hIPPYlib: An Extensible Software Framework for Large-scale Inverse Problems

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Introduction

Motivation

- The **inverse problem** seeks to extract knowledge from data via models, and is a critical precursor to computational prediction with rigorously quantified uncertainties.
- Bayesian inference provides a comprehensive and systematic framework for formulating and solving inverse problems under uncertainty.
- Bayesian inversion with conventional algorithms and software is prohibitive for complex models and high dimensional parameter spaces.
- Intensive research efforts are creating advanced algorithms that exploit the structure of the posterior, resulting in orders of magnitude speedups.
- However, these new algorithms have not been made accessible to a broad community of scientists and engineers interested in solving inverse problems.

Goals

- Develop, deploy, & support robust, scalable, high-performance, open-source software.
- Provide reference implementations of advanced Bayesian inversion algorithms.
- Enable the solution of Bayesian inverse problems of unprecendented size and realism.
- Facilitate the wider adoption of Bayesian tools in simulation-driven science.
- Any scientist interested in integrating data with models to quantify and reduce uncertainties in model predictions is a potential user.

Bayesian Formulation of Inverse Problems

- **Goal:** given (noisy, indirect) data and a deterministic or stochastic forward model, infer model parameters and update model predictions.
- *Solving* the inverse problem then amounts to *characterizing* the posterior distribution: drawing samples; estimating the mean, covariance, or higher moments; evaluating the posterior probabilities of particular events or quantities of interest.

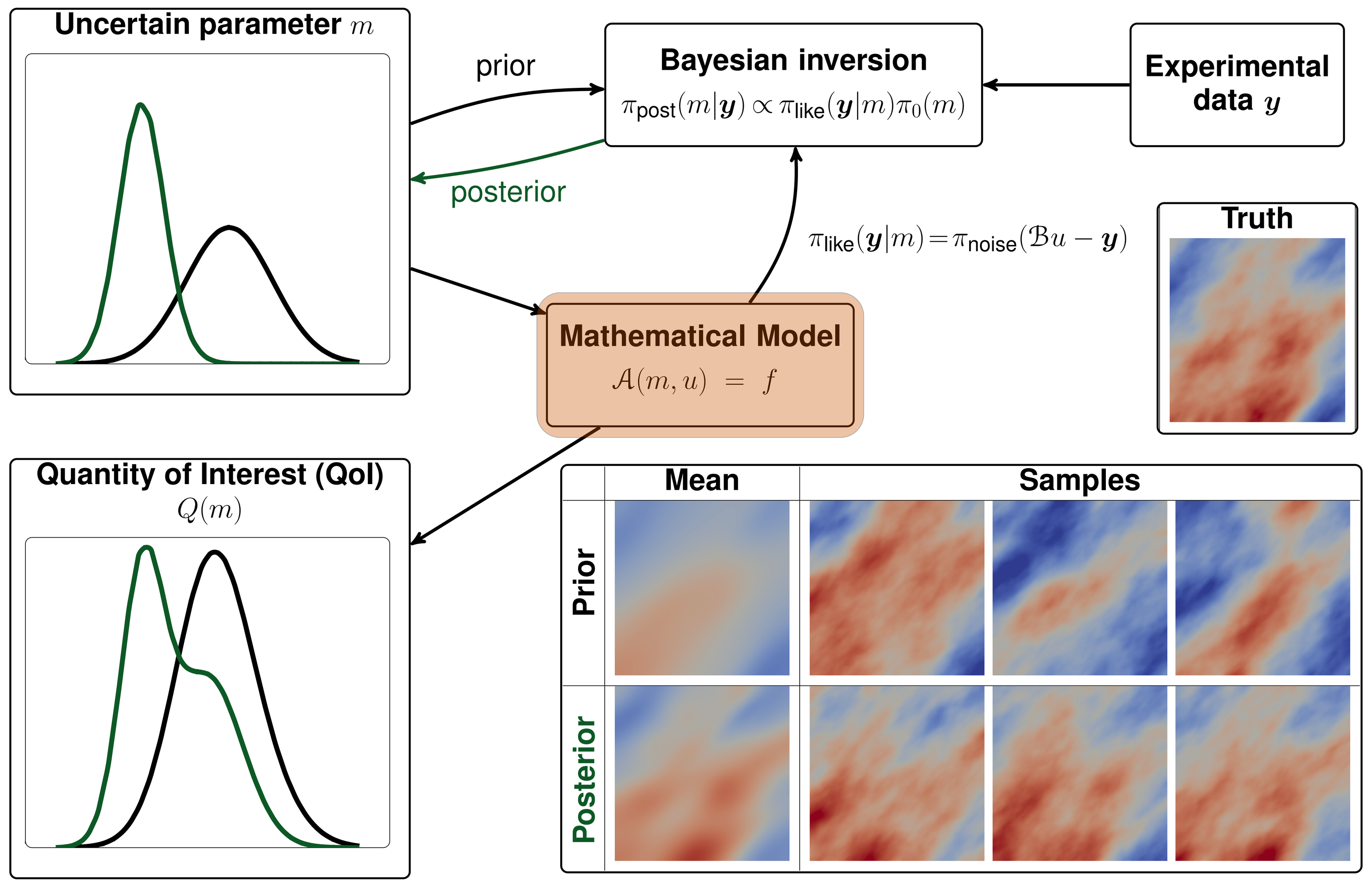


Figure: *The process of extracting knowledge from data by solving inverse problems*

hIPPYlib Software Framework

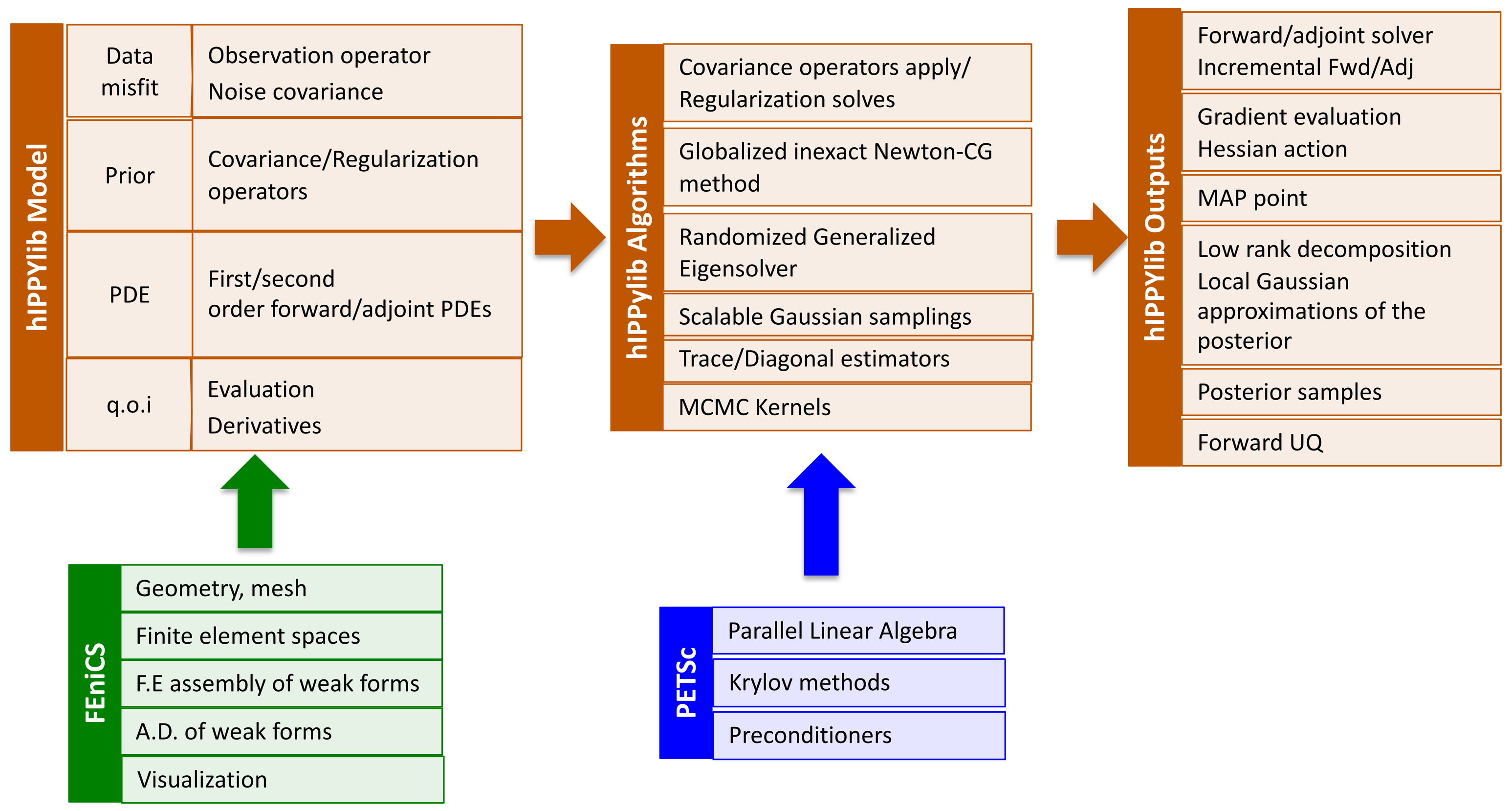


Figure: *Design of hIPPYlib (**I**nverse **P**roblems **Py**thon **lib**rary) [2].*

Application: Inverse Ice Sheet Problem Formulation

Here, we describe the inverse problem of estimating the posterior distribution of an unknown basal boundary condition β that characterizes ice sheet flow [1]. The parameter-to-observable map $\boldsymbol{u} = \boldsymbol{f}(\beta)$ involves the solution of a nonlinear Stokes system. We assume a Gaussian additive noise model for the observed velocities:

$$\boldsymbol{u}^{\text{obs}} = \boldsymbol{f}(\boldsymbol{\beta}) + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Gamma}_{\text{noise}})$$

If the prior is taken as Gaussian with mean β_{pr} and covariance $\boldsymbol{\Gamma}_{\text{pr}}$, then the posterior is:

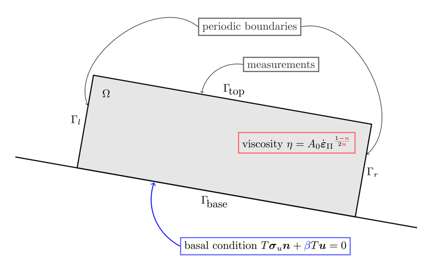
$$\pi_{\text{post}}(\beta) \propto \exp\left(-\tfrac{1}{2} \parallel \boldsymbol{f}(\boldsymbol{\beta}) - \boldsymbol{u}^{\text{obs}} \parallel^2_{\boldsymbol{\Gamma}^{-1}_{\text{noise}}} - \tfrac{1}{2} \parallel \boldsymbol{\beta} - \boldsymbol{\beta}_{\text{pr}} \parallel^2_{\boldsymbol{\Gamma}^{-1}_{\text{pr}}}\right)$$

The *maximum a posteriori* (MAP) point can be shown to be:

$$\boldsymbol{\beta}_{\text{MAP}} = \arg\min_{\boldsymbol{\beta}} \tfrac{1}{2} \parallel \boldsymbol{f}(\boldsymbol{\beta}) - \boldsymbol{u}^{\text{obs}} \parallel^2_{\boldsymbol{\Gamma}^{-1}_{\text{noise}}} + \tfrac{1}{2} \parallel \boldsymbol{\beta} - \boldsymbol{\beta}_{\text{pr}} \parallel^2_{\boldsymbol{\Gamma}^{-1}_{\text{pr}}}$$

This is an (appropriately weighted) deterministic inverse problem, which is solved with the inexact Newton-CG algorithm [1]. Each evaluation of $\boldsymbol{f}(\boldsymbol{\beta})$ requires solving a nonlinear Stokes system:

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0 && \text{in } \Omega \\ -\nabla \cdot \boldsymbol{\sigma}_{\mathbf{u}} &= \rho \mathbf{g} && \text{in } \Omega \\ \mathbf{u}|_{\Gamma_l} = \mathbf{u}|_{\Gamma_r} \text{ and } \boldsymbol{\sigma}_{\mathbf{u}}\mathbf{n}|_{\Gamma_l} &= \boldsymbol{\sigma}_{\mathbf{u}}\mathbf{n}|_{\Gamma_r} && \text{on } \Gamma_p \\ \boldsymbol{\sigma}_{\mathbf{u}}\mathbf{n} &= \mathbf{0} && \text{on } \Gamma_{\text{top}} \\ \mathbf{u}\cdot\mathbf{n} = 0, \ \mathrm{T}\boldsymbol{\sigma}_{\mathbf{u}}\mathbf{n} + \beta \mathrm{T}\mathbf{u} &= \mathbf{0} && \text{on } \Gamma_{\text{base}}, \end{aligned}$$



where Γ_{top} and Γ_{base} are the top and bottom surfaces of the ice sheet Ω, Γ_p is a periodic boundary, and the variables are:

- $\mathbf{u}$ velocity, p pressure
- $\boldsymbol{\sigma}_{\mathbf{u}} = -\mathbf{I}p + 2\eta(\boldsymbol{u}, n)\dot{\boldsymbol{\varepsilon}}_{\mathbf{u}}$ stress tensor
- $\eta(\boldsymbol{u}, n)$ viscosity
- $\dot{\boldsymbol{\varepsilon}}_{\mathbf{u}} = \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$ strain rate tensor
- $\mathrm{T} = \mathbf{I} - \mathbf{n} \otimes \mathbf{n}$ the tangential operator
- ρ density
- $\mathbf{g}$ gravitational acceleration vector
- $\mathbf{n}$ the unit normal vector
- β the slipperiness coefficient.

Application: Inverse Ice Sheet Problem Results

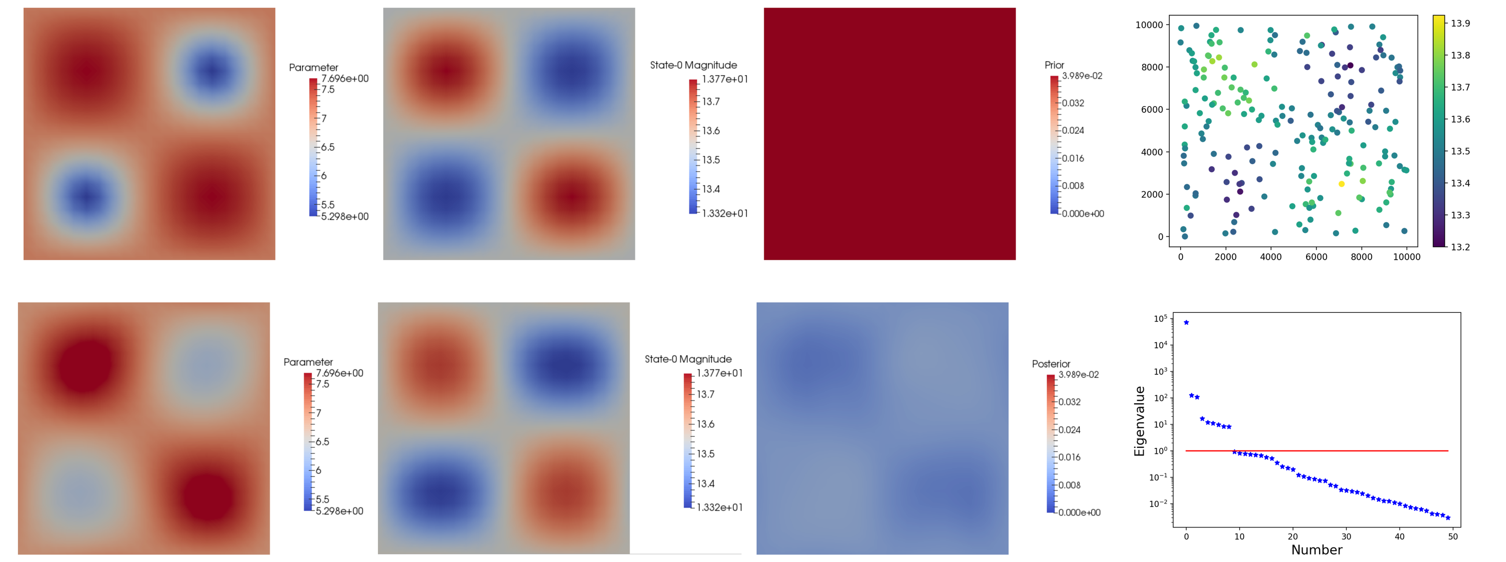


Figure: *Top: True parameter field (left), true velocity (center left), prior variance (center right), and observations (right). Bottom: Reconstructed parameter field (left), recovered velocity (center left), posterior variance (center right), and spectrum of the prior preconditioned Hessian of the negative log posterior misfit term (right).*

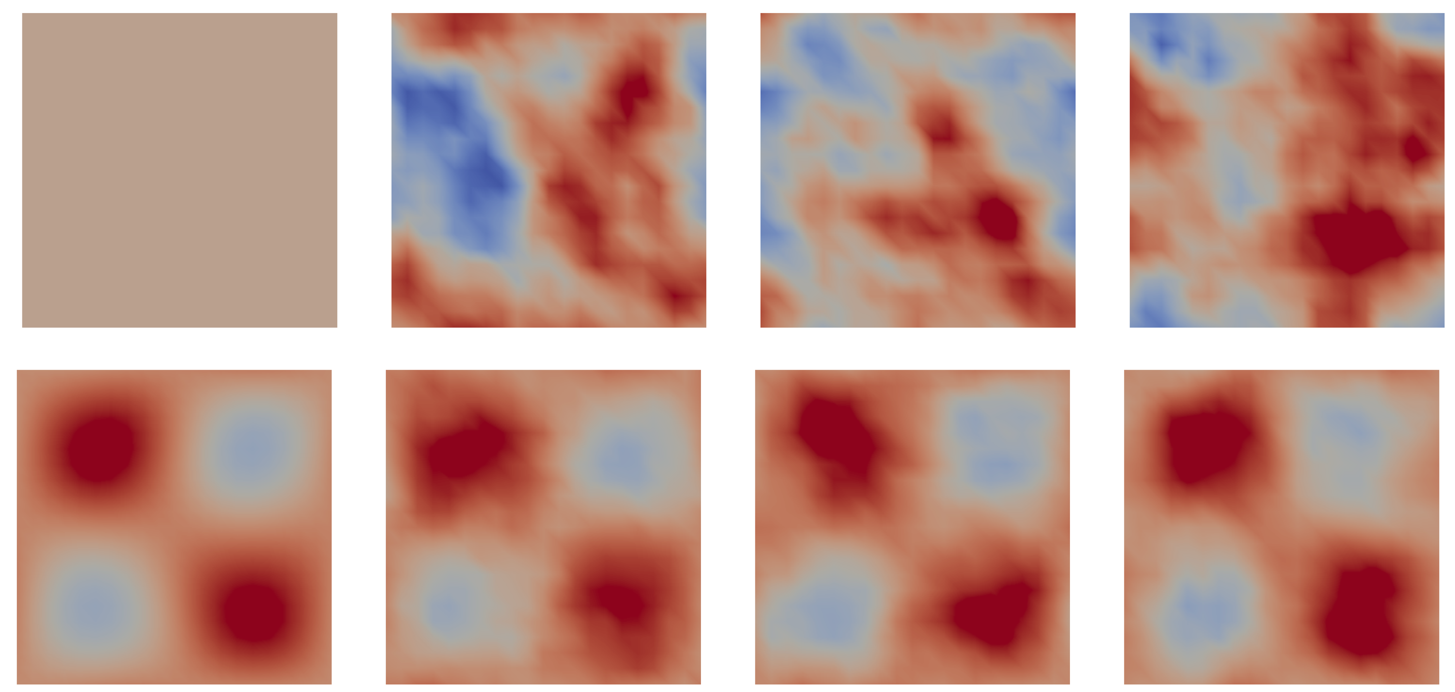


Figure: *Top row: Prior mean (left image), and three samples from the prior distribution. Bottom row: Posterior mean (left image), and three samples from the posterior distribution.*

Other applications in hIPPYlib

- Goal-oriented inference for reservoir models with complex features including faults (UT).
- Joint seismic-electromagnetic inversion (UT).
- Inference of constitutive laws in mechanics of nano-scale filaments (UC Merced)
- Inversion for coupled ice-ocean interaction (UT).

Code repository

- `http://hippylib.github.io`

Acknowledgement

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References

[1] Isaac, T., Petra, N., Stadler, G., and Ghattas, O. (2015). Scalable and efficient algorithms for the propagation of uncertainty from data through inference to prediction for large-scale problems, with application to flow of the antarctic ice sheet. *Journal of Computational Physics*, 296:348–368.

[2] Villa, U., Petra, N., and Ghattas, O. (2018). hIPPYlib: an Extensible Software Framework for Large-scale Deterministic and Bayesian Inverse Problems. *Journal of Open Source Software*, 3(30).