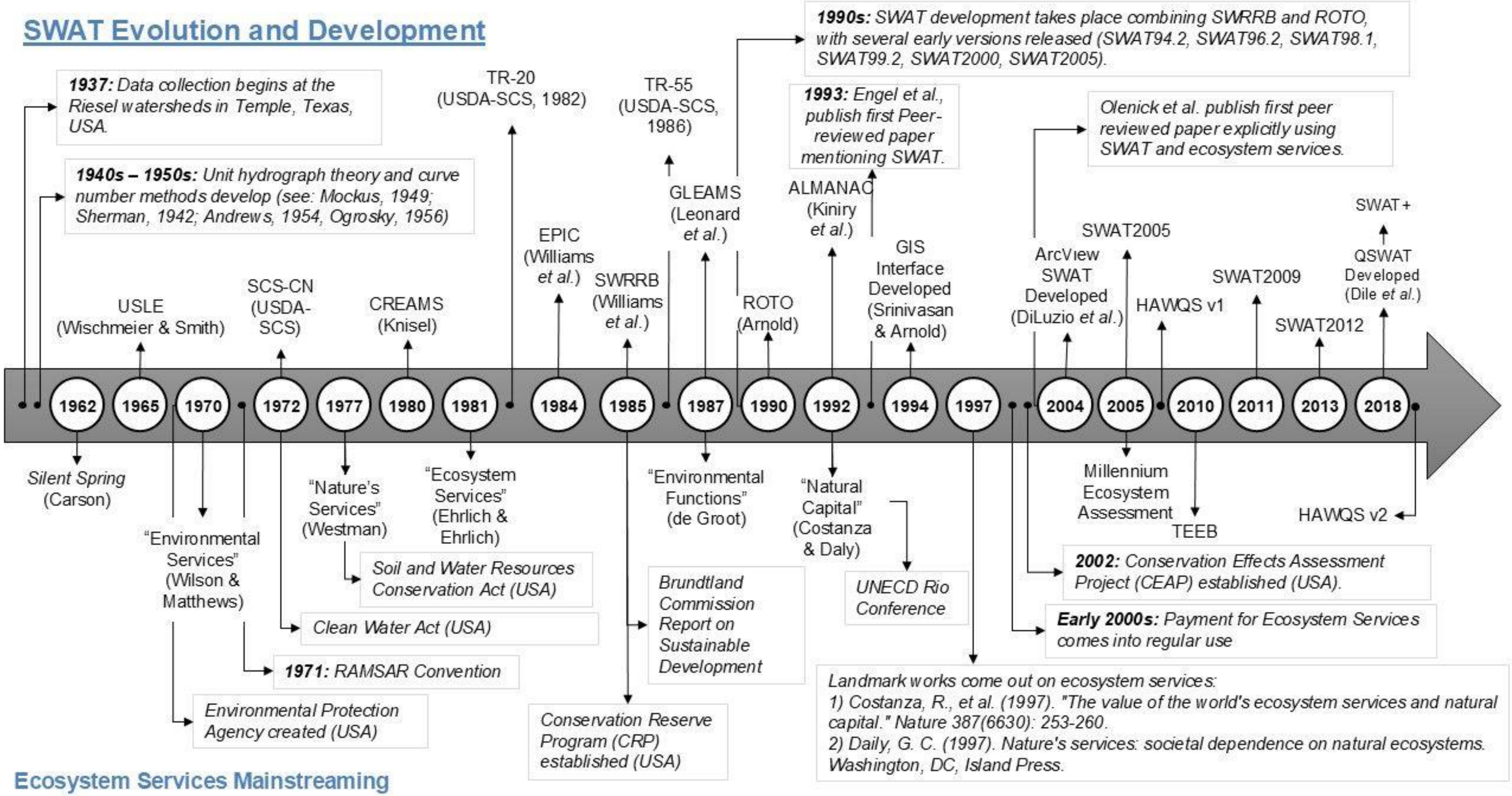
Development history

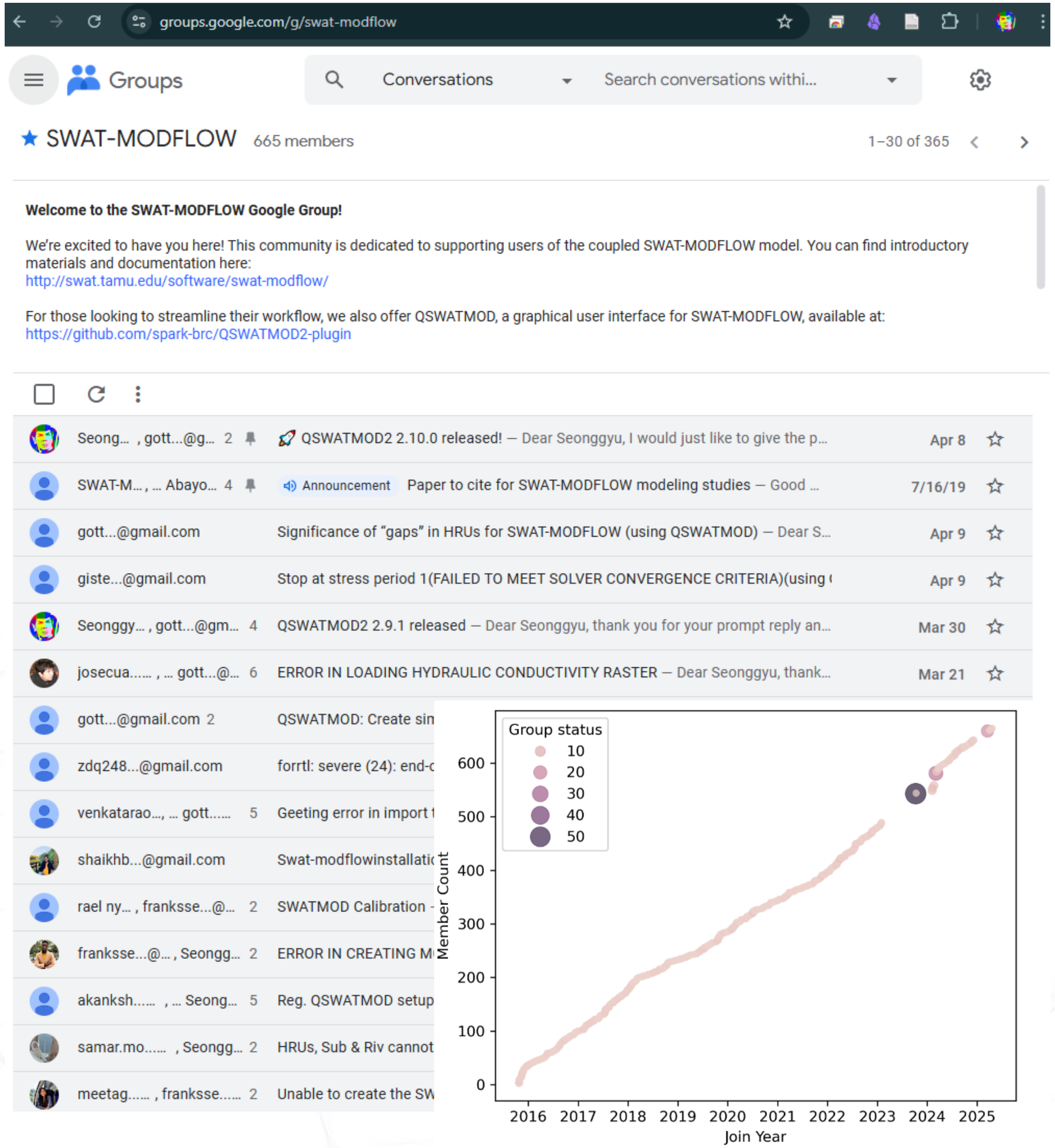
SWAT+
SOIL & WATER ASSESSMENT TOOL

Product of over **45 years** of U.S. Department of Agriculture and Texas A&M University model development, with multiple additions from the international user-community

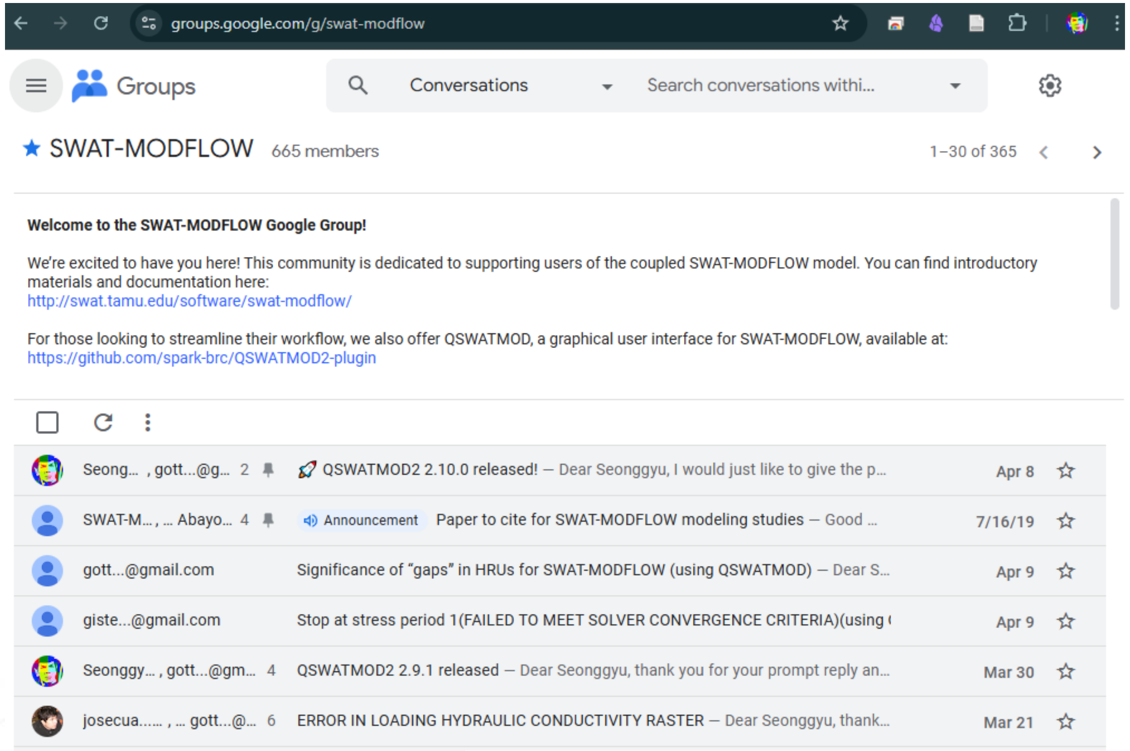


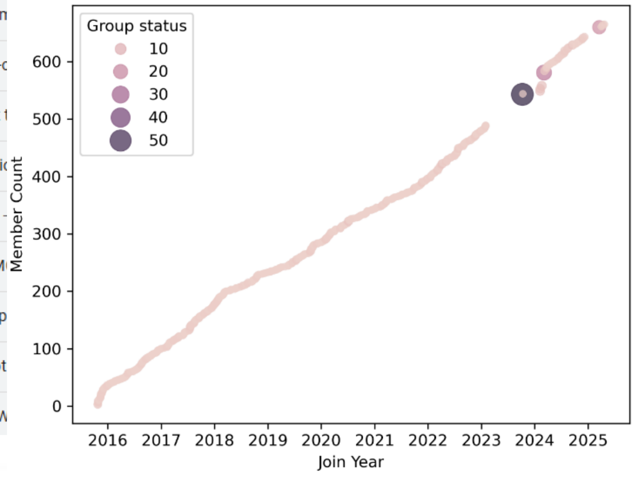
SWAT has a more than 80-year history of rigorous hydrological research and development on experimental watersheds behind it

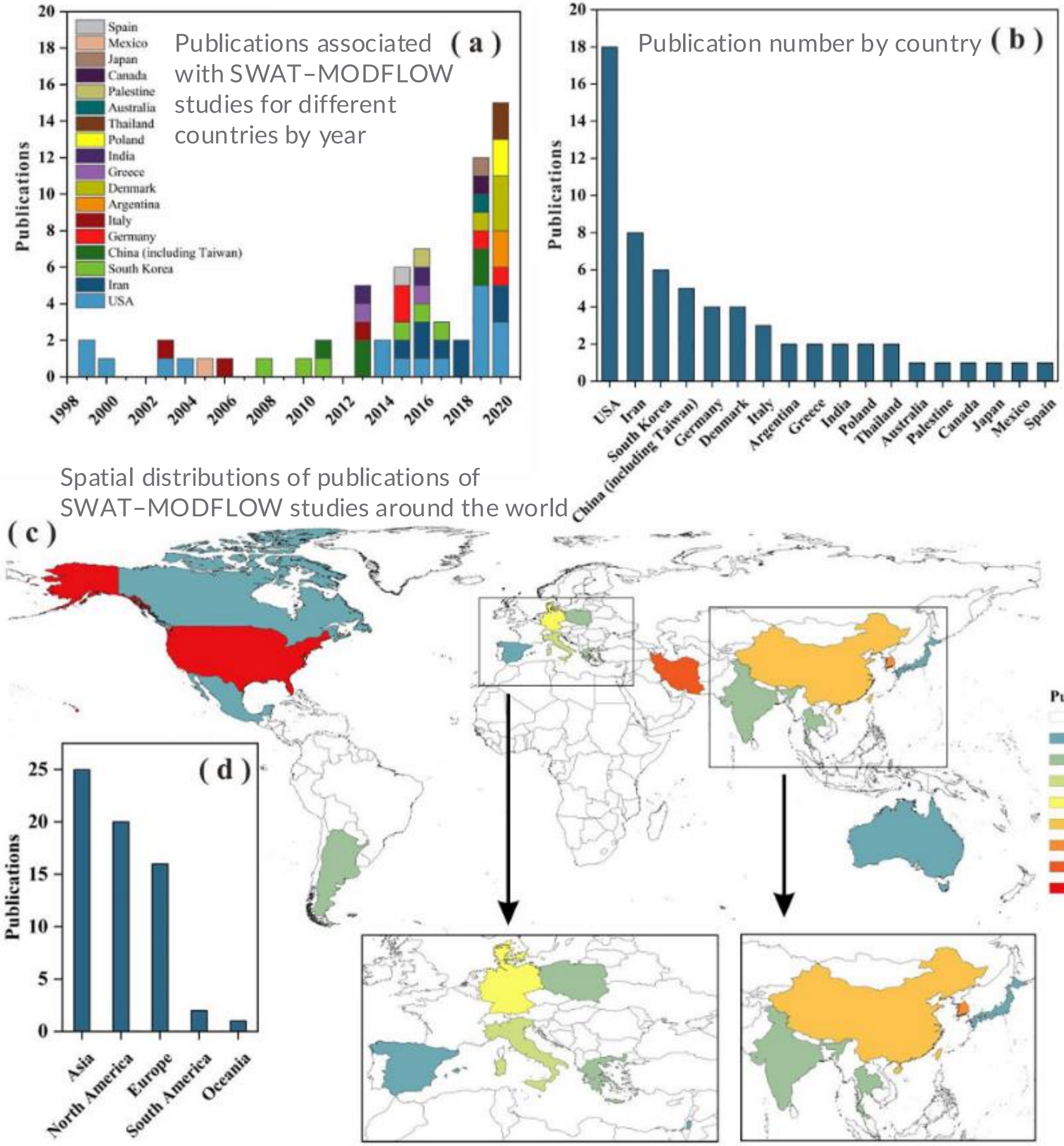
User Accessibility | Collaboration and Service



User Accessibility | Collaboration and Service







Sum of publication number by continent

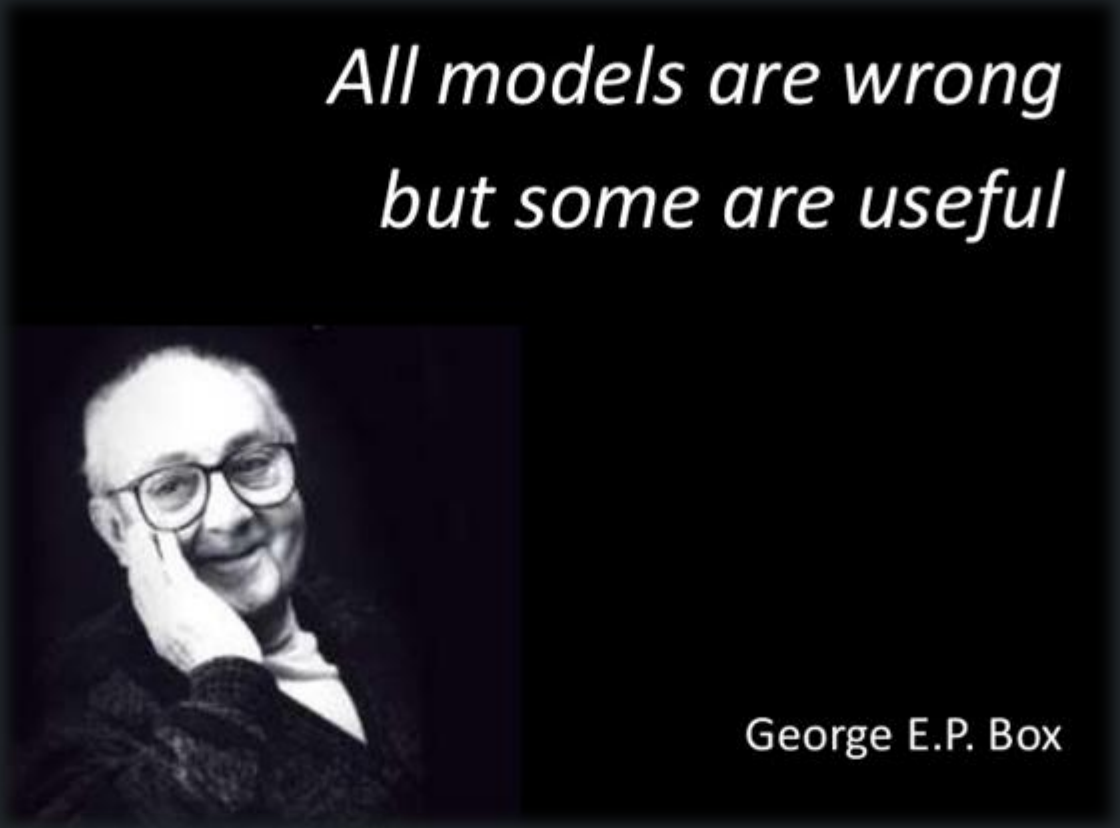
Wang, Y., Chen, N., 2021.
https://doi.org/10.1016/j.wsee.2021.04.001

Day 2

Hands-On Practice for Uncertainty Analysis

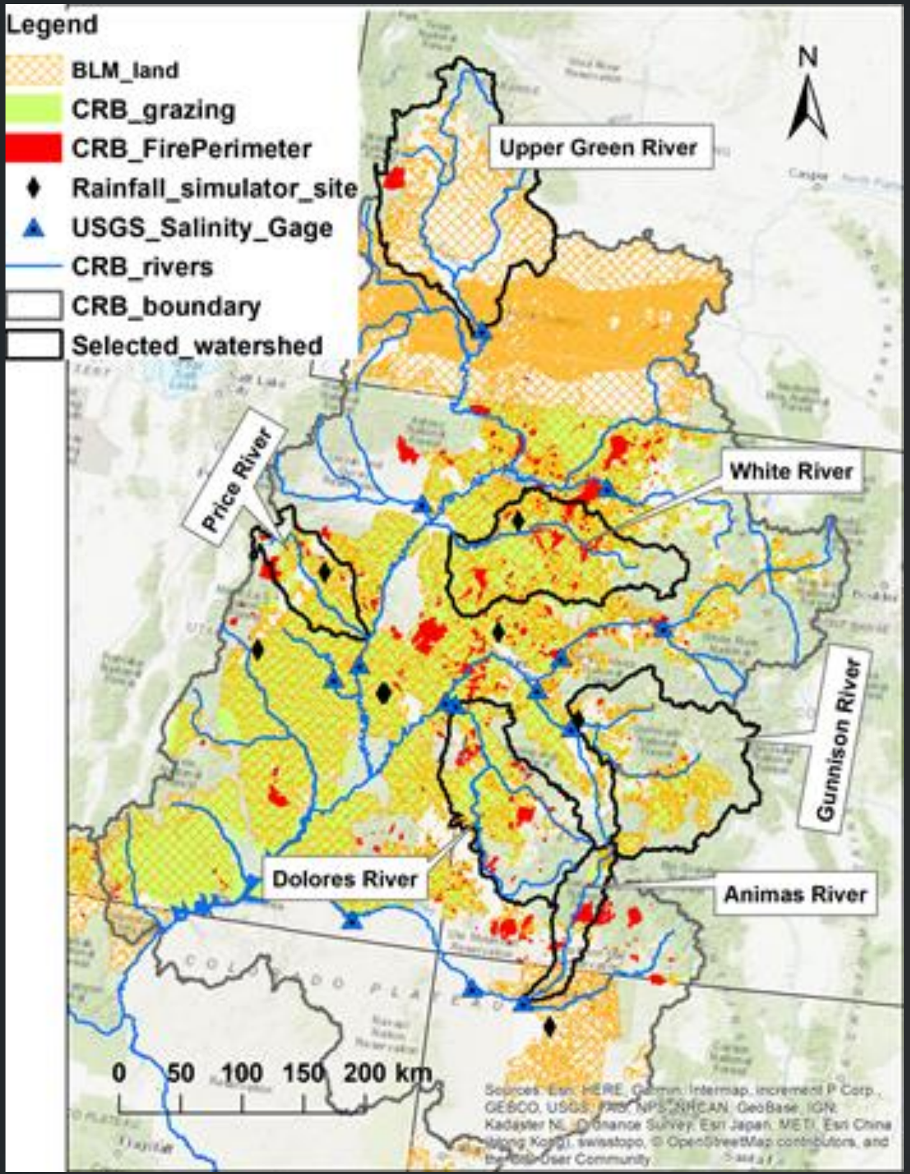
- PEST (Parameter EStimation Tool)
  - PEST official website: https://pesthomepage.org/
  - Tutorial Videos: https://pesthomepage.org/videos
  - Youtube: https://www.youtube.com/@gmdsi
  - Practice with Jupyter notebooks: https://github.com/gmdsi/GMDSI_notebooks
  - Groundwater Modeling Decision Support Initiative https://gmdsi.org/
- swatp_pst
  - Workflow: https://github.com/spark-brc/swatp_pst_wf

All models are wrong!



All models are approximations. Essentially, all models are wrong, but some are useful. However, the approximate nature of the model must always be borne in mind.

Project Background



- Colorado river transports **7-9 million tons** of salt annually to the Gulf of California.
- **Irrigated agricultural districts** causes **highly saline conditions.**
- Salinity contributes to more than **$300 million dollars per year** in economic damage.
  - **Assess** the sources of salinity and its transportation in the Colorado River Basin and
  - **Develop** effective management strategies.

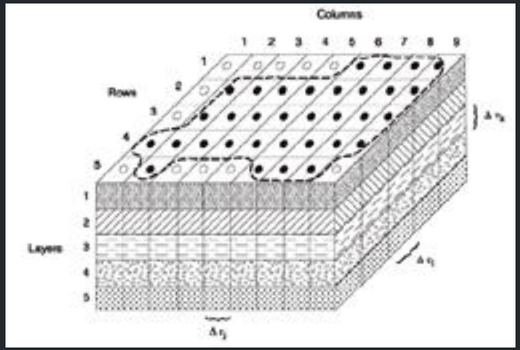
Approaches | Model Integration & Development

developed and maintained by

USDA United States Department of Agriculture

TEXAS A&M AGRILIFE RESEARCH

- The Agricultural Policy / Environmental eXtender (APEX) model was developed and included
  - crop growth algorithms
  - nutrient cycling in the soil profile
  - nutrient transport and
  - loading to streams in surface runoff, soil lateral flow, and groundwater flow, and in-stream transport.



developed and maintained by

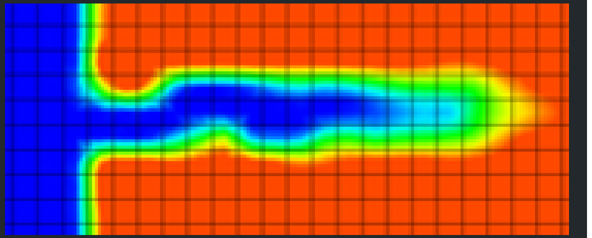
USGS science for a changing world

Partial Differential Equation: develop water balance for each point (cell) in the aquifer

$$\frac{\partial}{\partial x}\left(hK_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(hK_y\frac{\partial h}{\partial y}\right)+Q_{rech}-Q_{pump}-Q_{ET}=S_y\frac{\partial h}{\partial t}$$

- MODFLOW is the U.S. Geological Survey modular finite-difference flow model
  - solve the groundwater flow equation,
  - simulate the flow of groundwater through aquifers.

Reactive Transport in 3 Dimensions



Pacific Northwest NATIONAL LABORATORY

https://www.pnnl.gov/downloads-rt3d (Pacific Northwest National Laboratory)

NO_3:

$$\frac{\partial C_{NO_3}}{\partial t}=\underbrace{-\frac{\partial}{\partial x_i}(v_i C_{NO_3})}_{\text{Advection}}+\underbrace{\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C_{NO_3}}{\partial x_j}\right)}_{\text{Dispersion}}+\underbrace{\frac{q_s}{\phi}C_{s_{NO_3}}}_{\text{Source/Sink}}\underbrace{-k_{NO_3}C_{NO_3}\left(\frac{C_{NO_3}}{K_{NO_3}+C_{NO_3}}\right)}_{\text{Denitrification}}$$

P:

$$\frac{\partial C_P}{\partial t}\underbrace{R_P}_{\text{Sorption}}=\underbrace{-\frac{\partial}{\partial x_i}(v_i C_P)}_{\text{Advection}}+\underbrace{\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C_P}{\partial x_j}\right)}_{\text{Dispersion}}+\underbrace{\frac{q_s}{\phi}C_{s_P}}_{\text{Source/Sink}}$$

+ Salinity Module 8 major ions (SO_4, Ca, Mg, Na, Cl, K, CO_3, HCO_3)

Approaches | Model Integration & Development

developed and maintained by

- The Agricultural Policy / Environmental eXtender (APEX) model was developed and included
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  - loading to streams in surface runoff, soil lateral flow, and groundwater flow, and in-stream transport.


Environmental Modelling and Software 143 (2021) 105093

Contents lists available at ScienceDirect

Environmental Modelling and Software

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

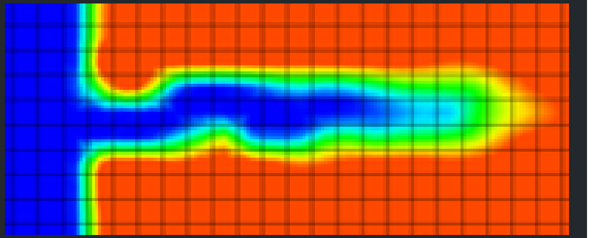
APEX-MODFLOW: A New integrated model to simulate hydrological processes in watershed systems

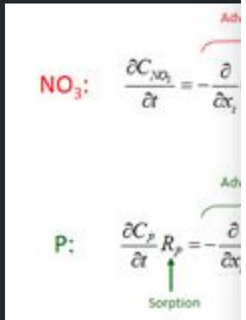
Ryan T. Bailey[a,*], Ali Tasdighi[a], Seonggyu Park[b], Saman Tavakoli-Kivi, PhD[a,d], Tadesse Abitew[b], Jaehak Jeong[b], Colleen H.M. Green[c], Abeyou W. Worqlul[b]

difference flow model

- solve the groundwater flow equation,
- simulate the flow of groundwater through aquifers.

Reactive Transport in 3 Dimensions






Journal of Hydrology 610 (2022) 127873

Contents lists available at ScienceDirect

Journal of Hydrology

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

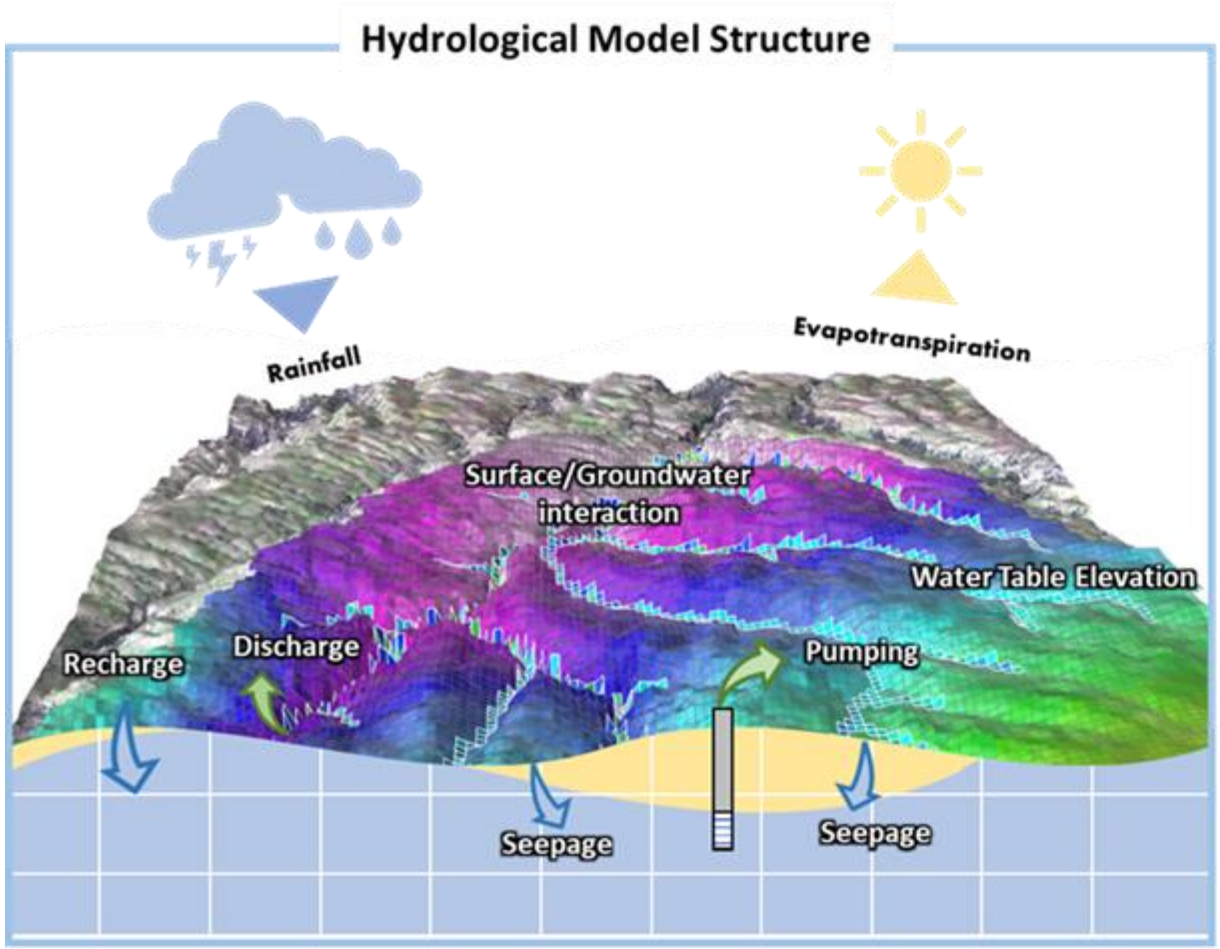
Research papers

Simulating salinity transport in High-Desert landscapes using APEX-MODFLOW-Salt

Ryan T. Bailey[a,*], Jaehak Jeong[b], Seonggyu Park[b], Colleen H.M. Green[c]

https://www.pnnl.gov/downloads-rt3d (Pacific Northwest National Laboratory)

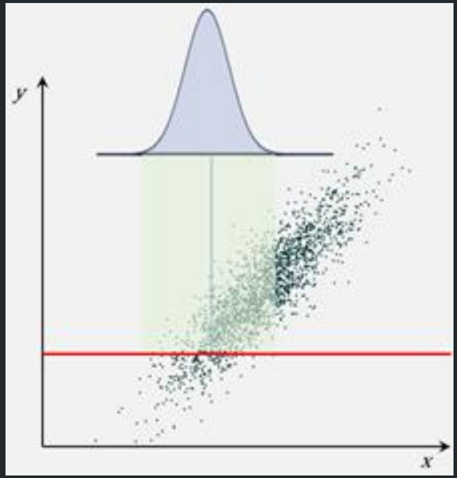
Challenges | Source of uncertainty



Parameters for APEX-MODFLOW-RT3D-Salt (Source of Uncertainty)

- Field Parameters: Available water capacity of the soil layer, Runoff curve number, Soil evaporation coefficient, Transmissivity (T), Hydraulic Conductivity (K), Specific Storage (Ss), Specific Yield (Sy)
- Boundary Parameters: Initial Head Boundary, Riverbed Conductance, Thickness
- Decision Parameters: Rainfall, Recharge, Evapotranspiration, Pumping and Injection Rates
- Numerical Algorithm: Spatio-Temporal Variation
- Salinity: Initial Salt Ion Concentrations / fractions

Uncertainty Analysis | Bayes Theorem



$$P(\theta|X) = P(X|\theta)P(\theta)$$

- Conditional Probability
- Prior
- Posterior
- Likelihood

Uncertainty Analysis | Sampling the posterior parameter probability distribution

- Populate a model with realizations of parameter fields
- Filter realizations based a metric of likelihood function

Uncertainty Analysis | Sampling the posterior parameter probability distribution

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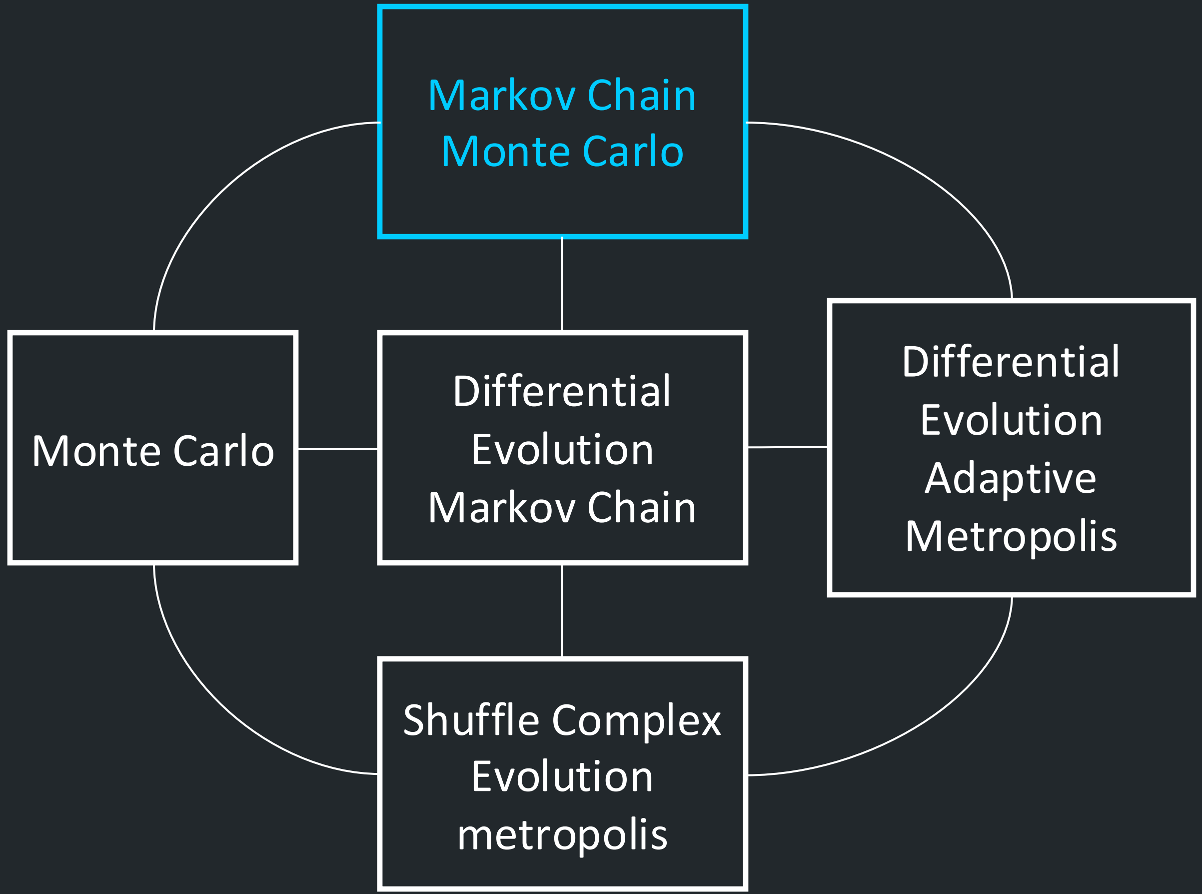

- Less than 1000 parameters
- Short model run time
- Long convergence time

Uncertainty Analysis | Ensemble Method

- Fundamental Concept:

  approximate model-based relations with ensembles

- Ensemble methods: optimization (minimization) algorithms that use ensembles to approximate first-order (partial first derivatives) between parameters and outputs to enable (very) high-dimensional data assimilation (White et al, 2018)

Ensembles: a collection of randomly-sampled model inputs and the corresponding collection of model outputs

Ensemble Methods: Monte Carlo + Linear Algebra

Uncertainty Analysis | Ensemble Method

- Model-based relations of interest:
    - Covariance between measured and unmeasured model outputs
        - State estimation
    - Cross-covariance (e.g. gradient) between model inputs and outputs
        - Parameter estimation
- What's Great: uncertainty analysis and history matching in a single algorithmic workflow
- What's Great: forces you to think about model input uncertainty from the very beginning!

Uncertainty Analysis | Iterative Ensemble Smoother (IES)

P (ne x npar)

	hk	mineral fraction	Initial sconc
real1	0.123	0.9	12.3
real2	0.321	0.0001	32.1
real3	0.987	0.2	69.0
real N	0.789	0.2345	54.1

model runs = ne (number reals)
(e.g. Monte Carlo)

$\mathbf{D}_{sim}$ (ne x nobs)

	head	sload instream	sconc inaqufier
real1	1.11	0.0001	3.21
real2	2.22	0.003	1.23
real3	3.33	0.0003	9.6
realN	4.44	0.001	1.45

Uncertainty Analysis | Iterative Ensemble Smoother (IES)

$$\Delta_P \propto (P - \bar{P})$$

$$J \propto \Delta_{D_{sim}}^T \Delta_P^{-1}$$

$$\Delta_{D_{sim}} \propto (D_{sim} - \bar{D}_{sim})$$

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Uncertainty Analysis | Iterative Ensemble Smoother (IES)

$$P_{\Delta} = -((J^T \Sigma_{\varepsilon}^{-1} J) + (1+\lambda)\Sigma_P^{-1})^{-1}(\Sigma_P^{-1}(P - P_0) + J^T \Sigma_{\varepsilon}^{-1}(D_{sim} - D_{obs}))$$

upgraded parameter matrix

Approx Hessian

dampening

parameter change matrix

residual vector

$$\Delta_P \propto (P - \bar{P})$$

$$J \propto \Delta_{D_{sim}}^T \Delta_P^{-1}$$

$$\Delta_{D_{sim}} \propto (D_{sim} - \bar{D}_{sim})$$

P (ne x npar)

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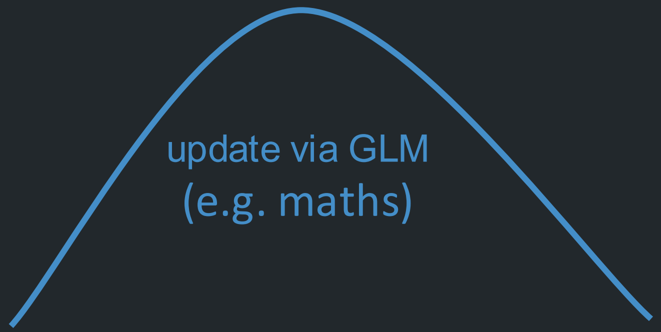

model runs = ne (number reals)

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Uncertainty Analysis | Iterative Ensemble Smoother (IES)

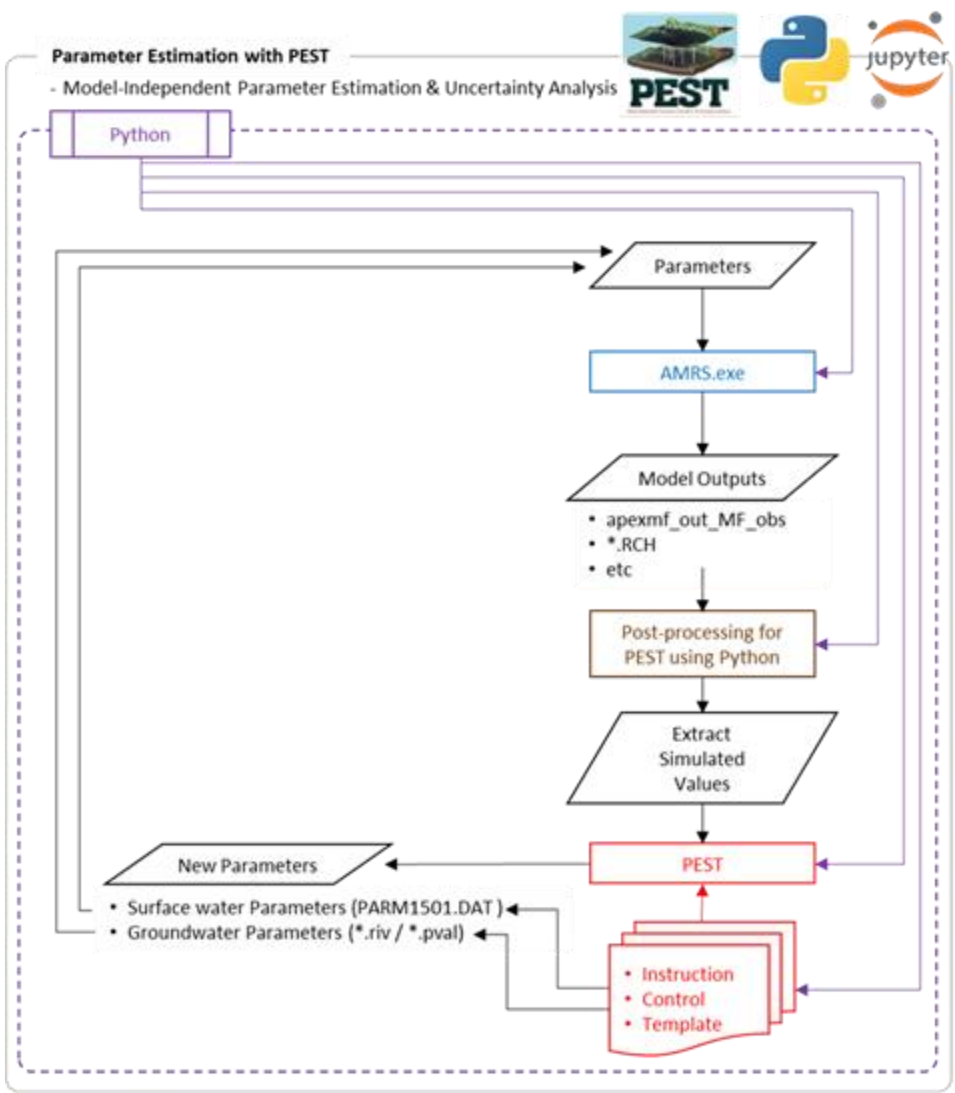
- Number of forward model runs required is controlled by the number of realizations.

Uncertainty Analysis | Iterative Ensemble Smoother (IES)

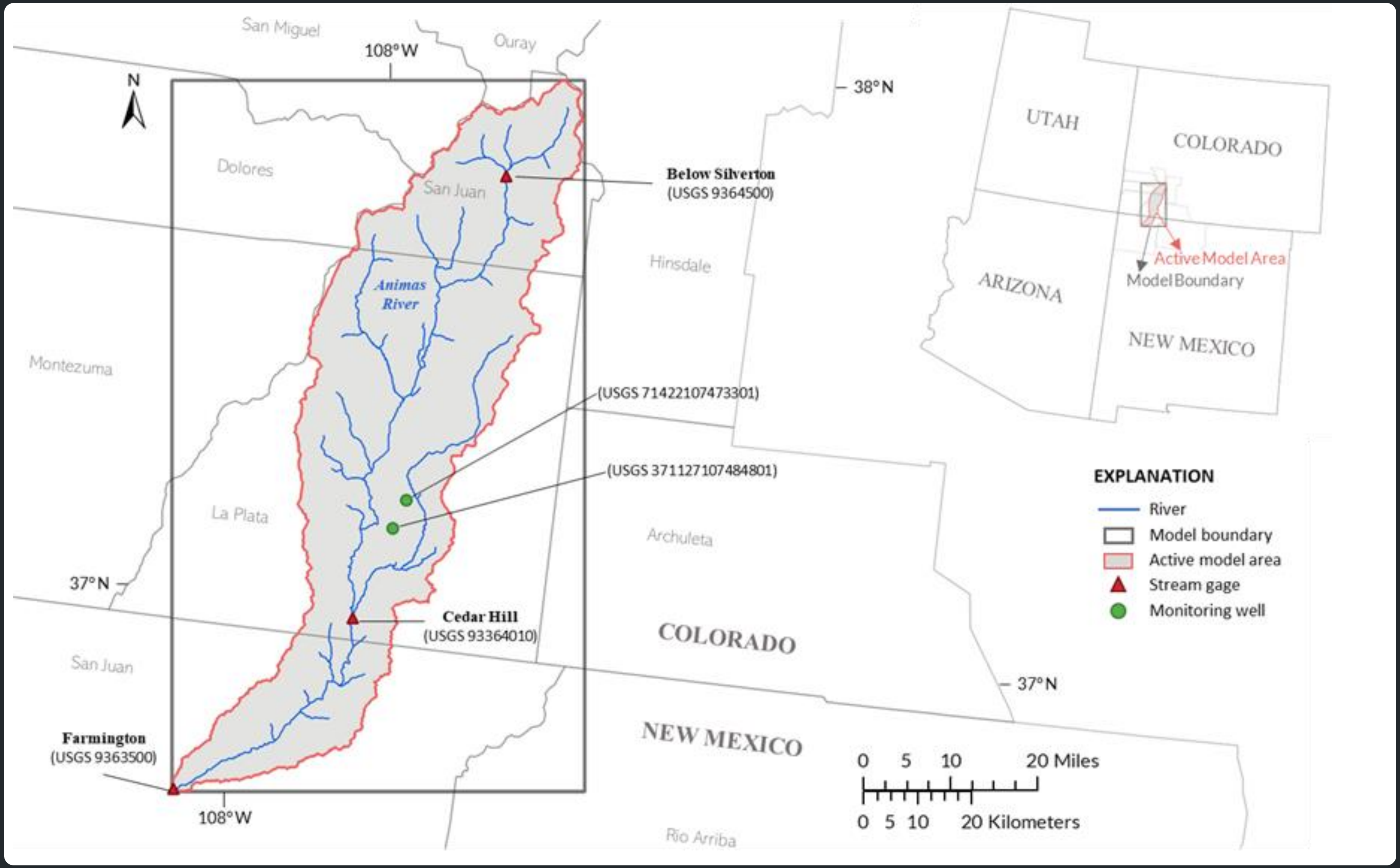
- Number of forward model runs required is controlled by the number of realizations.
- The parameter ensemble is a sample of the posterior parameter distribution which we can use for uncertainty analysis.

Uncertainty Analysis | Framework

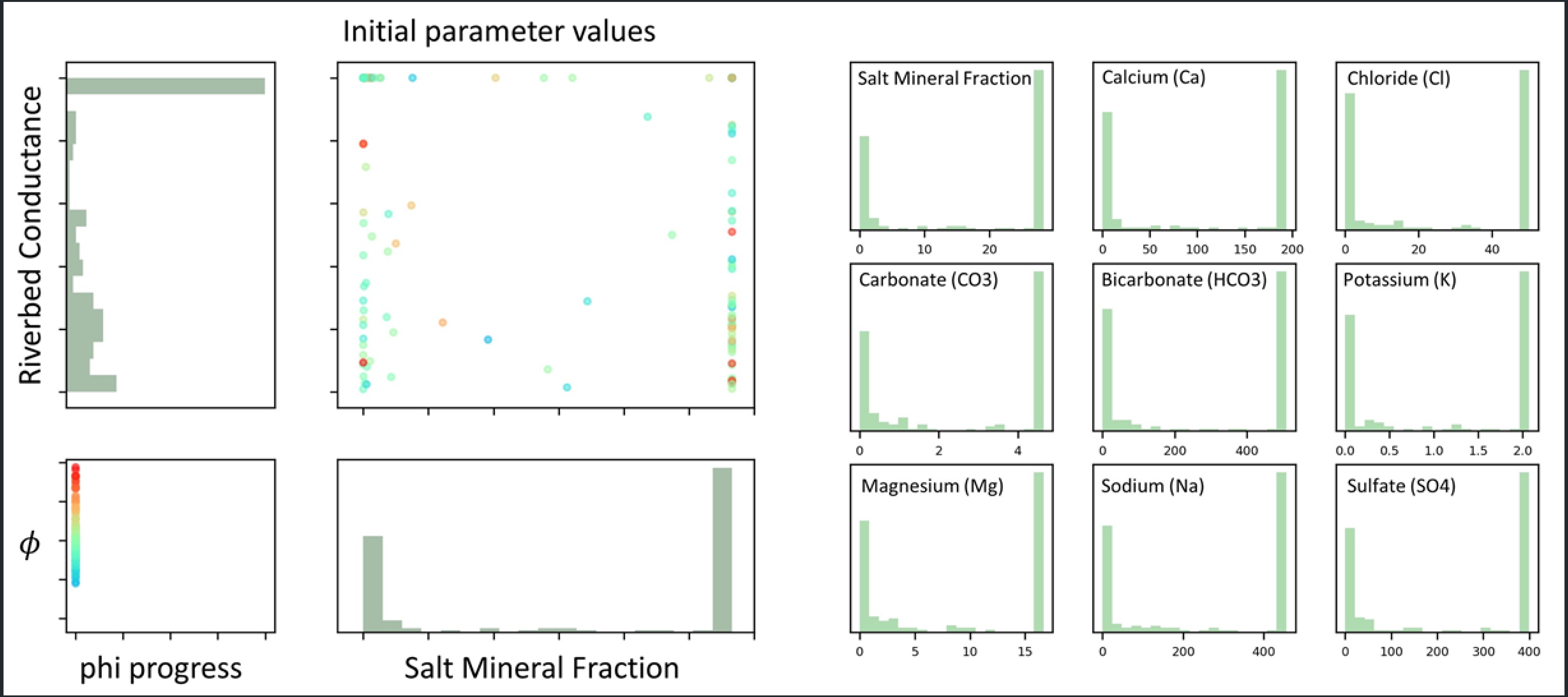
pyEMU + FloPy + apexmf



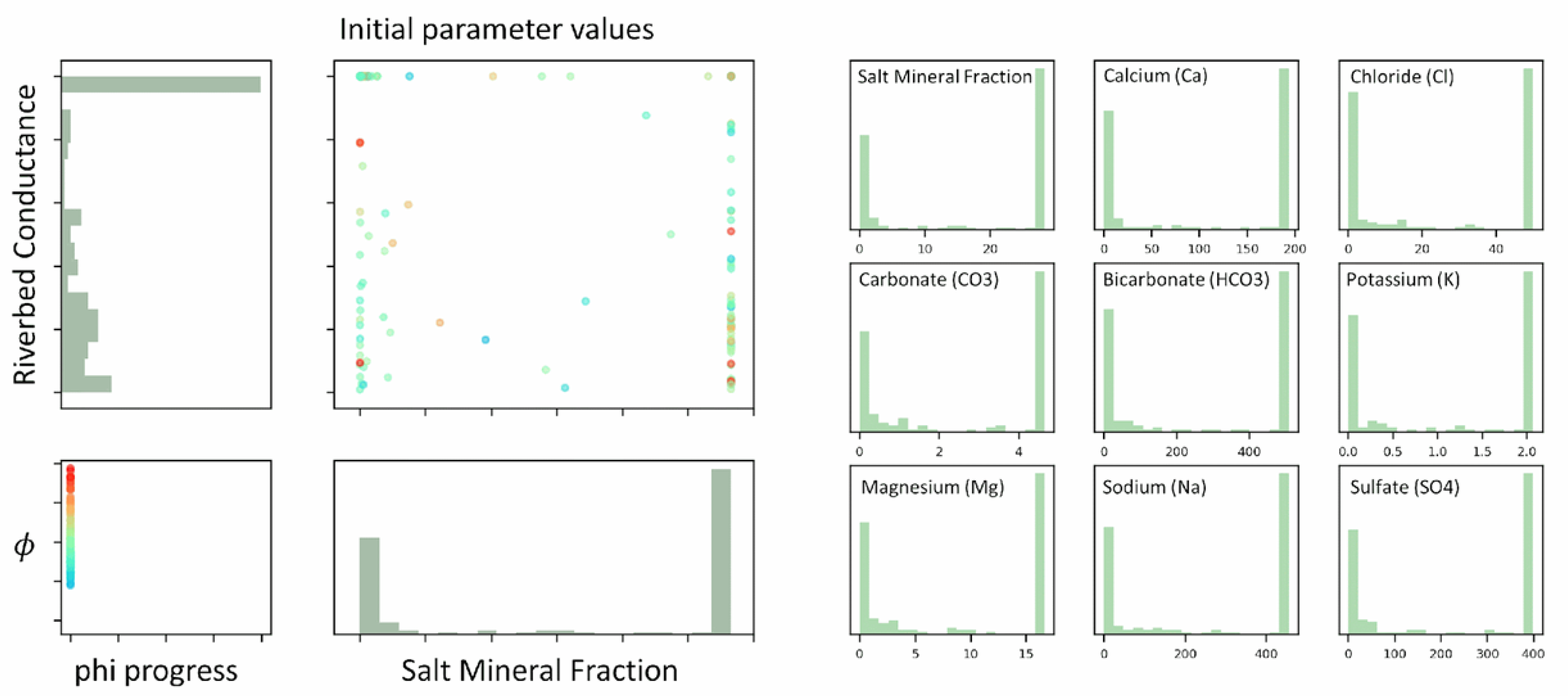
A Worked Example | Animas River Watershed



A Worked Example | Animas River Watershed

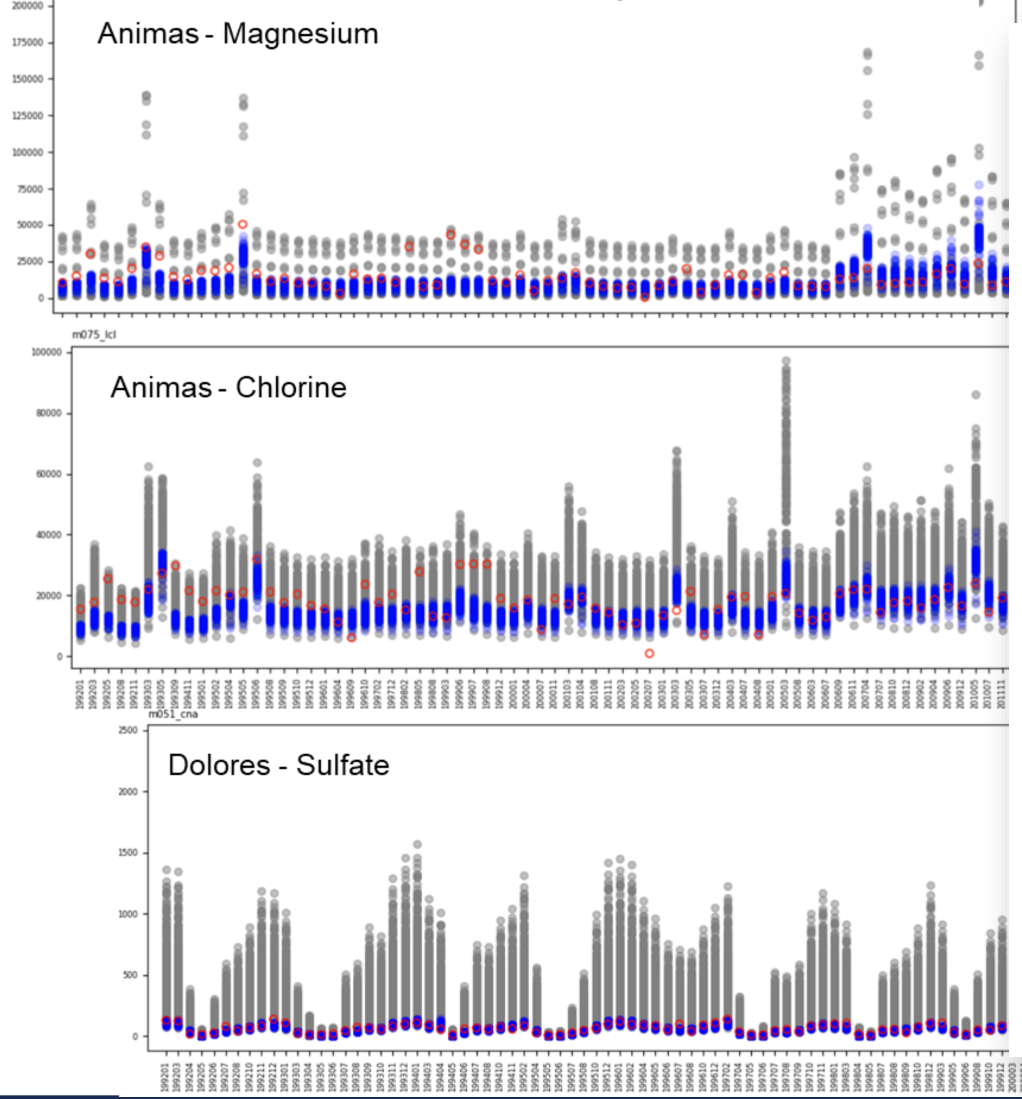


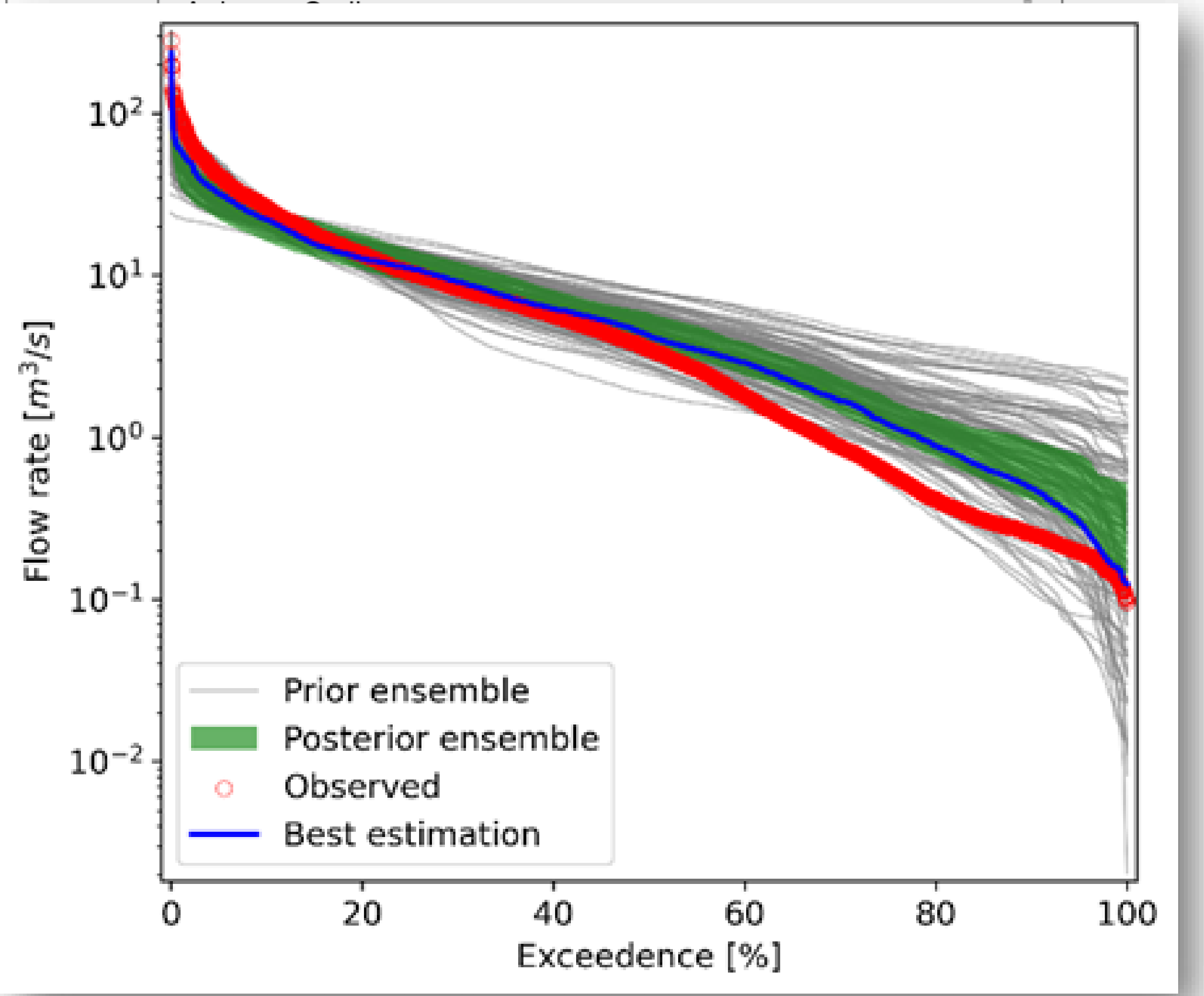
A Worked Example | Animas River Watershed



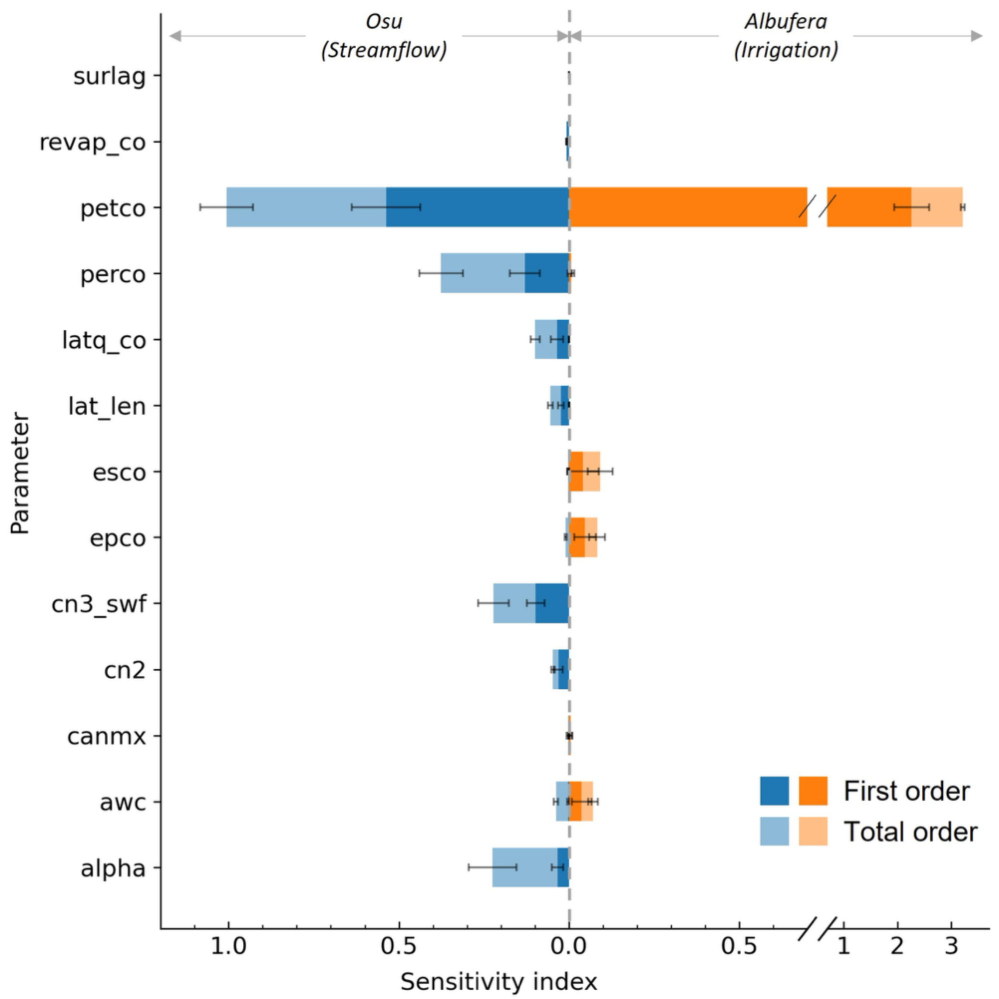
A Worked Example | Animas River Watershed

- Predictive Uncertainty Quantification

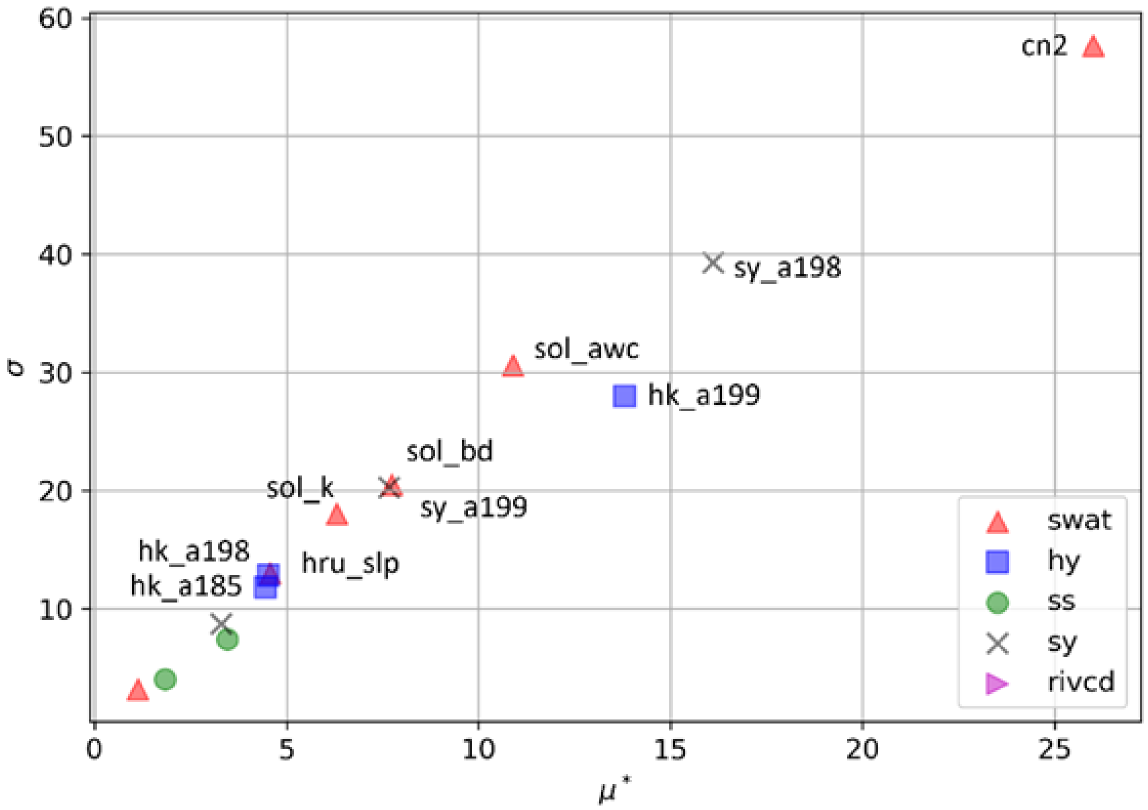




A Worked Example | Sensitivity Analysis



Sobol's first-order and total-order sensitivity indices were estimated for the selected 13 parameters. Error bars correspond to a 95% confidence interval.



Morris Screening Result:
Only the most sensitive parameters are labeled for clarity.
The σ values indicate the degree of nonlinearity or factor interaction, while μ* represents the sensitivity measure.

References

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  - SPOTPY: https://spotpy.readthedocs.io/en/latest/Algorithm_guide/
- Bayesian Theorem:
  - Probabilistic-Programming-and-Bayesian-Methods-for-Hackers: https://github.com/CamDavidsonPilon/Probabilistic-Programming-and-Bayesian-Methods-for-Hackers
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- DREAM:
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  - Tasdighi, A., Arabi, M., Harmel, D., Line, D., 2018. A Bayesian total uncertainty analysis framework for assessment of management practices using watershed models. Environmental Modelling & Software 108, 240–252. https://doi.org/10.1016/j.envsoft.2018.08.006
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