Applied Groundwater Model Calibration and Uncertainty Analysis Curriculum

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remove before flight – link to old syllabus with some notes
https://docs.google.com/document/d/12xPPWcSAGryn1aWi3tZ8-Nrk45SKbXDzIcIKXEqdd5s/edit
MONDAY

1. **Introductions of students/instructors [MNF].** Goals for the week and framing
    (a) The mechanics and theory
    (b) Learning by doing
    (c) Please speak up! Everyone learns from discussion
    (d) Work in pairs
    (e) Python, GUIs, and all that
2. **Shortish Historical Background #1 and Introductory material** [RJH]. What is "inverse"? How did we get here? The concepts of model usage, forecasting, how type of forecast influences uncertainty, learning, uncertainty analysis and the role of calibration. PE is a tool to an endpoint - not inviolate. A perfect fit for Stepwise modeling: a tool for automated trial-and-error, and tweak at end. MAIN COURSE POINT: There is no model of a part of the world, it is ALWAYS a simplification of reality and our job is to tune the simplifications for the forecasts of interest
3. **Logistics and airing of the IT grievances** [MNF]:
    (a) Did everyone get the software installed?
    (b) Pull the class from github and make a copy
    (c) Brief Git tutorial
4. **intro_to_regression** [MNF] Linear regression overview---illustration with fitting a polynomial to noisy data including the role of SSE (response curve), degrees of freedom, the gradient of that surface (Jacobian) overfitting (give fish) MAIN COURSE POINT: Not magic, automated trial-and-error (Maths!!!). The models will get more involved, need a more powerful tool (PEST++)
5. **freyberg_model_intro** [MNF]: Introduce Freyberg model outlining the role of forecasts, the increase in parameterization. Introduce forecasts of interest: head, sw-gw flux, travel time
6. **freyberg_trialerror** [JTW] Messing around with a pre-setup version of the Freyberg model using trial and error to explore fitting a couple parameters looking at both calibration and forecast implications. Find parameter values that best fit the calibration heads, and also parameters that fit the travel time forecast
7. **freyberg_pest_setup** [RJH]: Mechanics and Details on PEST++, how to run, control file (refer to annotated print out), model run command (mention importance of a forward run script), TPL and INS files and controlling MODFLOW; PESTCHEK: use TEMPCHEK and INSCHEK to write simple input and output for the freyberg single K model. Run PESTCHEK and then run PEST++. Have control file made for simple 1 par case, specify par and obs names. Show how forecasts can be observations in control file.
8. **freyberg_pestcheck_trouble** [RJH] fix a troubled PEST control file (trouble.pst), see an error that is not caught but by PESTCHEK but is caught when PEST++ is run, make them uncomment a PEST++ comment line to get their forecast back in the rec file
9. **Why we model** [JTW] Outlining forecasts to be made in first model runs and relate to why we model, and why looking at calibration is often not enough for good forecasts. Underscore MAIN COURSE POINT: we are focused on forecasts- model purpose. What does parameter estimation teach us about the model and its forecasts? Tie back to previous example/activity

(a) Models are built because of uncertainty Quantities of interest(QOIs)/forecasts/predictions can't be observed To properly "model", we should then have a "learning" framework: Learning == reduction in uncertainty Model analyses combine information our knowledge about the system Observations of the system (deterministic) parameter estimation is a small piece of modeling analyses Part of the "learning"-from-observations process But parameter estimation itself does not help us learn about QOIs Before "calibration" the QOIs a have a single "value" After "calibration" the QOIs have a (new) single "value" Tuesday

10. **introduction_to_GLM** [MNF] Derivation of the Gauss-Levenberg-Marquardt Algorithm part I. The maths

    TUESDAY

11. **freyberg_k** [RJH] Review the PEST++ control file...refer to annotated print out (provided) (need to decide balance of details day 1 - day 2). Use PEST++ to calibrate with only a single hydraulic conductivity (K) zone and head observations: we provide fully hooked-up MODFLOW files. We will walk through the pest setup components (TPL, INS, PST). Look at .rec file for parameter and forecast uncertainty. Explore how parameter bounds and observation weights influence the resulting forecast uncertainty. Reintroduce parameter estimation conceptually (tying back to regression, and highlighting forecasts). Parameter estimation is just a means to extract info from obs and store in parameters...we don't know how that information flowed until uncertainty analysis. GUI equivalent - hit the wall.

12. **Short Interlude - what does a response surface tell us?** [RJH] Quick and dirty activity, intro on response function, setup grid-based sampling and use sweep util to gen runs - allow them to specify their own weights for obs and PI - should give different response surface - nonuniqueness!!!

13. **xsec_response_surface_GLM** [MNF] Derivation of the Gauss-Levenberg-Marquardt Algorithm part II: response surface. Discussion of the algorithm in terms of the response surface, GLM, Use previous response surface to show steepest vs newton direction and how lambda works and why lambda is a regularization device.

14. **freyberg_k_and_r** [JTW] use PEST++ to calibrate both K and recharge (R) with head observations. Have premade files for this. DIY - have students add recharge parameter. With so many head targets why isn't this overdetermined? Why did forecast uncertainty go up?

15. **freyberg_k_and_r_response_surface** [MNF] Correlation and non-uniqueness in regression--Response surface illustration (using the Freyberg model): the need for diverse data. Discuss how the flux observation made a more unique solution and what this additional information does to uncertainty — going toward a good compromise (MAIN COURSE POINT: observations don't cost us runs; good practice put in as many observation types as possible). Show updated response surface with lovely bullseye replacing banana canyon

16. **freyberg_k_and_r_fluxobs** [RJH] use PEST++ to calibrate K and R with a flux observation and heads (we provide all files). MAIN COURSE POINT: Burning silicon can't make up for poorly thought out problems

17. **Adding a flux target in GWV GUI digression** [RJH] example of PEST++ file generation, GUI only as starting point. Include fluxobs unfix "rch_1" and look at how including future climate uncertainty impacts forecast uncertainty. Recharge is most sensitive parameter for calibration, makes sense it is important for forecasting the future. Fixing it implies we know the future perfectly.

18. **freyberg_reweighting** [MNF] The role of weighting and how to balance objective function. Doing it at the beginning - not the end (pyEMU, pie charts, weight-o-matic). Tie back to previous response surface activity.

19. **intro_to_sweep** [JTW] Show that response surface was not a built-in PEST utility. Sweep is general and allows you to setup whatever parameter sweep you want. Demo with a single parameter set csv. Demo YAMR - have students rerun k+r calibration, manually starting master and workers.

20. **freyberg_k_and_r_mc** [RJH] run MC on the K and R model but drawing from prior — talk about nonuniqueness and rejection sampling (GLUE). MAIN COURSE POINT: MC is a stakeholder friendly, easy-to-understand uncertainty technique, but incurs a huge computational burden for real problems. How many realizations are "acceptable" in terms of phi? How does the best "phi" compare to the calibrated phi? Including Monte Carlo analysis---we can't calibrate future recharge, but we can quantify how much it matters. The posterior for rch_1 is the same as the prior - why is that?

    WEDNESDAY

21. **freyberg_zones** [MNF] Set up zones for K and calibrate with PEST++. Using a given zonation and a zone-burner python script.

22. **freyberg_global_sensitivity** [RJH] How can we extend diagnosis with SVD -- which parameters are informed by the data? Scale, offset, tying, fixing. What matters?

23. **intro_to_bayes** [MNF] Really, calibration is a small component of Bayes' Rule (and model usage)—parameters are conditional on information (types and amounts of information) and model structure ("calibrated" parameters aren't transferable)- if forecast depends on those parameters, then we learn about the forecast. Put another way, discuss the process in terms of learning as a reduction in uncertainty.

24. **freyberg_zones_DIY_mc** [JTW] run both FOSM and MC on the zoned freyberg model - Compare FOSM and MC for both performance and results. Also explore identifiability

25. **intro_to_FOSM** [JTW] FOSM as an alternative to MC (rejection sampling). Implications of "implied" calibration, linearization, speed. MAIN COURSE POINT: MC is often easy to communicate results, but FOSM is much cheaper. How can FOSM be completed before history matching? It's magic!

26. **intro_to_dataworth** [MNF] FOSM- huh, good god y'all. What is it good for? Absolutely nothing! Quantification of prior and posterior forecast uncertainty (the value of calibration), but more importantly, data worth considerations. Linearity assumption may not be a good approximation in all cases, but still useful to eval the value of different calibration, different data, etc. What parameters are important to uncertainty in forecasts (modern alternative to "sensitivity analysis" (USGS-type)) PEST lingo = PREDUNC/GENLINPRED

27. **freyberg_zones_dw** [MNF] Data worth with the zoned model. Next best observation location to measure to reduce forecast uncertainty. We provide an alternate zonation option. Discuss the ramifications of various zonations on both forecasts The value of flexibility in parameter fields with special emphasis on avoiding overfitting--we fit to extract maximum info from the observations while also capturing parameter contributions to forecast uncertainty.

28. **GUI_demo_with_GW_Vistas** [RJH] Overview of how to use GW Vistas for setting up, running, and post-processing zoned model.

29. **intro_to_geostatistics** [MNF] Exploring the idea of a model of spatial correlation (e.g. covariance matrix). Variograms as a basis for interpolation, the use of factors, "spatially weighted averaging", all this wrapped up in Kriging. Function for creation and viz. In pyemu. Namecheck sGems, Surfer, TPRogs

    THURSDAY

30. **intro_to_pyemu** [JTW/MNF] The mechanics behind the beast. Control file handling and manipulation, matrix/cov/jco handling. Res handling, etc. Setting up the interface with flopy models. Pilot points, geostats, prior info construction, starting local slaves. FOSM (schur and error variance), MC/ensemble handling, various output setup and apply routines (hob, hyd, list file, hds).

31. **freyberg_pilot_points_1** [JTW] Create a pilot point network and run pestpp. YAMR for parallel processing on laptops. Cover the implementation of setting a pp network and setting geostats factors. No regularization...way over fit Perhaps need a brief intro to pilot points to explain the concept, history, importance of representative starting values, and high parameter flexibility does not equal high complexity

32. **intro_to_singular_value_decomposition** [MNF] an aside backing up the theory and practice of SVD and a little on SVDA because now that we are moving to PP land we need a crutch. Concepts of relinearization - think of a boss analogy. Make sure to discuss fundamental subspaces. Give chain of PEST developments that were caused by pilot points. Also TSVD and "super parameters" Need to talk about TSVD as a regularization device - the MAP implementation of GLM Need thought experiments with MAXSING and EIGTHRESH - what happens conceptually with these...

33. **freyberg_sensitivity_identifiability** [RJH] How can we extend diagnosis with SVD -- which parameters are informed by the data? What matters? What's the value of ID vs. Sensitivity. Correlation issues. Compare the two.

34. **intro_to_regularization** [RJH] introduction to the concepts, theory and implementation of Tikhonov regularization. Need to talk about TSVD as a regularization - they will see this in the next exercise Bringing in geostats concepts. Need to talk about constrained optimization with Lagrange multiplier?

35. **freyberg_pilot_points_2** [RJH] Add prior information and switch to regularization mode. What happens now? Talk about overfitting: parameters and forecasts.

36. **freyberg_pp_GUI** [RJH] GUI digression for creating PP network with regularization; debug file of steps. Maybe some discussion of other approaches

37. **parallel_processing** [JTW/MNF] As an aside, while running the above, show YAMR manually, maybe HTCondor too.

    FRIDAY

38. **freyberg_pp_dw** [JTW] Revisiting FOSM and data worth with the pilot point model--fare thee well artifacts. Diagonal prior was based on bounds. Have a full prior built for use also - plot for demystification. Why does uncertainty go up when a non-diagonal prior is used?

39. **freyberg_pp_monte_carlo** and **freyberg_pp_advanced_monte_carlo** [JTW] Monte Carlo with various sampling strategies to increase number of realization retained. Three strategies are: 0) sample Schur-derived posterior, 1) vanilla style with the prior full covariance.

40. **Discussion** [ALL] what other model inputs could be parameters (what is not known perfectly)? The importance of parameterization: "If it's not a parameter, it must be known perfectly". What are other sources of uncertainty? Future stresses as parameters?

41. **freyberg_grid_ies** [JTW] iterative ensemble smoothers. Allow all BCs, future stresses, etc. to be parameters and explore uncertainty with FOSM. Use the pyemu example freyberg notebook for this. JTW