

# PSimPy - Predictive and probabilistic simulation with Python



Hu Zhao, Anil Yildiz, Nazanin Bagherinejad, Julia Kowalski

Chair of Methods for Model-based Development in Computational Engineering, RWTH Aachen University, Germany

Gaussian Process, Multiphysics Simulation

## Simulate & Emulate

Scale up your simulator in just a few steps

- Plug in your simulator via a Python wrapper
- Run serial or parallel without changing your model
- Train a Robust GP emulator to mimic your simulator's outputs
- Use the emulator as a lightweight substitute for fast evaluations

## Quant. uncertainty

Identify key drivers. Calibrate with data.

- Run sensitivity analysis using Sobol indices
- Sample efficiently using Saltelli, LHS, or Metropolis Hastings
- Estimate posterior distributions using Bayesian Inference
- Use active learning to choose the most informative next simulations

Want to build unified,  
robust and sustainable  
UQ workflows? [1]

**PSimPy**

- Set up a Bayesian problem
- Kick off with a small batch of simulations and a GP Emulator
- Active learning automatically picks the next input points to improve calibration
- Estimate the posterior from the emulator and visualize it

Active-learning calibration

## Example

## Bibliography

- [1] H. Zhao, A. Yildiz, N. Bagherinejad, and J. Kowalski, “PSimPy: GP emulation-based sensitivity analysis, uncertainty quantification and calibration of landslide simulators,” in *14th International Conference on Applications of Statistics and Probability in Civil Engineering, ICASP14*, Dublin, Ireland, 2023.

## Bibliography