SAND2015-2494C

# From Deterministic Inversion to Uncertainty Quantification: Planning a Long Journey in Ice Sheet Modeling

M. Eledred, J. Jakeman, M. Perego, A. Salinger, I. K. Tezaur [SNL],

P. Heimbach, C. Jackson [UT Austin],

M. Hoffman, S. Price [LANL],

G. Stadler [Courant]

QUEST Workshop, Los Angeles, April 2, 2015

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**PISCEES**, funded by SciDAC Scientific Discovery through Advanced Computing

# Problem definition

**Quantity of Interest in ice sheet modeling:**

***total ice mass loss/gain by, e.g. 2200*** **→ sea level rise prediction**

**Main sources of uncertainty:**

- climate forcings (e.g. Surface Mass Balance)
- **basal friction**
- bedrock topography
- geothermal heat flux
- model parameters (e.g. Glen's Flow Law exponent)

# Problem definition

**Goal:** Uncertainty Quantification of QoI

**(Main) Issue**: Huge number of parameters ($10^5$-$10^7$)

Work flow:

- Perform adjoint-based deterministic inversion to estimate initial ice sheet state. (i.e. characterize the present state of ice sheet to be used for performing prediction runs).
- Use deterministic inversion to build a Gaussian posterior in the inverse problem (based on recovered fields and the Hessian).
- Bayesian Calibration: construct the posterior distribution using Markov Chain Monte Carlo run on an emulator of the forward model.
- Forward Propagation: sample the obtained distribution and perform ensemble of forward propagation runs to compute the uncertainty on the QoI.

# Deterministic Inversion

## GOAL

Find ice sheet initial state that

- matches observations (e.g. surface velocity, temperature, etc.)
- matches present-day geometry (elevation, thickness)
- is in "equilibrium" with climate forcings (SMB)

by inverting for unknown/uncertain ice sheet model parameters.

Significantly reduce non physical transients without spin-up.

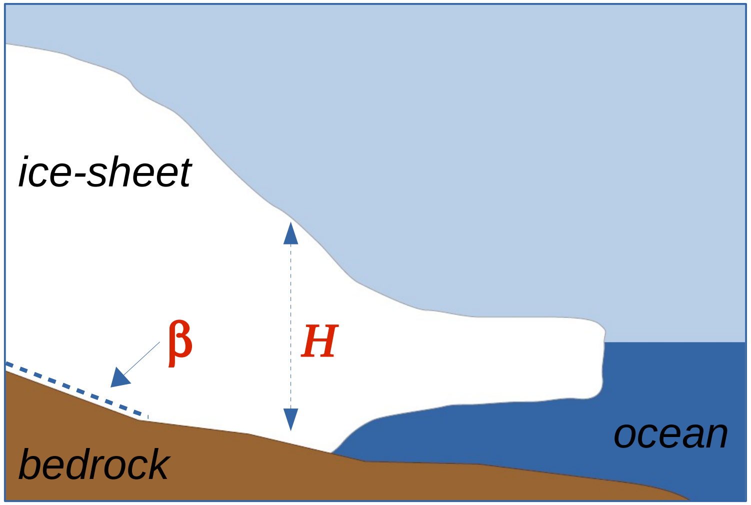
Bibliography


- *Arthern, Gudmundsson*, J. Glaciology, 2010
- *Price, Payne, Howat and Smith*, PNAS, 2011
- *Petra, Zhu, Stadler, Hughes, Ghattas*, J. Glaciology, 2012
- *Pollard DeConto*, TCD, 2012
- W. J. J.Van Pelt et al., The Cryosphere, 2013
- *Morlighem et al.* Geophysical Research Letters, 2013
- *Goldberg and Heimbach*, The Cryosphere, 2013
- *Michel et al.*, Computers & Geosciences, 2014

*Perego, Price, Stadler,* **Journal of Geophysical Research**, 2014

# Deterministic Inversion

## Problem details




**Available data/measurements**

- *ice extension and surface topography*
- ***surface velocity***
- ***Surface Mass Balance (SMB)***
- ***ice thickness H (sparse measurements)***

**Fields to be estimated**

- ***ice thickness H (allowed to vary but weighted by observational uncertainties)***
- ***basal friction β (spatially variable proxy for all basal processes)***

**Modeling Assumptions**

- *ice flow described by **nonlinear Stokes equation***
- *ice is close to **mechanical equilibrium***

**Additional Assumption (for now)**

- *given **temperature field***

*Perego, Price, Stadler,* **Journal of Geophysical Research**, 2014

Sandia National Laboratories

# Deterministic Inversion

PDE-constrained optimization problem: cost functional

**Problem**: find initial conditions such that the ice is close to thermo-mechanical equilibrium, given the geometry and the SMB, and matches available observations.

**Optimization problem**:

find $\beta$ and $H$ that minimizes the functional $\mathcal{J}$

$$\mathcal{J}(\beta, H) = \int_\Sigma \frac{1}{\sigma_u^2} |\mathbf{u} - \mathbf{u}^{obs}|^2 \, ds$$

surface velocity mismatch — *Common*

$$+ \int_\Sigma \frac{1}{\sigma_\tau^2} |\mathrm{div}(\boldsymbol{U} H) - \tau_s|^2 \, ds$$

SMB mismatch

$$+ \int_\Sigma \frac{1}{\sigma_H^2} |H - H^{obs}|^2 \, ds$$

thickness mismatch

(surface velocity, SMB and thickness mismatch together: *Proposed*)

$$+\mathcal{R}(\beta, H)$$

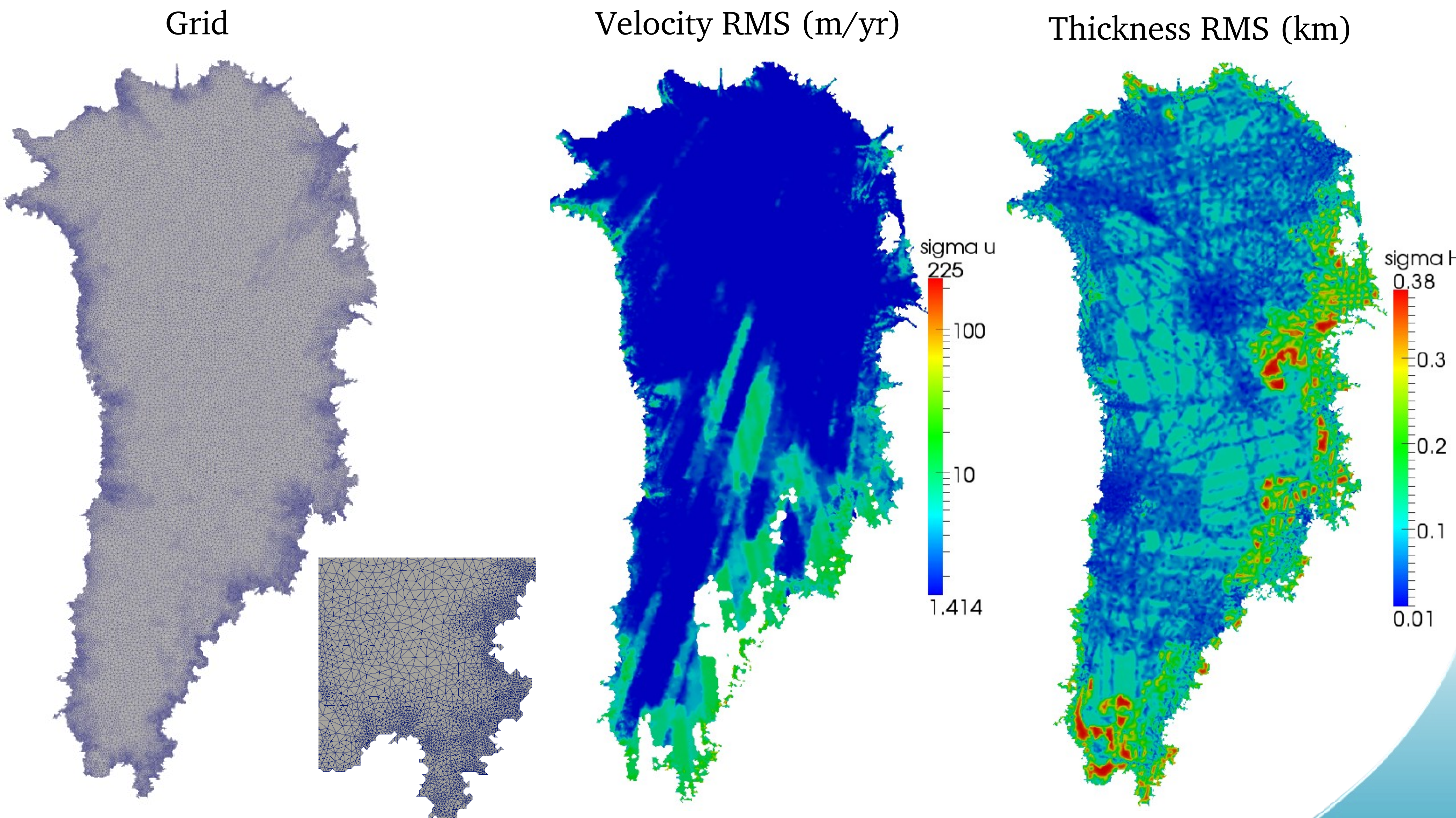
regularization terms.

subject to ice sheet model equations (FO or Stokes)

$\boldsymbol{U}$: computed depth averaged velocity
$H$: ice thickness
$\beta$: basal sliding friction coefficient
$\tau_s$: SMB
$\mathcal{R}(\beta)$ regularization term

# Deterministic Inversion for Greenland ice sheet

Grid and RMS of velocity and errors associated with velocity and thickness observations

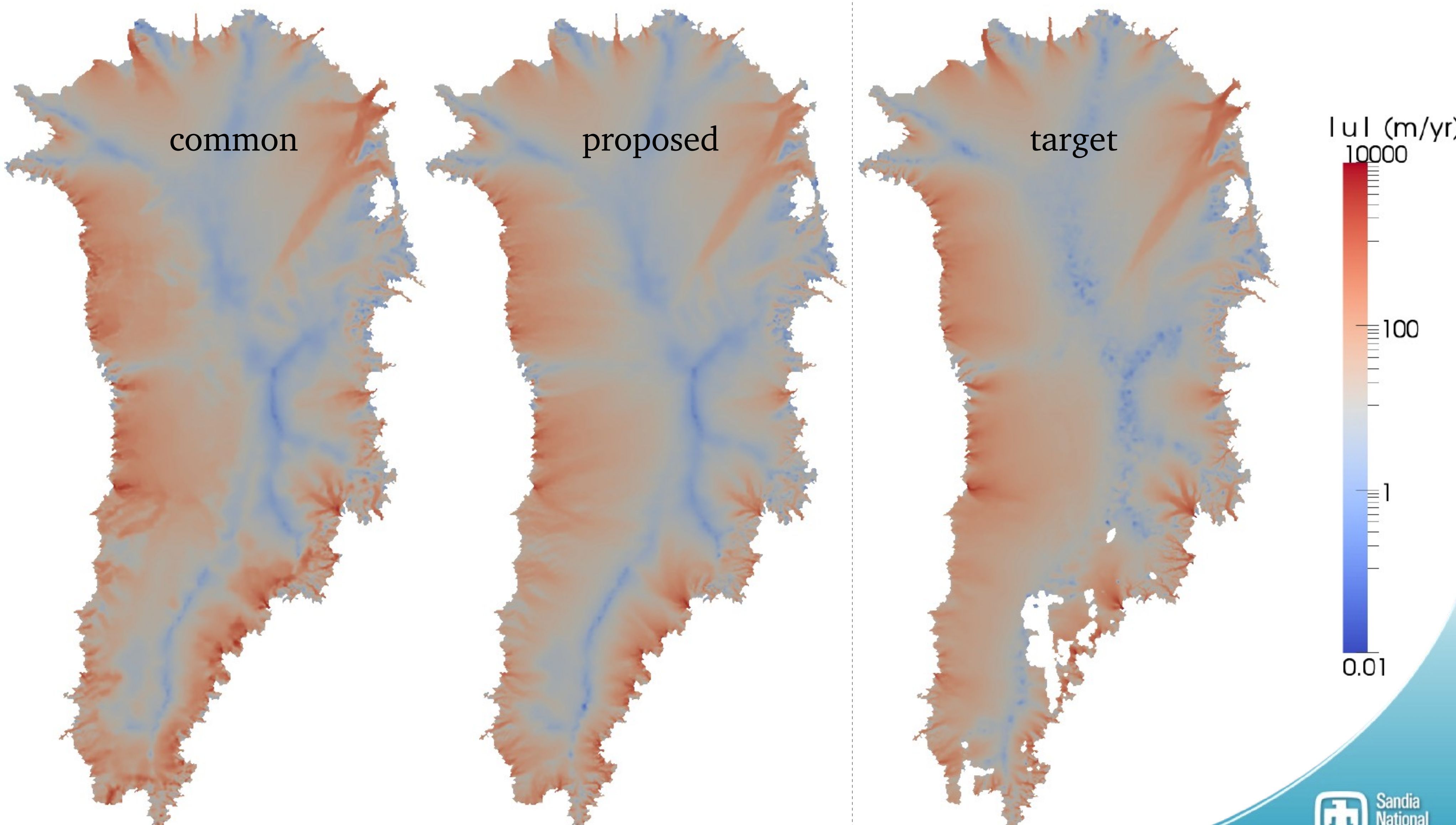



Geometry and fields Bamber et al.[2013], temperature computed with CISM (Shannon et al. [2013])

# Deterministic Inversion for Greenland ice sheet

## Inversion results: surface velocities

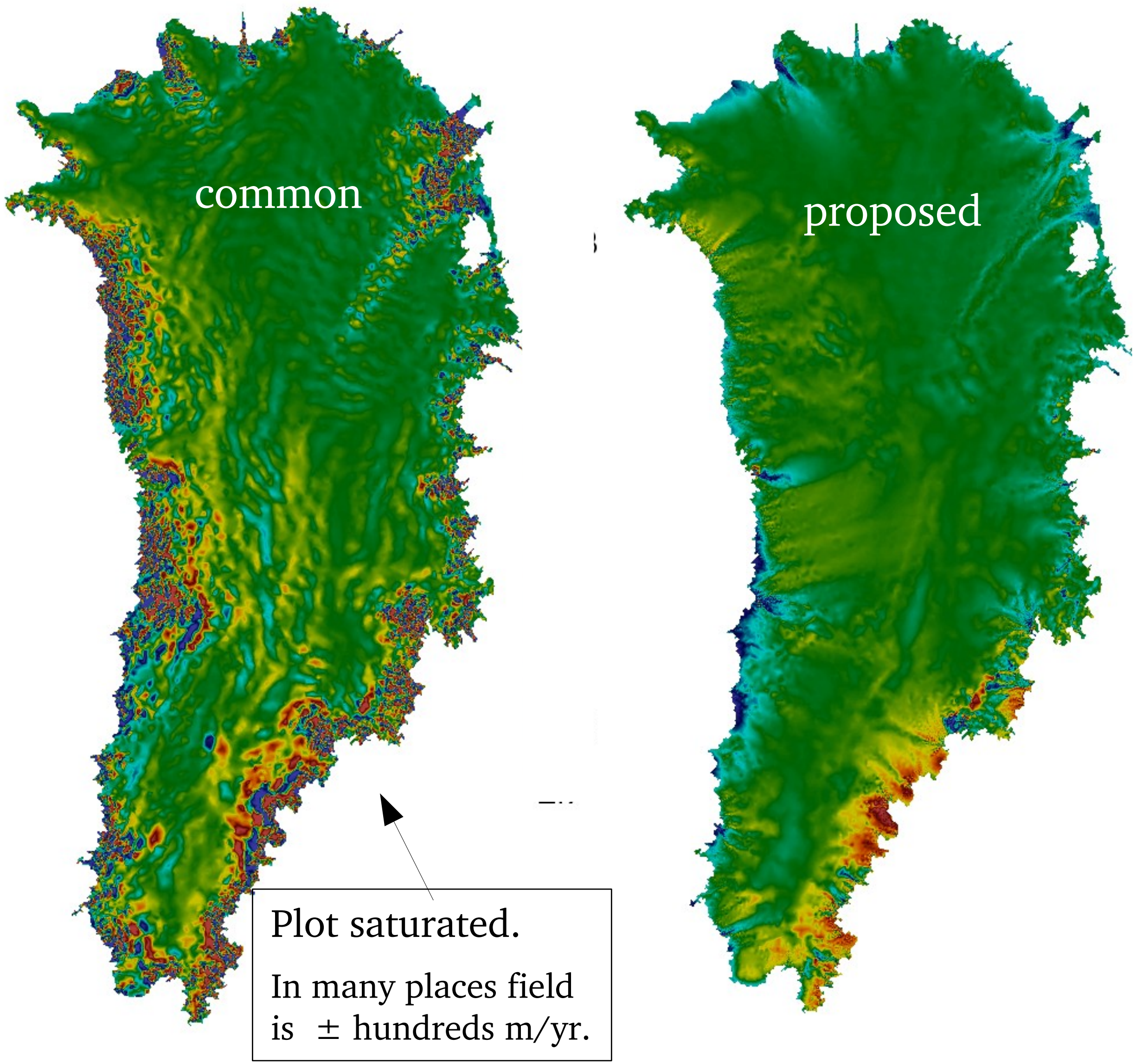
computed surface velocity | observed surface velocity



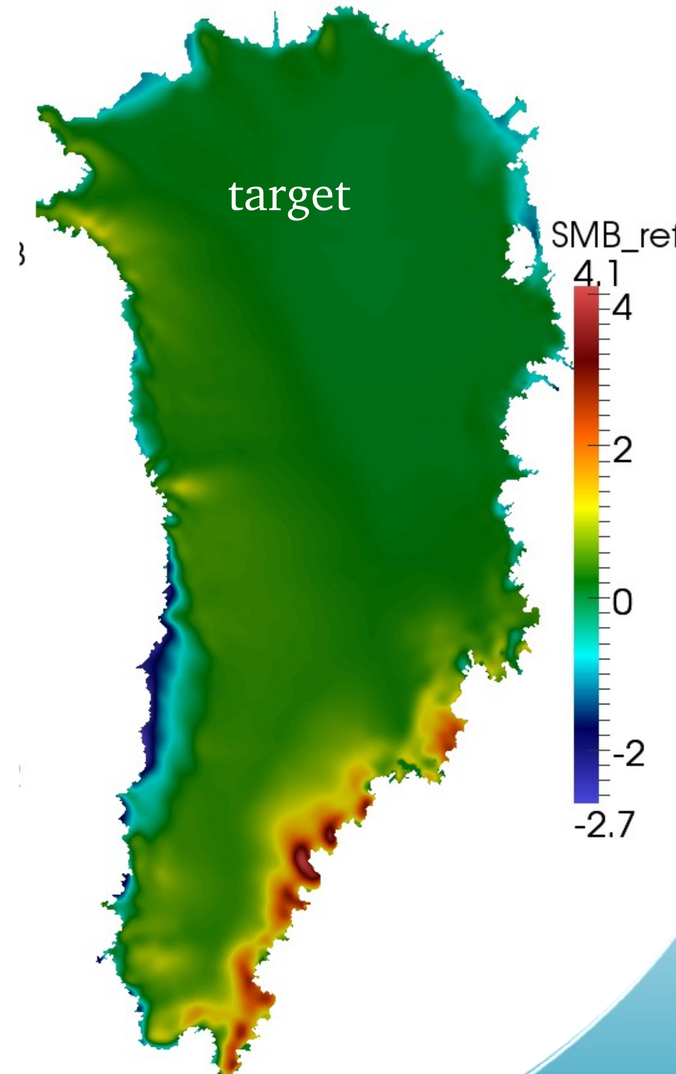
# Deterministic Inversion for Greenland ice sheet

## Inversion results: surface mass balance (SMB)

SMB (m/yr) needed for equilibrium



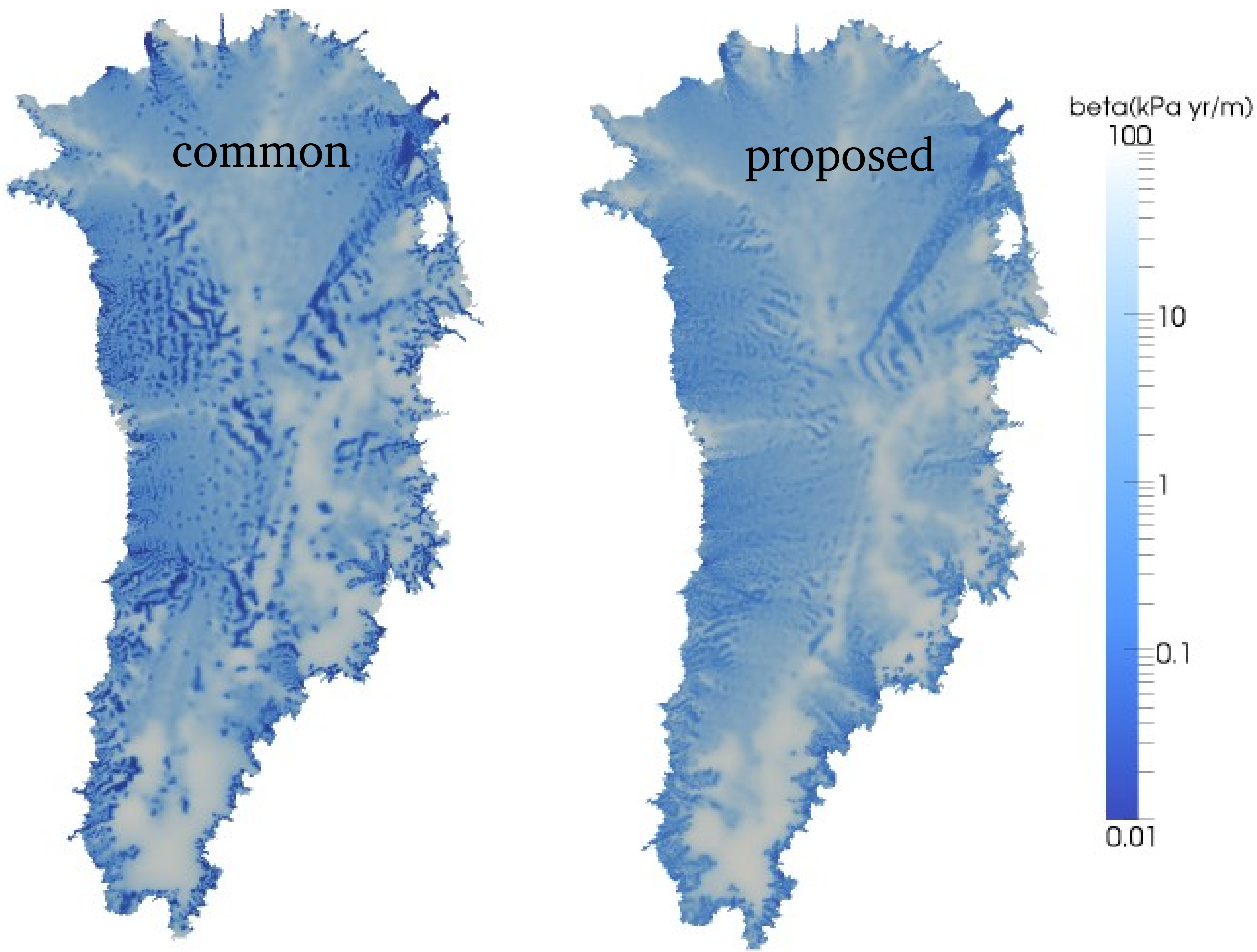

SMB from climate model
(Ettema et al. 2009, RACMO2/GR)



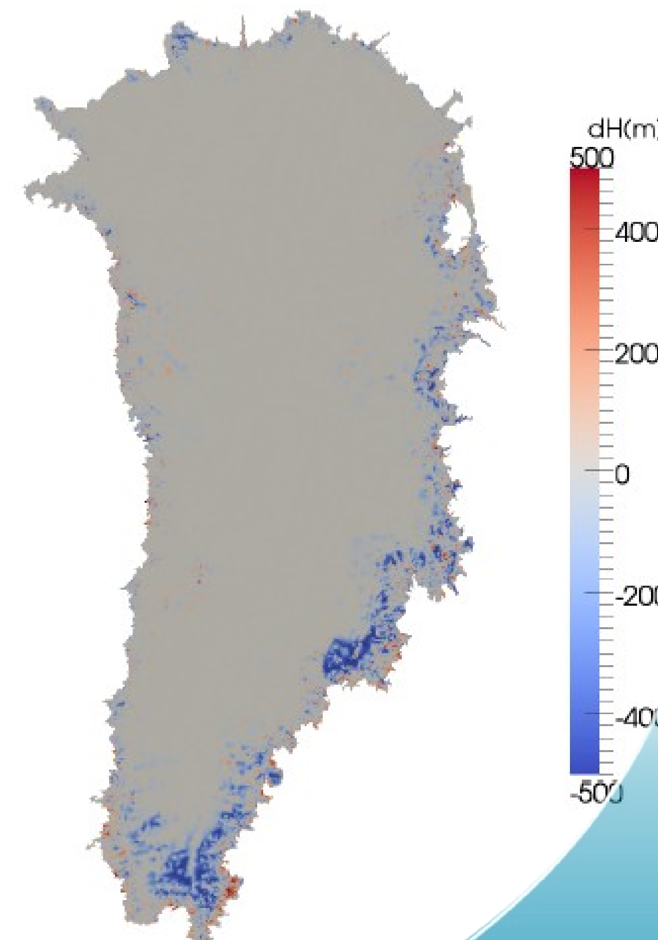
# Deterministic Inversion for Greenland ice sheet

## Estimated beta and change in topography

recovered basal friction




difference between recovered and observed thickness



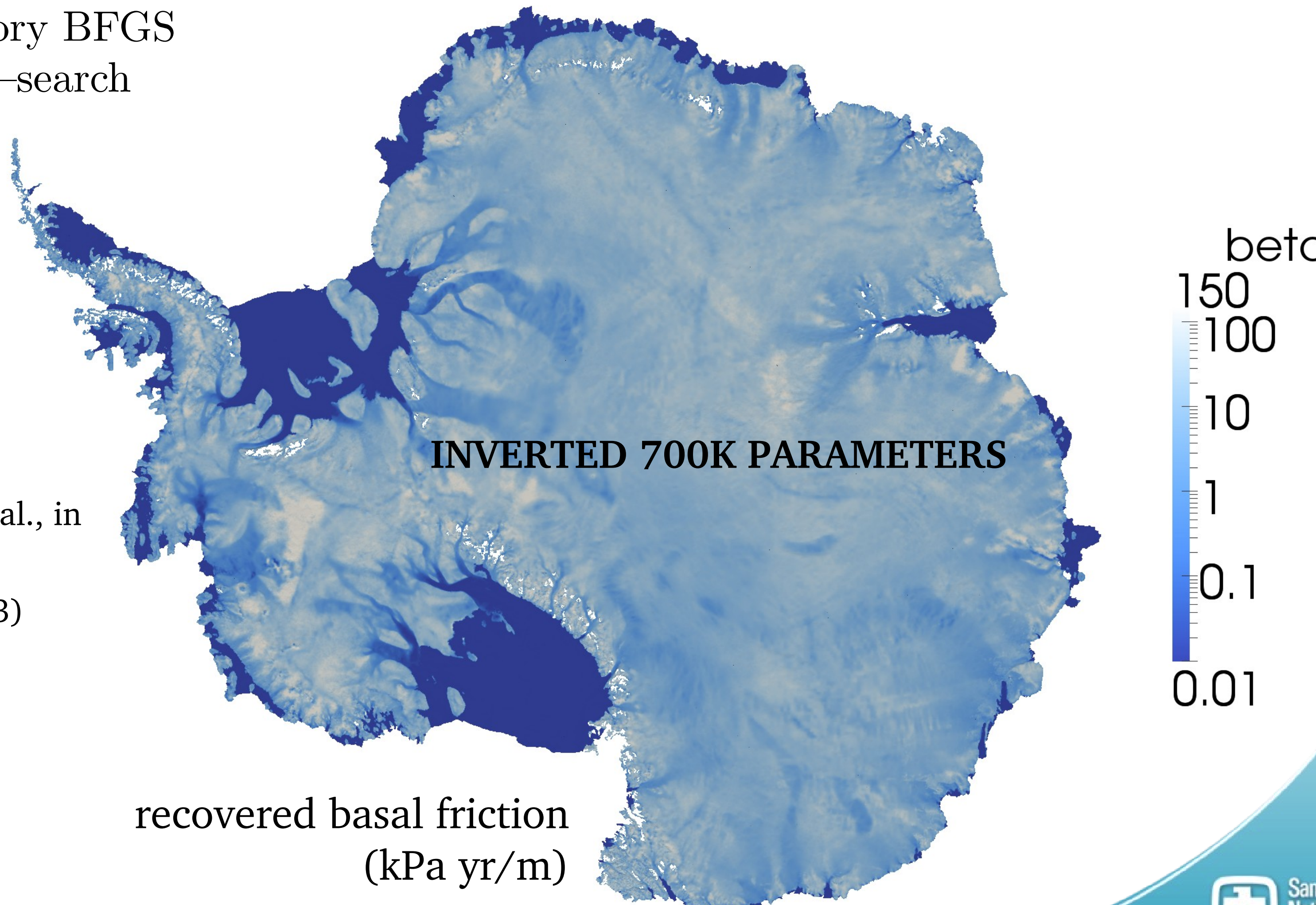

Sandia National Laboratories

# Antarctica Inversion (only for basal friction)

Objective functional: $\mathcal{J}(\mathbf{u}(\beta),\ \beta) = \int_\Sigma \frac{1}{\sigma_u^2} |\mathbf{u} - \mathbf{u}^{obs}|^2\, ds + \ \alpha \int_\Sigma |\nabla\beta|^2\, ds$

ROL algorithm:

- Limited–Memory BFGS
- Backtrack line–search




recovered basal friction (kPa yr/m)

Gometry (Cornford, Martin et al., in prep.)

Bedmap2 (Fretwell et al., 2013)

Temperature (Pattyn, 2010)

# Bayesian Calibration (proof of concept w/ KLE)

Difficulty in UQ approach: *"Curse of dimensionality"*.
At relevant model resolutions, the basal friction parameter space can have $O(10^6)$ parameters.
However, the effective dimension of the problem is smaller.

1. Assume analytic covariance kernel $\Gamma_{\text{prior}} = \exp\left(-\frac{|r_1 - r_2|^2}{L^2}\right)$. First attempt, we intend to use Hessian based covariance in the future.
2. Perform eigenvalue decomposition of $\Gamma_{\text{prior}}$.
3. Take the mean $\bar{\beta}$ to be the deterministic solution and expand $\beta$ in basis of eigenvector $\{\phi_k\}$ of $\Gamma_{\text{prior}}$, with random variables $\{\xi_k\}$

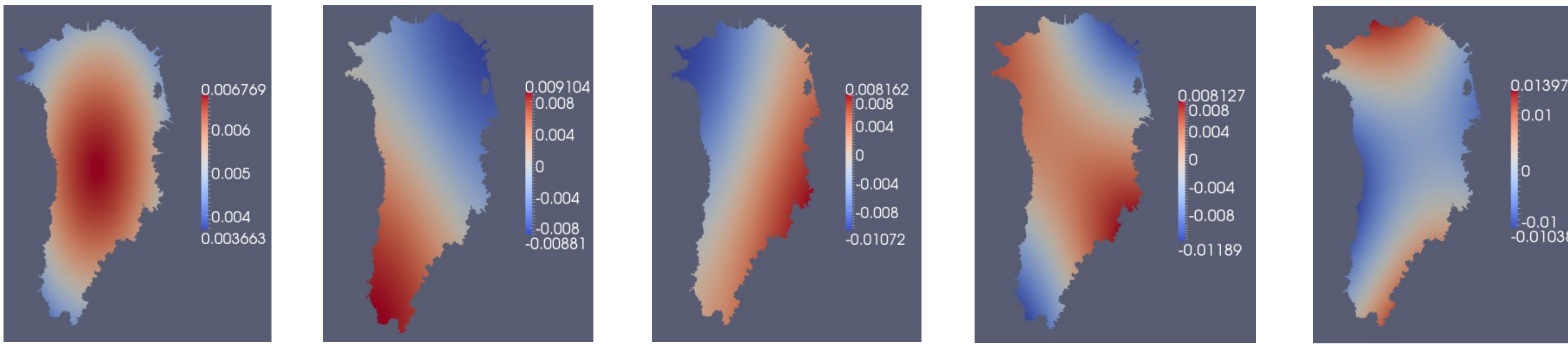
$$\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{\lambda_k}\phi_k \xi_k(\omega)$$

*Expansion done on $\log(\beta)$ to avoid negative values for $\beta$.

# Bayesian Calibration (proof of concept w/ KLE)

KLE modes, emulator build, inversion

- 5 KLE modes capture 95% of covariance energy – consequence of chosen covariance (parallel C++/Trilinos code **Anasazi**).




Only spatial correlation has been considered.

- Mismatch (**ALBANY**): $\mathcal{J}(\beta) = \int_{\Sigma} \frac{1}{\sigma_u^2} |\mathbf{u} - \mathbf{u}^{obs}|^2 \, ds$

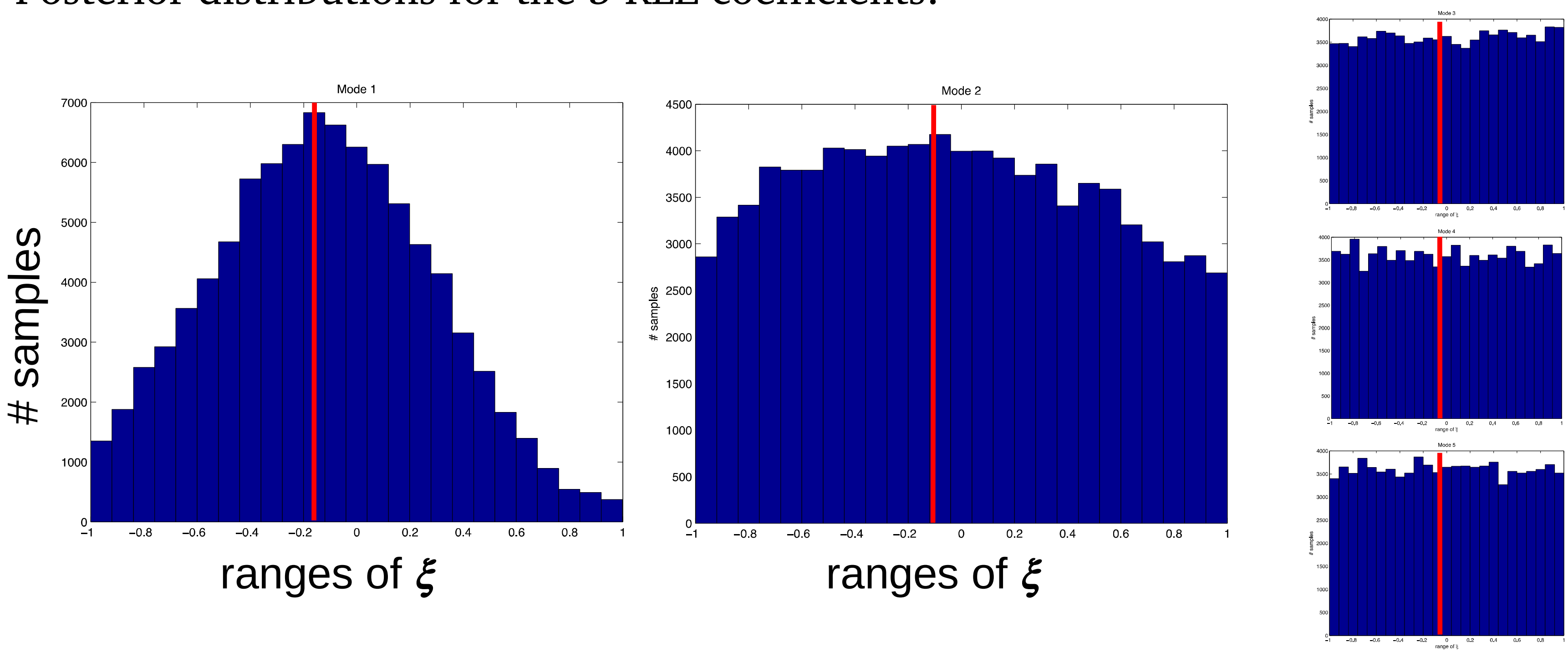
- ***Build Emulator.*** Polynomial chaos expansion (**PCE**) was formed for the mismatch over random variables using uniform prior distributions. **DAKOTA**.

- **Inversion/Calibration**. Markov Chain Monte Carlo (**MCMC**) was performed on the PCE with 100K samples **QUESO**.

# Bayesian Calibration (proof of concept w/ KLE)

## Numerical results

Posterior distributions for the 5 KLE coefficients:




*MAP solution:* $\xi = (-0.16, -0.08, 0, 0, 0)$

True $\beta$ field

Reconstructed $\beta$ field

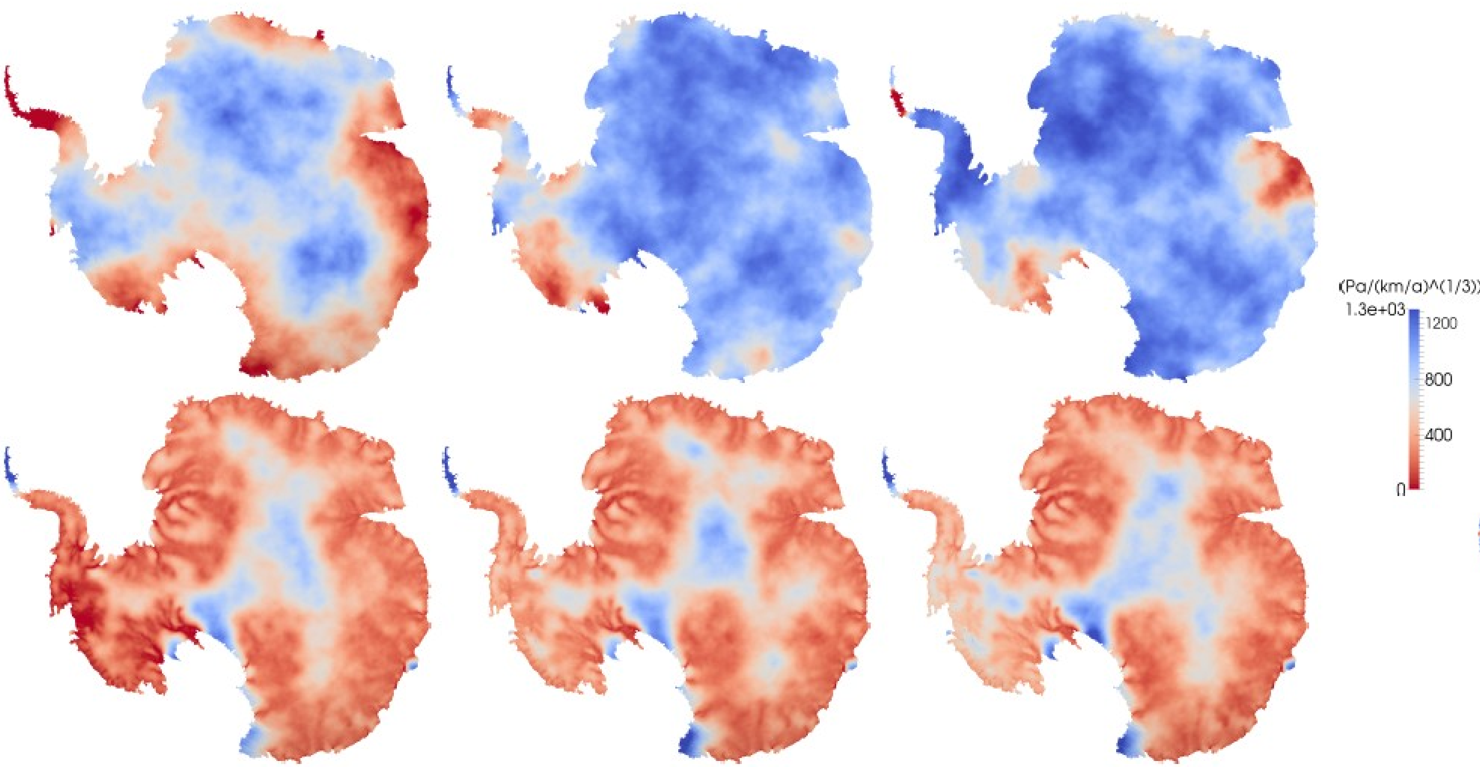
Sandia National Laboratories

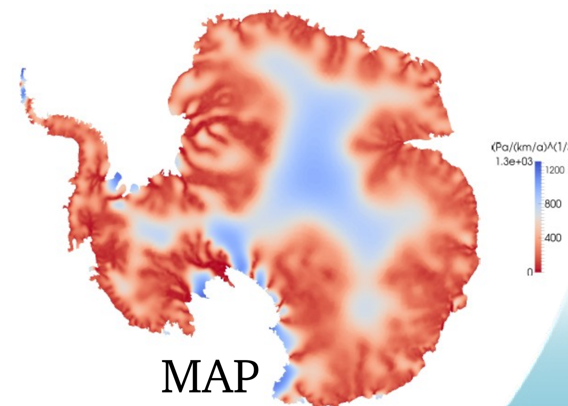
# Building the Gaussian posterior approximation using Hessian from deterministic inversion

Hessian provide a way to compute the Covariance of the Gaussian posterior.

$$\Gamma_{\text{post}} = \left(\Gamma_{\text{prior}} H_{\text{misfit}} + I\right)^{-1} \Gamma_{\text{prior}}$$

Courtesy of O. Ghattas group



MAP

Samples from the prior (top row) and Gaussianized posterior (bottom row) distributions for the basal sliding parameter field. ***Isaac et al. 2004***.

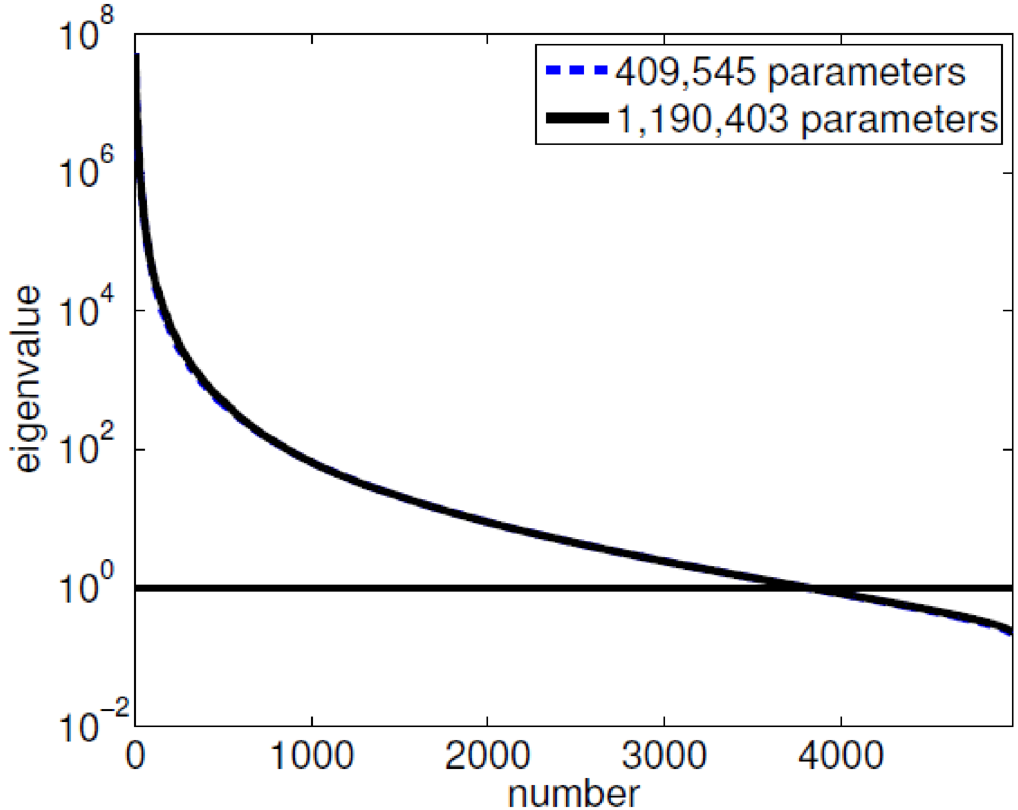
# Building the Gaussian posterior approximation using Hessian from deterministic inversion

Hessian provide a way to compute the Covariance of the Gaussian posterior.

$$\Gamma_{\text{post}} = \left(\Gamma_{\text{prior}} H_{\text{misfit}} + I\right)^{-1} \Gamma_{\text{prior}}$$

We want to limit to only the most important directions of the covariance matrix.

Issue: significant eigenvalues are **still too many (~ 1000)**.




Courtesy of O. Ghattas group

$$\text{Err}^{\text{post}} = \mathcal{O}\left(\sum_{i=r+1}^{n} \frac{\lambda_i^{\text{prior}}}{1+\lambda_i^{\text{prior}}}\right)$$

Log-linear plot of spectrum of prior-preconditioned data misfit Hessian for two successively finer parameter/state meshes of the inverse ice sheet problem. ***Isaac et al. 2004***.

# Perform Uncertainty Propagation using compressed sensing

**Build emulator**
(Polynomial Chaos Expansion, PCE)

**Dakota/Albany**

$$\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{\lambda_k} \phi_k \xi_k(\omega)$$

Model realizations → $\mathrm{QoI}(\beta)$
Forward propagation
(e.g. 2000-2100)

total ice
mass loss

- Parameter distribution can be either assumed to be Gaussian (based on Hessian information) or can be the result of the Bayesian calibration.
- The emulator is built using Dakota coupled with Albany for forward runs.

  - use **compressed sensing technique*** to adaptively select significant modes and the basis for the parameter space. The hope is that only few modes affect the QoI.
  - possibly use cheap physical models to reduce the time of computing the forward model.
- Use MCMC to perform Uncertainty propagation.

*Jakeman, Eldred, Sargsyan, JCP, 2015

Albany DAKOTA QUEST Trilinos Sandia National Laboratories

Thank you!