Subsurface characterization for large scale systems: A Python-based inversion tool for TOUGH2

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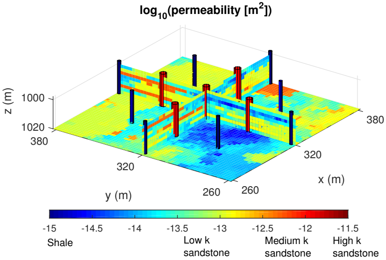
Outline

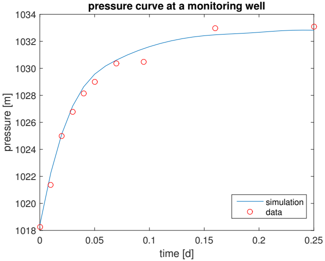
- Introduction
- Geostatistical inverse modeling
- pyPCGA-TOUGH: structure and advantages
- Test case results
- Conclusions

Introduction

Geostatistical Inverse Modeling: a Bayesian framework to estimate grid-scale, spatially distributed model parameters using indirect observations



Unknown parameter



Local, noisy observations

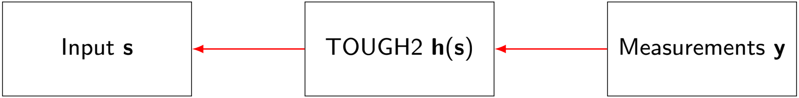
- Subsurface characterization (e.g. hydraulic tomography)
- Real-time estimation (e.g. contaminant tracking)
- Optimization (e.g. pumping schedule estimation)

Introduction: Inverse Problem

$$\boxed{\text{Input } \mathbf{s}} \longrightarrow \boxed{\text{TOUGH2 } \mathbf{h}(\mathbf{s})} \longrightarrow \boxed{\text{Output } \mathbf{y}}$$

- In the **forward problem**, given model parameters, **s**, TOUGH2 predicts the state of the system **y**
- **s** is typically permeability, but could be other rock properties, or boundary conditions
- **y** are the primary variables of the EOS module

Introduction: Inverse Problem



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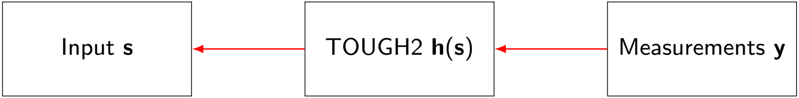

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- In the **inverse** problem, we use measurements of **y** to estimate **s**
- TOUGH2 is now used to calculate the sensitivity of measurements to parameters $\mathbf{H} = \frac{\partial \mathbf{y}}{\partial \mathbf{s}}$

Inverse Problem in Hierarchical Bayesian Framework

Consider the measurement equation

$$y = h(s) + v \qquad v \sim \mathcal{N}(0, \mathbf{R})$$

$\mathbf{y} := n_{obs} \times 1$ noisy measurements	pressure, temperature
$h :=$ forward model	TOUGH2
$v :=$ measurement and model error	uncertainty and error
$\mathbf{s} := n_{unknowns} \times 1$	permeability

$$s \sim \mathcal{N}(s_{prior}, \mathbf{Q}_{prior})$$

- Parameters are treated as random variables in a statistical framework (e.g., Gelman, Calin, and Stern, 2013; Kitanidis, 2010, Kitanidis, 1995)
- Use covariances **Q** and **R** to represent variability and uncertainty
- Objective: **A best estimate of unknowns and corresponding uncertainty at each grid cell of the TOUGH2 model, given a set of measurements**

Inverse Problem in Hierarchical Bayesian Framework

Consider the measurement equation

$$y = h(s) + v \qquad v \sim \mathcal{N}(0, \mathbf{R})$$

Using Bayes' rule, the posterior pdf is

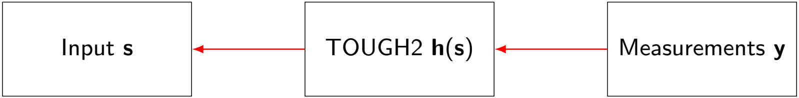
$$p(s|y) \quad \propto \quad \underbrace{p(y|s)}_{\text{Data misfit}} \underbrace{p(s)}_{\text{Prior}}$$

- Data misfit - How well the model reproduces data
- Prior - Prior knowledge of unknown field structure

Best estimate is obtained by maximizing the likelihood of **s** given a set of measurements **y**, using GN optimization:

$$p(\mathbf{s}) \sim \exp\left(\underbrace{-\frac{1}{2}(\mathbf{y} - \mathbf{h}(\mathbf{s}))^\top \mathbf{R}^{-1}(\mathbf{y} - \mathbf{h}(\mathbf{s}))}_{likelihood} \underbrace{-\frac{1}{2}(\mathbf{s} - \mathbf{s}_{prior})^\top \mathbf{Q}_{\text{prior}}^{-1}(\mathbf{s} - \mathbf{s}_{prior})}_{prior} \right)$$

Inverse Problem: the challenges for large systems



For large-scale systems:

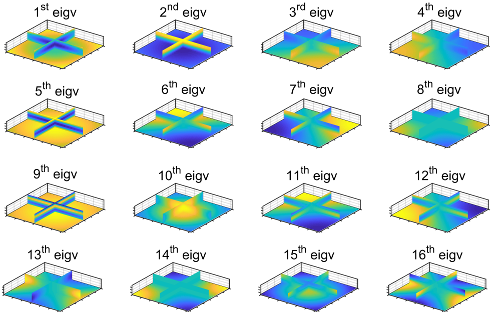
- Typically many unknowns, few measurements $n_{obs} \ll n_{unknowns}$
- Requires $\mathcal{O}(min(n_{obs}, n_{unknowns}))$ TOUGH2 runs or more
- High dimensional matrix operations

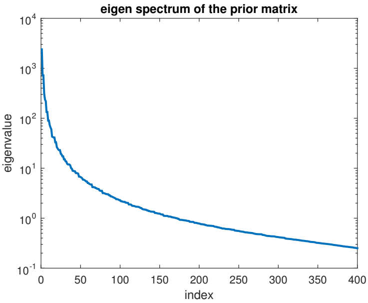
Therefore:

- Fast Linear Algebra is necessary to enable computations and storage
  - Matrix-matrix, matrix-vector multiplications
- Reduce number of forward runs
- Finetuning and evaluation of the inversion design and parameters is critical

pyPCGA: Geostatistical inversion in Python

Principal **C**omponent **G**eostatistical **A**pproach:
A computationally efficient algorithm for geostatistical inversion based on compression of covariance matrices and Jacobian-free evaluation of sensitivity. [1]





[1] Lee and Kitanidis, 2014, Kitanidis and Lee, 2014

pyPCGA: Geostatistical inversion in Python

Compression of the covariance matrix reduces the number of matrix-vector multiplications to $\mathcal{O}(n_{pc})$:

$$\mathbf{Q}_{prior} \approx \mathbf{U}\mathbf{\Sigma}\mathbf{U}^T$$

Calculation of sensitivity matrix requires TOUGH2 runs, black-box style, using the finite difference approach:

$$\mathbf{Hs} = \frac{h(\mathbf{s} + \Delta s) - h(\mathbf{s})}{\Delta s}$$

Computations involving large matrices (**Q**, **H**) utilize fast linear algebra that allows **fully parallelizable, fast matrix-vector multiplications**:

- Fast Fourier Transform (FFT) approach for regular grids [2]
- Fast Multipole Method (FMM) and Hierachical Matrices Approach for unstructured grids [3]

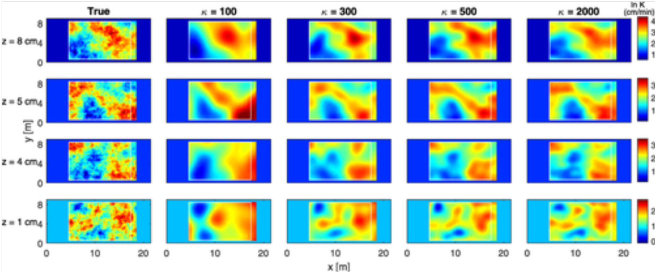
[2] https://github.com/arvindks/kle

[3] https://github.com/ruoxi-wang/PBBFMM3D

pyPCGA: Geostatistical inversion in Python

Computational gain:

- Matrix computations scale linearly with number of unknowns
- $\sim \mathcal{O}(100)$ forward model runs for large domains ($\sim 10^6$ unknowns)
- Parallelization further accelerates inversion



- **Linear scaling makes possible the inversion of domains with millions of unknowns and observations [4].**

[4] Lee et al., 2016

An inversion package for TOUGH2 users

- pyPCGA-TOUGH: An open-source package for geostatistical inversion
  - Compatible with pyTOUGH, extension of pyTOUGH
  - Tutorial-like templates with visualizations, to get started
  - Tool for designing monitoring, and assessing information content of data

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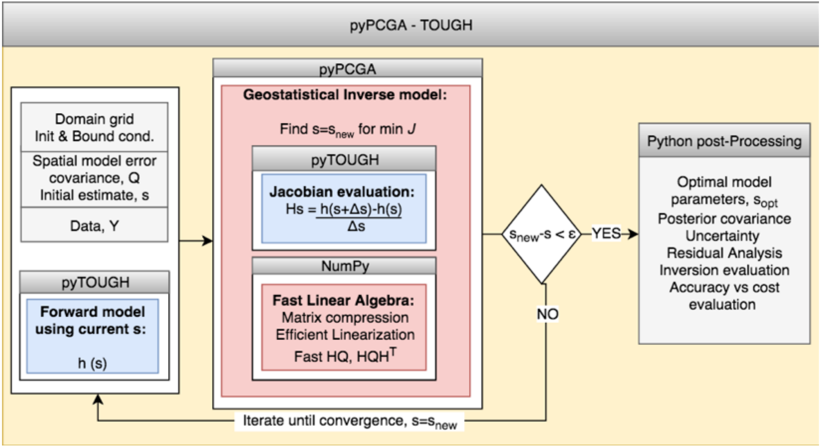
  - Tutorial-like templates with visualizations, to get started
  - Tool for designing monitoring, and assessing information content of data
- Framework for powerful statistical estimation for TOUGH2 models
  - Connects with packages for fast linear algebra tools
  - Can be extended with other types of inversion
  - Allows reproducibility and method comparison

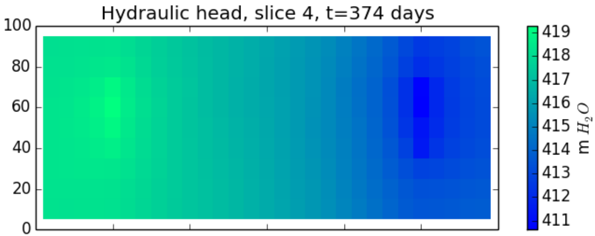
▸ pyPCGA-Demo

pyPCGA-TOUGH: Geostatistical inversion for TOUGH2



pyPCGA-TOUGH: Getting started

0. Set up the forward and inverse problem
   - Is the problem physically (numerically) feasible?
   - Are measurements sensitive to parameters?
   - What is a reasonable first guess for the unknowns?
   - Implementation for consistent "obs" for runs with different parameters?



pyPCGA-TOUGH: Getting started

pyPCGA: Python Interface of PCGA algorithm

```
params = {'R': (0.5) ** 2, 'n_pc': 50,
          'maxiter': 10, 'restol': 0.01,
          'matvec': 'FFT', 'xmin': xmin, 'xmax': xmax, 'N': N,
          'prior_std': prior_std, 'prior_cov_scale': prior_cov_scale,
          'kernel': kernel, 'post_cov': "diag",
          'precond': True, 'LM': True,
          'parallel': True, 'linesearch': True,
          'forward_model_verbose': False, 'verbose': False,
          'iter_save': True}
```

pyPCGA-TOUGH: Getting started

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```

Integrated with pyTOUGH

```
# TOUGH2 Simulation parameters:
# Table 4.9 page 78 pytough tutorial and Appendix E of TOUGH2 tutorial
# data.parameter is a dictionary
# each parameter can be called as dat.parameter['parameter name']
dat.parameter.update(
    {'max_timesteps': 9000,                # maximum number of time steps
     'tstop': 0.32342126E+08,              # stop time
     'const_timestep': 6,                  # time step length
     'max_timestep':86400,                 # maximum time step size
     'absolute_error': 1,                  # absolute convergence tolerance
     'relative_error': 5.e-6,              # relative convergence tolerance
     'print_interval': 9000,               # time step interval for printing
     'timestep_reduction': 3.,             # time step reduction factor
     'gravity': 9.81,                      # gravitational acceleration
     'default_incons': [100.e4, 10]})      # default initial conditions
    # Pressure in Pa, 100 m water = 10.e5 Pa water, 10 is the temperature in Celcius
dat.start = True
```

pyPCGA-TOUGH: Running the inversion

1. Read inversion parameters

```
prob = PCGA(forward_model, s_init, pts, params, s_true, obs)
```

```
##### PCGA Inversion #####
##### 1. Initialize forward and inversion parameters
------------ Inversion Parameters -------------------------
   Number of unknowns                                   : 10001
   Number of observations                               : 100
   Number of principal components (n_pc)                : 50
   Prior model                                          : def kernel(r): return (prior_std ** 2) * np.
exp(-r)

   Prior variance                                       : 1.600000e-03
   Prior scale (correlation) parameter                  : [200.]
   Posterior cov computation                            : diag
   Posterior variance computation                       : Direct
   Number of CPU cores (n_core)                         : 4
   Maximum GN iterations                                : 10
   machine precision (delta = sqrt(precision))          : 1.000000e-08
   Tol for iterations (norm(sol_diff)/norm(sol))        : 1.000000e-02
   Levenberg-Marquardt (LM)                             : True
   LM solution range constraints (LM_smin, LM_smax)     : None, None
   Line search                                          : True
-----------------------------------------------------------
```

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   LM solution range constraints (LM_smin, LM_smax)      : None, None
   Line search                                           : True
-----------------------------------------------------------
```

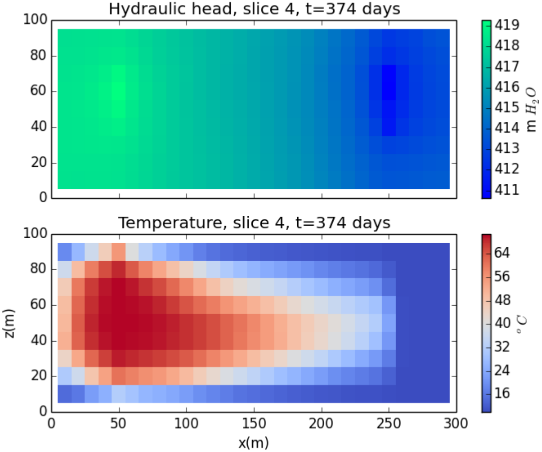
2. Run inversion

```
# run inversion
s_hat, simul_obs, post_diagv, iter_best = prob.Run()
```

```
##### 2. Construct Prior Covariance Matrix
- time for covariance matrix construction (m = 10001) is 0 sec
##### 3. Eigendecomposition of Prior Covariance
- time for eigendecomposition with k = 50 is 0 sec
- 1st eigv : 5.29487, 50-th eigv : 0.00674062, ratio: 0.00127305
##### 4. Start PCGA Inversion #####
-- evaluate initial solution
obs. RMSE (norm(obs. diff.)/sqrt(nobs)): 0.776609, normalized obs. RMSE (norm(obs. diff./sqrtR)/sq
rt(nobs)): 19.4152
```

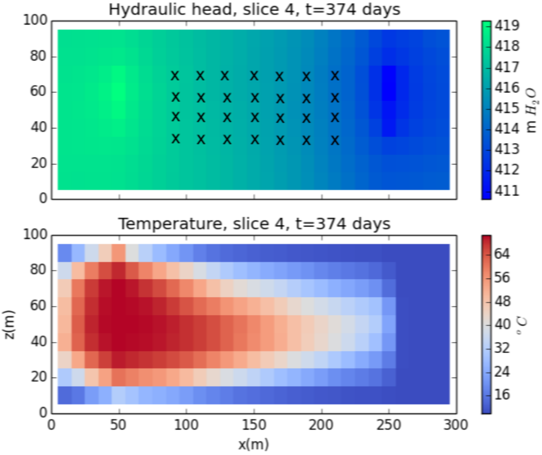
pyPCGA-TOUGH: Test Case

Synthetic case: $300m \times 100m \times 100m$, Log-normal permeability
Boundary conditions: injection-extraction system, warm water injected
Simulation time: 374 days



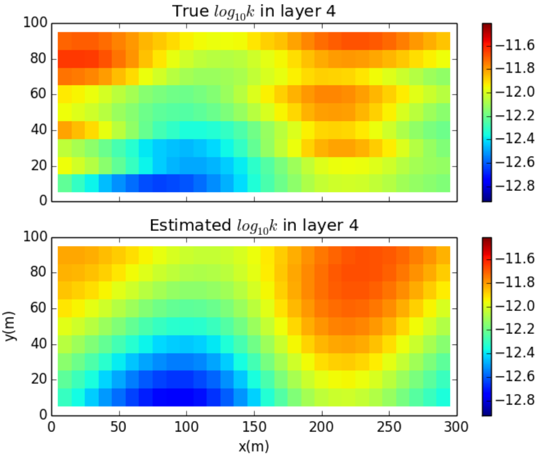
pyPCGA-TOUGH: Test Case

Unknowns: 3000 permeabilities (pmx values)
Measurements: Pressure collected every $\sim$ 5 days at 128 monitoring locations between the injection and extraction well ($n_{press.obs.} = 7400$)



pyPCGA-TOUGH: Test Case

Unknowns: 3000 permeabilities
Measurements: 7400 pressure measurements
Principal components: 30
Time to run (with parallelization): 10 minutes on 36-cores



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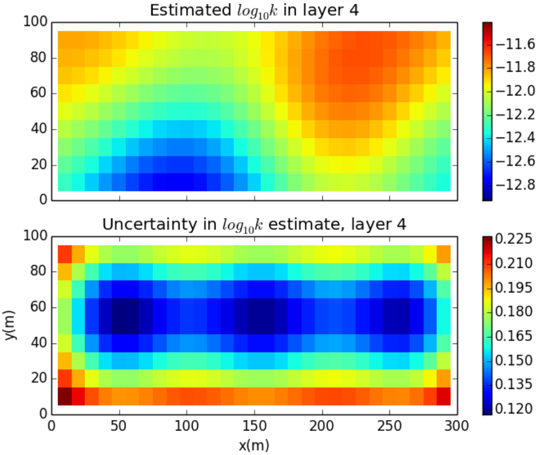
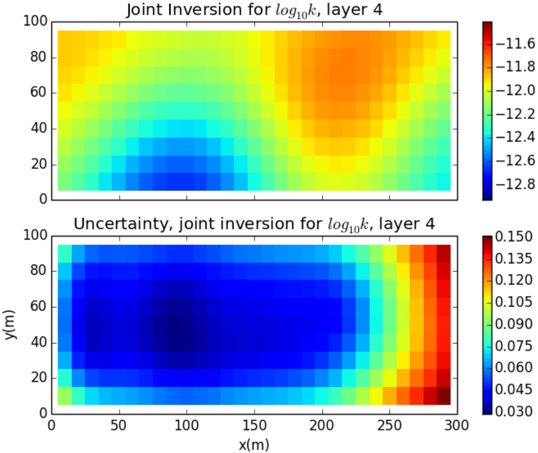


pyPCGA-TOUGH: Test Case 2 (Joint inversion)

Unknowns: 3000 permeabilities

Measurements: pressure and temperature measurements

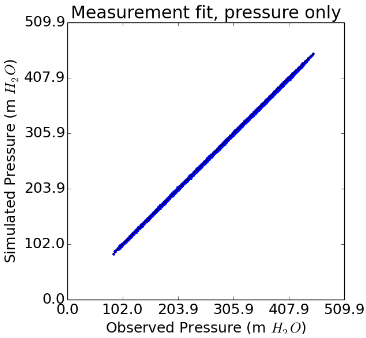
- Joint inversion of P,T data reduces the uncertainty.
- Useful for design of monitoring network.

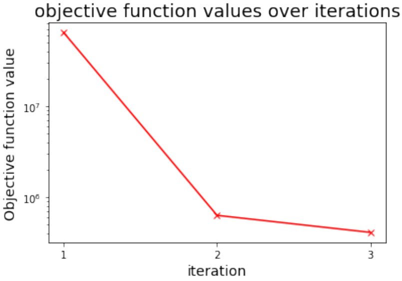


pyPCGA-TOUGH: Test Case

Inversion evaluation: Measurement fit (RMSE), objective function, L2-norm w.r.t. true field, convergence behavior

Post-processing of inversion results allows finetuning of parameters (model error, tolerance, finite difference δ, prior covariance parameters)





pyPCGA-TOUGH: An inversion package for TOUGH2 users

pyPCGA-TOUGH offers an open-source package for geostatistical inversion for TOUGH2-MP models. Package development is ongoing.

Upcoming additions include:

- Extension of pyTOUGH with tools for sensitivity evaluation
- Tutorial templates for inversion using EOS1, EOS3, ECO2N
- Visualization tools fast predictive model validation using cR/Q2 criteria
  - automatic covariance model parameter calibration
- New faster linear algebra for unstructured grids (PBBFMM3D, and HMatrix)
- Level-set and total variation method for sharp boundaries estimation

`https://github.com/jonghyunharrylee/pyPCGA`
`https://github.com/hojjatgh/pyPCGA-TOUGH`

PCGA: method development and applications

- Lee, Kokkinaki and Kitanidis, Fast Large-Scale Joint Inversion for Deep Aquifer Characterization Using Pressure and Heat Tracer Measurements. Transport in Porous Media, 123(3): 533-543, 2018
- Lee, J., Ghorbanidehno, H., Farthing, M. W., Hesser, T. J., Darve, E. F., & Kitanidis, P. K. Riverine bathymetry imaging with indirect observations. Water Resources Research, 54. https://doi.org/10.1029/ 2017WR021649, 2018
- P. K. Kang, J. Lee, X. Fu, S. Lee, P. K. Kitanidis, and J. Ruben, Improved Characterization of Heterogeneous Permeability in Saline Aquifers from Transient Pressure Data during Freshwater Injection Water Resources Research, 53(5): 4444-458, 2017
- Lee, Yoon, Kitanidis, Werth, and Valocchi, Scalable subsurface inverse modeling of huge data sets with an application to tracer concentration breakthrough data from magnetic resonance imaging Water Resources Research, 52(7), 5213-5231, 2016
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Thank you!