Accelerating Preconditioned MCMC via Multiscale Sampling

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Motivation

Subsurface characterization: What lies in an underground volume?

Need for the subsurface characterization: To make decisions regarding economic, environmental, or health and safety concerns.

- Oil Recovery
  Forecasting the output of oil production.
- Environmental Contamination
  Dynamics of contaminant concentration in groundwater.
- Geological sequestration of CO_2
  Prediction of movement of CO_2 plumes in the underground.

Challenges in Subsurface Characterization

A reliable characterization of subsurface is one of the most challenging tasks.

The challenges arise in several aspects:

- Nonlinear system of PDEs
- Hyperbolic dominated problem
- Very large computational problem
- Stochastic coefficients/uncertainty
- Uncertainty reduction: conditioning of reservoir properties to dynamic and/or static data

Model Problem: Elliptic Equation

Using Darcy's law, we write the elliptic problem as follows:

$$\boldsymbol{v}(\boldsymbol{x}) = -k(\boldsymbol{x}, \omega)\nabla p(\boldsymbol{x}),$$
$$\nabla \cdot \boldsymbol{v}(\boldsymbol{x}) = f, \quad \boldsymbol{x} \in \Omega,$$

and appropriate Boundary Conditions,

where,
f: source term
$k(\boldsymbol{x}, \omega)$: unknown permeability of the porous medium
$\boldsymbol{v}(\boldsymbol{x})$: Darcy velocity
$p(\boldsymbol{x})$: pressure of the fluid.

Numerical Simulator: Uses a mixed finite element formulation on Graphics Processing Units (GPUs).

Subsurface Characterization

Bayes' Theorem

We sample the permeability field, $\log k(x) = \eta$, conditioned on available pressure data, R_p, i.e., from $P(\eta|R_p)$.

Bayes' Theorem: $P\left(\eta|R_p\right) \propto P\left(R_p|\eta\right)\, P(\eta)$

- $P\left(R_p|\eta\right)$ is the likelihood function. We assume the form

  $$P(R_p|\boldsymbol{\eta}) \propto \exp\Big(-\left(R_p - R_{\boldsymbol{\eta}}\right)^\top \Sigma (R_p - R_{\boldsymbol{\eta}})\Big),$$

  where $R_{\boldsymbol{\eta}}$ denotes the simulated pressure data, and $\Sigma = \boldsymbol{I}/2\sigma_R^2$. It deals with the statistical distribution involving the solution of the elliptic equation.
- $P(\eta)$ is the prior distribution (has to be provided).

Many samples of the permeability field may yield the same/similar pressure data (not one-to-one mapping). Therefore, this is an ill-posed inverse problem.

The Prior Distribution

Consider a Gaussian field $Y(x,\omega)$.

It is characterized by $R(x,z) = \Big\langle Y(x,\omega)Y(z,\omega)\Big\rangle \qquad \Big\langle Y(x,\omega)\Big\rangle = 0.$

Example: $R(x,z) = \sigma_Y^2 \exp\left(-\sum_{i=1}^{2} \frac{(x_i - z_i)^2}{2L_i^2} \right)$

We set, as a simple model for rock permeability,

$$k(x,\omega) = \exp(Y(x,\omega)).$$

Difficulty in Characterization

Typical permeability field is defined over the underlying grid where the number of grid blocks can be large.

Direct sampling of the permeability field over these grid blocks yields a very large dimensional parameter space.

The Karhunen-Loève Expansion is used to efficiently parametrize the permeability field, resulting in greatly reduced parameter space dimension [Loève, 1977].

Karhunen-Loève Expansion

It relies on decomposing Y using basis functions satisfying

$$\int_\Omega R(x,z)\varphi_n(z)\,dz = \lambda_n\varphi_n(x).$$

The Karhunen-Loève Expansion is

$$Y(x,\omega) = \sum_{n=1}^{\infty} \theta_n(\omega)\sqrt{\lambda_n}\,\varphi_n(x).$$

The parameter reduction is achieved by truncating the series:

$$Y(x,\omega) \approx \sum_{n=1}^{N} \theta_n(\omega)\sqrt{\lambda_n}\,\varphi_n(x)$$

Karhunen-Loève Expansion

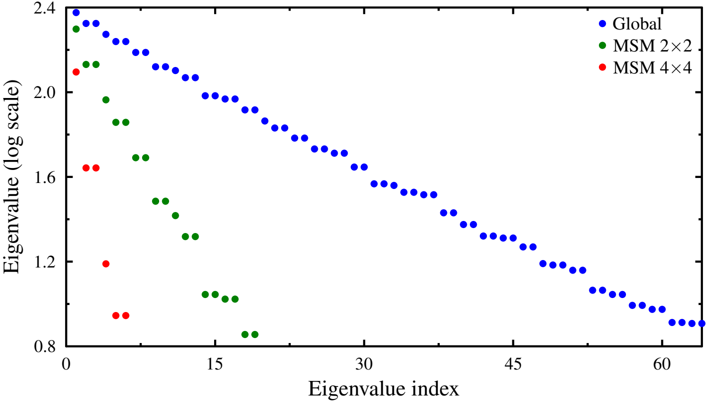

Fig. 1. Decay of eigenvalues for the global and multiscale sampling methods.

Markov Chain Monte Carlo Methods

Metropolis-Hasting Markov Chain Monte Carlo

Goal: To sample from the posterior dist. $P(\boldsymbol{\eta}|R_p)$, $\boldsymbol{\eta} = \mathsf{KLE}[\boldsymbol{\theta}]$

Strategy: Construct a Markov chain such that $P(\boldsymbol{\eta}|R_p)$ is the equilibrium distribution of the chain.

Drawbacks:

It is inherently a serial process with low acceptance rates.

Proposed Alternatives:

- Preconditioned (Two-stage) MCMC, which uses a coarse scale filter [Christen and Fox, 2005; Efendiev et al., 2005].
- Parallelize a single MCMC chain by Prefetching [Brockwell, 2006].
- Multiple MCMC chains.

Multiscale Sampling Method

- MSM combines the simplicity of the preconditioned MCMC with a new multiscale sampling algorithm.
- The algorithm decomposes the stochastic space in orthogonal complement subspaces, through a one-to-one mapping to a non-overlapping domain decomposition of the region of interest.
- The localization of the search is performed by Gibbs sampling: we apply a KL expansion locally, at the subdomain level.

The Mapping: Prior Distribution and Subdomains

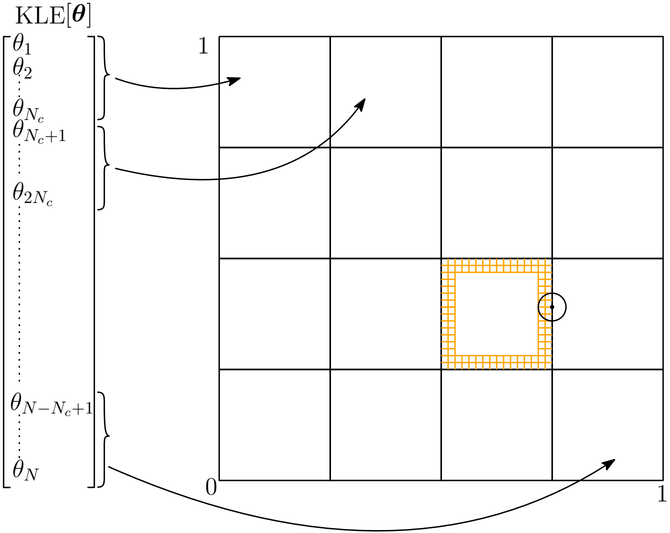

Fig. 2. Decomposition of the theta vector (left) and the domain (right).

Convergence Analysis of Multiple MCMC Chains

- Start multiple MCMC chains from different initial conditions and make sure that the chains mix together sufficiently.
- Two most commonly used convergence measures: Potential Scale Reduction Factor (PSRF) and its multivariate extension (MPSRF).
- The PSRF takes into account only a subset of parameters; The MPSRF incorporates the convergence information of all the parameters and their interactions [Brooks and Gelman, 1998].

Simulation Study

Problem Setup

- Consider a unit square-shaped physical domain; Solve the elliptic equation in the domain.
- Source Term: Set $f = 0$.
- Boundary Conditions: Impose Dirichlet boundary conditions, $p = 1$ and $p = 0$, on the left and right boundaries, respectively; Set no-flow boundary condition everywhere else on the boundaries of the domain.
- Subsurface Characterization: Use MCMC simulations to characterize the permeability field using available pressure data.

Numerical Results

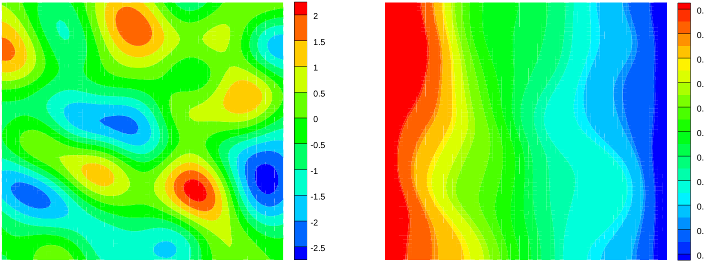

Fig. 3. Reference log permeability field (left) and the corresponding reference pressure field (right)

Numerical Results

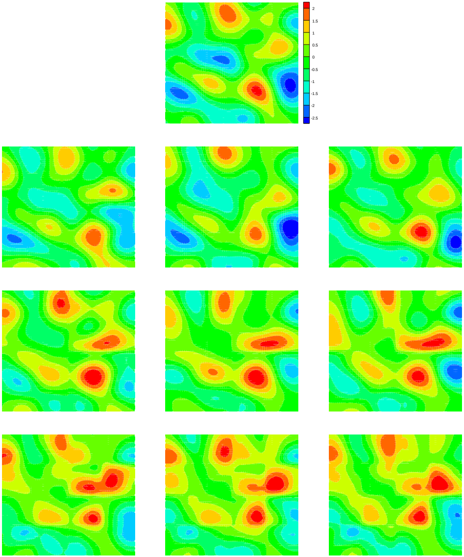

Fig. 4. First row: Reference log permeability field. Second row: Accepted permeability fields in the global sampling method. Third row: Accepted permeability fields in MSM 2×2. Fourth row: Accepted permeability fields in MSM 4×4. From left to right, log permeability fields at 80000, 160000 and 240000 iterations, respectively.

PSRF and MPSRF Curves

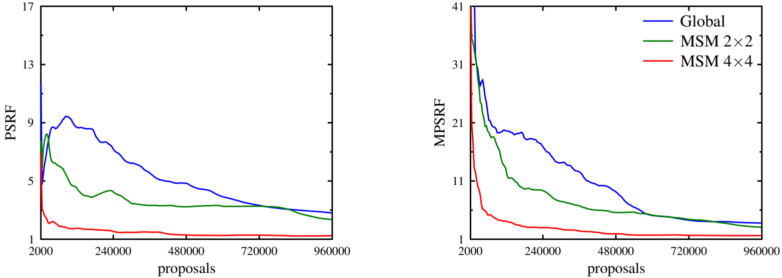

Fig. 5. The maximum of PSRFs and MPSRF for the MCMC method with and without multiscale sampling.

Multiscale sampling methods show an improved convergence.

Conclusions

- We have presented a novel multiscale sampling method for subsurface characterization.
- The proposed method is based on a non-overlapping partition of the domain of the governing partial differential equation that leads to the localization of the search in the underlying stochastic space.
- Our results show that the new multiscale sampling method considerably improves the convergence rate of the preconditioned Markov Chain Monte Carlo algorithm.
- We will extend the multiscale sampling method to solve the inverse problems associated with single and multiphase flows in porous media.

Reference

- A. Ali, A. Al-Mamun, F. Pereira, A. Rahunanthan, Multiscale sampling for the inverse modeling of partial differential equations, Journal of Computational Physics, Volume 497, 2024, 112609, ISSN 0021-9991, https://doi.org/10.1016/j.jcp.2023.112609.