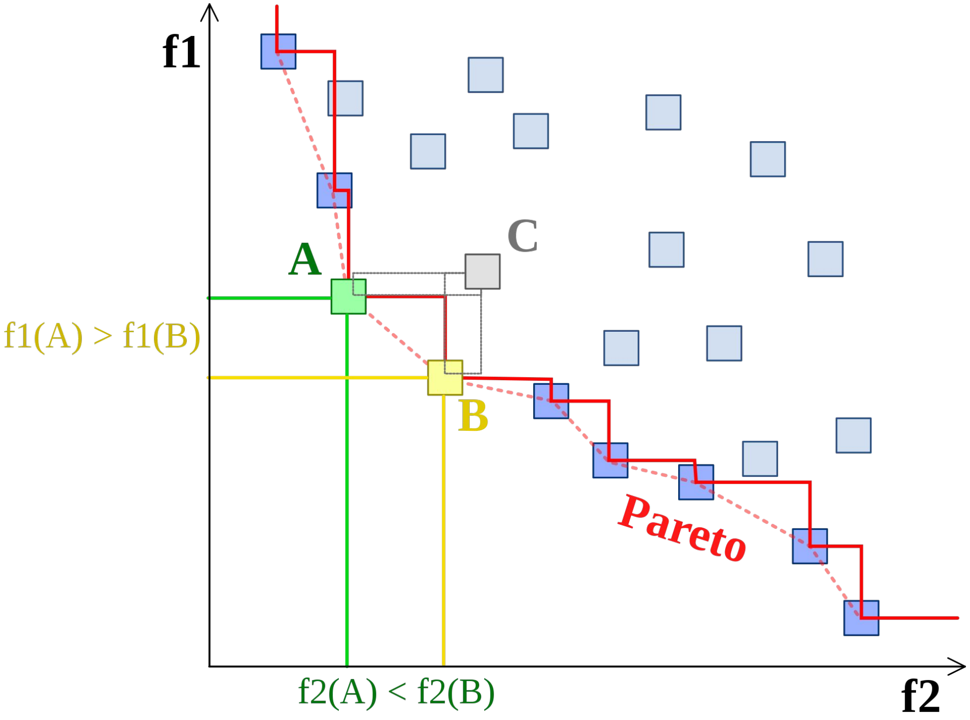


Parameter optimization: multi-objective

"A solution is called nondominated, Pareto optimal, Pareto efficient or noninferior, if none of the objective functions can be improved in value without degrading some of the other objective values"

For example, in the right figure, for points (e.g., A and B) at the Pareto frontier, you cannot find other points that have better f1 and f2 at the same time.

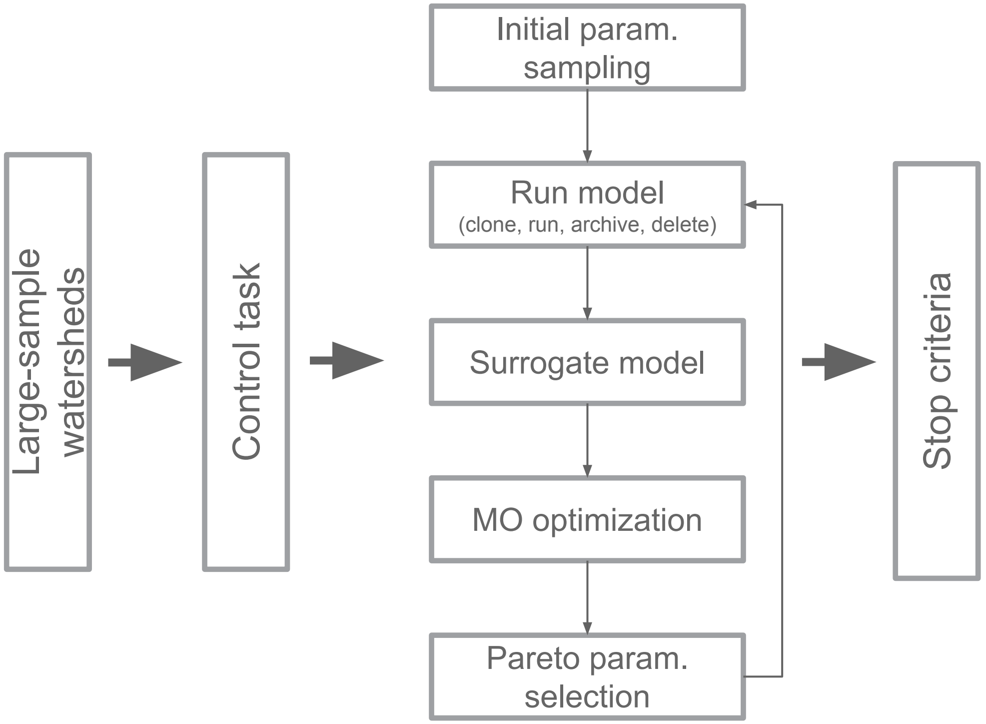
Example of a Pareto frontier
f1 and f2 are objective functions to be minimized (e.g., accuracy metrics for runoff or GPP)



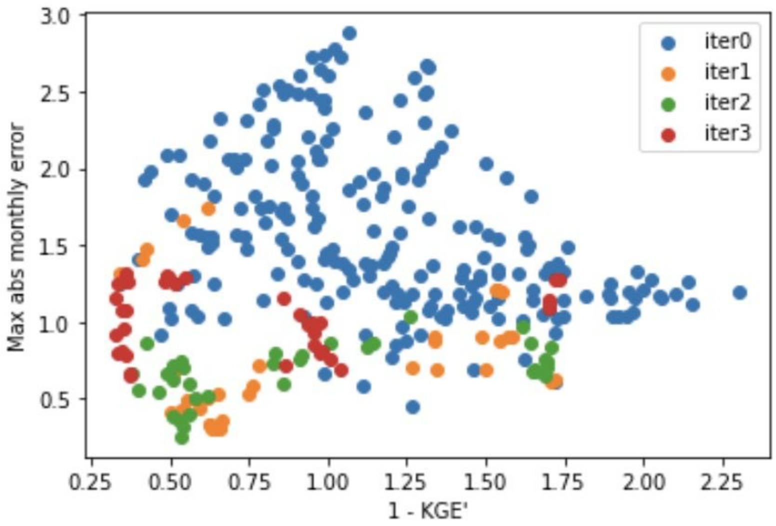
Source: Wikipedia

MO-ASMO: Moving towards multi-objective optimization

Multi-Objective Adaptive Surrogate Based Modeling Optimization (MO-ASMO)



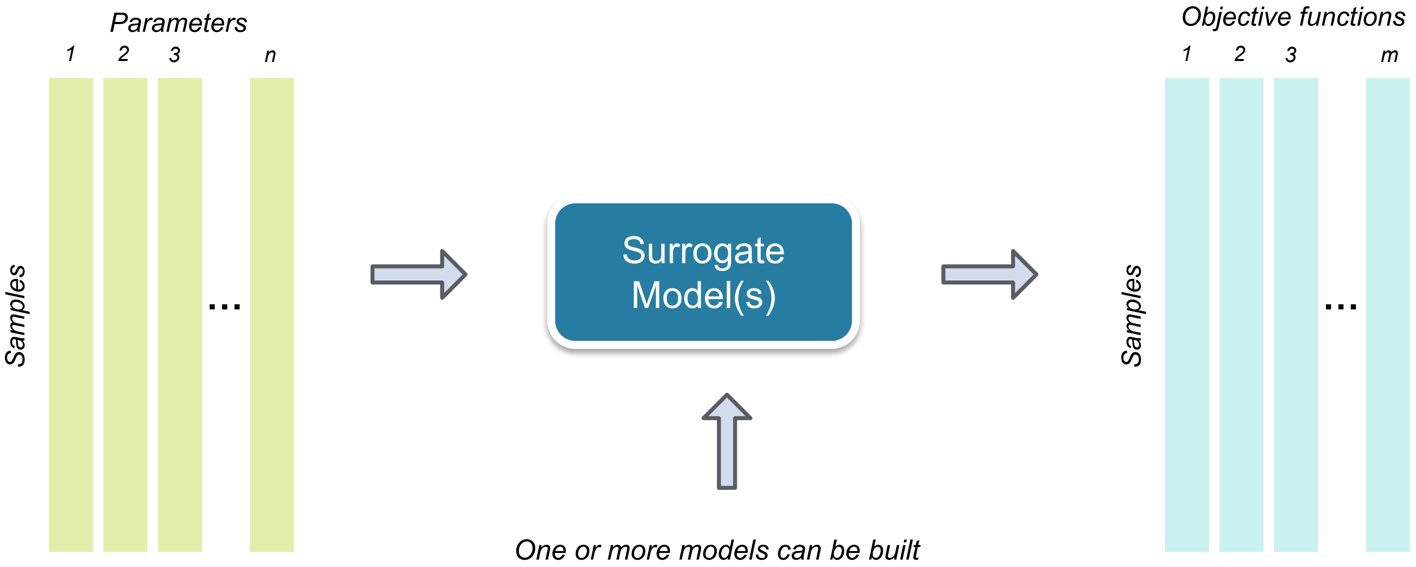
A test example of the workflow output using random forest as the surrogate model



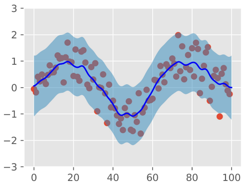
We aim to streamline hands-on model setup and calibration effort by developing the MO-ASMO workflow for large-sample watersheds.

Multi-objective calibration

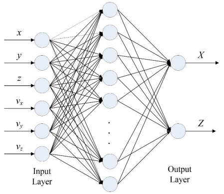
A surrogate model is used to map parameters to objective functions



Gaussian Processes Regression



BP neural network

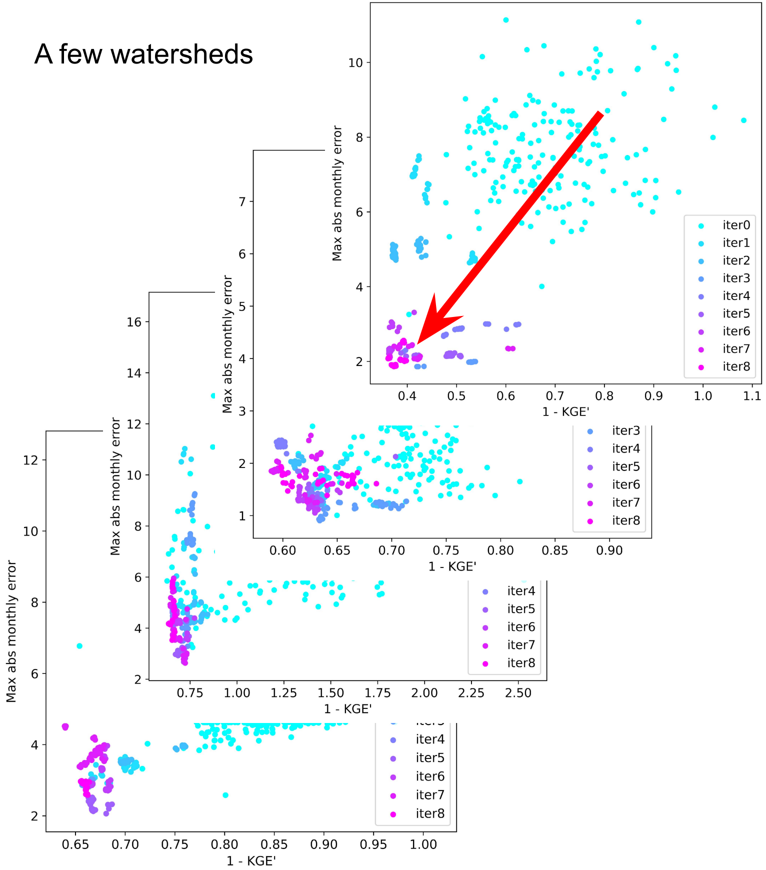


Random forest

...

MO-ASMO: Moving towards multi-objective optimization

A few watersheds



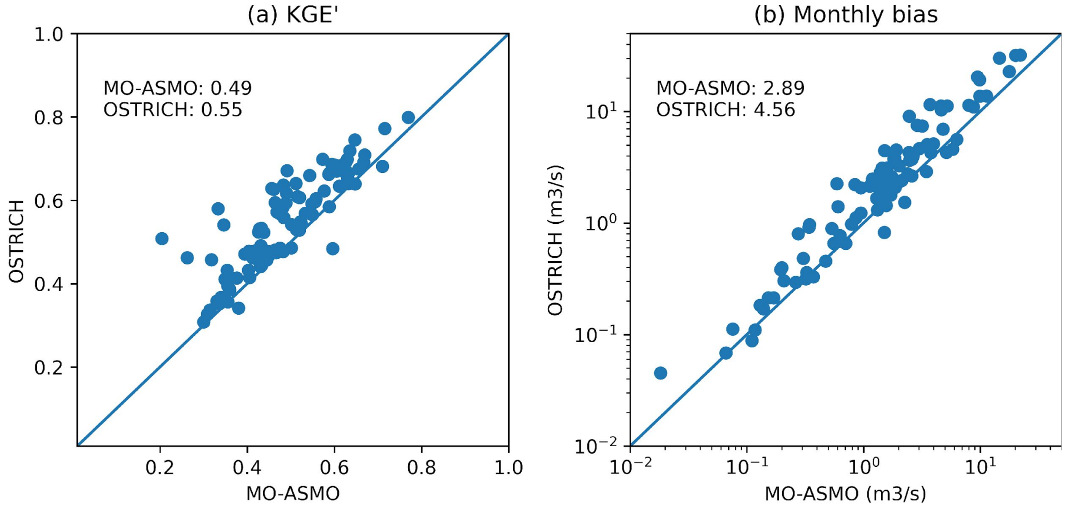
In MO-ASMO optimization, each parameter set is ranked separately for both objectives, from lowest to highest performance. We sum these ranks for each set. The set with the lowest total rank is chosen as optimal.

Compared to Ostrich, MO-ASMO shows

- worse KGE' (**0.49 VS 0.55**)
- better monthly bias (**2.89 VS 4.56**)

This is expected because the KGE' is not the only calibration objective in multi-objective optimization (versus our single-obj. optimization)

MO-ASMO and Ostrich comparison over 100 basins



Summary and Next Steps

We analyze the sensitivity of CLM parameters to runoff over the 627 CAMELS headwater basins in CONUS:

- The five most sensitive parameters are fff, FMAX, sucsat_sf, hksat_sf, and medlynslope.
- The sensitivity shows notable spatial variability.
- The sensitivity is different from the CLM PPE results. The significant variation observed in some parameters can be partly attributed to the constraints of Latin hypercube sampling, especially when the default parameter does not align with the midpoint of the parameter range.
- The calibration significantly improves the runoff simulation.

Next steps:

- Select 10-15 parameters from the sensitivity analysis results
- Perform multi-objective optimization
- Investigate different CLM configurations (particularly varying soil layers and depths; PFT strategies; hillslope choices)
- Develop general two phase approach: regional followed by individual
- Investigate the hydrological robustness to forced climate changes of both CLM and SUMMA models

Thank you!

Contacts

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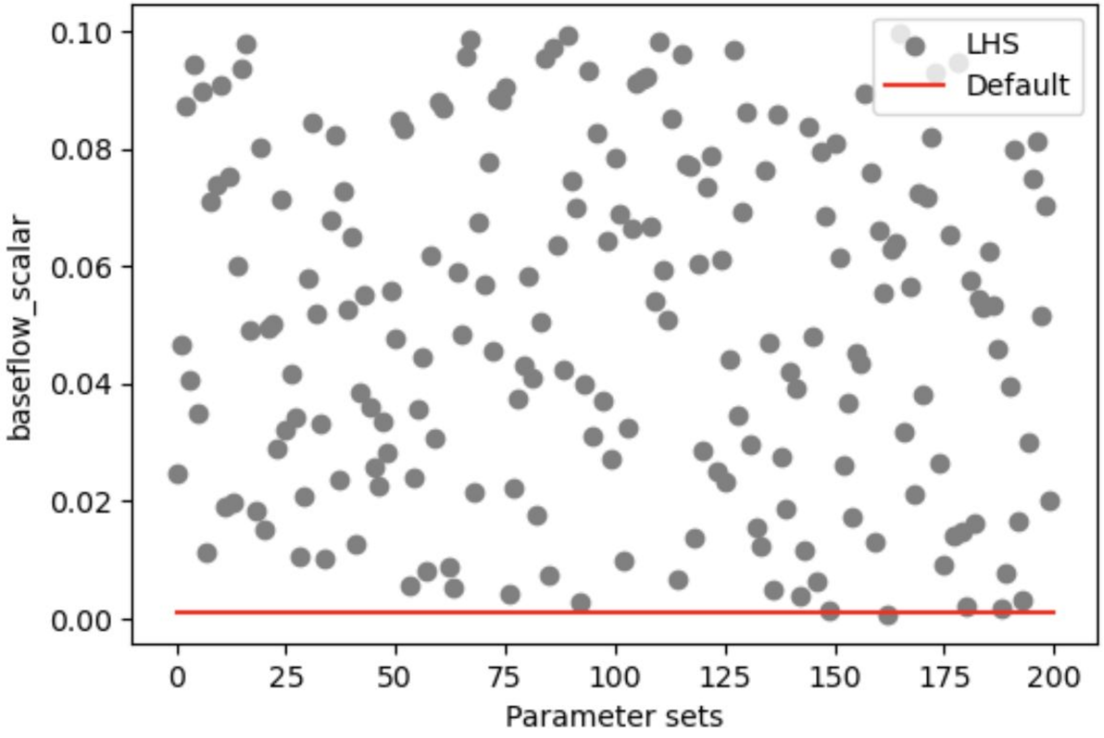
Comparison between CLM PPE and runoff sensitivity analysis

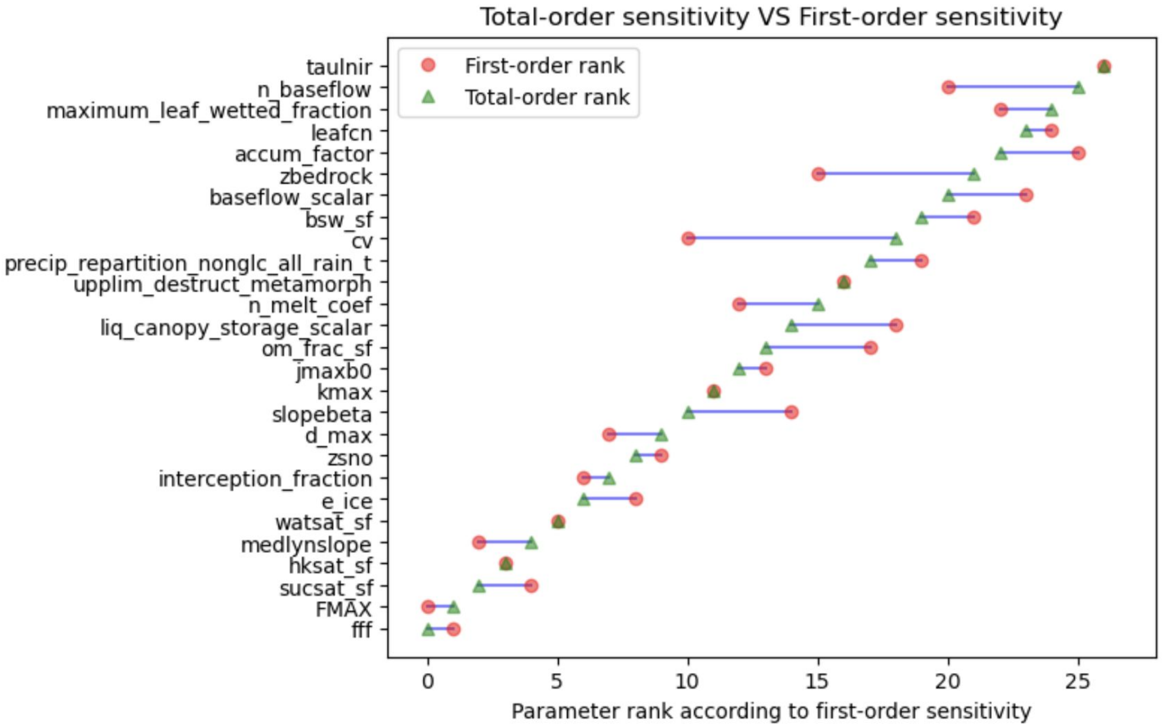
Parameter	Default	Lower	Upper
baseflow_scalar	0.001	0.0005	0.1



The uniform sampling method used by LHS cannot cover the desired space well if the default parameter is not located in the center of the minimum-maximum range.

Using baseflow_scalar as an example, the default value is too close to the lower limit. Only one among the 200 parameters is smaller than the default parameter.

Comparison between first-order and total-order sensitivity

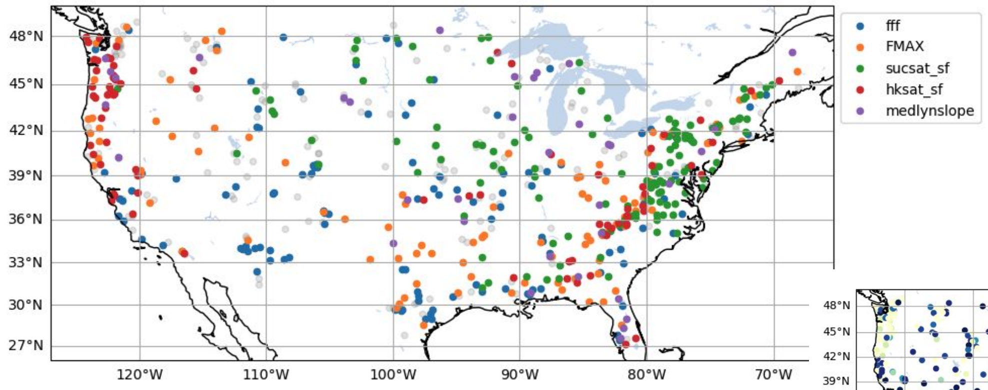


Overall, the total-order and first-order sensitivity agrees with each other.

Param	Fir	Tot
slopebeta	14	10
om_frac_sf	17	13
cv	10	18
zbedrock	15	21
n_baseflow	20	25

Spatial pattern of sensitive parameters

Most sensitive parameters in each basin



Rank of four parameters in each basin