



Theory and Practice of Applied Predictive Groundwater Modeling

When: October 8th and 9th

Where: Freys Hotel & Konferens, Stockholm

Instructors: Dr. Rui Hugman and Dr. Jeremy White

Overview: Applied predictive groundwater modeling is the science and practice of using groundwater models as decision support tools to help stakeholders and decision makers manage important groundwater resources. This type of groundwater modeling is distinct from more traditional explanatory groundwater modeling. Predictive groundwater modeling focuses heavily on statistical learning from available (imprecise) data and estimating uncertainty in important predictive outcomes. In this way, applied predictive modeling is more similar to the practice of data-driven modeling and so-called "machine-learning".

In this 2-day short course, attendees will be exposed to the theory and concepts that enable predictive groundwater modeling, such as automated parameter estimation/data assimilation, uncertainty analysis, data-worth analysis, geostatistics, and management optimization, among others. Day 2 will provide the opportunity to practice the application of many of these concepts in hands-on exercises using free and open source software, including:

- MODFLOW-6: https://github.com/MODFLOW-USGS/modflow6
- FloPy: https://github.com/modflowpy/flopy
- PEST++: https://github.com/usgs/pestpp
- pyEMU: https://github.com/pypest/pyemu
- GMDSI notebooks: https://github.com/gmdsi/GMDSI notebooks

Most importantly, we want this course to be a forum where attendees are free to discuss their experiences and how groundwater modeling does and doesn't serve its role as a decision support tool within the context of Sweden's groundwater resource management framework. Attendees can choose to participate in both days or just the first day.

Aspirational outline:

1. Day 1: Concepts, Theory and Experiences

- a. Overview: Why we are here and setting the stage with a local perspective
- b. Introduction Predictive vs explanatory modeling and model complexity
- c. Open discussion/group therapy sharing stories of modelling pain and suffering
- d. Intro to Uncertainty
 - i. Bayes and learning from data
 - ii. Getting to the airport thought experiment
- e. Uncertainty in groundwater modelling
 - i. Where does it come from?
 - ii. Why does it matter?
 - iii. What can we do about it?
- f. Heterogeneity and why it matters
 - i. Geostatistics, pilot points, and representing heterogeneity
 - ii. Uncertainty in heterogeneity
 - iii. The parameter parsimony fallacy / the non-uniqueness boogeyman
- g. Reducing uncertainty
 - i. Inverse problems, calibration, history matching and data assimilation
 - ii. GLM algorithm
 - iii. Ensemble methods
 - iv. (bonus) Data Space Inversion and other emulators

v. Applied examples

- h. The value of data
 - i. Data worth analysis
 - ii. Ensemble variance analysis
 - iii. Applied example
- i. Management optimisation
 - i. Optimal solution versus scenario testing
 - ii. Optimisation under uncertainty
 - iii. Applied example
- j. Open discussion and additional topics
 - i. Model complexity
 - ii. Tradeoffs with scripting and automation
 - iii. Rapid, reproducible, and robust
 - iv. Considerations on data-driven (AI/ML) vs physics-based models
 - v. The role of problem decomposition
 - vi. "I pay for models, what should I ask for?"

2. Day 2: Hands-on Practice with Decision Support Modelling Software

- a. Intros and making sure IT is working (or not...)
- b. GUI's and scripting
 - i. Brief overview of common GUI support for PEST/PEST++
 - ii. Brief discussion of the value of scripting and replicable workflows
 - iii. Mention GIT
- c. Introduce our synthetic decision support case (Freyberg) and model
 - i. History of the freyberg model
 - ii. Building a model that simulates the past and the future all at once
- d. Mechanics of pestpp
 - i. pestpp control, template and instruction files
 - ii. How to construct them yourself
 - iii. Hands on: build a template, instruction and control file, debug as needed
- e. How to run pestpp
 - i. What's a command line?
 - ii. What to do when things go wrong
 - iii. Understanding parallelization
 - iv. Hands on: run a pestpp code using the interface you setup
- f. Live demo pyemu
 - i. Show all of the above with PstFrom
 - ii. Pilot points and multipliers
- g. History matching and UA with pestpp-ies
 - i. Run pestpp-ies in parallel
 - ii. Post-process results
 - iii. Observation noise
 - iv. Prior data conflict
 - v. **Hands-on:** run pestpp-ies on the interface you setup
- h. Live demo scripted
 - i. From zero to hero with a few lines of code
- i. (Bonus) Optimisation with pespp-opt/mou
 - i. Decision variables, objectives and constraints
 - ii. See how many model runs it takes...