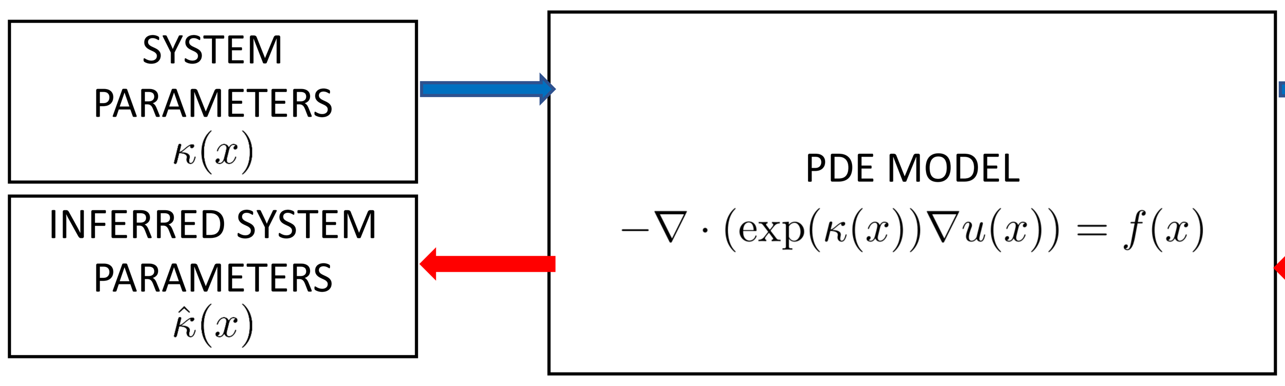
Variational Bayes: Scalable Uncertainty Quantification for PDE Inverse Problems

CSIC Cambridge Centre for Smart Infrastructure & Construction

Motivation

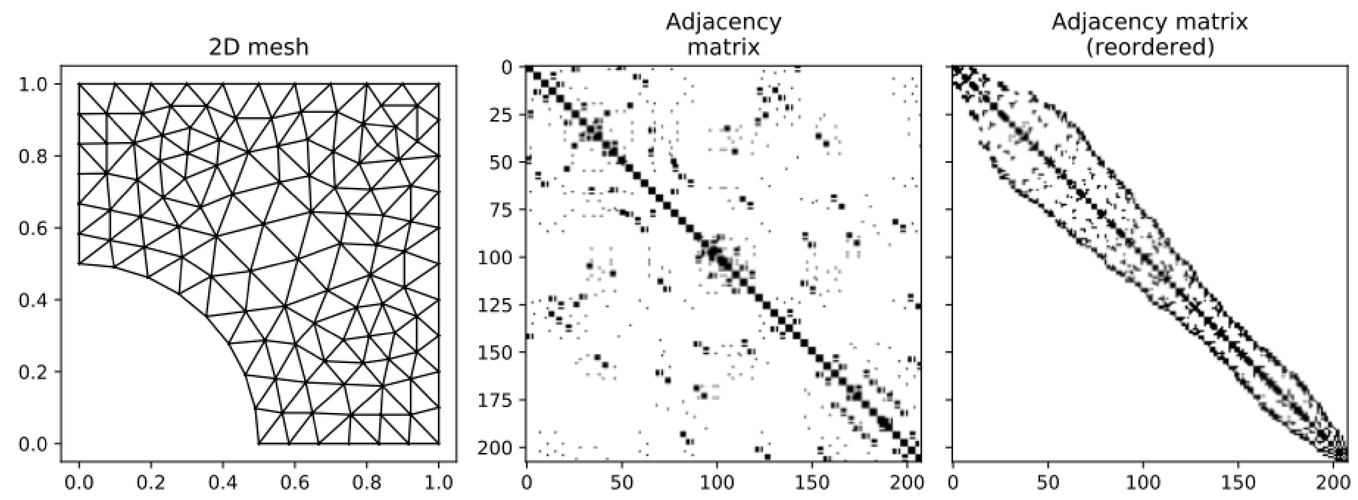
- Many phenomena in Science and Engineering are modelled using Partial Differential Equations (PDEs)
- For example, we may model material properties using elasticity equations, resulting in a PDE formulation.
- Subsequently, we may be interested in either simulating material behaviour under different circumstances (aka **forward problem**), or in inferring material properties from experiments such as tensile tests (this is termed the **inverse problem**).



- We focus on the **inverse problem**, which is often under-constrained; many possible solutions exist due to inferring a continuous function from finite observations. Thus we constrain the search space to find a specific solution.
- We follow the **Bayesian approach** which allows for incorporating expert prior knowledge and uncertainty quantification of the inferred quantities.
- The posterior distribution for $\kappa(x)$ is analytically intractable, so approximation methods must be used. Traditionally, simulation-based methods such as Markov Chain Monte Carlo (MCMC) have been used.
- We advocate for Variational Bayes (VB) as an alternative by reformulating the integration problem in MCMC as an **optimisation problem**.

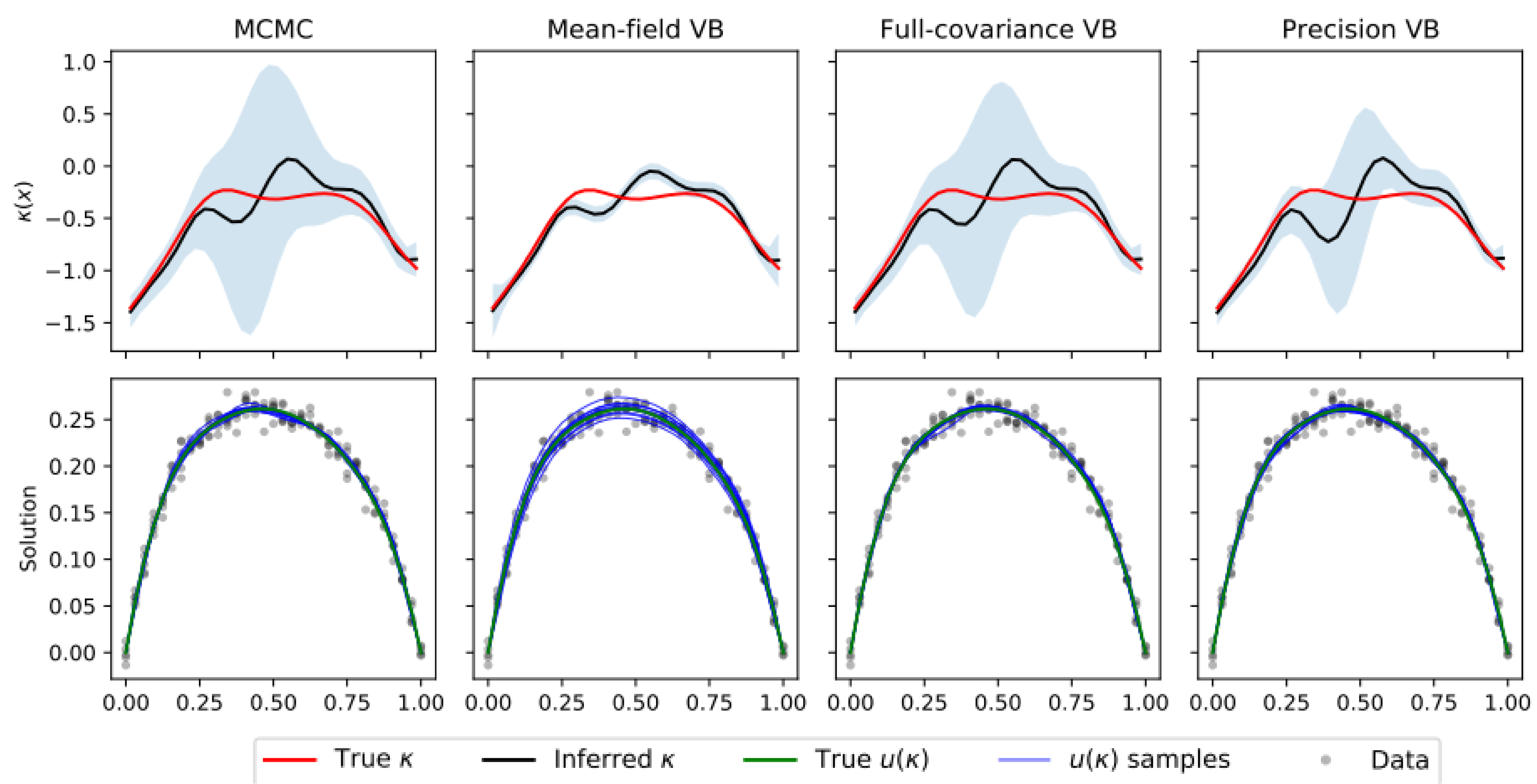
Method

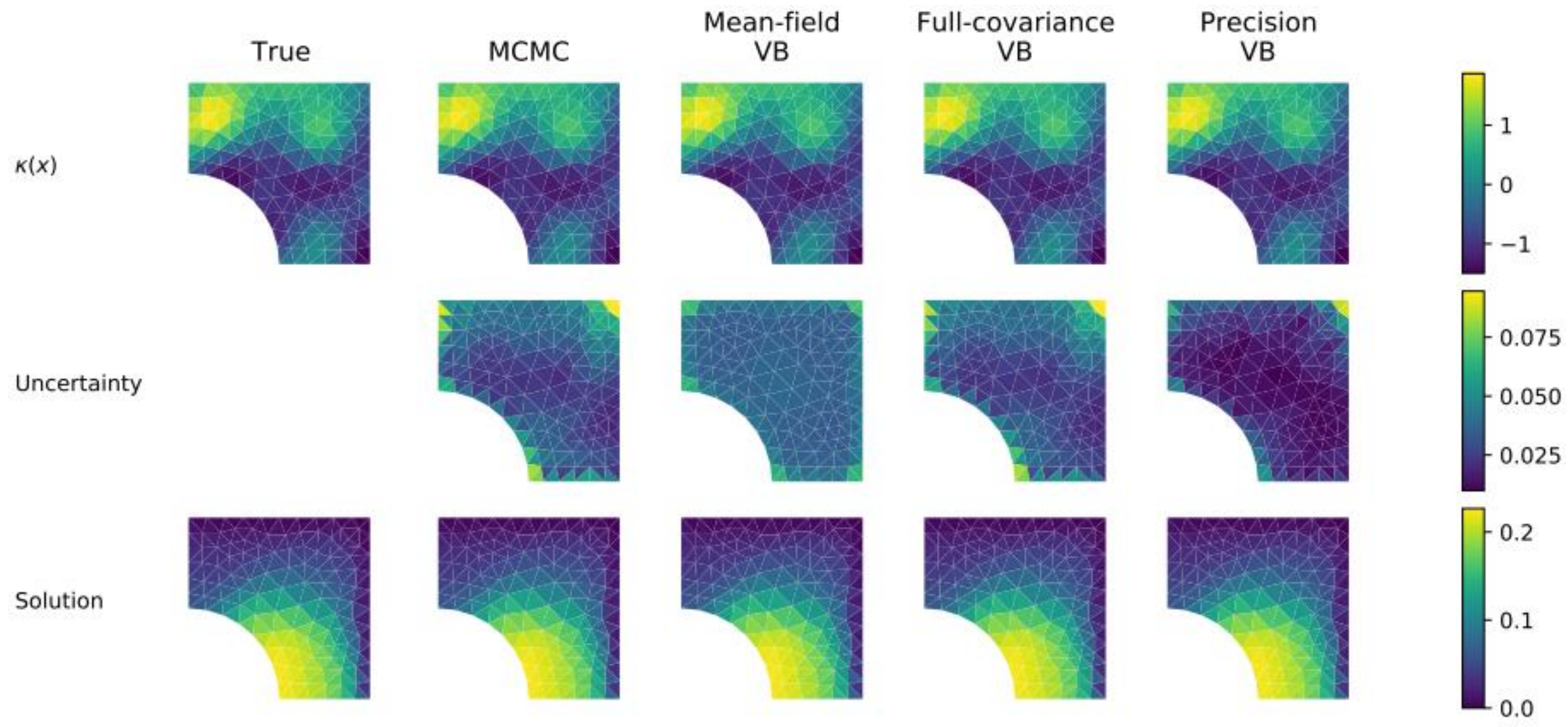
- In VB, we choose a family of approximating distributions over which we optimise.
- The complexity of the family determines how much of the dependence of the posterior distribution is captured by the approximation.
- We use multivariate Gaussian to model the components of the discretization of $\kappa(x)$
- When specifying the covariance matrix of the approximating distribution, we take advantage of the structure of the discretized problem to decide which components are conditionally independent.
- The resulting sparse matrix allows for faster linear algebra and fewer optimization parameters.



Contributions and Results

- Variational Bayes offers a **computationally tractable** alternative to the intractable MCMC methods and provides **consistent mean and uncertainty estimates** on the problems inspired by questions in computational mechanics.
- The variational approximation with a full-covariance structure and the structured precision structure **adequately estimates posterior variance** when compared to MCMC which are known to be asymptotically correct.
- It is naturally **integrated with existing FEM solvers**, using the gradient calculations from the FEM solvers to optimize the VB objective.
- Parameterizing the multivariate Gaussian distribution using **a sparse precision matrix** provides a way to balance the trade-off between computational complexity and the ability to capture dependencies in the posterior distribution.
- VB provides a good estimate for the mean and the variance of the posterior distribution in a time that is **an order of magnitude faster** than MCMC methods.
- The VB estimates may be used effectively in **downstream tasks** to estimate various quantities of interest.





Jan Povala, Ieva Kazlauskaite, Eky Febrianto, Fehmi Cirak, Mark Girolami

ik394@cam.ac.uk

@CSIC-IKC www.smartinfrastructure.eng.cam.ac.uk

University of Cambridge | UKRI Innovate UK | UKRI Engineering and Physical Sciences Research Council