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Computational Challenges in Ice Sheet Modeling

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joint collaboration with
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Center for Computing Research

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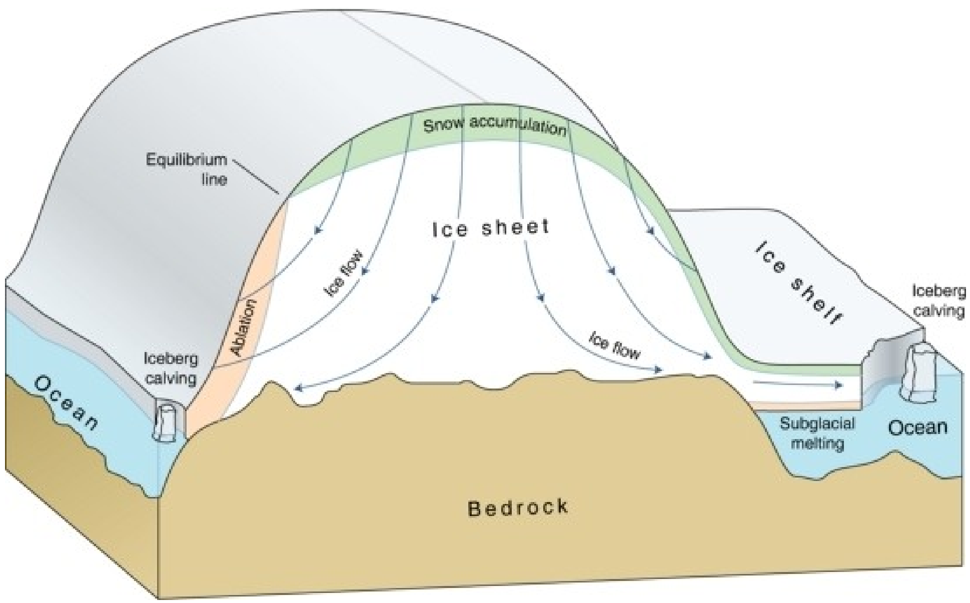
Brief introduction and motivation

- Modeling ice sheets (Greenland and Antarctica) dynamics is essential to provide estimates for sea level rise in next decades to centuries.
- Ice behaves like a very viscous shear-thinning fluid (similar to lava flow) and can be modeled with nonlinear Stokes equation.



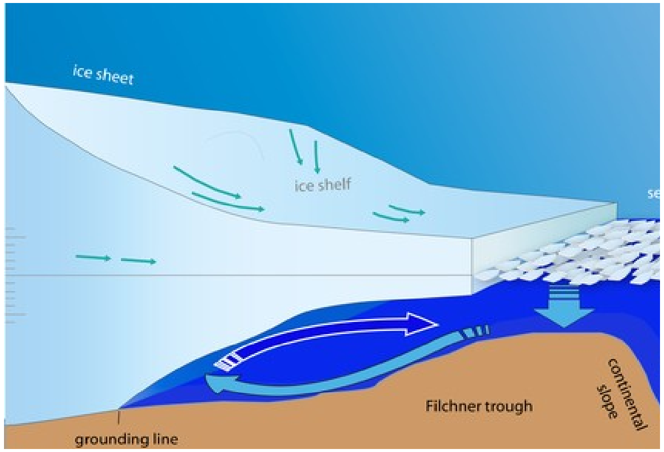
from http://www.climate.be

Brief motivation and introduction

- Modeling ice sheets (Greenland and Antarctica) dynamics is essential to provide estimates for sea level rise in next decades to centuries.
- Ice behaves like a very viscous shear-thinning fluid (similar to lava flow) and can be modeled with nonlinear Stokes equation.
- Greenland and Antarctica ice sheets have a shallow geometry (thickness up to 3km, horizontal extensions of thousands of km).
- Several ice sheet models are derived relying on the fact that the domain is shallow and they handle differently horizontal coordinates (x-y) and vertical coordinate z. However, ice sheets lie on earth surface and are not planar.
- Here we investigate the effect of assuming planar geometry in approximate models.

(Numerical) Modeling Issues

- Computationally challenging, due to complexity of models, of geometries and large domains
  - design of linear/nonlinear solvers, preconditioners, etc.
  - mesh adaptivity especially close to the grounding line
  - modeling of ice advance/retreat



- Boundary conditions / coupling (e.g. with ocean)
  - Floating/calving
  - Basal friction at the bedrock,
  - Subglacial hydrology,
  - Heat exchange / phase change

- Initialization / parameter estimation

- Uncertainty quantification

Problem definition

Our Quantity of Interest (QoI) in ice sheet modeling:

total ice mass loss/gain by, e.g., 2100 **→** **sea level rise prediction**

Main sources of uncertainty:

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

Problem definition

Ultimate goal:
quantify the QoI and related uncertainties

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 characterize the parameter distribution (i.e, use the inverted field as mean field of the parameter distribution and approximate its covariance using sensitivities/Hessian).
- Perform *Bayesian Calibration*: construct the posterior distribution using Markov Chain Monte Carlo runs on an emulator of the forward model.
- Perform *Forward Propagation*: sample the obtained distribution and perform ensemble of forward propagation runs to compute the uncertainty on the QoI.

Ice Sheet Modeling

Main components of an ice model:

- Ice flow equations (momentum and mass balance)

$$\begin{cases} \rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) - \nabla\cdot\sigma = \rho\mathbf{g} \\ \nabla\cdot\mathbf{u} = 0 \end{cases}$$

Ice Sheet Modeling

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Ice Sheet Modeling

Main components of an ice model:

- **Ice flow equations** (momentum and mass balance)

$$\begin{cases} -\nabla \cdot \sigma = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

with:

$$\sigma = 2\mu \mathbf{D} - \Phi I, \qquad \mathbf{D}_{ij}(\mathbf{u}) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

nonlinear viscosity:

$$\mu = \frac{1}{2}\alpha(T)\,|\mathbf{D}(\mathbf{u})|^{(p-2)}, \quad p \in (1,2] \quad (\text{tipically } p \simeq \frac{4}{3})$$

viscosity is singular when ice is not deforming

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Ice Sheet Modeling

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$$\begin{cases} -\nabla \cdot \sigma = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

Ice Sheet Modeling

Main components of an ice model:

- **Ice flow equations** (momentum and mass balance)

$$\begin{cases} -\nabla \cdot \sigma = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

- **Model for the evolution of the boundaries** (thickness evolution equation)

$$\frac{\partial H}{\partial t} = H_{flux} - \nabla \cdot \int_z \mathbf{u}\, dz$$

- **Temperature equation**

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z}\right) - \rho c \mathbf{u} \cdot \nabla T + 2\dot{\varepsilon}\sigma$$

- **Coupling with other climate components (e.g. ocean, atmosphere)**

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Stokes Approximations

"Reference" model: **STOKES**[1]

$O(\delta^2)$ ***FO,*** Blatter-Pattyn first order model[2] (3D PDE, in horizontal velocities)

$O(\delta)$ Zeroth order, depth integrated models:
SIA, Shallow Ice Approximation (slow sliding regimes) ,
SSA Shallow Shelf Approximation (2D PDE) (fast sliding regimes)

$\simeq O(\delta^2)$ Higher order, depth integrated (2D) models: ***L1L2***[3], (L1L1)...

$\delta :=$ ratio between ice thickness and ice horizontal extension

[1]Gagliardini and Zwinger, 2008. The Cryosphere.

[2]Dukowicz, Price and Lipscomb, 2010. J. Glaciol.

[3]Schoof and Hindmarsh, 2010. Q. J. Mech. Appl. Math.

Stokes approximations in different regimes

$\text{Stokes}(\mathbf{u}, p)$

$$\begin{cases} -\nabla \cdot (2\mu \mathbf{D}(\mathbf{u}) - p\mathbf{I}) = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

$\text{FO}(u, v)$

First Order* or
Blatter-Pattyn model

$$-\nabla \cdot \left(2\mu \tilde{\mathbf{D}} - \rho g (s - z)\mathbf{I}\right) = \mathbf{0}$$

**Dukowicz, Price and Lipscomb, 2010. J. Glaciol*

Stokes approximations in different regimes

$$\text{Stokes}(\mathbf{u}, p)$$

$$\begin{cases} -\nabla \cdot (2\mu \mathbf{D}(\mathbf{u}) - p\mathbf{I}) = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

Drop terms using **scaling argument** based on the fact that ice sheets are shallow

$$\mathbf{D}(\mathbf{u}) = \begin{bmatrix} u_x & \frac{1}{2}(u_y + v_x) & \frac{1}{2}(u_z + \cancel{w_x}) \\ \frac{1}{2}(u_y + v_x) & v_y & \frac{1}{2}(v_z + \cancel{w_y}) \\ \frac{1}{2}(u_z + \cancel{w_x}) & \frac{1}{2}(v_z + \cancel{w_y}) & w_z \end{bmatrix} \qquad \text{u} := \begin{bmatrix} u \\ v \\ w \end{bmatrix}$$

$$\mu = \mu(|\mathbf{D}(\mathbf{u})|)$$

$$\text{FO}(u, v)$$

First Order* or Blatter-Pattyn model

Dukowicz, Price and Lipscomb, 2010. J. Glaciol

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$$\mu = \mu(|\mathbf{D}(\mathbf{u})|)$$

Quasi-hydrostatic approximation

3rd momentum equation

$$-\cancel{\partial_x(\mu u_z)} - \cancel{\partial_y(\mu v_z)} - \partial_z(2\mu w_z - p) = -\rho g,$$

continuity equation

$$w_z = -(u_x + v_y)$$

$$\Longrightarrow p = \rho g(s - z) - 2\mu(u_x + v_y)$$

$\text{FO}(u, v)$

First Order* or Blatter-Pattyn model

*Dukowicz, Price and Lipscomb, 2010. J. Glaciol

Stokes approximations in different regimes

$$\text{Stokes}(\mathbf{u}, p)$$

$$\begin{cases} -\nabla \cdot (2\mu \mathbf{D}(\mathbf{u}) - p\mathbf{I}) = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

Drop terms using **scaling argument** based on the fact that ice sheets are shallow

$$\mathbf{D}(u,v) = \begin{bmatrix} u_x & \frac{1}{2}(u_y + v_x) & \frac{1}{2}(u_z + \cancel{w_x}) \\ \frac{1}{2}(u_y + v_x) & v_y & \frac{1}{2}(v_z + \cancel{w_y}) \\ \frac{1}{2}(u_z + \cancel{w_x}) & \frac{1}{2}(v_z + \cancel{w_y}) & -(u_x + v_y) \end{bmatrix} \qquad \mathrm{u} := \begin{bmatrix} u \\ v \\ w \end{bmatrix}$$

$$\mu = \mu(|\mathbf{D}(u,v)|)$$

Quasi-hydrostatic approximation

3rd momentum equation

$$-\cancel{\partial_x(\mu u_z)} - \cancel{\partial_y(\mu v_z)} - \partial_z(2\mu w_z - p) = -\rho g,$$

continuity equation

$$w_z = -(u_x + v_y)$$

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$$\text{FO}(u, v)$$

First Order* or Blatter-Pattyn model

$$-\nabla \cdot \left(2\mu \tilde{\mathbf{D}} - \rho g(s - z)\mathbf{I}\right) = \mathbf{0}$$

$$\text{with } \tilde{\mathbf{D}}(u,v) = \begin{bmatrix} 2u_x + v_y & \frac{1}{2}(u_y + v_x) & \frac{1}{2}u_z \\ \frac{1}{2}(u_y + v_x) & u_x + 2v_y & \frac{1}{2}v_z \end{bmatrix}$$

**Dukowicz, Price and Lipscomb, 2010. J. Glaciol*

Estimation of ice sheet initial state

Steady state equations and basal sliding conditions

How to prescribe ice sheet mechanical equilibrium:

flux divergence

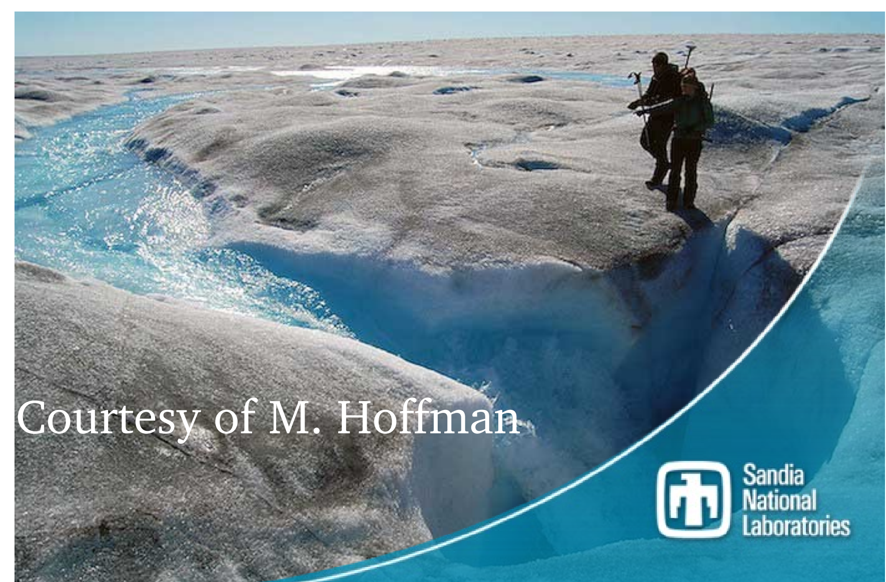
$$\frac{\partial H}{\partial t} = -\mathrm{div}\,(\mathbf{U}H) + \tau_{\mathrm{smb}}, \qquad \mathbf{U} = \frac{1}{H}\int_z \mathbf{u}\,dz.$$

Surface Mass Balance

$$\boxed{\mathrm{div}\,(\mathbf{U}H) - \tau_{\mathrm{smb}} + \left\{\frac{\partial H}{\partial t}\right\}^{\mathrm{obs}} = 0}$$

Boundary condition at ice-bedrock interface :

$$(\sigma \mathbf{n} + \beta \mathbf{u})_{||} = \mathbf{0} \quad \text{on} \quad \Gamma_\beta$$



Deterministic Inversion

GOAL

1. 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.

2. 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

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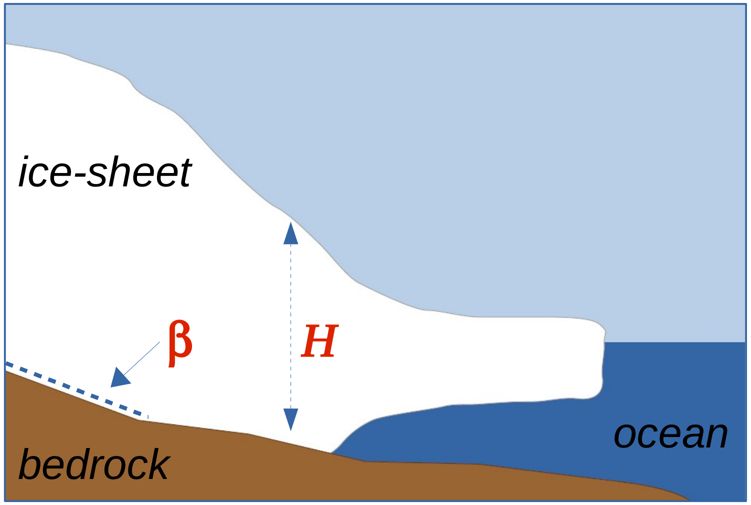
Deterministic Inversion

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 close to* ***mechanical equilibrium***

Additional Assumption (for now)

- *given* ***temperature field***

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

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 β and H that minimize the functional $\mathcal{J}$

$$\begin{aligned} \mathcal{J}(\beta, H) &= \int_\Sigma \frac{1}{\sigma_u^2} |\mathbf{u} - \mathbf{u}^{obs}|^2 \, ds && \text{surface velocity mismatch} \\ &+ \int_\Sigma \frac{1}{\sigma_\tau^2} |\mathrm{div}(\boldsymbol{U} H) - \tau_s|^2 \, ds && \text{SMB mismatch} \\ &+ \int_\Sigma \frac{1}{\sigma_H^2} |H - H^{obs}|^2 \, ds && \text{thickness mismatch} \\ &+ \mathcal{R}(\beta, H) && \text{regularization terms.} \end{aligned}$$

subject to ice sheet model equations (FO or Stokes)

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

Inverse Problem

Estimation of ice-sheet initial state

PDE-constraint optimization problem: gradient computation

$$\text{Find } (\beta, H) \text{ that minimize } \quad \mathcal{J}(\beta, H, \mathbf{u})$$
$$\text{subject to } \quad \mathcal{F}(\mathbf{u}, \beta, H) = 0 \quad \leftarrow \quad \text{flow model}$$

How to compute **total derivatives** of the functional w.r.t. the parameters?

Solve State System $\quad \mathcal{F}(\mathbf{u}, \beta, H) = 0$

Solve Adjoint System $\quad \langle \mathcal{F}^*_{\mathbf{u}}(\boldsymbol{\lambda}), \boldsymbol{\delta}_{\mathbf{u}} \rangle = \mathcal{J}_{\mathbf{u}}(\boldsymbol{\delta}), \quad \forall \boldsymbol{\delta}_{\mathbf{u}}$

Total derivatives $\quad \mathcal{G}(\delta_\beta, \delta_H) = \mathcal{J}_{(\beta,H)}(\delta_\beta, \delta_H) - \langle \boldsymbol{\lambda}, \mathcal{F}_{(\beta,H)}(\delta_\beta, \delta_H) \rangle$

Derivative w.r.t. β $\quad \mathcal{G}_1(\delta_\beta) = \alpha_\beta \int_\Sigma \nabla\beta \cdot \nabla\delta_\beta \, ds - \int_\Sigma \delta_\beta \, \mathbf{u} \cdot \boldsymbol{\lambda} \, ds$

Estimation of ice sheet initial state

Algorithm and Software tools used

ALGORITHM	SOFTWARE TOOLS
Linear Finite Elements on hexahedra	Albany
Quasi-Newton optimization (L-BFGS)	ROL
Nonlinear solver (Newton method)	NOX
Krylov linear solvers/Prec	AztecOO/ML

Albany: C++ finite element library built on Trilinos to enable multiple capabilities:

- Jacobian/adjoints assembled using automatic differentiation (SACADO).
- nonlinear and parameter continuation solvers (NOX/LOCA)
- large scale PDE constrained optimization (Piro/ROL)
- Uncertainty Quantification (using Dakota)
- linear solver and preconditioners (Belos/AztecOO, ML/MeuLu/Ifpack)

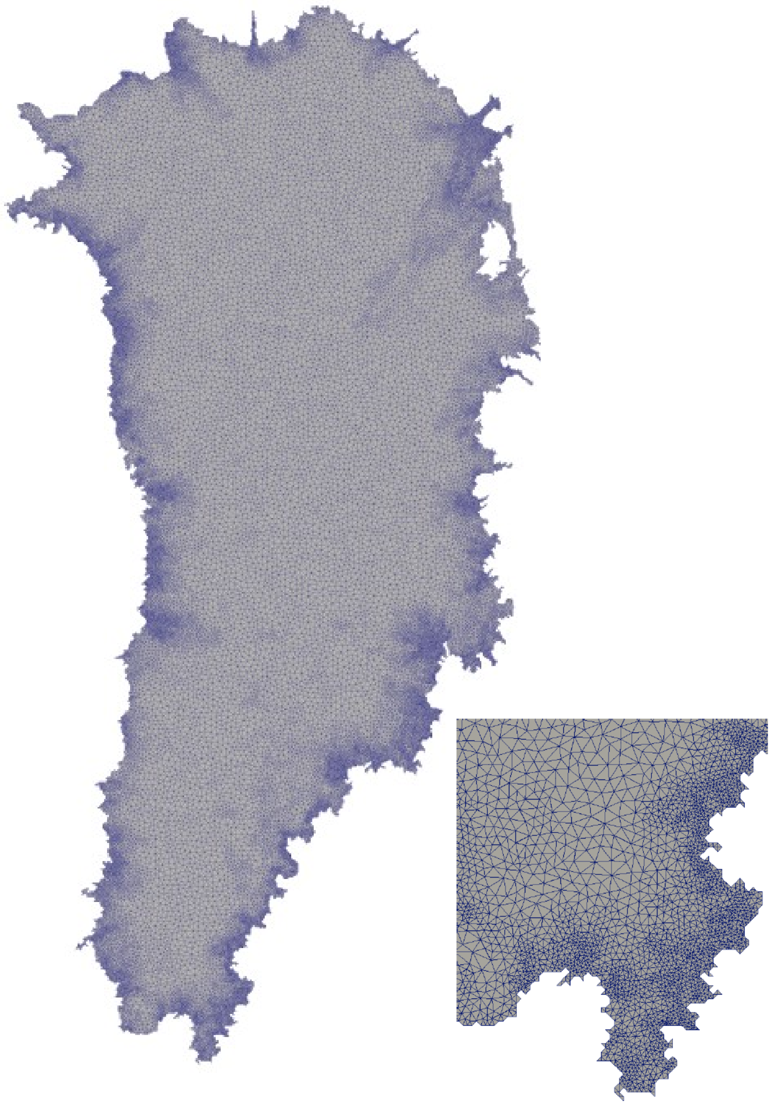
Optimization algorithm:

Reduce Gradient optimization, using L-BFGS.
Storage: 200, Linesearch: backtrack

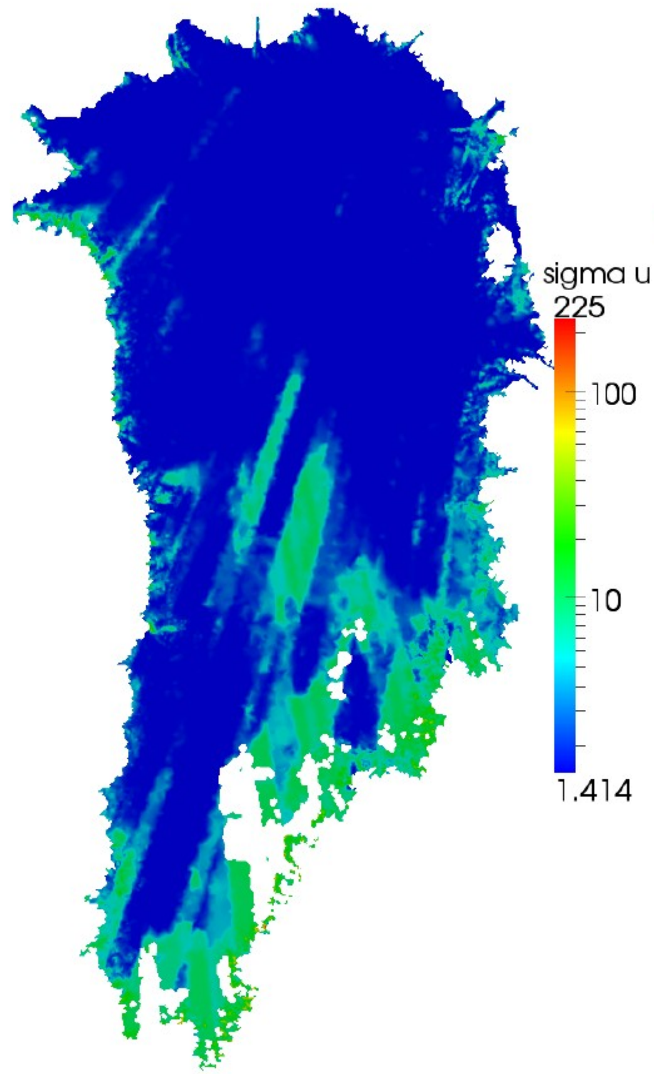
Deterministic Inversion for Greenland ice sheet

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

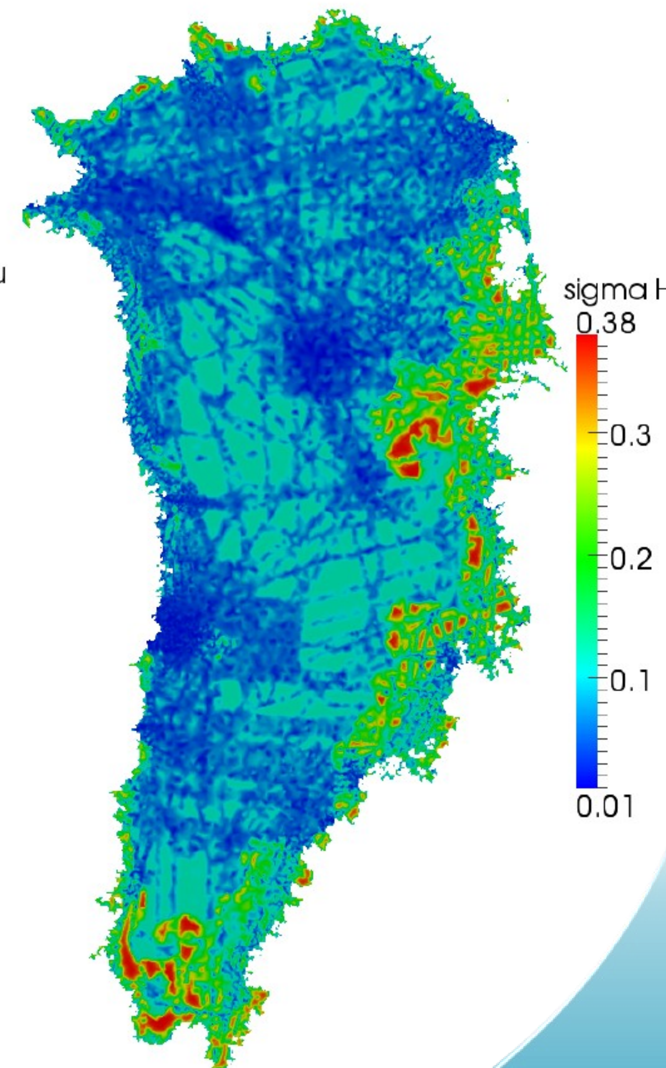
Grid



Velocity RMS (m/yr)



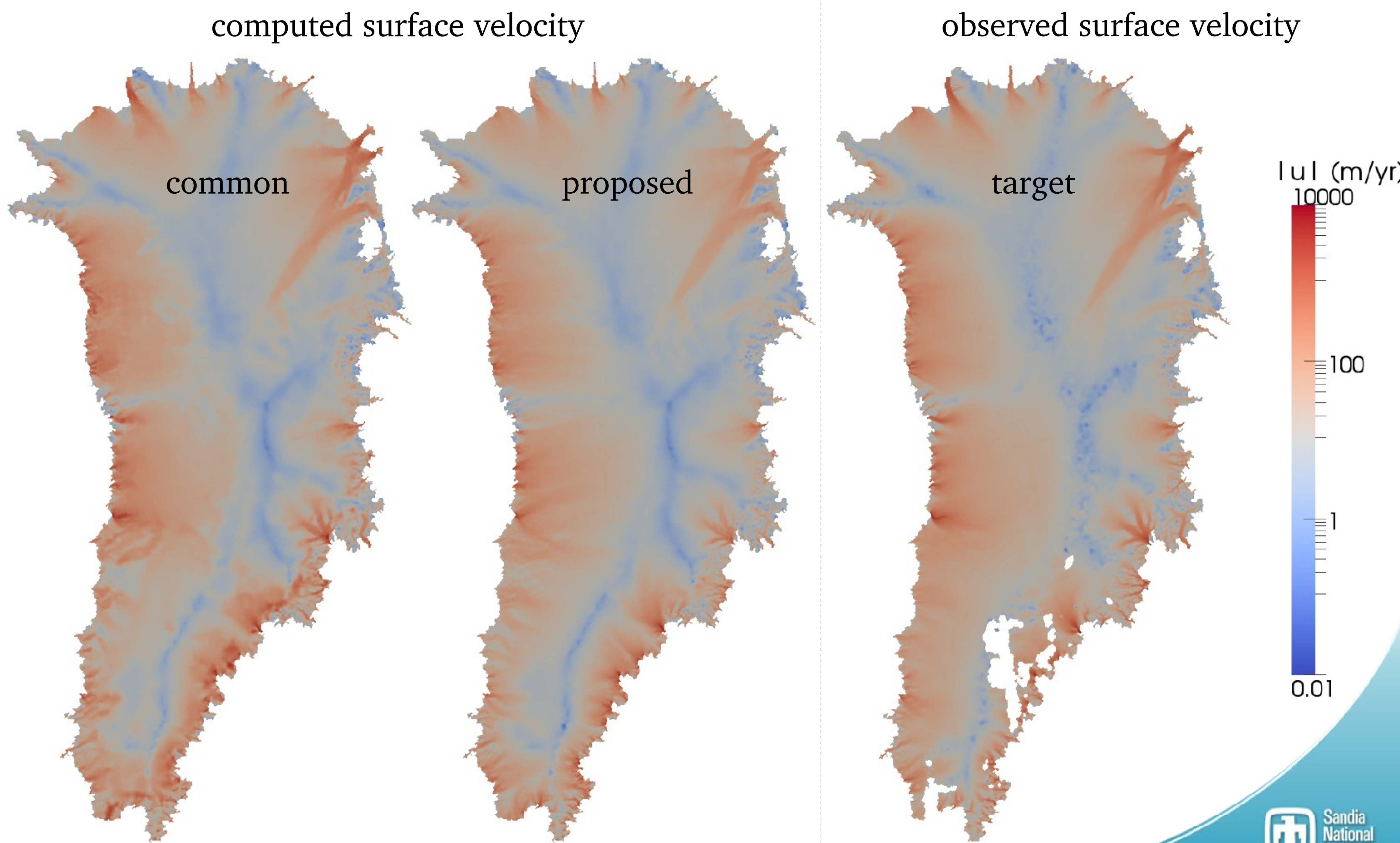
Thickness RMS (km)



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



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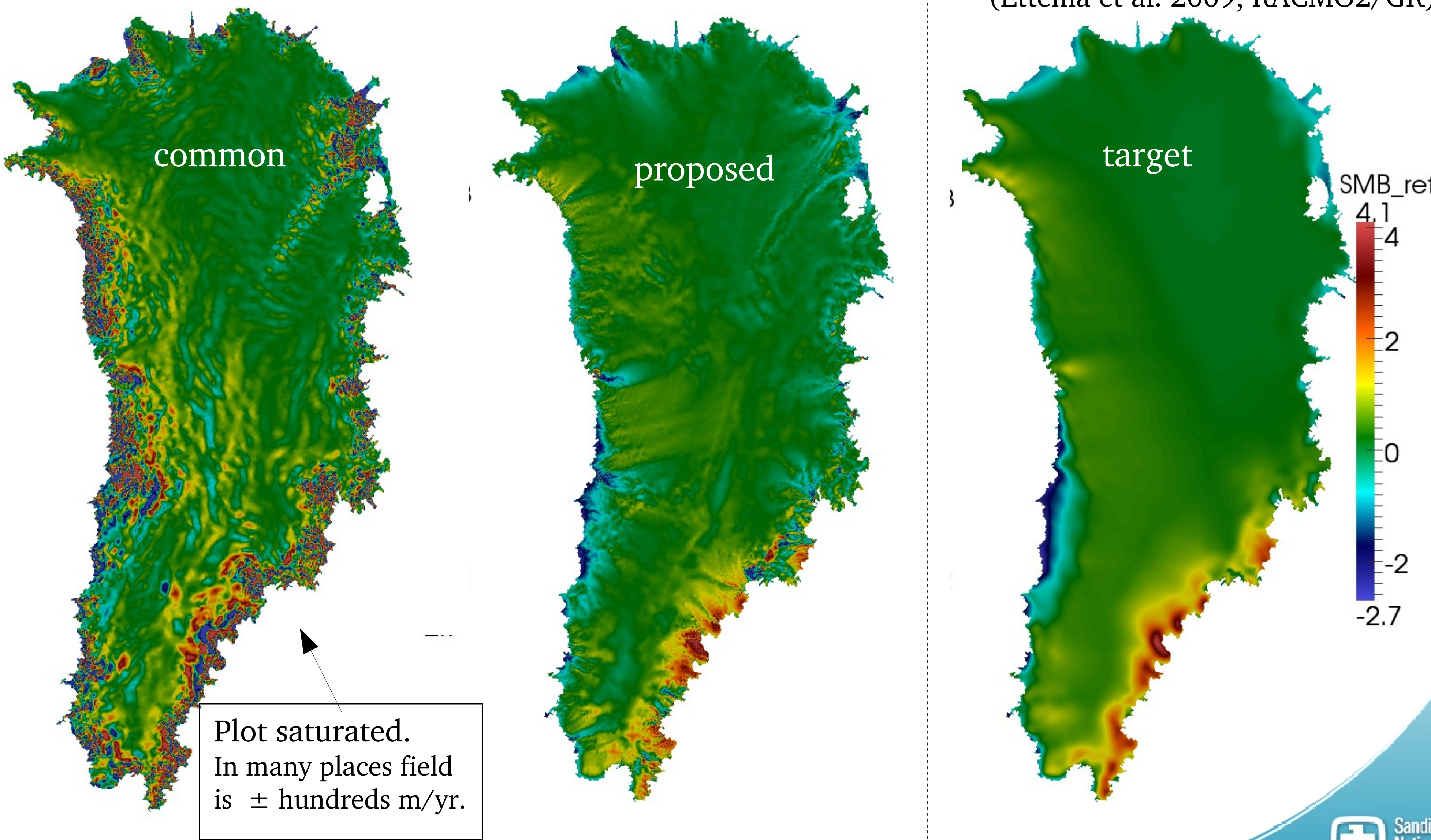
Deterministic Inversion for Greenland ice sheet

Inversion results: surface mass balance (SMB)

SMB (m/yr) needed for equilibrium

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

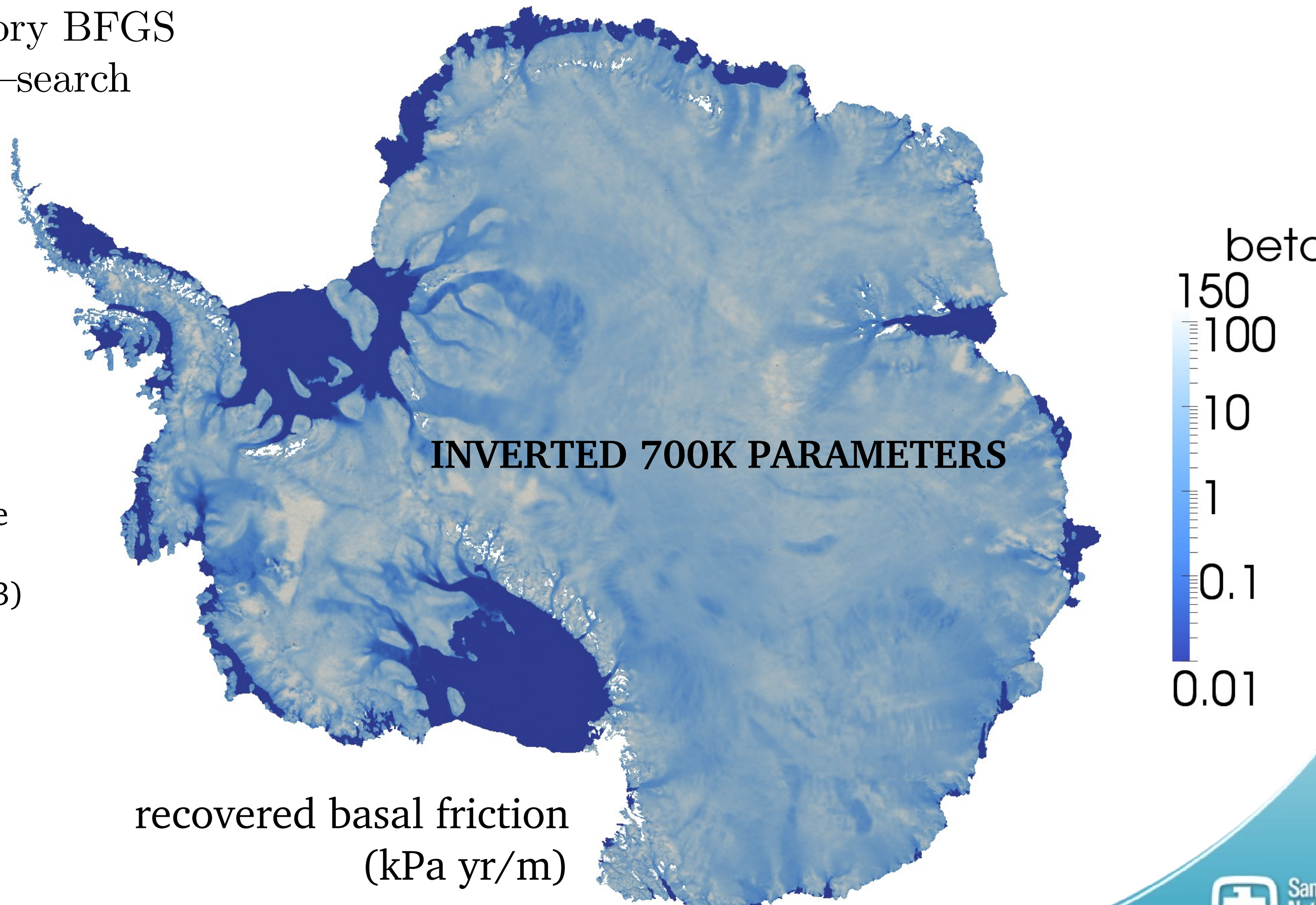


Antarctica Inversion (only for basal friction)

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

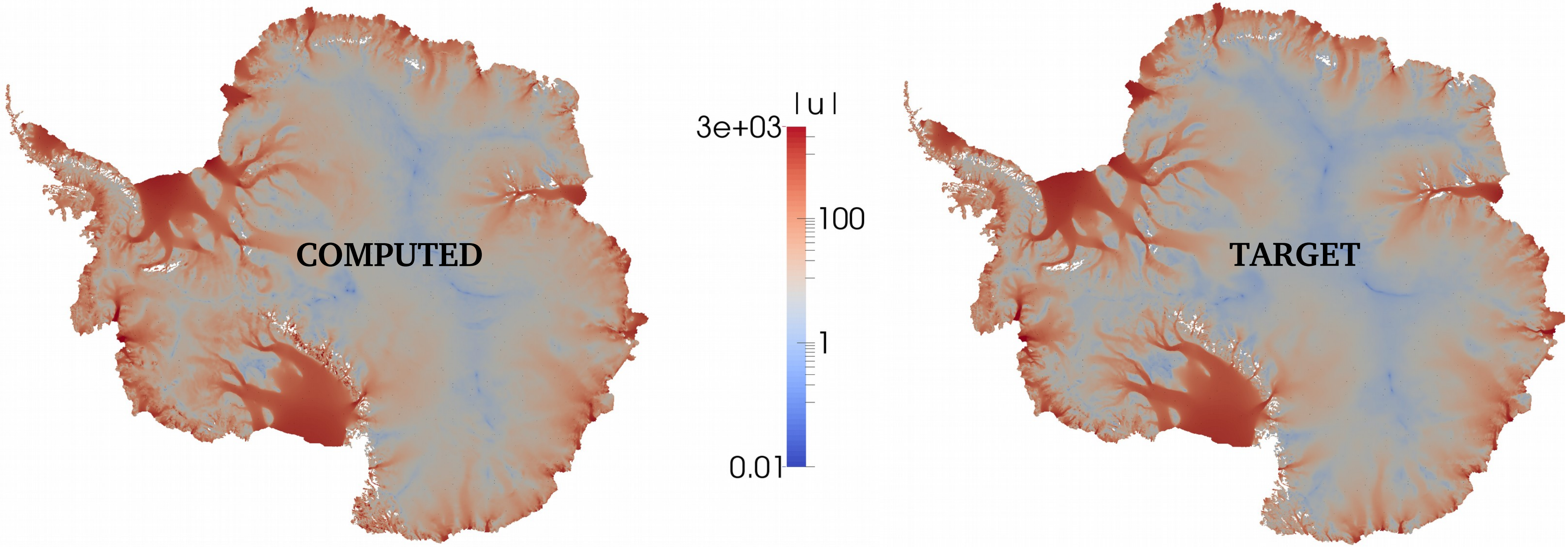


recovered basal friction (kPa yr/m)

Geometry (Cornford et al., The Cryosphere, 2015)
Bedmap2 (Fretwell et al., 2013)
Temperature (Pattyn, 2010)

Antarctica Inversion (only for basal friction)

comparison surface velocities, computed vs. target

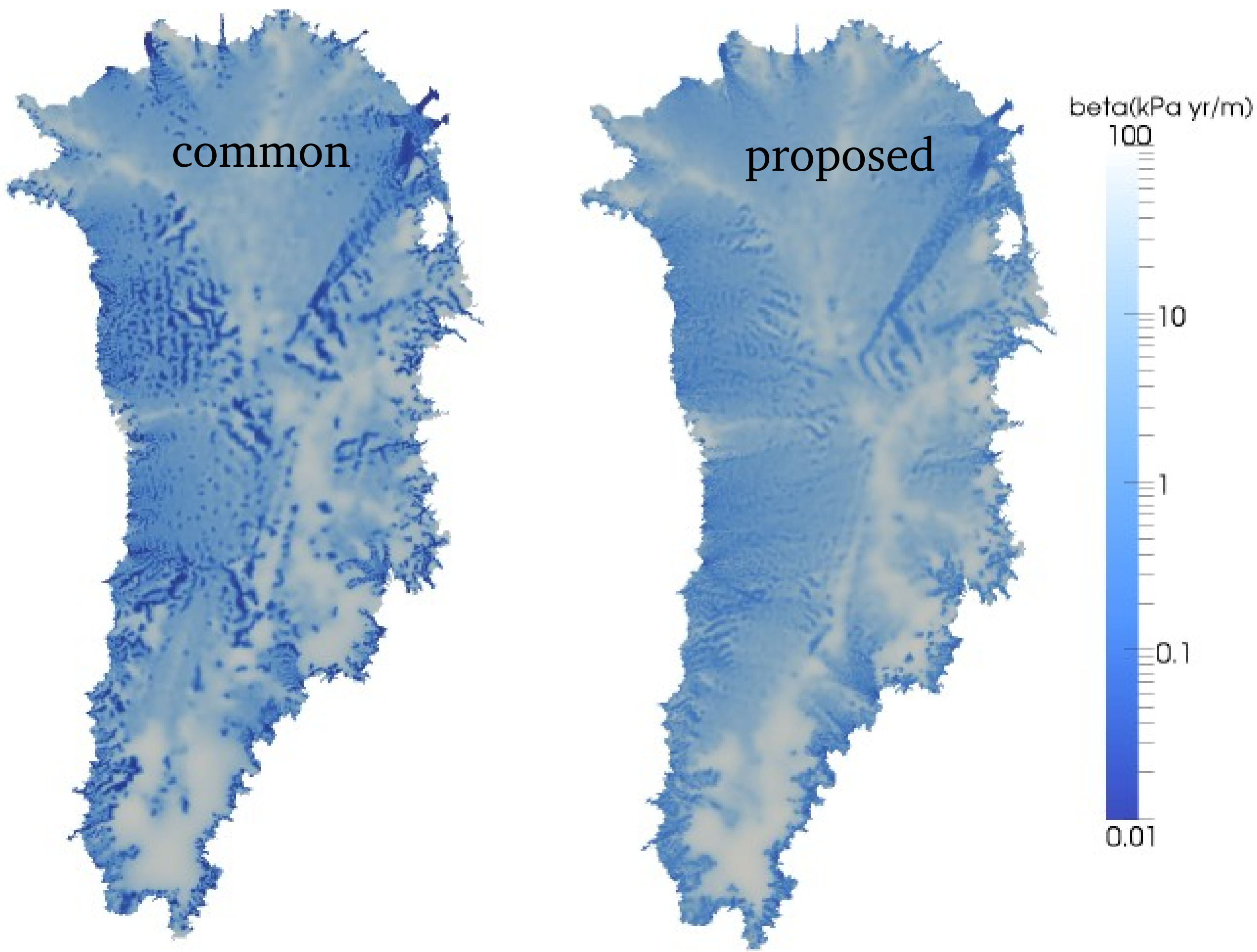


surface velocity magnitude (m/yr)

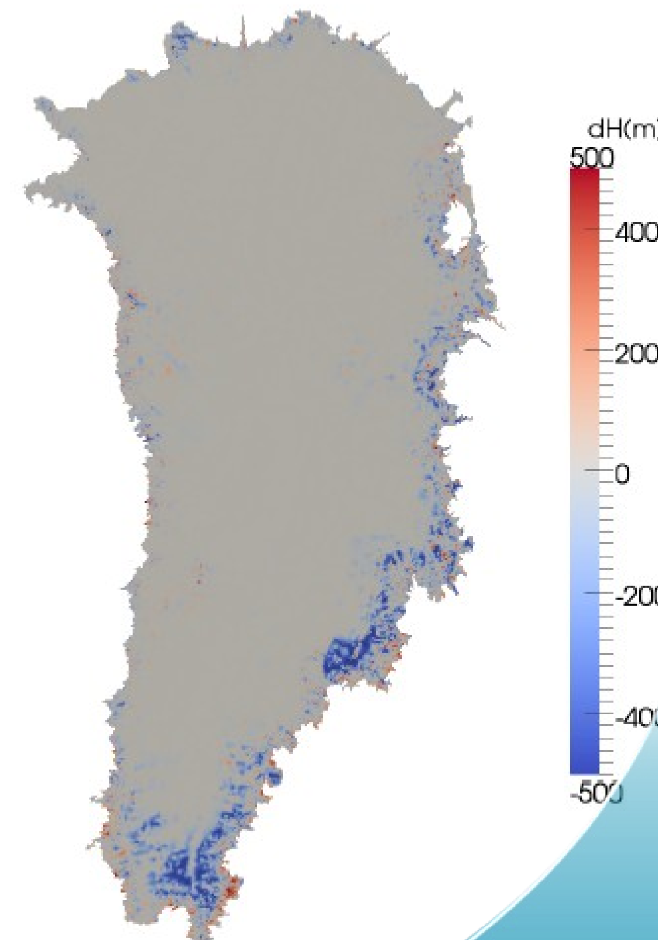
Deterministic Inversion for Greenland ice sheet

Estimated beta and change in topography

recovered basal friction



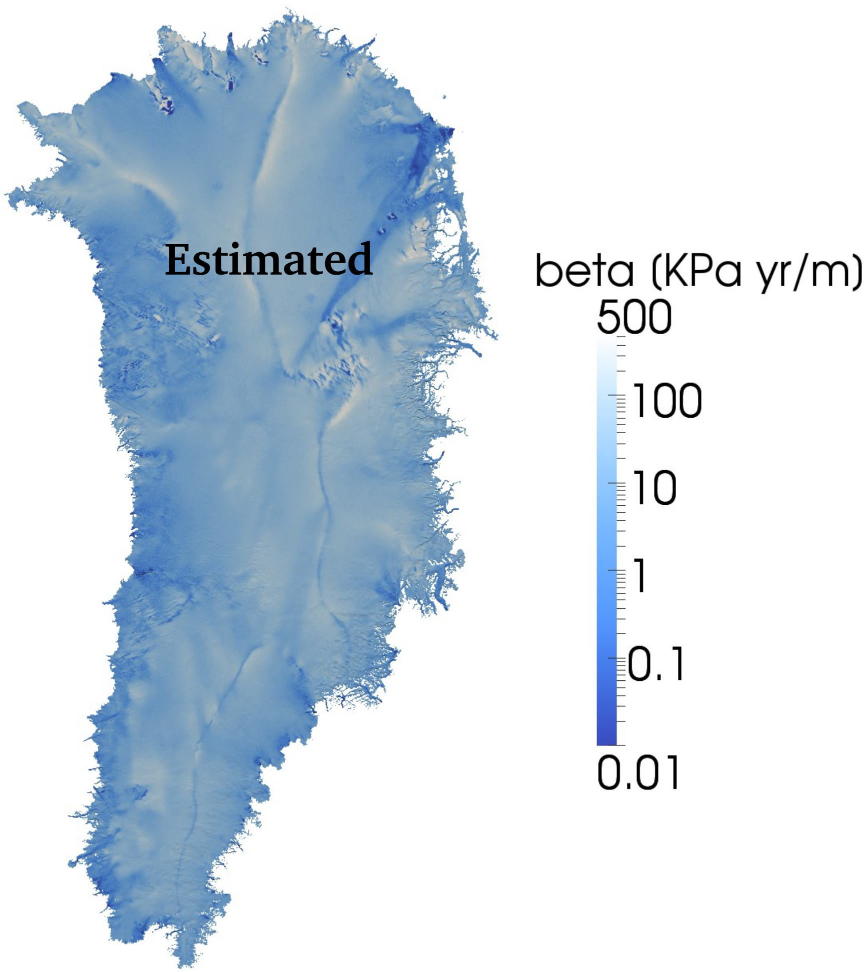
difference between recovered and observed thickness



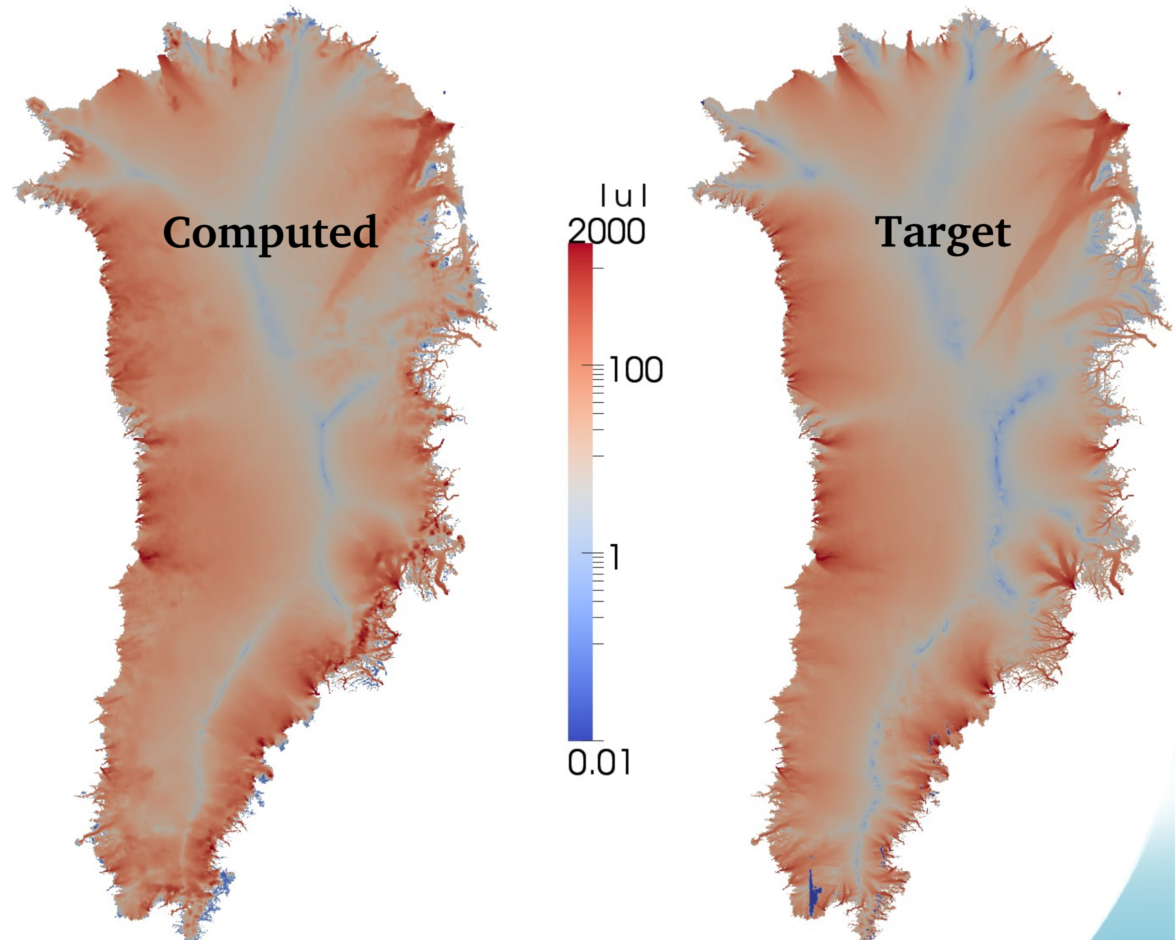
Geometry (Morlighem et al., Nature Geo., 2014)

Greenland Inversion using Albany-Piro-ROL

Inversion with 1.6M parameters



Basal friction coefficient (m/yr)



surface velocity magnitude (m/yr)

Geometry (Morlighem et al., Nature Geo., 2014)

Discussion on inversion

Optimization helps finding an initial state that is somewhat in compliance with observed velocities and with observed climate forcing and ice transients.

The mismatch found is larger then ideal (computed quantities on average 3-4 sigmas away from observations). Possible causes are:

- Temperature is assumed as given, with no uncertainty associated with it.
- Observations of velocity, surface mass balance, bedrock topography do not come from the same dataset and hence effective uncertainty might be bigger than the one provided with the measurement.
- Consider other source of uncertainty, e.g. model parameters (e.g. Glen’s law exponent) or the model itself.

Another limit of the current inversion is that the basal friction law does not account for variation in time of the basal friction due to subglacial hydrology.

Bayesian Calibration and Uncertainty Propagation

(feasibility study)

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 Γ_{prior}.

3. Take the mean $\bar{\beta}$ to be the deterministic solution and expand β in basis of eigenvector $\{\phi_k\}$ of Γ_{prior}, with random variables $\{\xi_k\}$

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

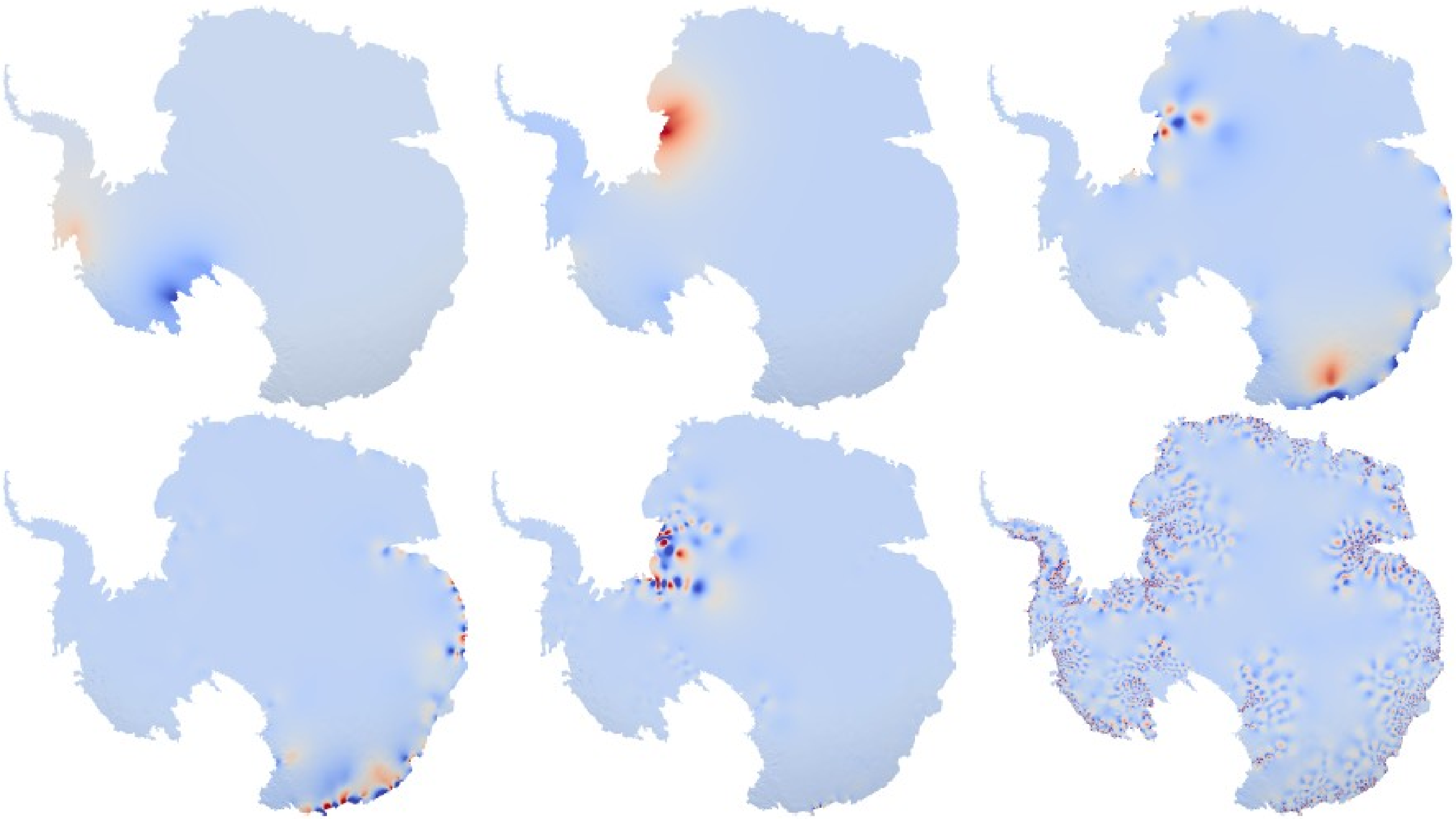
*Expansion done on $\log(\beta)$ to avoid negative values for β.

Building the Gaussian distribution using Hessian from deterministic inversion

Compute the Covariance of the Gaussian posterior using Hessian of merit functional.

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

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



Courtesy of O. Ghattas group

Eigenvectors of the prior-preconditioned data misfit Hessian corresponding to the 1st, 2nd, 100th, 200th, 500th, and 4000th eigenvalues. ***Isaac et al. 2004.***

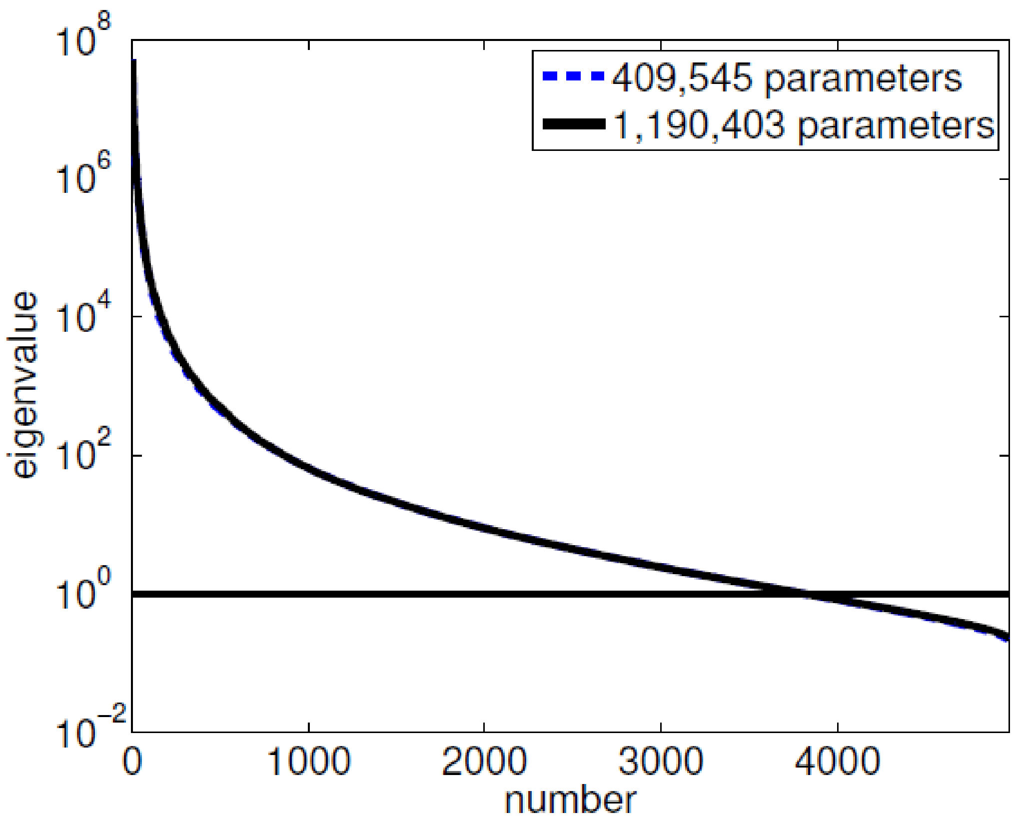
Building the Gaussian posterior approximation using Hessian from deterministic inversion

The Hessian provides 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 ($\sim$ 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***.

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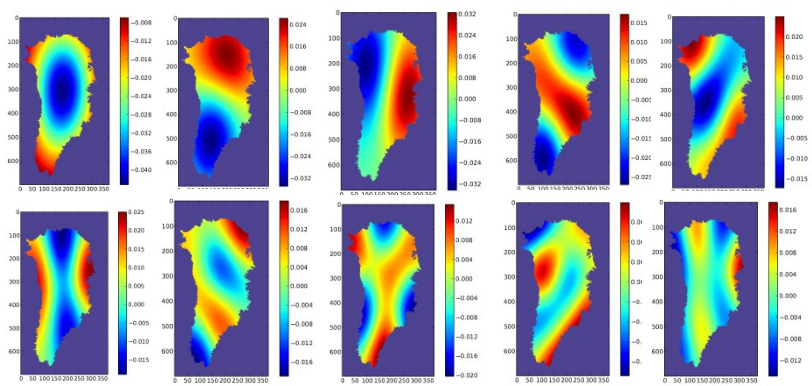
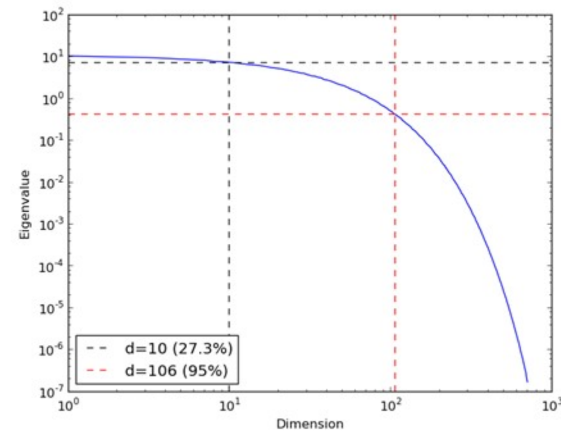
Bayesian Calibration and Uncertainty Propagation

(feasibility study)

- First 10 KLE modes
  (parallel C++/Trilinos code **Anasazi**).



Eigenvalues Decay
(100 eigenvalues capture 95% energy)



Only spatial correlation has been considered.

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

- ***Build Emulator.*** Polynomial chaos expansion (**PCE**) was formed for the mismatch over random variables with uniform prior distributions using almost 300 steady-state simulations. (**DAKOTA)**

Emulator (Polynomial Chaos Expansion):

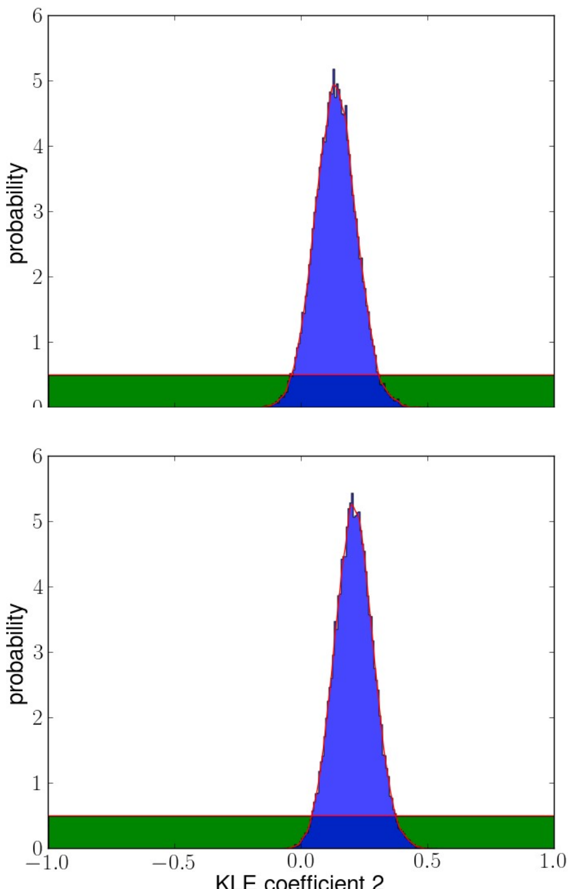
$$\beta(\omega) = \bar{\beta} + \exp\left\{ \sum_{k=1}^{K} \sqrt{\lambda_k} \phi_k \xi_k(\omega) \right\}$$

Bayesian Calibration and Uncertainty Propagation

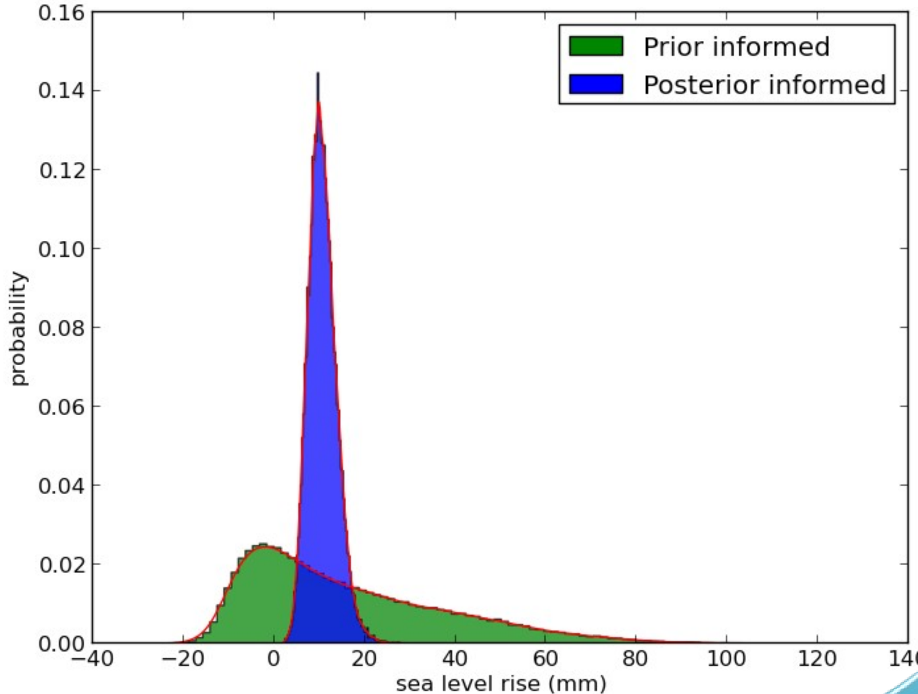
(feasibility study)

- **Inversion/Calibration**. Markov Chain Monte Carlo (**MCMC**), delayed rejection adaptive metropolis (DRAM), was performed on the PCE (**QUESO**).
- **Uncertainty propagation**. Used Gaussian process to build surrogate using 66 transient simulations.

Posterior distributions



Uncertainty propagation:
Sea level rise prediction in 50 years



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Bayesian Calibration and Uncertainty Propagation

(feasibility study)

- Prior chosen is somewhat arbitrary, however it is possible to build an informed Gaussian distribution using the **Hessian of the deterministic inversion**.

- The prior distribution size is big (in real applications, million of parameters with thousands significant parameters) and so the KLE expansion needs several modes to retain most of the prior energy – in the results shown we only retained 27% of the prior energy!

- A lot of samples are needed to build the emulator. Cross correlation tests showed that the simulations we run for the uncertainty propagation was not sufficient for building the emulator.

- We might use techniques such as the **compressed sensing technique*** to adaptively select significant modes and the basis for the parameter space. The hope is that only few modes affect the low dimensional QoI (e.g. sea level rise).

- We might use cheap physical models (e.g. SIA) or low resolution solves to reduce the cost of building the emulator.

*Jakeman, Eldred, Sargsyan, JCP, 2015

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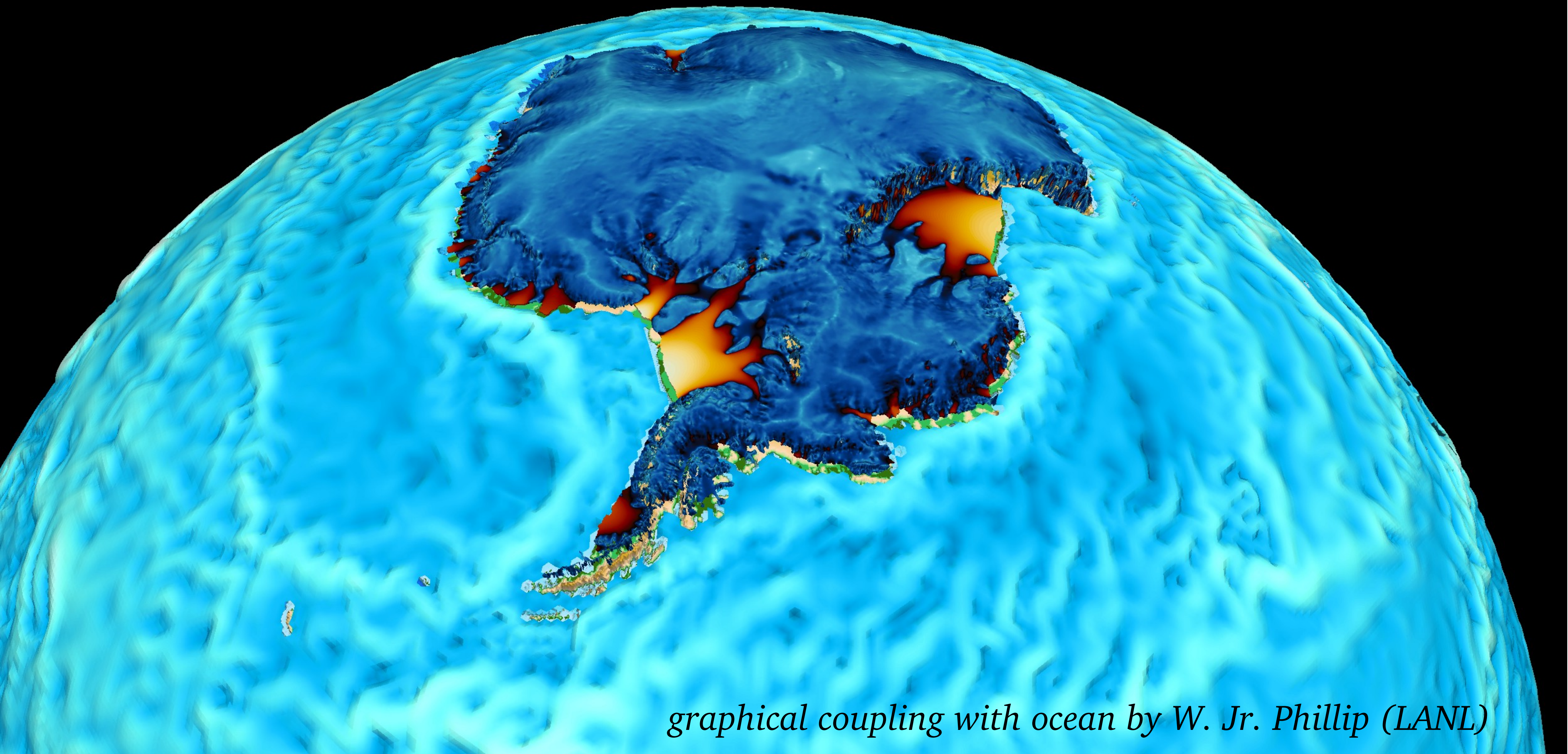
Thank you for your attention



graphical coupling with ocean by W. Jr. Phillip (LANL)