Tuesday Afternoon Panel: Uncertainty & Inverse Problems in Practice

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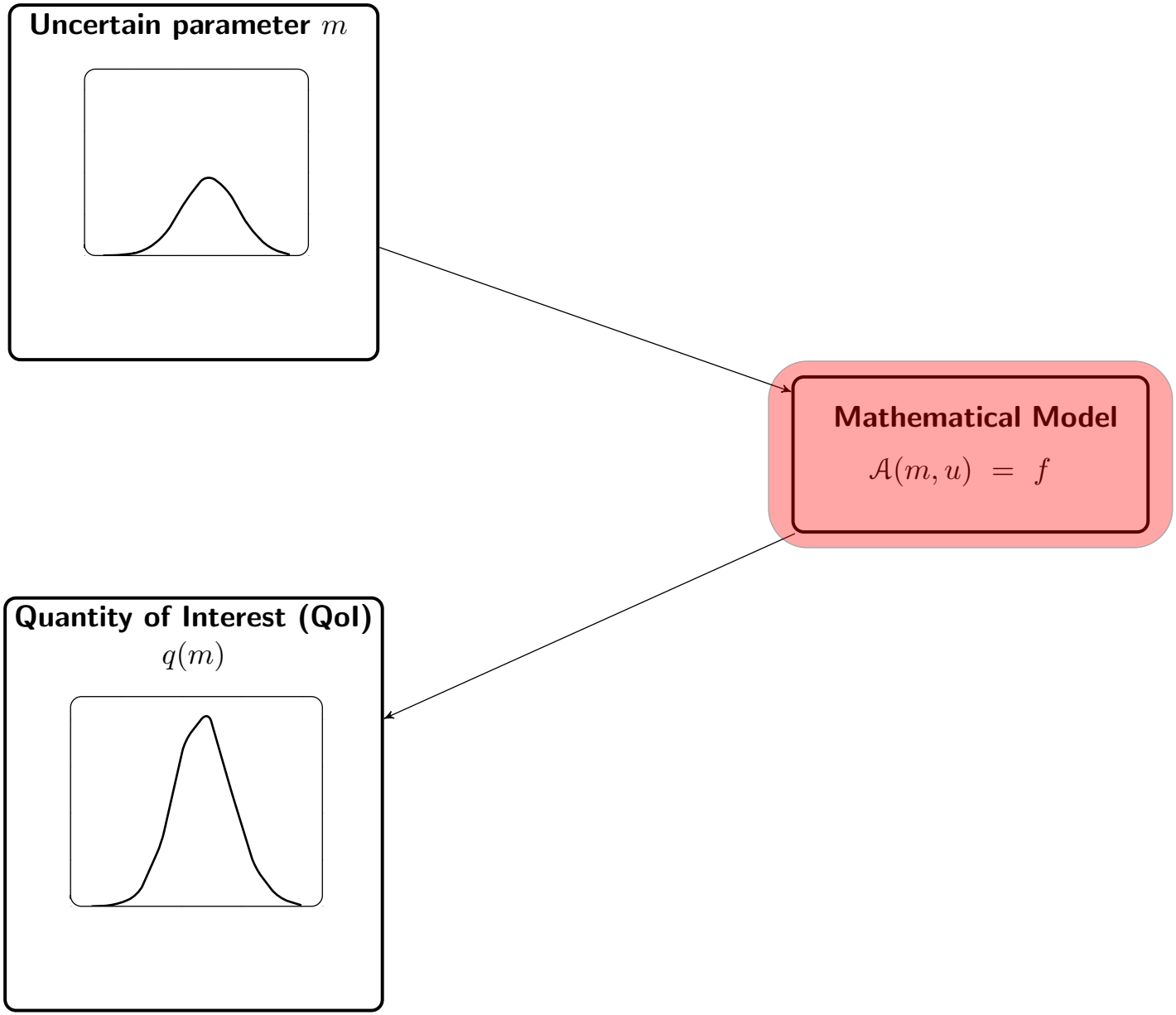
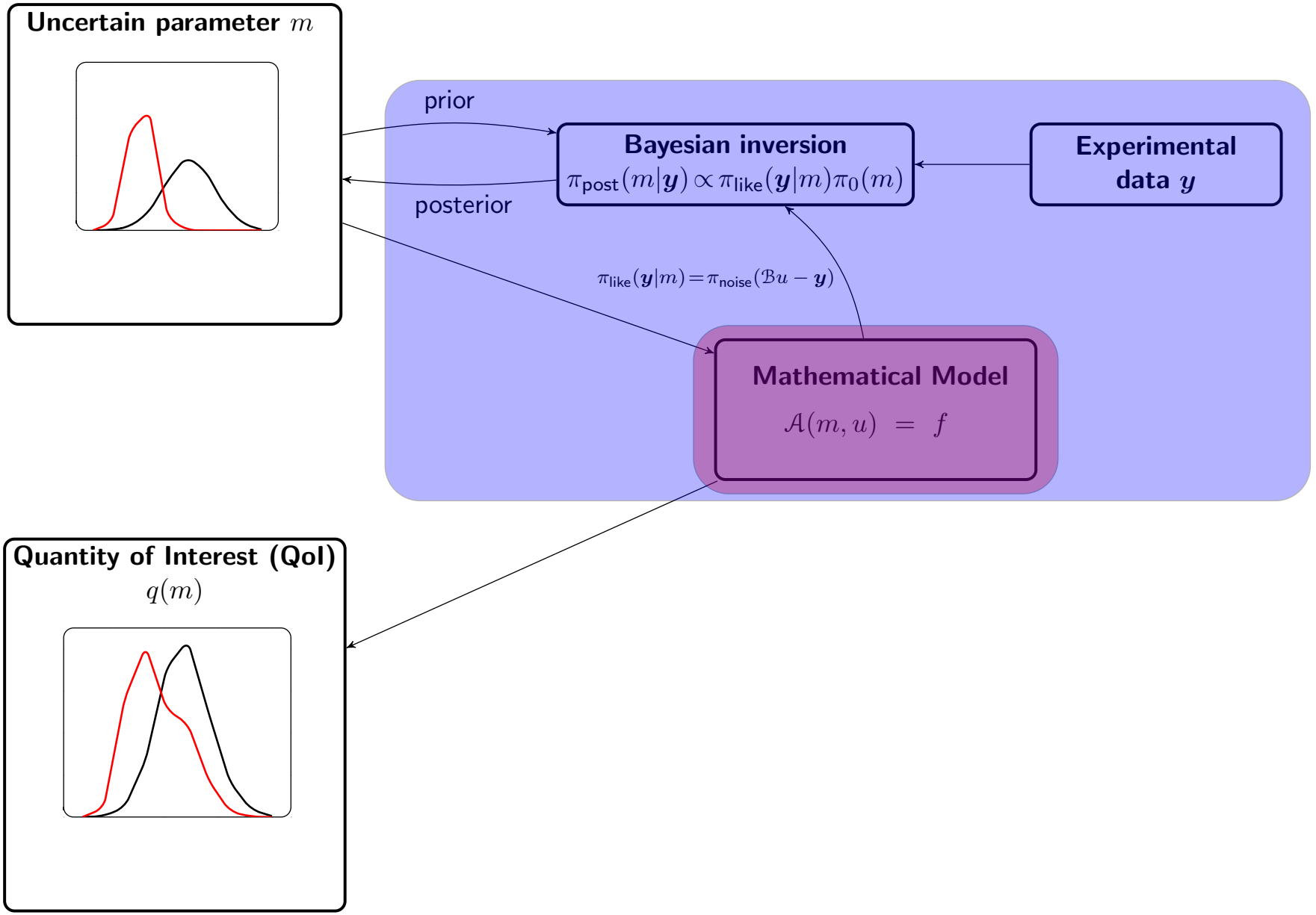
Inverse Problems and Uncertainty Quantification in Solid Earth Geophysics

- Solid earth geophysics is a poster child for inverse problems and UQ: we cannot directly observe the interior
- We must infer interior structure and processes from observations of surface phenomena
- This is formally a mathematical inverse problem, and usually ill-posed (many sets of parameters are consistent with the data to within the noise)
- Quantifying uncertainties in the inversion (and forward propagating them to predictions) thus becomes critical

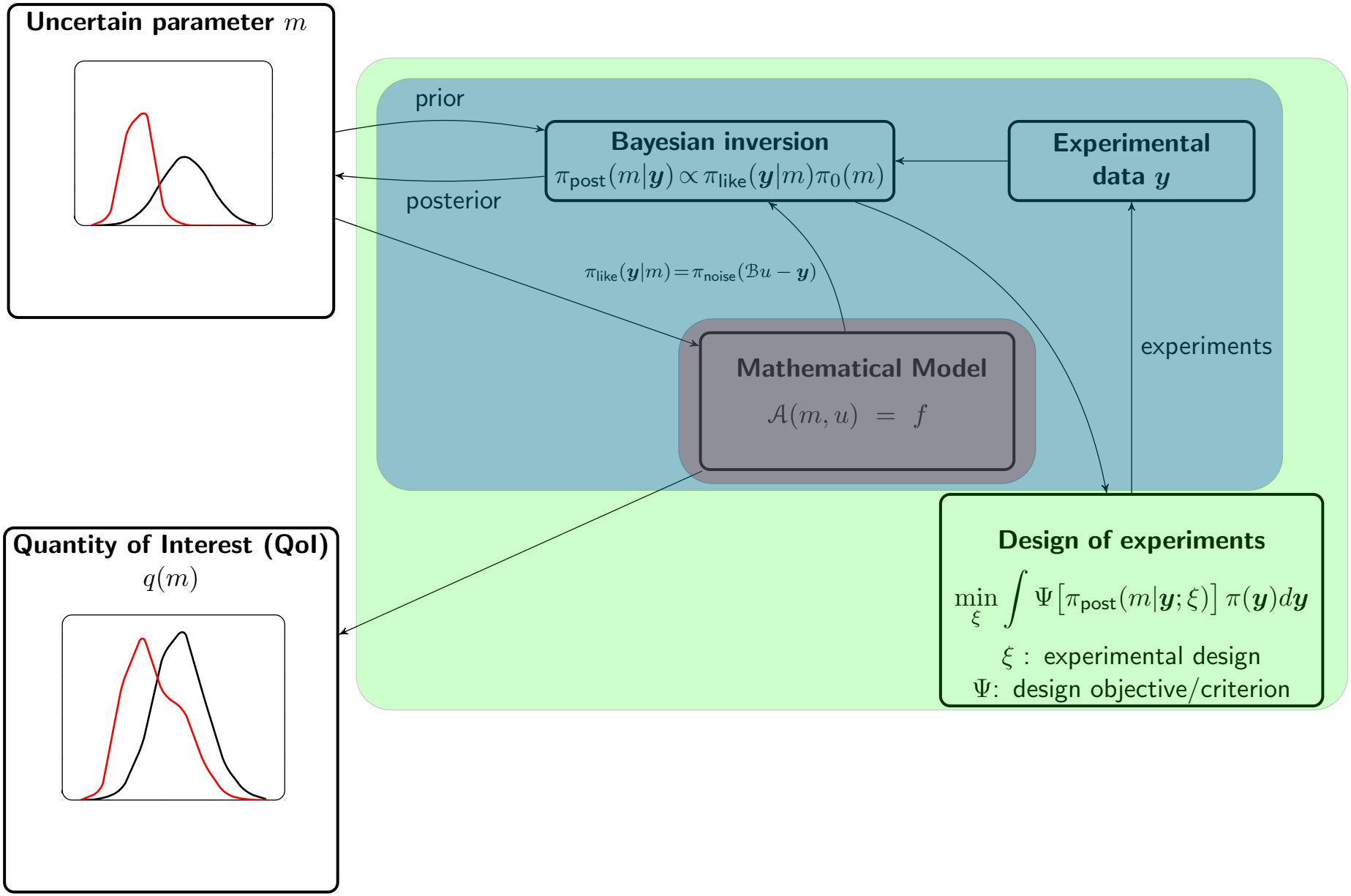
End-to-End Uncertainty Quantification



End-to-End Uncertainty Quantification

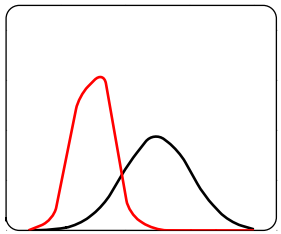


End-to-End Uncertainty Quantification



End-to-End Uncertainty Quantification

Uncertain parameter m



prior

posterior

Bayesian inversion

$\pi_{\text{post}}(m|\boldsymbol{y}) \propto \pi_{\text{like}}(\boldsymbol{y}|m)\pi_0(m)$

Experimental data $\boldsymbol{y}$

$\pi_{\text{like}}(\boldsymbol{y}|m) = \pi_{\text{noise}}(\mathcal{B}u - \boldsymbol{y})$

Mathematical Model

$\mathcal{A}(m,u) = f(\cdot;z)$

$z :=$ control function

experiments

Design of experiments

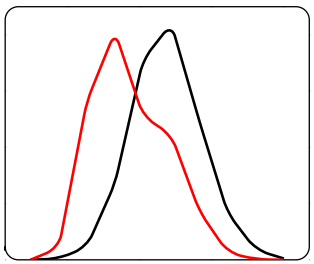
$$\min_{\xi} \int \Psi\left[\pi_{\text{post}}(m|\boldsymbol{y};\xi)\right] \pi(\boldsymbol{y}) d\boldsymbol{y}$$

ξ : experimental design

Ψ: design objective/criterion

Quantity of Interest (QoI)

$q(z,m)$



Optimal control/design under uncertainty

e.g. $\min_{z} \int q(z,m)\mu(dm)$

Three classes of uncertainty quantification problems

- Inverse problem
  - Given observations and their uncertainties, a model that maps input model parameters to output observables and its uncertainty, and a prior probability of model parameters, find posterior probability distribution of model parameters
- Prediction (or forward) problem
  - Given probability distributions of input parameters and a model that maps input model parameters to output quantities of interest, find probabilities of output quantities
- Optimal control/design problem
  - Given an objective function consisting of statistics of an output quantity of interest and a cost of the control/design, and a stochastic model that maps control/design variables to a probability distribution of the output, find the optimal control/design that minimize the objective

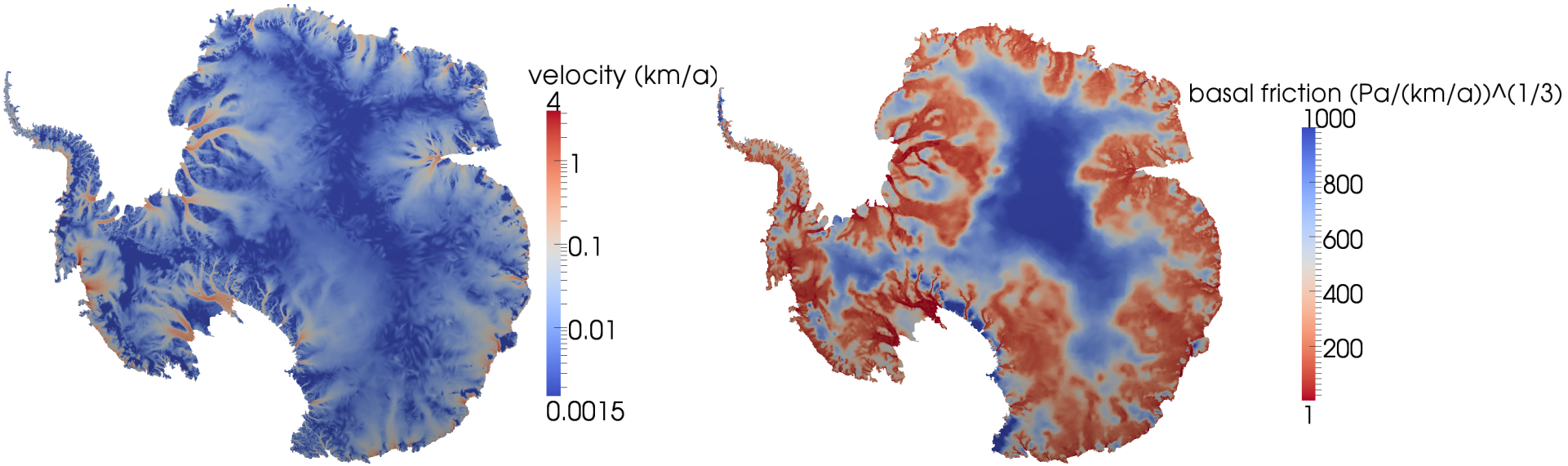
The bad news...

- UQ is fundamentally difficult: It involves exploring high dimensional parameter space, which is exponentially sparse ("the curse of dimensionality")
- When the uncertain parameters represent (infinite dimensional) fields such as initial conditions, boundary conditions, source terms, heterogeneous material parameters, the number of parameters can number in the millions or more after discretization
- For large-scale complex models, evaluating the probability of each point in parameter space entails an expensive simulation
- Conventional uncertainty quantification methods (e.g., Monte Carlo) fail for such high-dimensional, expensive UQ problems

The good news...

- Parameter space is often only formally high dimensional; many problems have intrinsically low dimensional structure
  - For inverse problem, data are often informative about a low-dimensional parameter space
- Expensive forward models can often be replaced by (parameterized) reduced order models (Taylor expansions, projection-based ROMs, etc.)
- Using these ideas, we can often exploit problem structure to overcome the challenges of UQ
- Applications to seismic inversion, ice sheet dynamics, electromagnetic scattering, subsurface flow, mantle convection, ...
- However no free lunch: Exploiting problem structure often requires adjoint-based gradients and Hessians

Deterministic inversion for basal sliding field in Antarctica

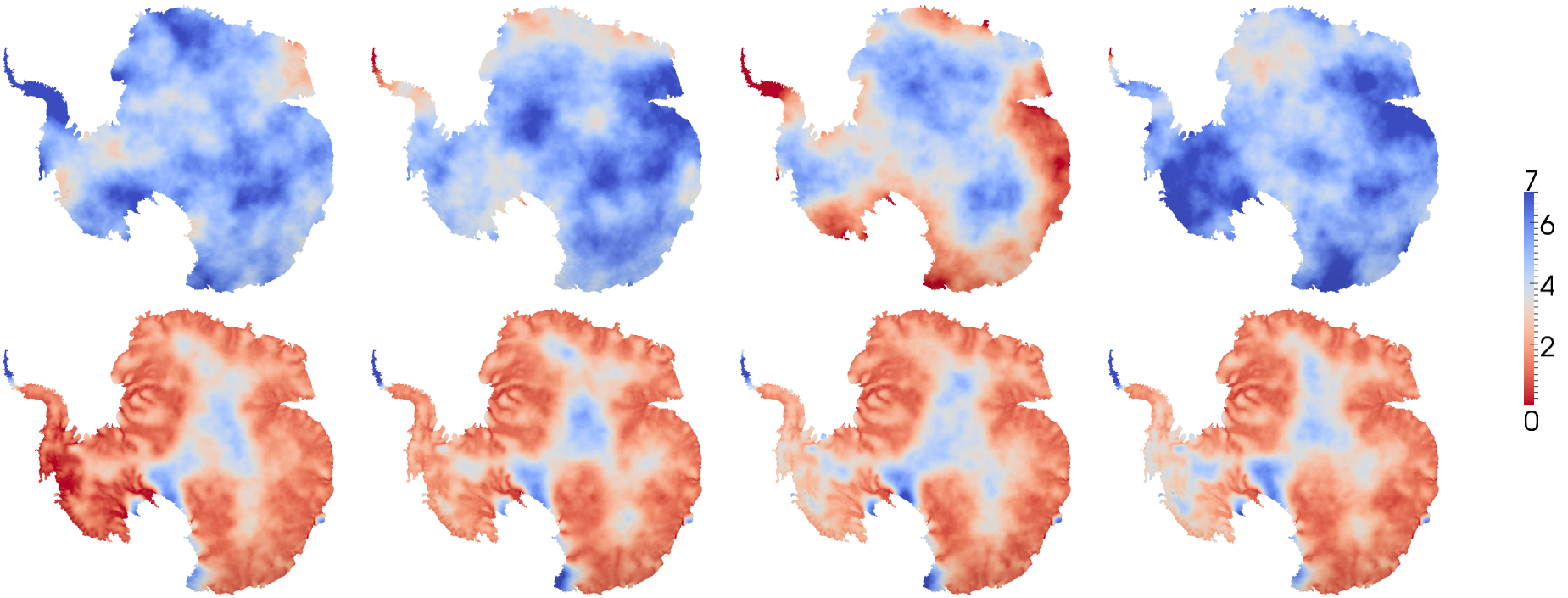


Left: Antarctica ice surface velocity observations from InSAR
Right: Inferred basal sliding field

$\Rightarrow$ Deterministic inversions do not convey the confidence we have in the inferred basal sliding parameter field

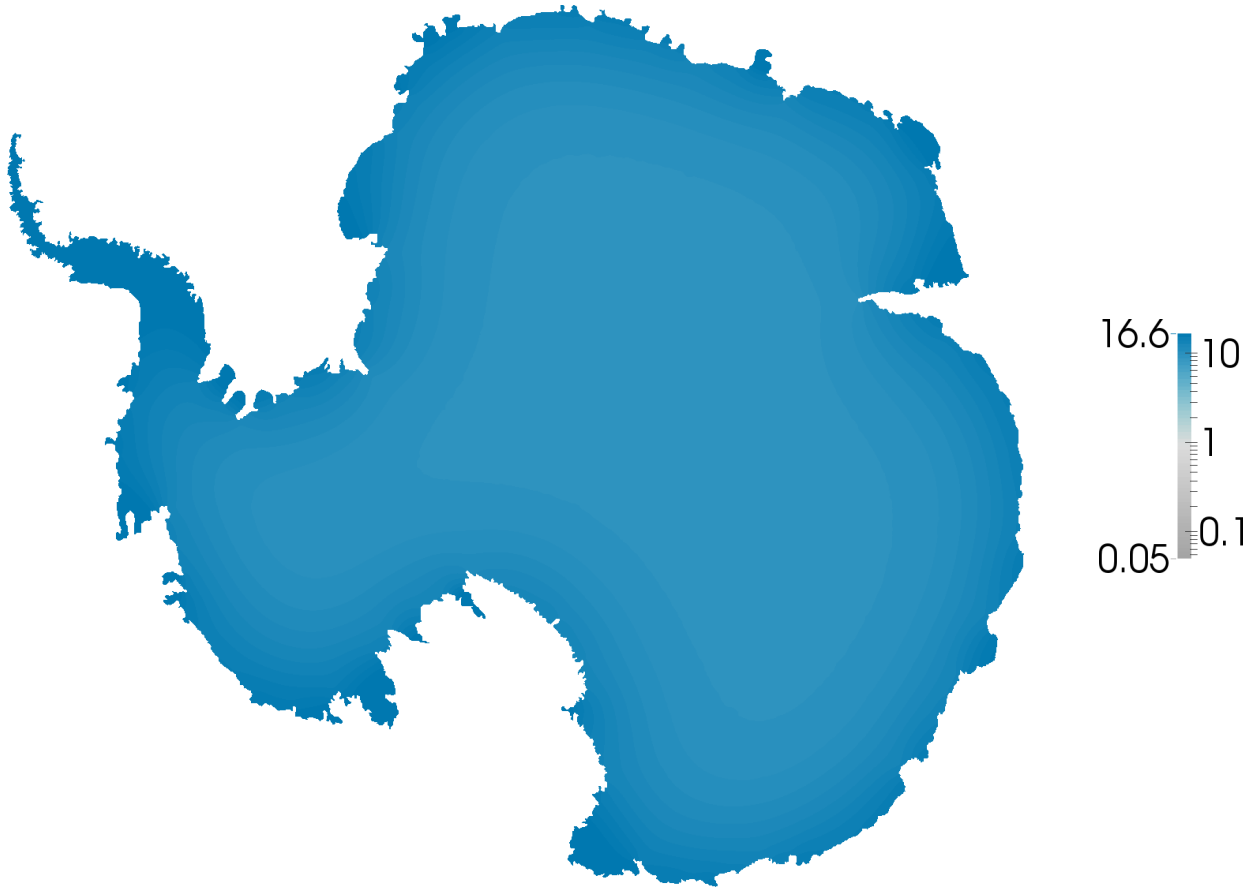
More details in: T. Isaac, N. Petra, G. Stadler, O. Ghattas, *Scalable and efficient algorithms for the propagation of uncertainty from data through inference to prediction for large-scale problems, with application to flow of the Antarctic ice sheet*, *J Comp Phys*, 2015.

Bayesian inversion: Samples from prior and posterior



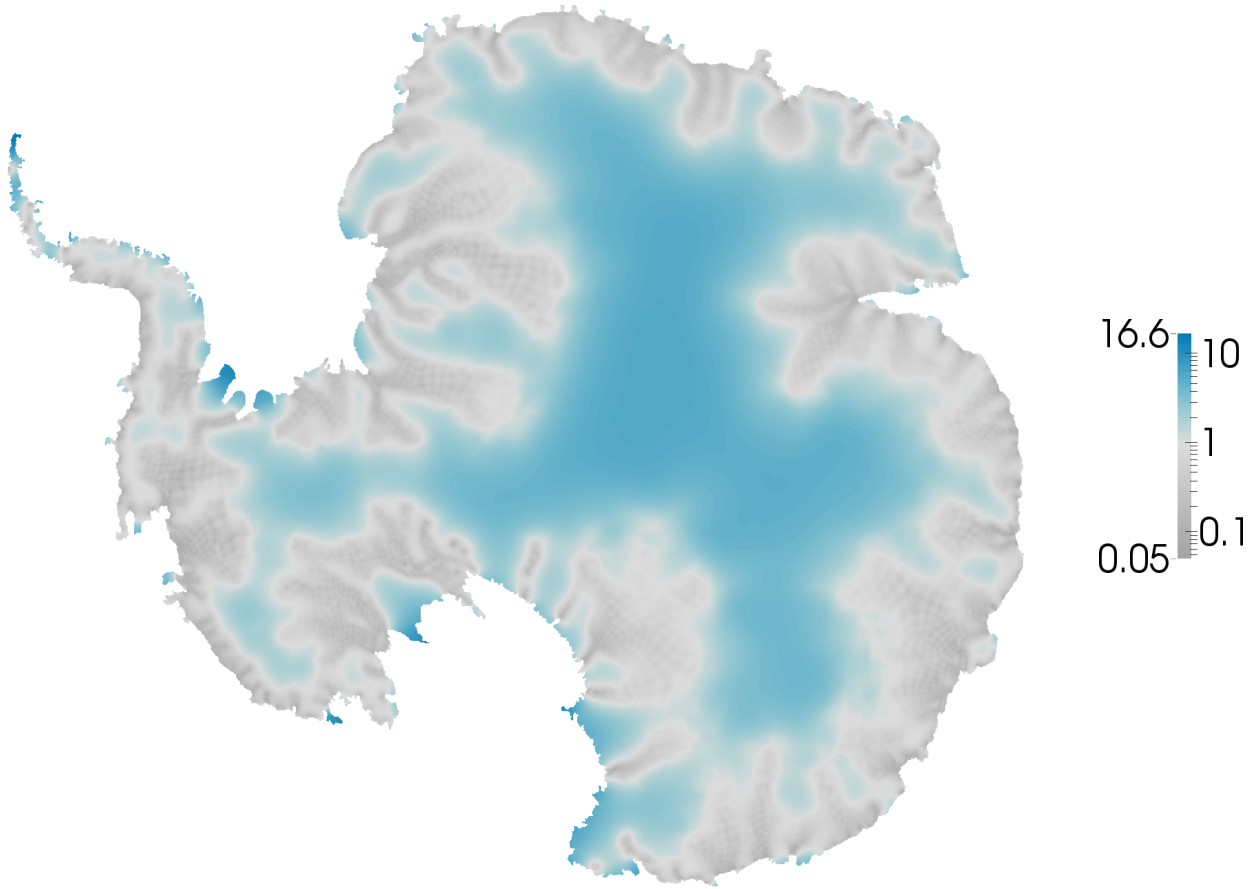
- Top: samples from prior
- Bottom: samples from posterior
- Difference between top and bottom reflects information gained (and uncertainty reduction) from data

Prior and posterior standard deviation of parameter field



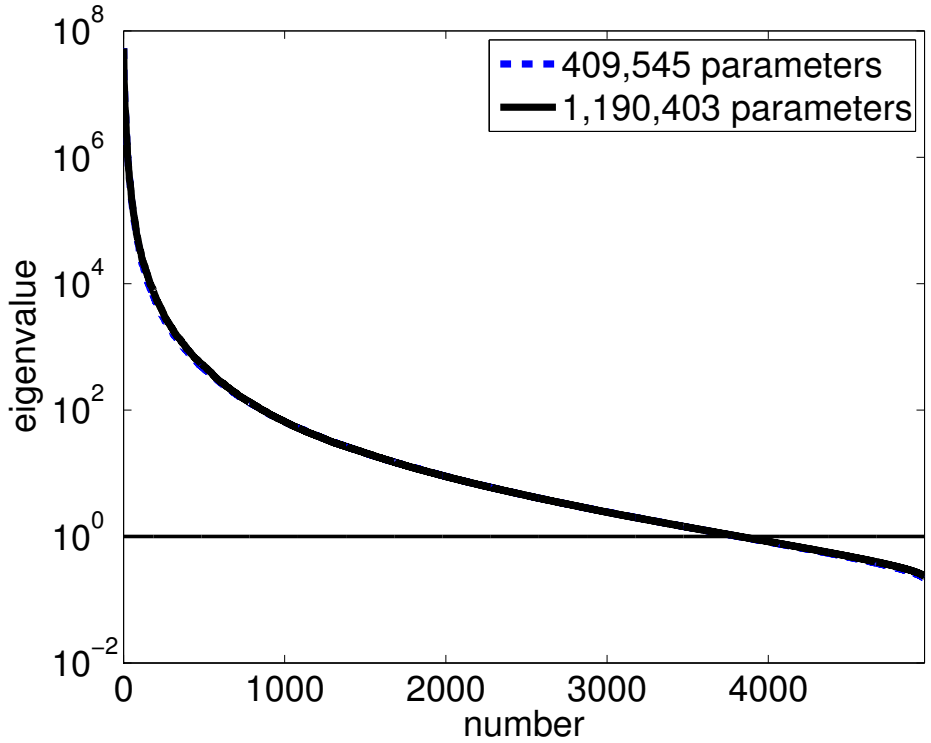
Prior standard deviation of log basal sliding parameter

Prior and posterior standard deviation of parameter field



Posterior standard deviation of log basal sliding parameter

Spectrum of data misfit operator



- Spectrum of data misfit Hessian for Antarctica inverse problem with 410K and 1.19M basal sliding parameters
- 4000 dominant modes, independent of parameter and data dimension
- Can be extracted at cost (measured in linearized model solves) that is independent of parameter dimensions
- Intrinsic problem dimension depends only on information content of data
- Still requires $O(4000)$ linearized ice sheet model solves

Prospects for adjoint-based gradients and Hessians

Theoretical cost:

- Adjoint operator is "transpose of Jacobian" of forward operator
- One (linear) adjoint solve per gradient or Hessian-vector evaluation
- Number of Hessian-vector multiplies depends on "information" dimension, not parameter or data dimensions

For legacy codes:

- Automatic/algorithmic differentiation: challenging for complex codes (multiphysics, message-passing, non-smoothness); expensive
- Partial refactoring + local application of AD may be best option

For new codes:

- Straightforwardly done at continuous level
- Must be careful when continuous and discrete adjoints do not coincide (e.g., non-Galerkin or DG discretizations, AMR and other adaptive numerics)
- Regularize nonsmooth model features (plasticity, contact, bounds, shocks...)

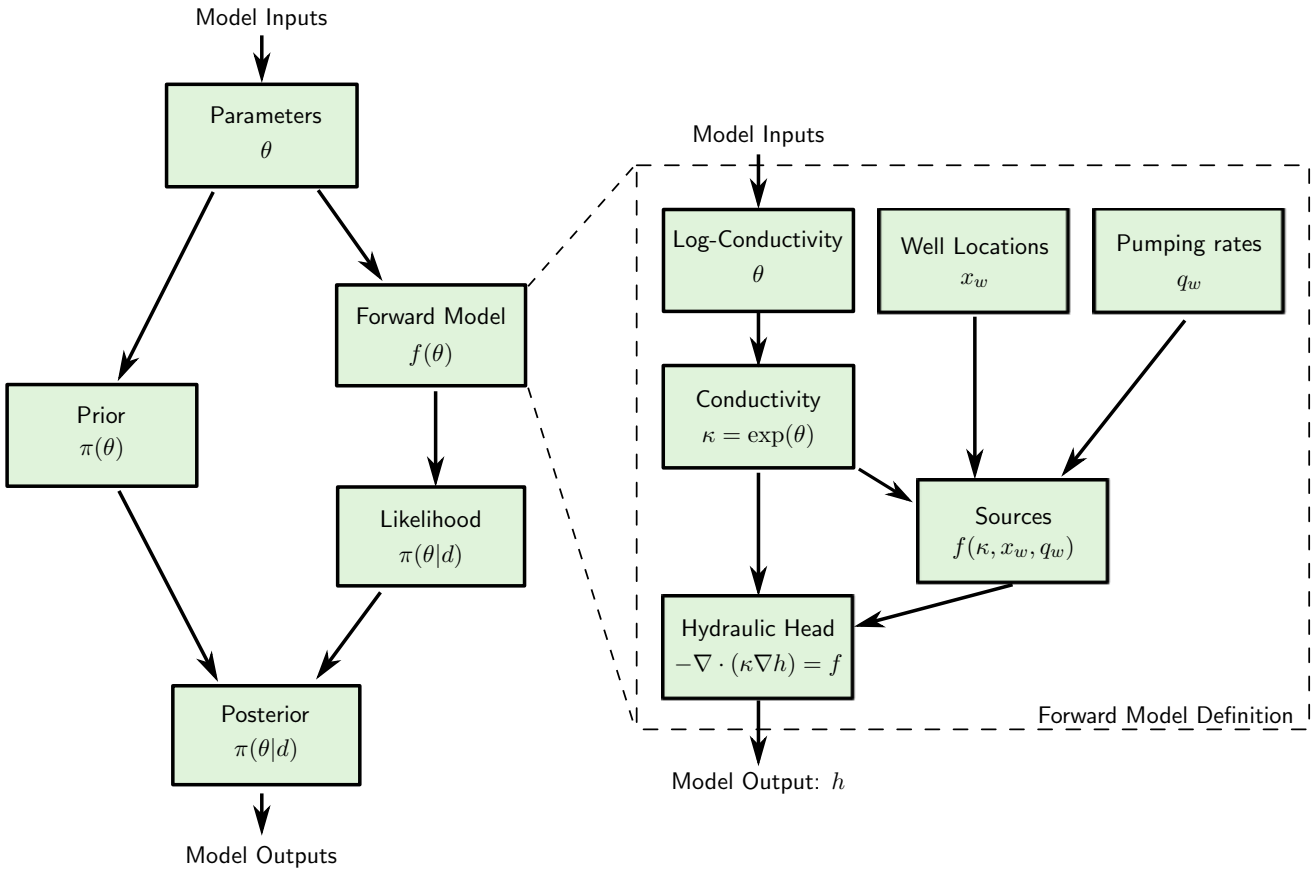
Advertisement: hIPPYlib and MUQ

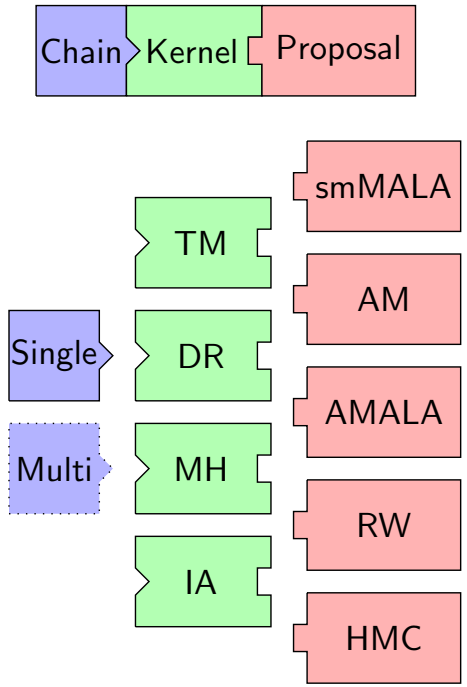
- hIPPYlib (Umberto Villa (UT) and Noemi Petra (UC Merced))
  - Implements state-of-the-art scalable adjoint-based algorithms for PDE-based deterministic and linearized Bayesian inverse problems
  - Builds on FEniCS for PDE discretization and PETSc for linear algebra and iterative solvers
  - Forthcoming release at `http://hippylib.github.io`
- MUQ: MIT Uncertainty Quantification library (Matt Parno, Andrew Davis, Youssef Marzouk (MIT))
  - Implements state-of-the-art Markov chain Monte Carlo samplers for nonlinear Bayesian inverse problems
  - Employs graphical modeling to allow experimentation with different modeling components and MCMC proposals and transition kernels
  - Available at `muq.mit.edu`
- hIPPYlib and MUQ will be integrated under a new NSF SI2–SSI grant

More on hIPPYlib

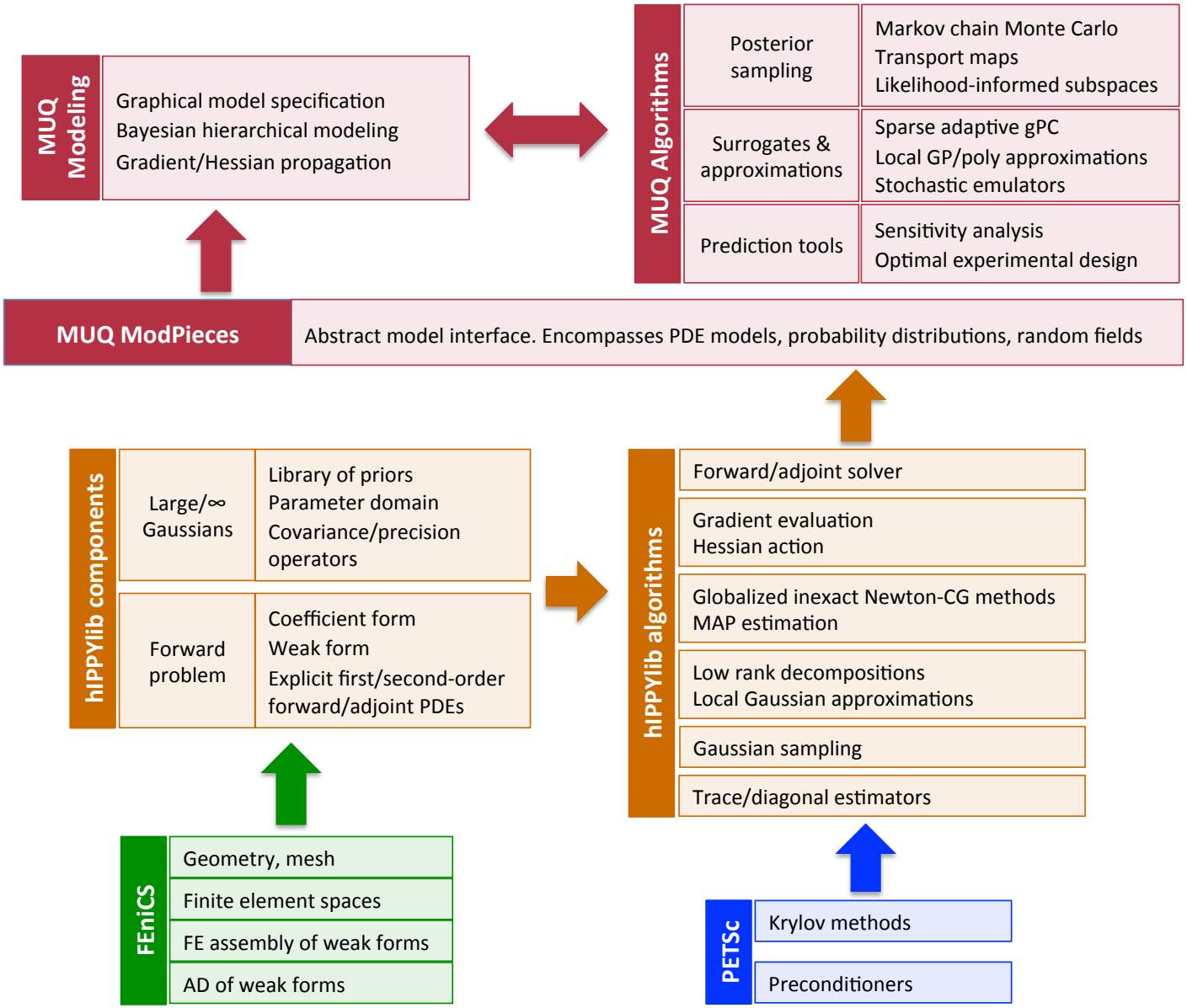
- Friendly, compact, near-mathematical FEniCS notation to express the PDE and likelihood in weak form
- Automatic generation of efficient code for the discretization of weak forms using FEniCS
- Symbolic differentiation of weak forms to generate derivatives and adjoint information
- Globalized inexact Newton-CG method to solve the inverse problem
- Randomized SVD to extract low rank approximation of data misfit Hessian
- Low rank-based representation of the posterior covariance
- Sampling from the prior and from the Gaussian approximation of the posterior
- Extract pointwise variance of prior and posterior
- Details in: U. Villa, N. Petra, and O. Ghattas, *hIPPYlib: An extensible software framework for PDE-constrained deterministic and linearized Bayesian inverse problems*, manuscript.

MUQ


Model Inputs
Parameters
θ
Prior
$\pi(\theta)$
Forward Model
$f(\theta)$
Likelihood
$\pi(\theta|d)$
Posterior
$\pi(\theta|d)$
Model Outputs
Model Inputs
Log-Conductivity
θ
Well Locations
x_w
Pumping rates
q_w
Conductivity
$\kappa = \exp(\theta)$
Sources
$f(\kappa, x_w, q_w)$
Hydraulic Head
$-\nabla \cdot (\kappa \nabla h) = f$
Forward Model Definition
Model Output: h


Chain
Kernel
Proposal
Single
Multi
TM
DR
MH
IA
smMALA
AM
AMALA
RW
HMC

hIPPYlib (and Integration with MUQ)



Questions for panel and audience

- What are the scientific drivers for moving from forward to inverse modeling?
- What are the scientific drivers for moving from deterministic to probabilistic models?
- How should the mathematical/computational challenges be overcome?
- How can the software issues be addressed?
- What should CIG's role be in supporting tools for UQ/IP? What about training?