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Improving predictive capability of land surface models through robust statistical calibration techniques

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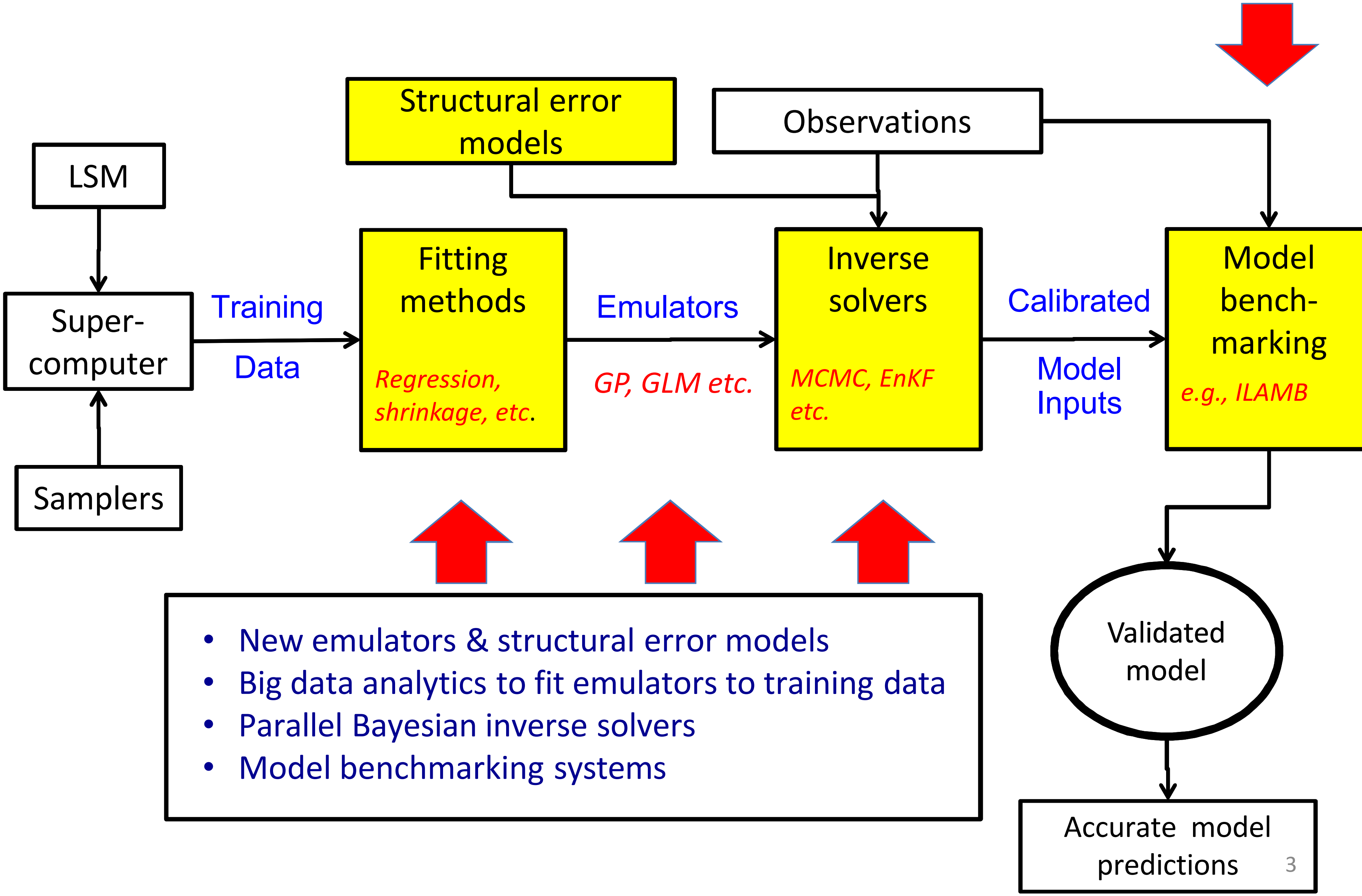
The need for model calibration

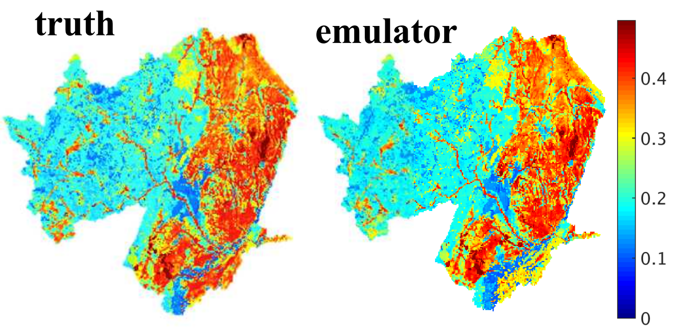
- Climate models, including Land Surface Models (LSMs) calibrated to perform well at the global scale
  - For practical planning, engineering and assessment of climate change, need predictions at a finer resolution e.g., county or provincial scale
- Many parameterizations in LSMs are scale-dependent
  - As spatial resolutions become finer, or when used at regional or site-level, need re-calibration
  - Calibration (observational) data is available at *site* scales
- Limited observational data and structural errors in LSMs hinder calibration
  - Have to continuously estimate uncertainty in calibrated parameters
  - Need to model structural errors in some form when performing calibration
  - Often have to consider vectors and fields as “parameters” being estimated, not just scalars E.g., CO_2 flux fields
- Some LSM calibration work performed; some idea of what might work

The calibration pipeline



Challenges in calibration

- Structural errors: In calibration, structural errors may be
  - Removed e.g., use better sub-model OR
  - Modeled and estimated from observations; need random field models
- Uncertainty quantification: Limited observational data demand that
  - We reduce dimensionality beforehand
  - Estimate model inputs along with their uncertainty



Including physics often improves emulators

- Emulators: curve-fits of model responses; used to address the computational expense of Bayesian methods
  - Not always possible to make accurate emulators
  - Emulators for fields (not scalars) tend to require huge training data
  - Rough model responses lack good parameterizations
- Scalability: Many statistical algos are parallelizable but tools are serial
  - Popular ones: R, Matlab, Dakota, UQTK

Solutions we need – 1/2

- Parallel MCMC methods for calibration
  - To calibrate using LSMs, not their emulators
  - Prototypes exist, but:
    - Scalability not proven (yet)
    - Don’t combine LSMs and their (perhaps inaccurate) emulators
    - No mature software base yet
- Emulators of different types
  - Many types of emulators exist when model response is *smooth*
    - But we need a “recipe” to decide what type fits a given training dataset
  - Need non-stationary RFMs for model responses that are *rough*
  - We also need classifiers to stay in the “physical” part of a parameter domain
    - Or at least, where an emulator is usable
  - Finally, we need scalable (> 1K cores) tools that can fit emulators to large datasets

Solutions we need – 2/2

- Non-stationary random field models
  - Fancy name for parameterizations that can capture rough fields
  - Needed when the length-scale of model response variation changes in perturbed parameter domain
    - Examples: wavelet-based, tree-based etc.
    - Basic idea is to chop the parametric domain into sub-domains (in a data-driven manner) and fit conventional emulators with compact support
  - They need specialized algorithms to fit to training data
- Need to use "big data analytics" for fitting emulators & RFMs
  - Fancy name for very scalable statistical tools
  - Contain scalable, statistical algos e.g., regression, shrinkage, NN, PCA, classifiers
  - Existing frameworks like Spark/MLlib and H20 scale to Google-sized problems - our emulator training dataset won't stretch them
- Finally, integration with a bench-marking system
  - Check the usefulness of calibration

Practicalities

- Prototypes of 3 / 5 solutions have been demonstrated (see 2 pager)
  - "big-data-analytics" in anything useful – not yet (2015 α-release)
  - No integration with a benchmarking system either
  - Scalable (MPI + R) tools to "do discovery" in climate datasets
    - U. Minnesota (NSF-funded); http://climatechange.cs.umn.edu;
    - No calibration or emulators
- Ongoing ASCR-funded work on developing RFMs and parallel MCMC
  - Prototypes/proof-of-concept; won't fund hardened tools
  - Have been demonstrated with LSMs
- Deliverables – to be useful in climate modeling, we need:
  - Libraries of scalable, multi-chain MCMC methods
  - Libraries of emulators that implement a pipeline:
    - Fit & simplify emulators to data using big-data-analytics (BDA) platforms
    - Select between them using ML model selection techniques
    - BDA infrastructure at supercomputing centers
  - Integration of calibration libraries with a benchmarking package

Synopsis

- We need a hardened software base for calibration of climate models
  - LSMs are the easiest target; there are preliminary results and prototype implementations of such a software base
- Calibration should yield the objects of interest as PDFs
  - Quantify the uncertainty due to limited data and/or structural errors
- The main constituents of this software base would be:
  - Methods to make and select emulators from very large training data
  - Use of big data analytics to fit emulators and RFMs to large data
  - Parallel calibration methods, in case we cannot make emulators
  - Integration with a benchmarking package
- In order to achieve this, we will need:
  - A use-case e.g., LSMs, to pose realistic calibration problems rather than theoretical ones
  - A team of climate scientists & ASCR-types to get this done
  - Funding would also be appreciated ☺

BACKGROUND

Calibration methods & shortcomings -1/2

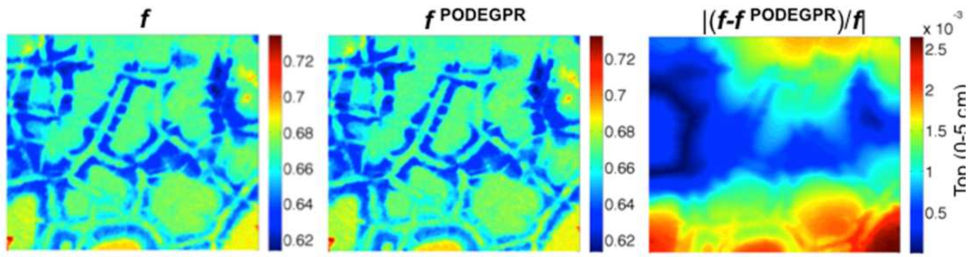
- During calibration, structural errors are incorporated in two ways
  - *Remove them:* e.g. use a detailed sub-surface simulator when using an LSM in calibration. E.g., use PFLOTRAN with CLM4
  - *Estimate them:* use a statistical parameterization for them and estimate them during calibration
- The effect of limited observational data is addressed in 2 ways
  - *Dimensionality reduction:* Estimate just the important model parameters
    - Use sensitivity analysis or shrinkage to discover them
  - *Bayesian calibration:* Use a Bayesian formulation and a method like Markov chain Monte Carlo (MCMC) or Ensemble Kalman Filters (EnKF) to estimate parameters as PDFs
    - PDFs provide you with a concise measure of estimation uncertainty
- Bayesian calibration is always more comp. expensive (10^2x-10^6x)
  - Sometimes, scalable methods exist e.g., EnKFs
  - Else, we need to use emulators (stat. curve-fits acting as proxies)

Calibration methods & shortcomings -2/2

- Emulators are **NOT** a silver bullet
  - Made by fitting response surfaces to training data from perturbed parameter runs
  - Limited to 1-10 parameters- huge training data requirements
- Often not possible to make *accurate* emulators (e.g., < 10%)
- Often need to model fields (not scalars) as a function of perturbed parameters
  - Both need parameterizations of surfaces in high dimensions (called random field models, RFMs)
- Tools to fit emulators usually serial (DAKOTA, Matlab, R)
  - Sometimes the training data *does not* fit in the memory (e.g., if emulating fields, not scalars)
  - We need:
    - Scalable, multi-processor statistical frameworks for fitting emulators
    - Calibration tools that will work if we fail to make emulators

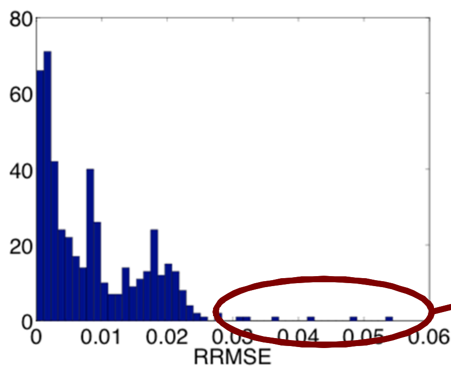
Representative results of emulators

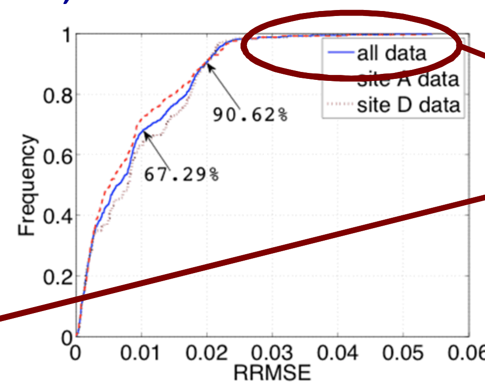
- Aim to reproduce moisture content distribution by combining data dimensional reduction technique (PCA) and Gaussian process regression.



Looks good for a single snapshot, BUT …

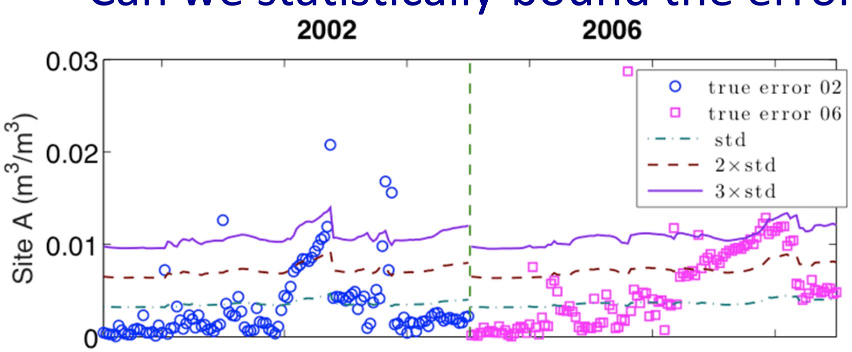
- Accuracy is not uniform, with some outliers.





What's the impact of these outliers on UQ analysis?

- Can we statistically bound the error?

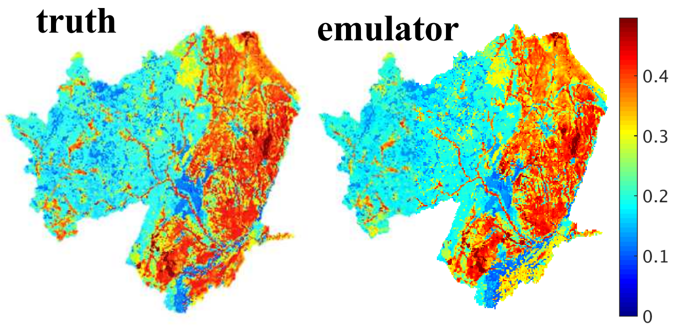


Somewhat. How do we use these estimates in an UQ analysis?

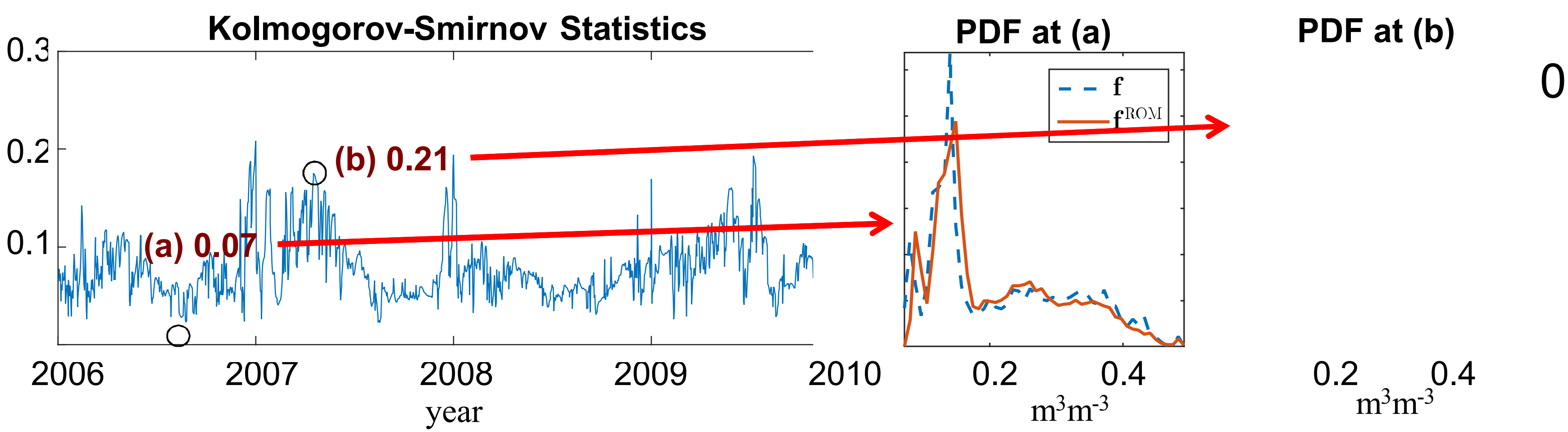
Source: Liu, Y., et al. (2015). "A hybrid reduced-order model of fine-resolution hydrologic simulations at a polygonal tundra site." Vadose Zone Journal. doi:10.2136/vzj2015.05.0068

Representative results of emulators

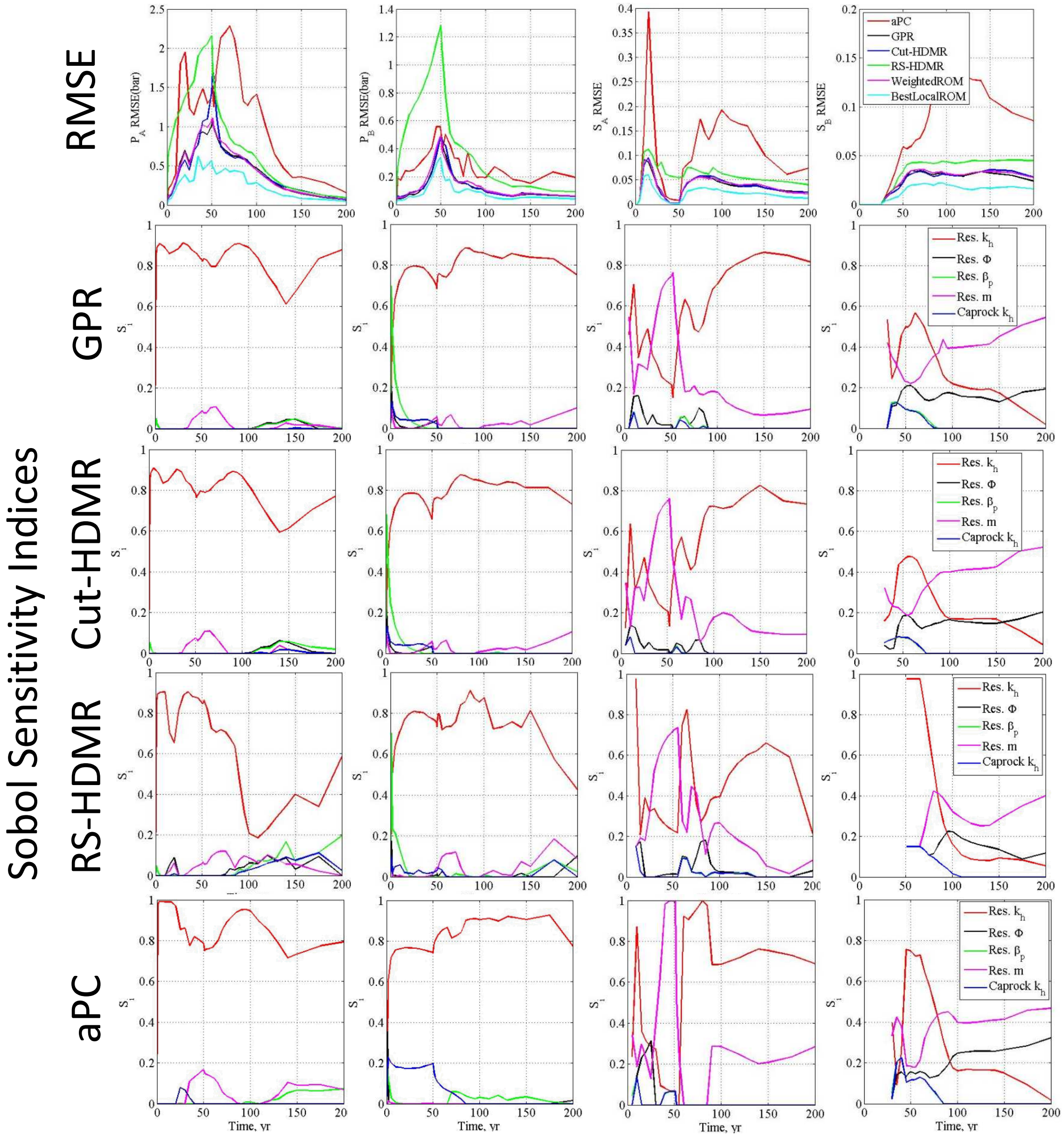
- A more heterogeneous problem require more advanced emulator technique: here based on coarse-grid simulation and PODMM downscaling technique.



Including physics-related information (through efficient coarse model) can improve the representation. Still, accuracy is not uniform.



Effects of ROM accuracy on Global SA



ROM studied:

- GPR: Gaussian Process Regression
- Cut-HDMR: Cut High Dimensional Model Reduction
- RS-HDMR: Random sampling HDMR
- aPC: arbitrary Polynomial Chaos

Accuracy of emulator depends

- type of ROMs: GPR and cut-HDMR have better accuracies.
- smoothness in the variables studied: pressure easier to estimate than saturation.

Accuracy of analysis

- Less sensitive to emulators if only qualitative analysis is needed.

Source: Zhang, Y, et al. (2016). "Evaluation of Multiple Reduced-Order Models to Enhance Confidence in Global Sensitivity Analyses." Submitted.