Fast large-scale joint inversion for deep aquifer characterization using pressure and heat tracer measurements

InterPore 2018 Poster

Contribution ID : 726

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Overview

With recent advances in sensor and computation technology, unprecedented large volumes of hydro-geophysical and geochemical data sets can be obtained and processed to achieve high-resolution images of subsurface properties for more accurate and reliable subsurface flow and reactive transport prediction. For such problems, the **Principal Component Geostatistical Approach (PCGA)** [1,2,3] has been proposed as:

- **Jacobian-free** : no need to compute/store full Jacobian
- **Forward model runs independent of the problem size** : often runs much smaller number of simulations in practice
- **Linear scalability** : Matrix computation and storage costs grow linearly with respect the problem size
- **Easy to implement** : linked with any **"black-box"** multi-physics simulation models **without invasive changes**

Principal Component Geostatistical Approach

With $\mathbf{m}$ unknowns, $\mathbf{n_{obs}}$ measurements, and forward model(s) $\mathbf{h}$, one needs:

- Jacobian matrix $\mathbf{H}$, *i.e.*, sensitivity of the data to unknown parameters $\frac{\partial \mathbf{h}}{\partial \mathbf{s}}$
- Jacobian products with the prior covariance matrix $\mathbf{Q}$, *i.e.*, $\mathbf{HQ}$ and $\mathbf{HQH}^\mathsf{T}$

For large-scale/joint inversions (large $\mathbf{m}$ and $\mathbf{n_{obs}}$), one faces several challenges such as

- time-consuming, invasive changes in multi-physics simulation code for efficient adjoint-state method implementation to evaluate Jacobian $\mathbf{H}$
- expensive Jacobian construction requiring $\mathbf{n_{obs}}$ ($\geq \mathcal{O}(10^4)$) simulations
- prohibitive large dense matrix multiplication/storage for large $\mathbf{m}$ ($\geq \mathcal{O}(10^6)$)

In order to tackle these challenges, we developed PCGA that avoids expensive Jacobian evaluation and its matrix products (cross-covariance) by using a **fast truncated decomposition** [2,3] of the prior covariance

$$\mathbf{Q} \approx \mathbf{Q}_\kappa = \Sigma_{i=1}^{\kappa} \zeta_i \zeta_i^\mathsf{T} \quad \Leftarrow \quad \textbf{scales linearly} \ (\text{Cost } \mathcal{O}(m\kappa^2))$$

and **finite-difference approximation**:

$$\mathbf{H}\zeta_i \approx \frac{1}{\delta}\left[h(\mathbf{s}+\delta\zeta_i) - h(\mathbf{s})\right], \quad \mathbf{HQ} \approx \Sigma_{i=1}^{\kappa} (H\zeta_i)\, \zeta_i^\mathsf{T} \quad \Leftarrow \quad \textbf{total } \kappa+1 \textbf{ simulations!}$$

Thus, PCGA can achieve **a significant speed-up with reasonable accuracy**, using simulation outputs **without modifying multi-physics simulation code**.

Python Software - pyPCGA

- pyPCGA: Python package for Principal Component Geostatistical Approach
- Supports $\mathcal{O}(N)$ fast linear algebra and (randomized) eigen-decomposition
- `https://github.com/jonghyunharrylee/pyPCGA`

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Synthetic Example : Frio site

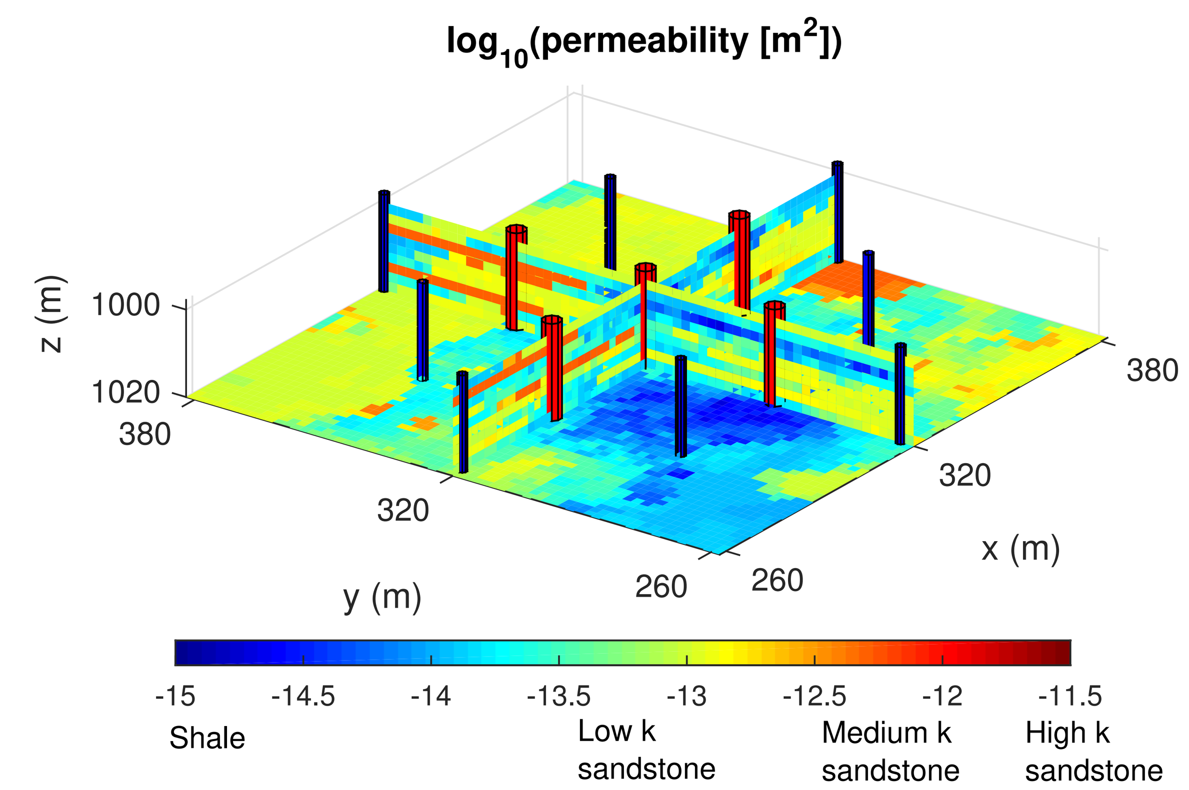

Figure: Synthetic true field generated by TProgS; pumping (red) and monitoring (blue) wells

TOUGH2-MP with module EOS1 was used for four dipole pumping tests between the center injection well and the other four wells. The monitoring network consists of a total of 8 multilevel monitoring wells with 10 monitoring ports. Transient pressure and zero-th moment of temperature ("total heat") data was used for the inversion performed on a Linux workstation with Intel 16 core 3.4 GHz processors and 100 GB RAM.

Results with pressure data inversion

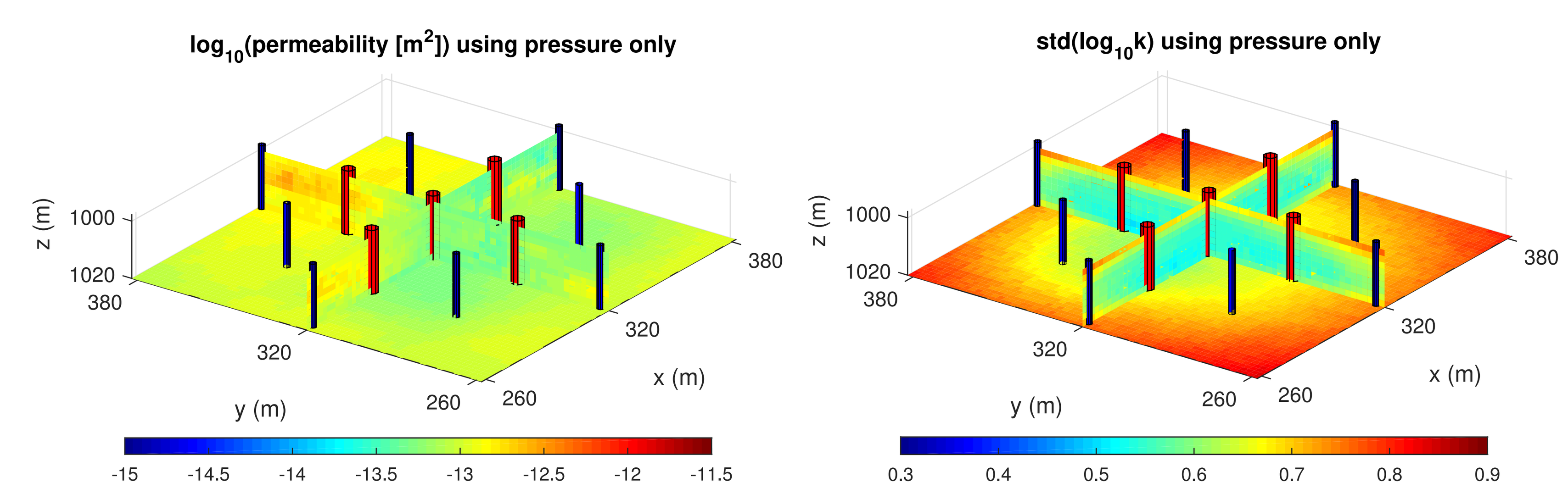

Figure: the best estimate (left) and its estimation uncertainty (right) for pressure data inversion

Results with joint pressure and heat data inversion

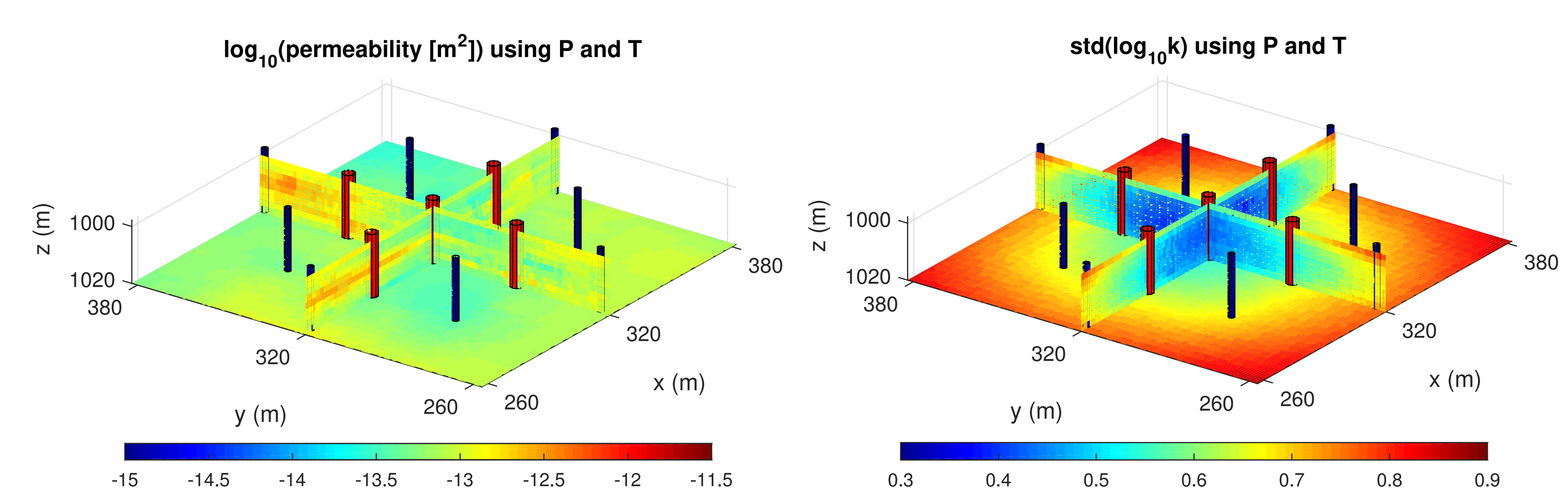

Figure: the best estimate (left) and its estimation uncertainty (right) for joint data inversion

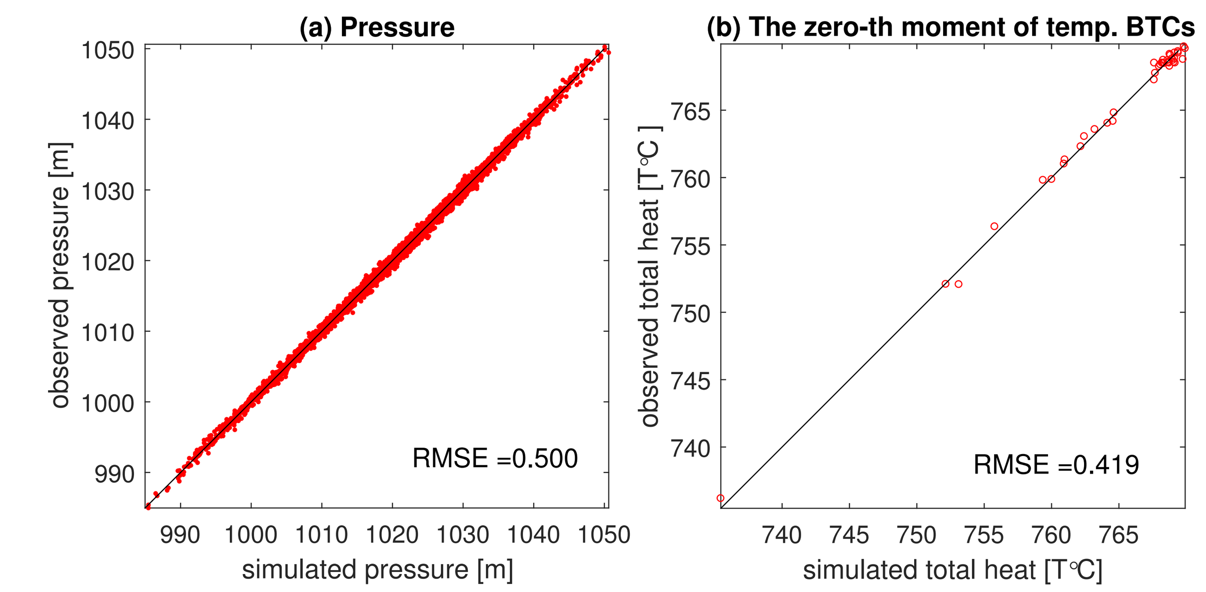

Figure: Data fitting for joint inversion; (a) observed vs. simulated pressure and (b) observed vs. simulated zero-th moment of temperature breakthrough curves.

Parameters	Results
Number of grids (unknowns)	29800
Number of wells	1 (injection), 4 (extraction), 8 (monitoring)
Number of measurements	4,000 (P only), 4,040 (P + 0-th moment of T)
Measurement error (std)	0.5 [m], 2.0 [°C]
Total number of TOUGH2 runs	1,353 (P only), 1,780 (P + T)
Inversion time (hours)	2.3 (P only), 8.0 (P + T)

pyPCGA + pyTOUGH

- *Coming soon!* a Python library for automating TOUGH2 simulations and parameter estimation for subsurface fluid and heat flow modeling: pyPCGA linked with pyTOUGH as a seemless computing environment.

Conclusion

- PCGA scales well with the number of observations to high-dimensional inverse problems with controlled accuracy (~ total $\mathcal{O}(100)$ per pumping test).
- Small-scale variability and low permeability inclusions are better identified with the addition of heat tracer test data.
- Computational efficiency of pyPCGA enables assessing the information content of complex monitoring datasets for large scale subsurface characterization.

References

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[4] `https://github.com/jonghyunharrylee/pyPCGA`

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Acknowledgment

This work was supported by Hawai'i Experimental Program to Stimulate Competitive Research (EPSCoR) provided by the National Science FoundationâĂŹs Research Infrastructure Improvement (RII) Track-1: 'Ike Wai: Securing Hawai'i's Water Future Award #OIA-1557349 and the AWS Cloud Credits for Research Program. We would like to thank Dr. Quanlin Zhou of Lawrence Berkeley National Laboratory for support on TOUGH2.