

# An Ensemble-Based Approach to Optimal Experimental Design for Large-Scale Nonlinear Inverse Problems

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# Overview

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- Ensemble Methods

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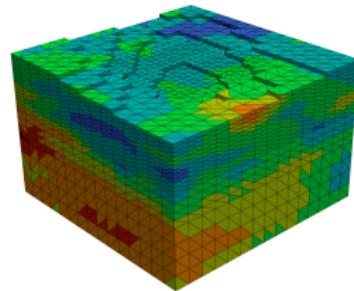


# Geothermal Reservoir Modelling

Computer modelling is an important mechanism for learning about the structure of geothermal systems and predicting the effect of proposed management plans.

Challenges associated with geothermal reservoir modelling include:

- High-dimensional parameter spaces
- Long simulation times (hours to weeks)
- Frequent simulation failures



# Bayesian Inference

We consider problems of the form

$$\mathbf{y} = \mathcal{G}(\boldsymbol{\theta}) + \boldsymbol{\epsilon},$$

where  $\boldsymbol{\theta} \sim \pi_0(\boldsymbol{\theta})$  denote unknown parameters, and  $\boldsymbol{\epsilon} \sim \pi_\epsilon(\boldsymbol{\epsilon})$  is an additive error term.

Assuming  $\boldsymbol{\theta} \perp \boldsymbol{\epsilon}$ , the density of  $\mathbf{y} | \boldsymbol{\theta}$  inherits the density of the error. Using Bayes' theorem, the posterior density of  $\boldsymbol{\theta} | \mathbf{y}$  is

$$\underbrace{\pi^y(\boldsymbol{\theta})}_{\text{posterior}} \propto \underbrace{\pi_\epsilon(\mathcal{G}(\boldsymbol{\theta}) - \mathbf{y})}_{\text{likelihood}} \underbrace{\pi_0(\boldsymbol{\theta})}_{\text{prior}}.$$



# Ensemble Methods

Ensemble methods iteratively update a set of *interacting particles* to produce an approximation to the posterior.

Ensemble methods are:

- **Derivative free:** gradients are estimated using the ensemble
- **Efficient:** they can produce accurate results using  $\mathcal{O}(10^3)$  simulations
- **Embarrassingly parallel:** the ensemble can be run simultaneously at each iteration

Widely-used ensemble methods include:

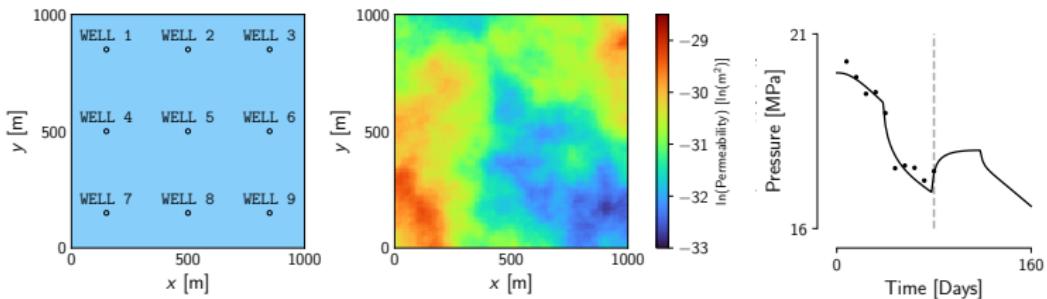
- **Ensemble Randomised Maximum Likelihood** (Chen and Oliver 2012, 2013)
- **Ensemble Smoother w/ Multiple Data Assimilation** (Emerick and Reynolds 2013)
- **Ensemble Kalman Inversion** (Iglesias *et al.* 2013; Iglesias and Yang 2021)
- **Ensemble Kalman Sampler** (Garbuno-Inigo *et al.* 2020a, 2020b)



# Oil Reservoir Benchmark: Problem

*Forward problem:*

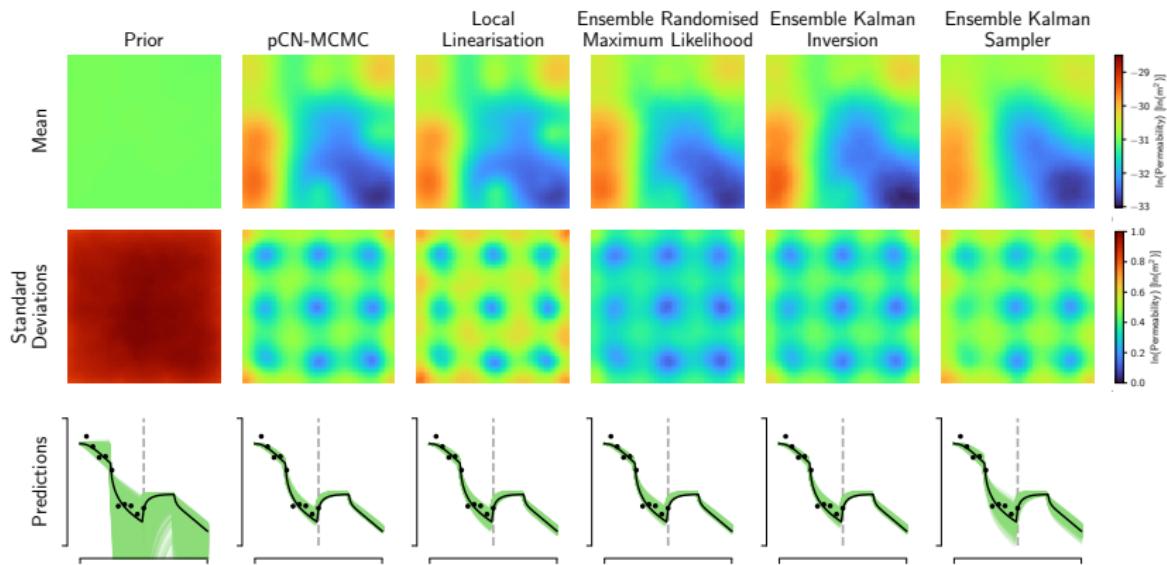
$$c\phi \frac{\partial p}{\partial t} - \frac{1}{\mu} \nabla \cdot (e^u \nabla p) = \sum_{i=1}^{n_w} q_i \delta_{x_i}(x), \quad x \in \Omega, t \in (0, T],$$
$$-e^u \nabla p \cdot n = 0, \quad x \in \partial\Omega, t \in (0, T],$$
$$p = p_0, \quad x \in \Omega, t = 0.$$



*Inverse problem:* estimate log-permeability,  $u = u(x)$ , using noisy measurements of pressure,  $p = p(x, t)$ .



# Oil Reservoir Benchmark: Results



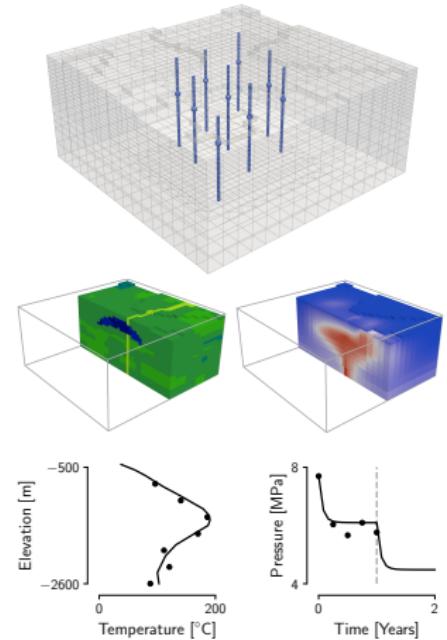
# Geothermal Case Study: Problem

*Forward problem:*

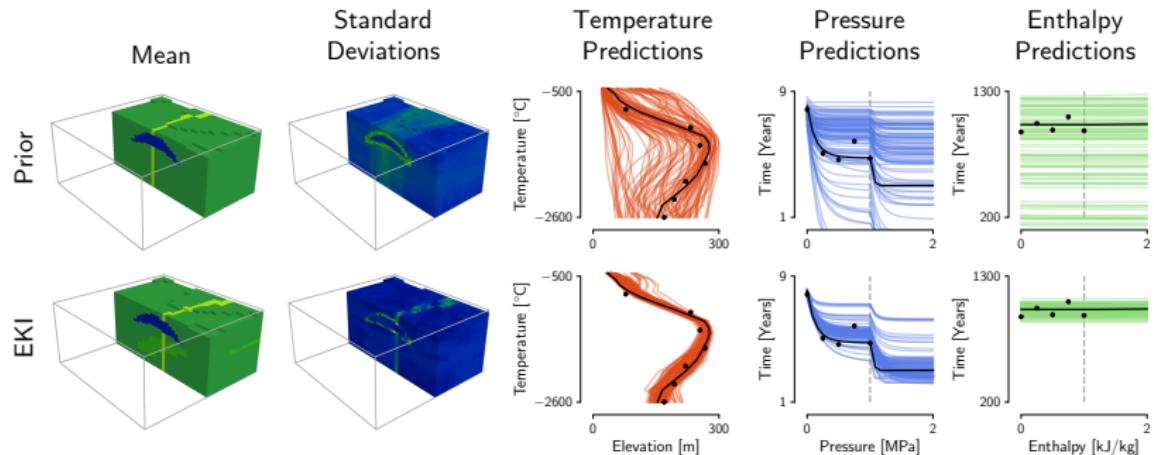
$$\frac{d}{dt} \int_{\Omega} M_m \, dx = - \int_{\partial\Omega} \mathbf{F}_m \cdot \mathbf{n} \, d\sigma + \int_{\Omega} q_m \, dx,$$

$$\frac{d}{dt} \int_{\Omega} M_e \, dx = - \int_{\partial\Omega} \mathbf{F}_e \cdot \mathbf{n} \, d\sigma + \int_{\Omega} q_e \, dx.$$

*Inverse problem:* estimate permeability structure and properties of hot mass upflow ( $\sim 20,000$  unknown parameters) using noisy downhole pressure, temperature and enthalpy measurements.



# Geothermal Case Study: Results



# Bayesian Optimal Experimental Design (OED)

Drilling geothermal wells costs millions of dollars. Where should we drill to learn the most about the system?

We can formulate this within the framework of OED.

## The Sensor Placement Problem

$$\min_{\mathbf{w} \in \{0,1\}^{n_s}} \Psi(\mathbf{w}), \quad \text{s.t. } \|\mathbf{w}\|_0 = k.$$

This is a challenging binary optimisation problem. We use a greedy approach to solve it.



# Design Criteria

We consider several design criteria:

- A-Optimality:  $\psi_A(\mathbf{y}, \mathbf{w}) := \text{tr}[\mathbf{C}^{y,w}]$ ,
- D-Optimality:  $\psi_D(\mathbf{y}, \mathbf{w}) := -\mathcal{D}_{KL}(\pi^{y,w} \parallel \pi_0)$ ,
- Normality:  $\psi_N(\mathbf{y}, \mathbf{w}) := \mathcal{D}_{KL}(\pi^{y,w} \parallel \pi_N^{y,w})$ .

We aim to *minimise* the expectations of each of these.

# Design Criteria

We compute approximations of posteriors using ensemble methods, and use sample average approximation to estimate the expectation of each criterion:

$$\mathbb{E}_{\theta,y|w}[\psi_A] \approx \hat{\Psi}_A^{n_y}(\mathbf{w}) := \frac{1}{n_y} \sum_{i=1}^{n_y} \text{tr}[\hat{\mathbf{C}}^{y_i, w}],$$

$$\mathbb{E}_{\theta,y|w}[\psi_D] \approx \hat{\Psi}_D^{n_y}(\mathbf{w}) := \frac{1}{n_y} \sum_{i=1}^{n_y} \left( \frac{1}{J} \sum_{j=1}^J \log \left( \frac{\pi_0(\boldsymbol{\theta}_j)}{\hat{\pi}^{y_i, w}(\boldsymbol{\theta}_j)} \right) \right),$$

$$\mathbb{E}_{\theta,y|w}[\psi_N] \approx \hat{\Psi}_N^{n_y}(\mathbf{w}) := \frac{1}{n_y} \sum_{i=1}^{n_y} \left( \frac{1}{J} \sum_{j=1}^J \log \left( \frac{\hat{\pi}^{y_i, w}(\boldsymbol{\theta}_j)}{\hat{\pi}_N^{y_i, w}(\boldsymbol{\theta}_j)} \right) \right).$$

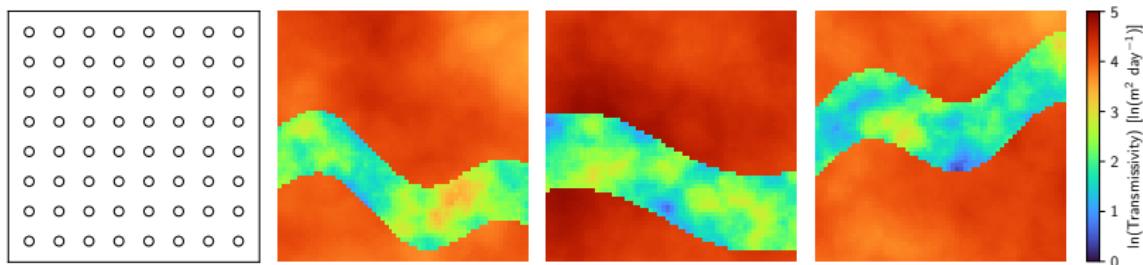
We compute a kernel density estimate of the posterior using the ensemble.



# Aquifer Case Study Part I: Problem

*Inverse problem:* estimate the transmissivity of a steady-state aquifer based on measurements of the hydraulic head.

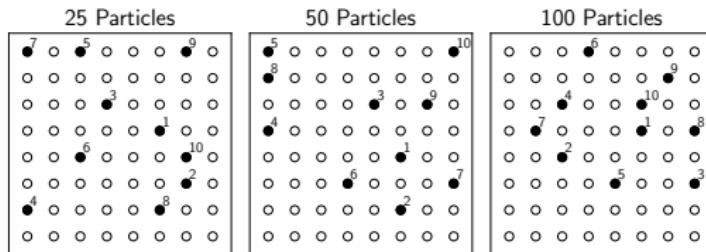
We consider an  $8 \times 8$  grid of possible sensor locations.



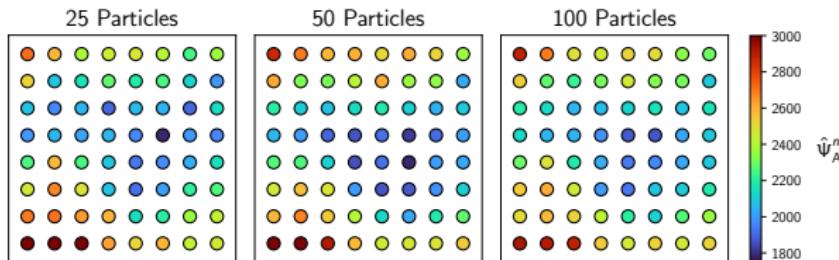
We aim to compute A-optimal designs using EKI.

# Aquifer Case Study Part I: Results

Designs using EKI with varying numbers of particles:

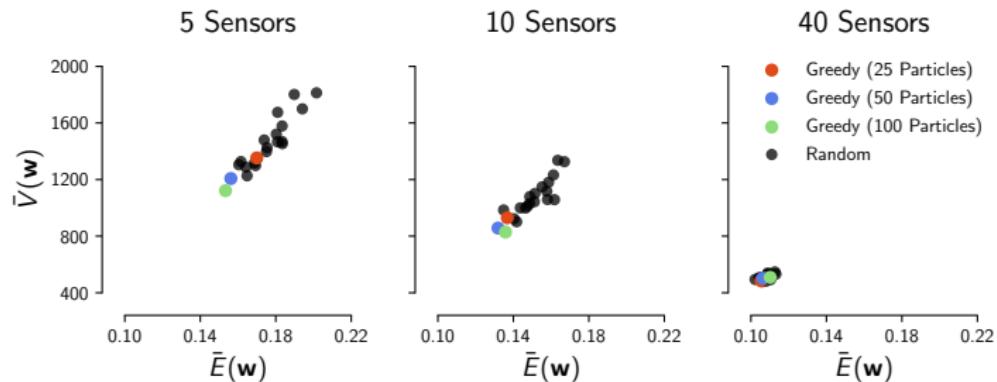


Estimates of  $\Psi_A$  at each location when selecting the first sensor:



# Aquifer Case Study Part I: Validation

Results using  $n_v = 20$  validation datasets and EKI with 200 particles:



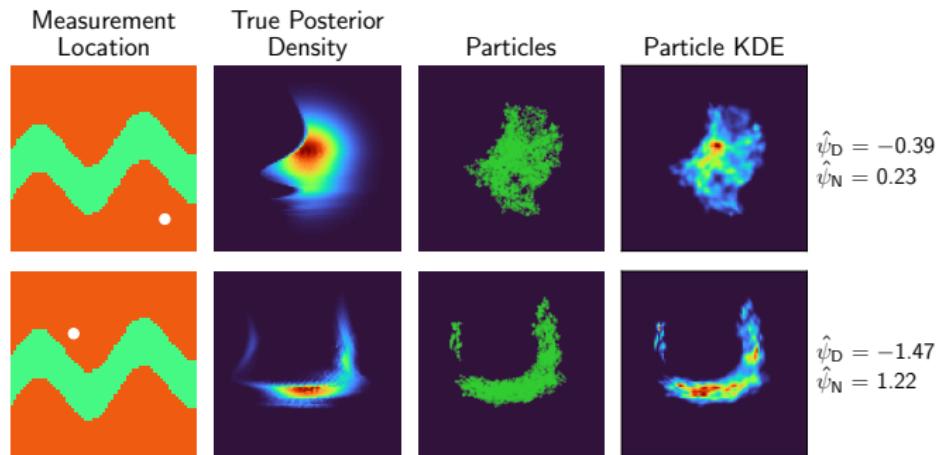
$$\underbrace{\bar{V}(\mathbf{w}) := \frac{1}{n_v} \sum_{i=1}^{n_v} \text{tr}[\hat{\mathbf{C}}^{y_i^v, \mathbf{w}}]}_{\text{A-Optimality}}, \quad \underbrace{\bar{E}(\mathbf{w}) := \frac{1}{n_v} \sum_{i=1}^{n_v} \frac{\|\hat{\mathbf{m}}^{y_i^v, \mathbf{w}} - \boldsymbol{\theta}_i^v\|}{\|\boldsymbol{\theta}_i^v\|}}_{\text{Accuracy of Estimate}}$$



# Aquifer Case Study Part II: Problem

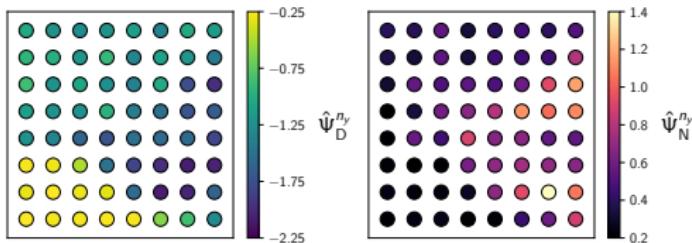
We now consider the D-optimality and normality criteria.

Here, we use an ensemble method proposed by Reich and Weissmann (2021), which is similar to the ensemble Kalman sampler but uses “locally-weighted” gradients.

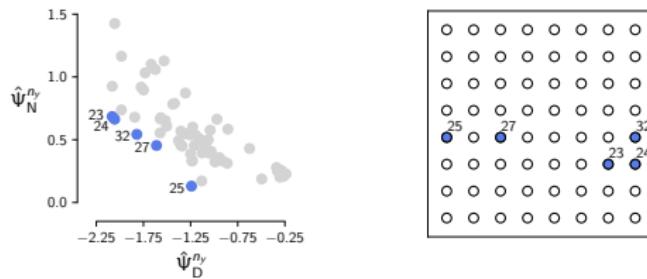


# Aquifer Case Study Part II: Results

Objectives at each location when selecting a single sensor:



Some *nondominated* locations:



# Conclusions and Future Work

Ensemble methods are flexible tools for solving geophysical inverse problems and OED problems.

Next steps include:

- Applying this methodology to real-world problems
- Pairing ensemble methods with dimension reduction techniques or surrogate models (Cleary *et al.* 2021; Dunbar *et al.* 2022)
- Using ensemble methods for goal-oriented OED



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