

# Towards Uncertainty Quantification in 21st Century Sea-Level Rise Predictions: PDE Constrained Optimization as a First Step in Bayesian Calibration and Forward Propagation

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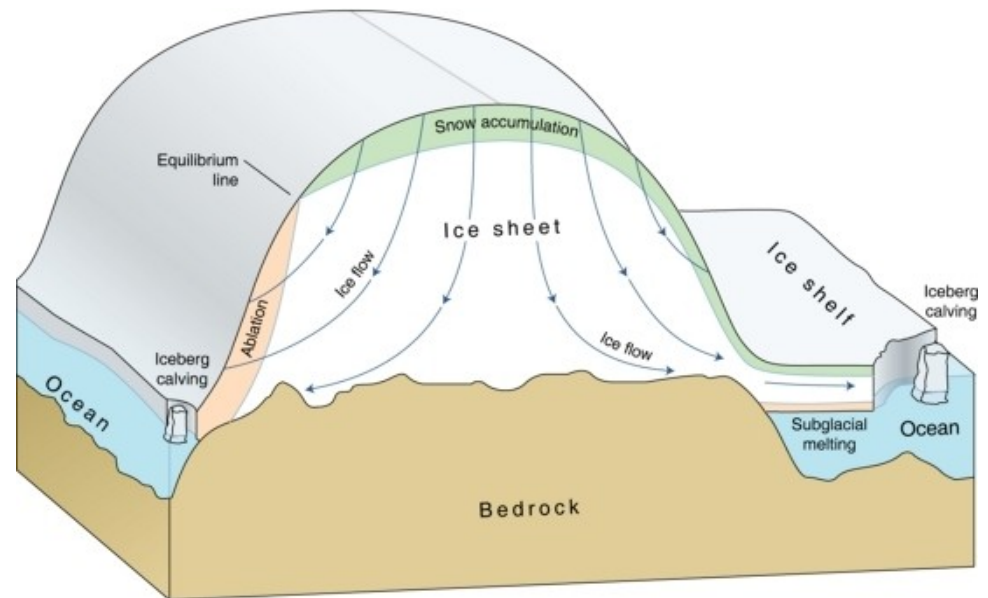
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## Brief introduction and motivation

- 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.

# 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* (see next talk by Irina Tezaur).
- Perform *Forward Propagation* (see next talk by Irina Tezaur).

# Ice Sheet Modeling

## Ice momentum equations

- Ice flow equations (momentum and mass balance)

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

with:

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

Nonlinear viscosity:

$$\mu = \frac{1}{2} \alpha(T) |\mathbf{D}(\mathbf{u})|^{\frac{1}{n}-1}, \quad n \geq 1, \quad (\text{typically } n \simeq 3)$$

Viscosity is singular when ice is not deforming



# Stokes approximations in different regimes

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

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



FO( $u, v$ )

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

First Order\* or  
Blatter-Pattyn model

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

# Stokes approximations in different regimes

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

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

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

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

3<sup>rd</sup> 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

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

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

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

Quasi-hydrostatic  
approximation

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# Stokes approximations in different regimes

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

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

Drop terms using  
**scaling argument**  
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$$-\cancel{\partial_x(\mu u_z)} - \cancel{\partial_y(\mu v_z)} - \partial_z(2\mu w_z - p) = -\rho g, \quad \text{continuity equation}$$

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

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

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

\*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:

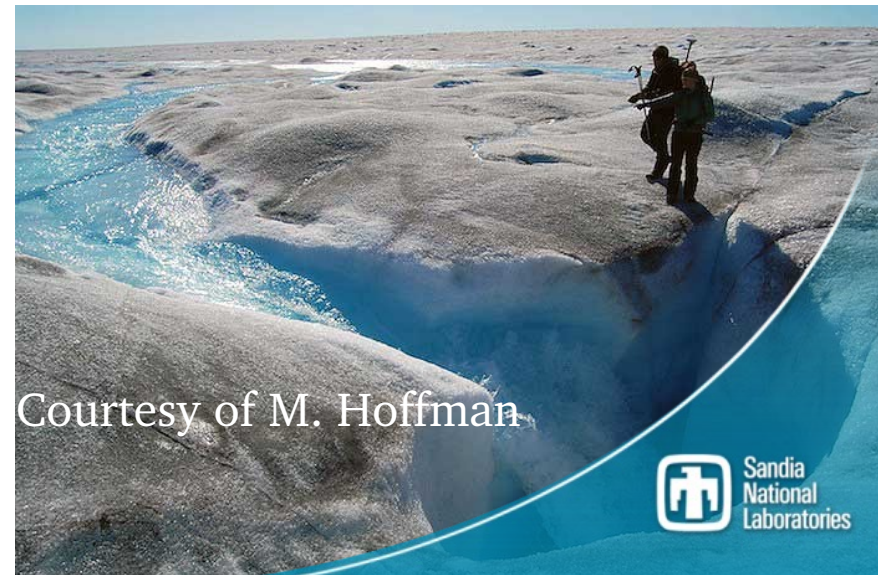
$$\frac{\partial H}{\partial t} = -\text{div}(\mathbf{U}H) + \tau_{\text{smb}}, \quad \mathbf{U} = \frac{1}{H} \int_z \mathbf{u} dz.$$

*flux divergence*  
↓  
*Surface Mass Balance* ↑

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

Boundary condition at ice-bedrock interface :

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



Courtesy of M. Hoffman

# 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

# 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

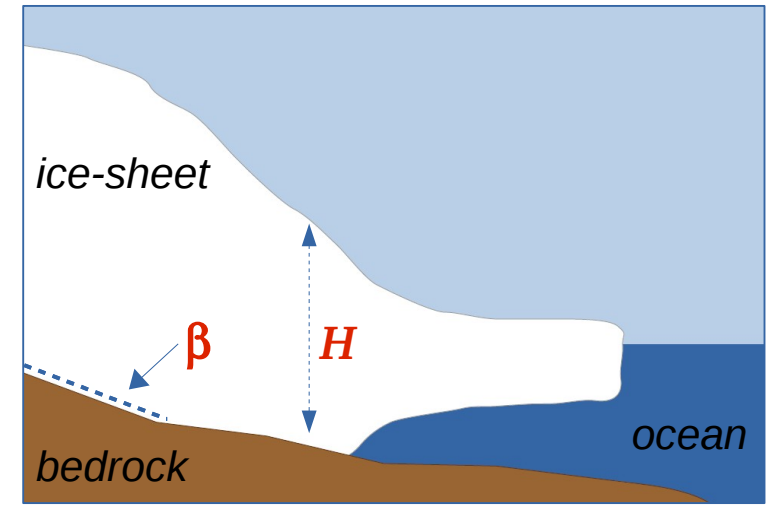
- *ice thickness  $H$  (allowed to vary but weighted by observational uncertainties)*
- *basal friction  $\beta$  (spatially variable proxy for all basal processes)*

### Modeling Assumptions

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

### Additional Assumption (for now)

- *given **temperature field***



# 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 minimize the functional  $\mathcal{J}$

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

subject to ice sheet model equations  
(FO or Stokes)

$\mathbf{U}$ : computed depth averaged velocity

$H$ : ice thickness

$\beta$ : basal sliding friction coefficient

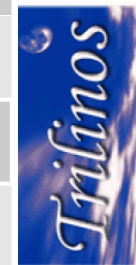
$\tau_s$ : SMB

$\mathcal{R}(\beta)$  regularization term

# 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, Line search: backtrack*

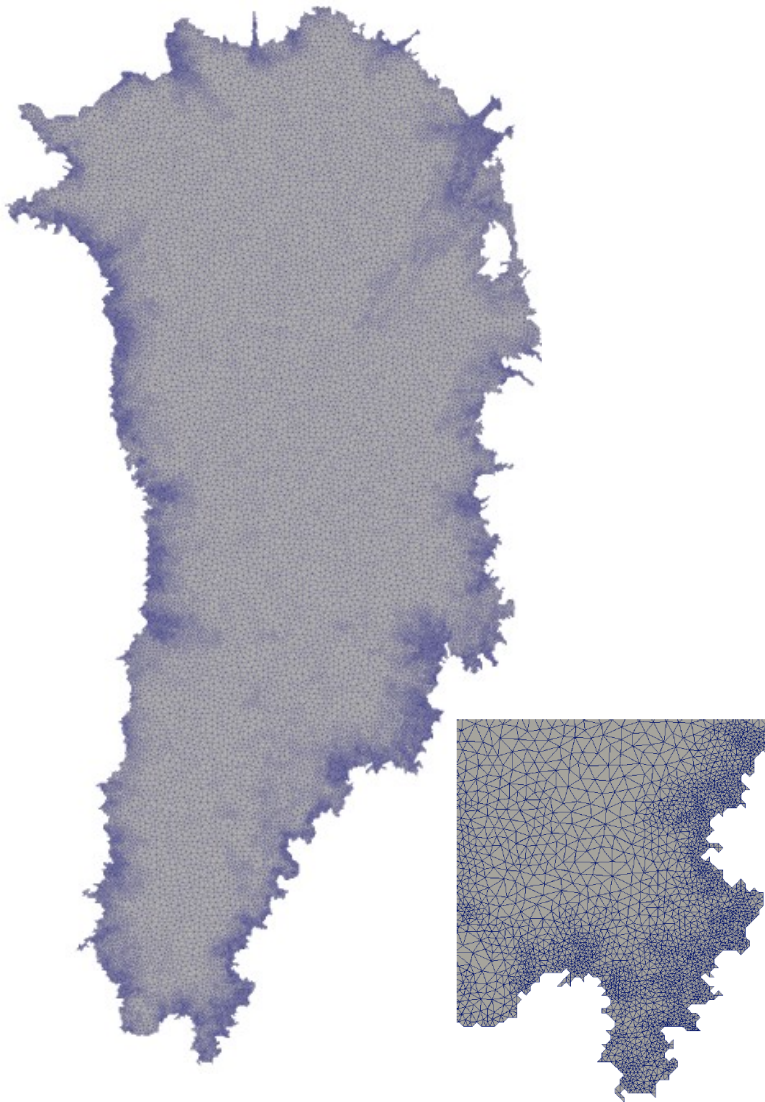




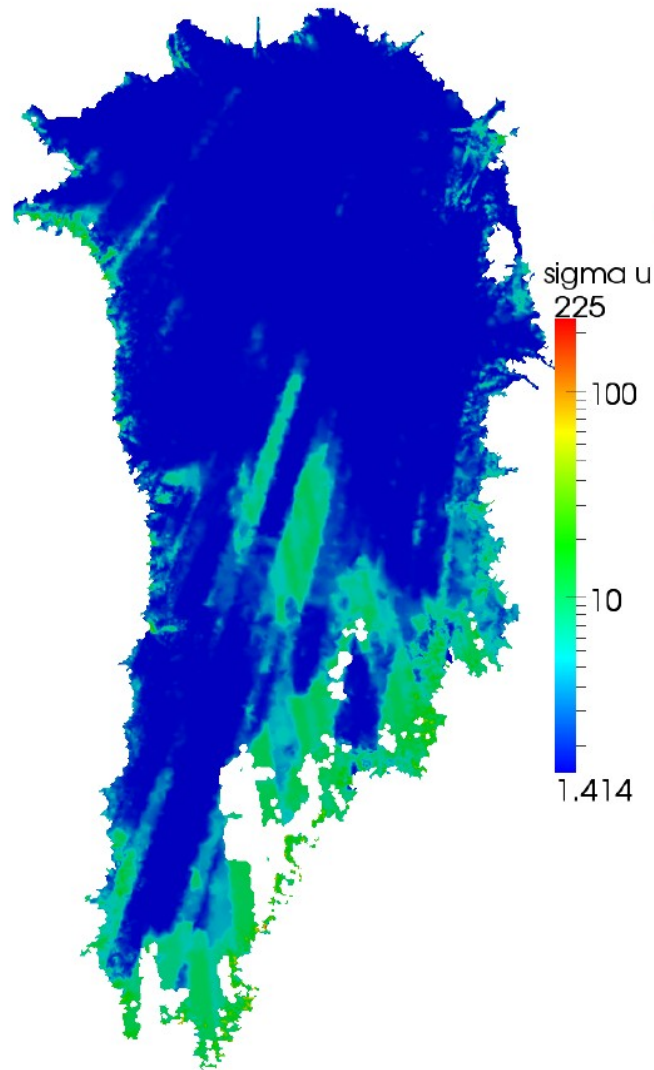
# Deterministic Inversion for Greenland ice sheet

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

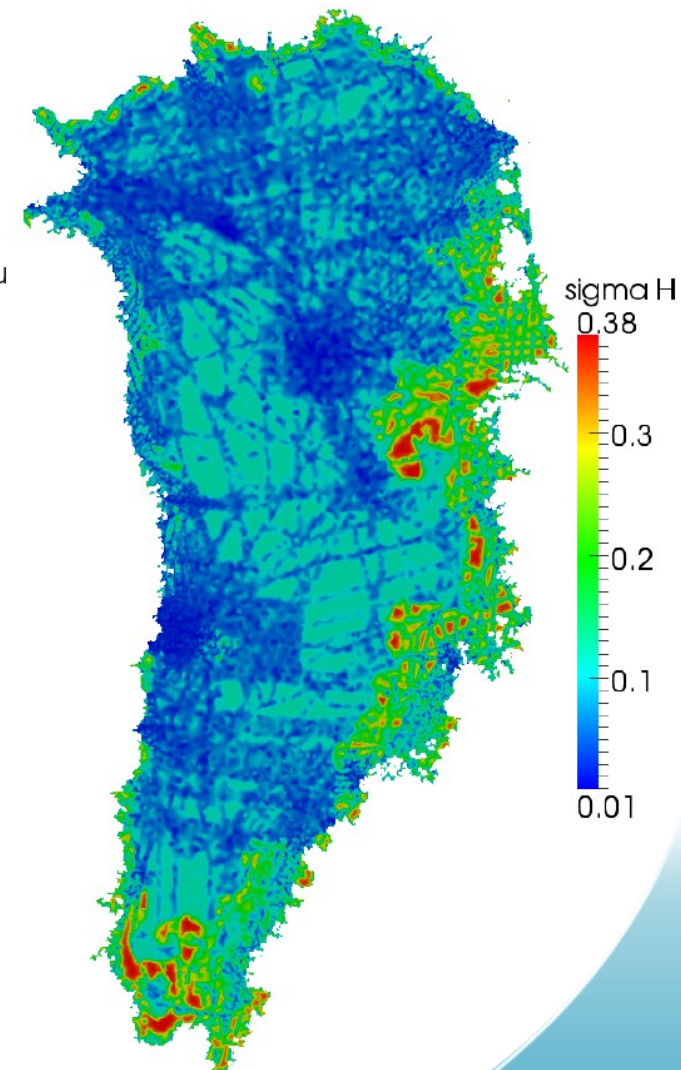
Grid



Velocity RMS (m/yr)



Thickness RMS (km)





# Deterministic Inversion for Greenland ice sheet

Inversion results: surface velocities

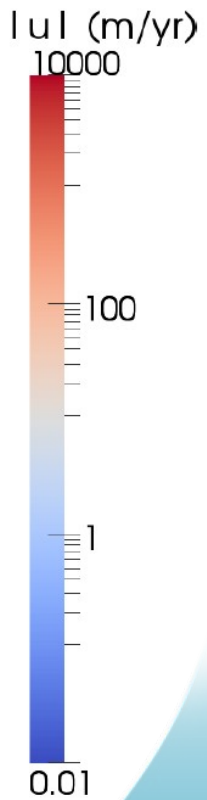
computed surface velocity

common

proposed

observed surface velocity

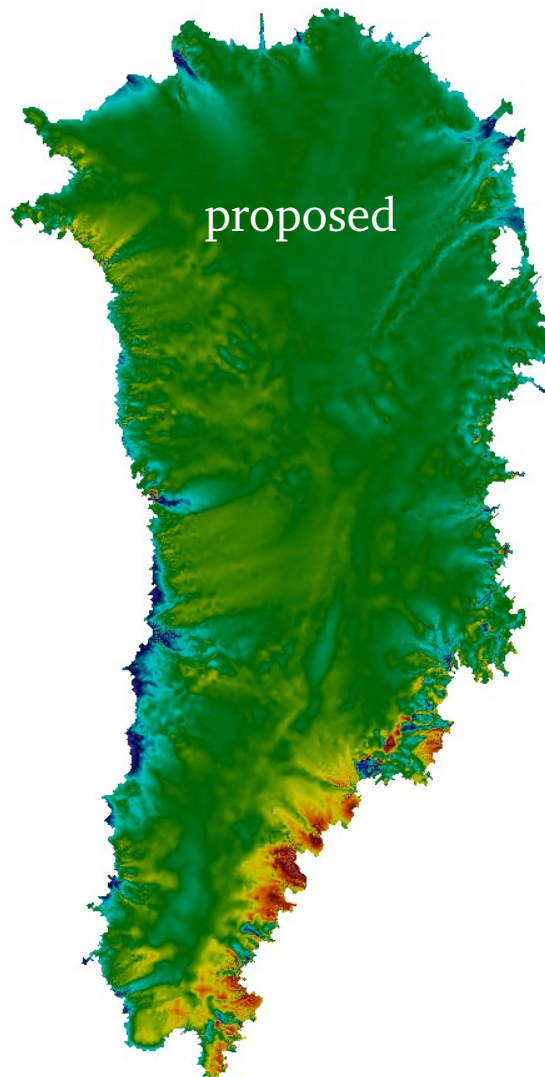
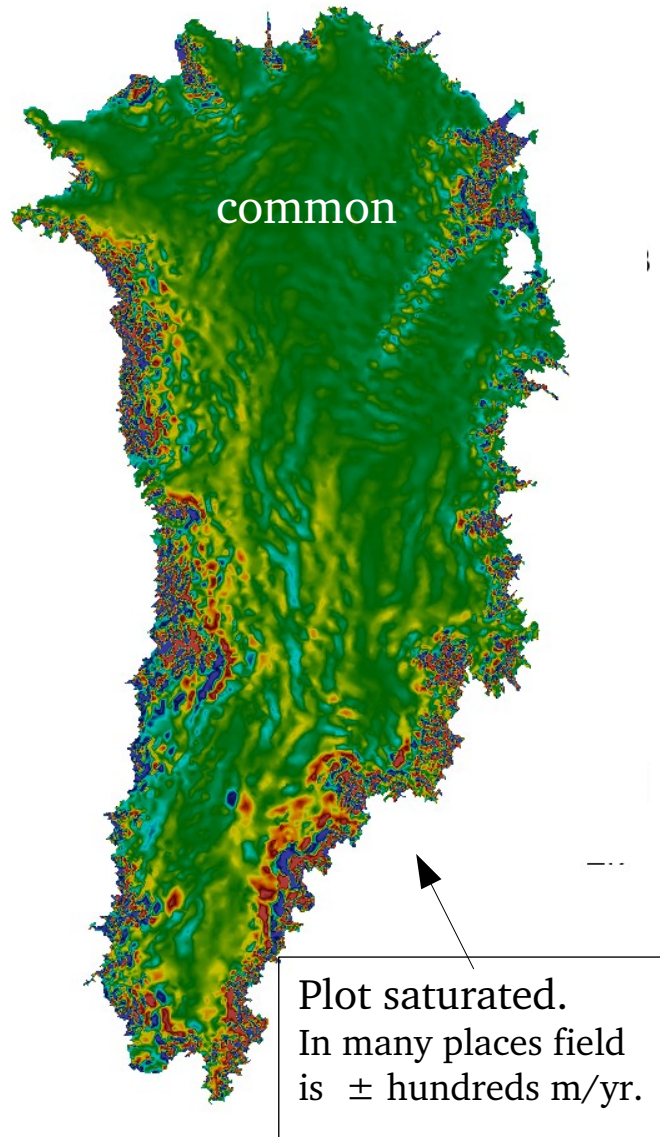
target



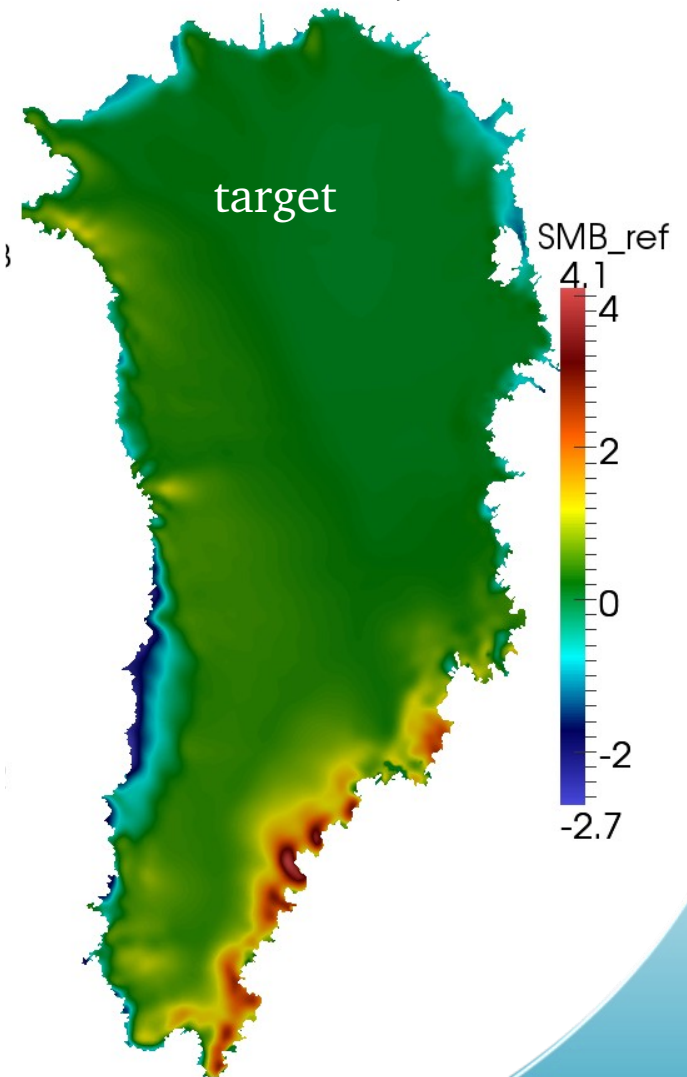
# Deterministic Inversion for Greenland ice sheet

Inversion results: surface mass balance (SMB)

SMB (m/yr) needed for equilibrium



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



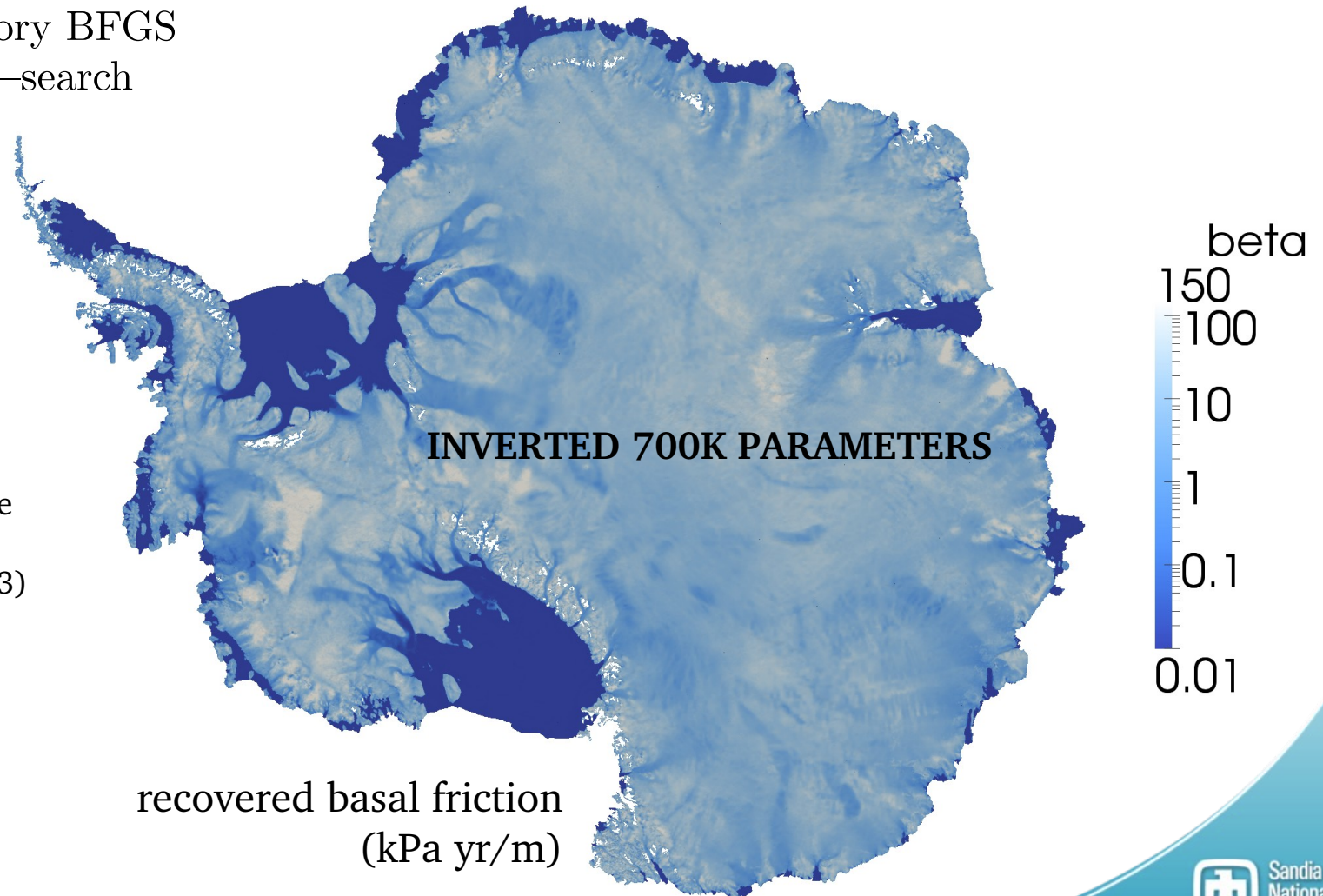


# Antarctica Inversion (only for basal friction)

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

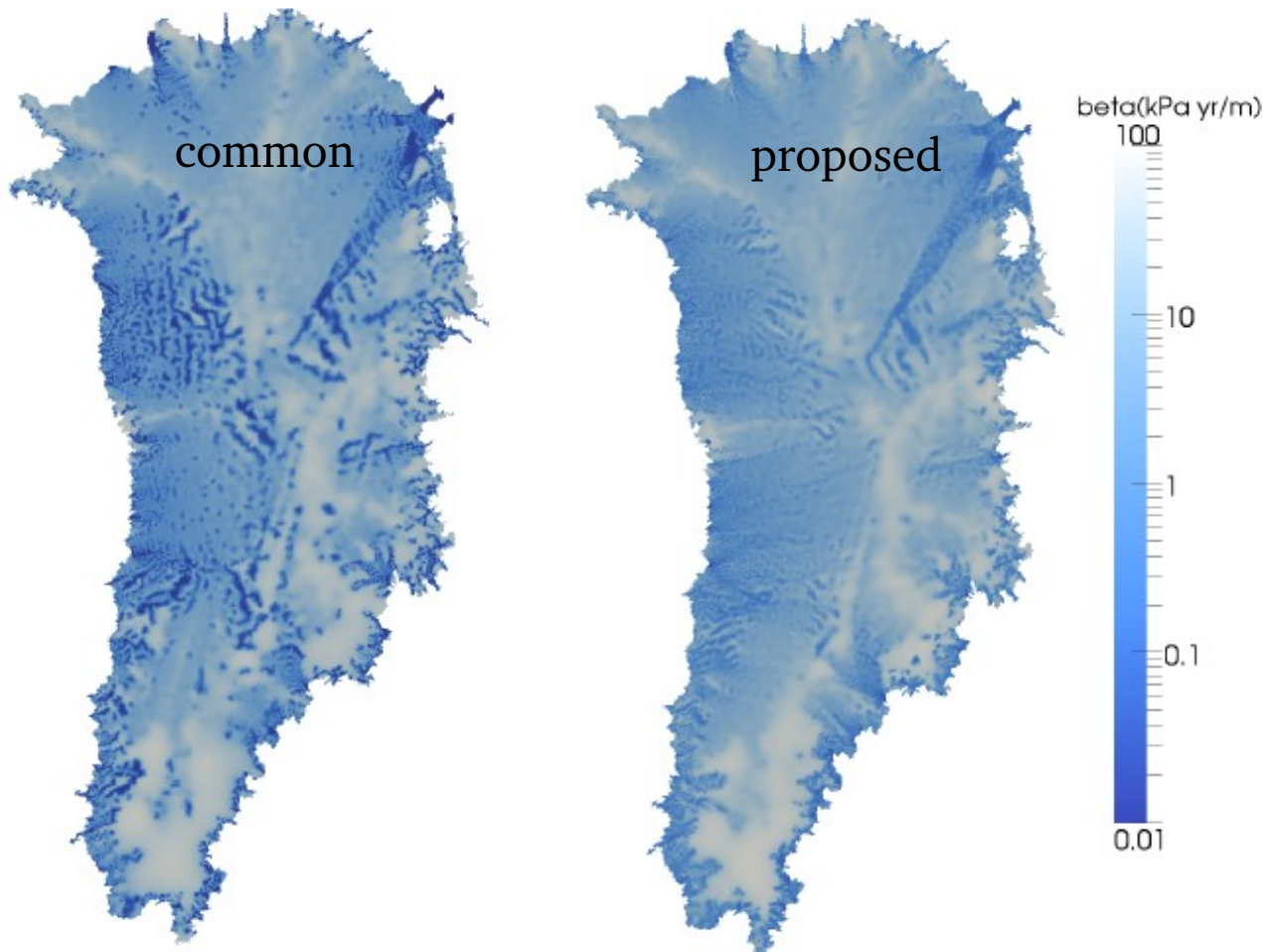


Geometry (Cornford et al., The Cryosphere, 2015)  
Bedmap2 (Fretwell et al., 2013)  
Temperature (Pattyn, 2010)

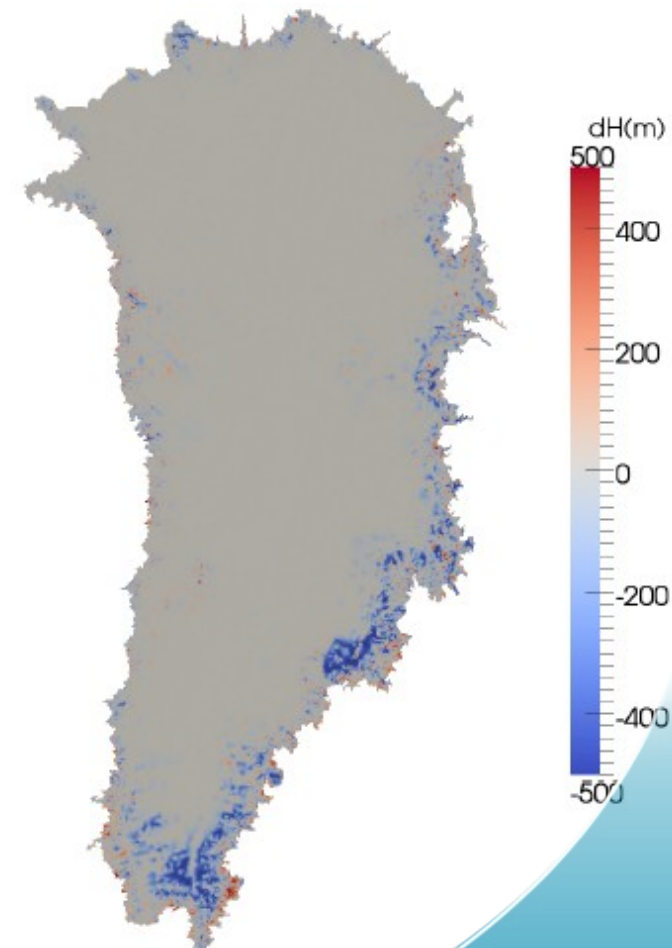
# Deterministic Inversion for Greenland ice sheet

Estimated beta and change in topography

recovered basal friction

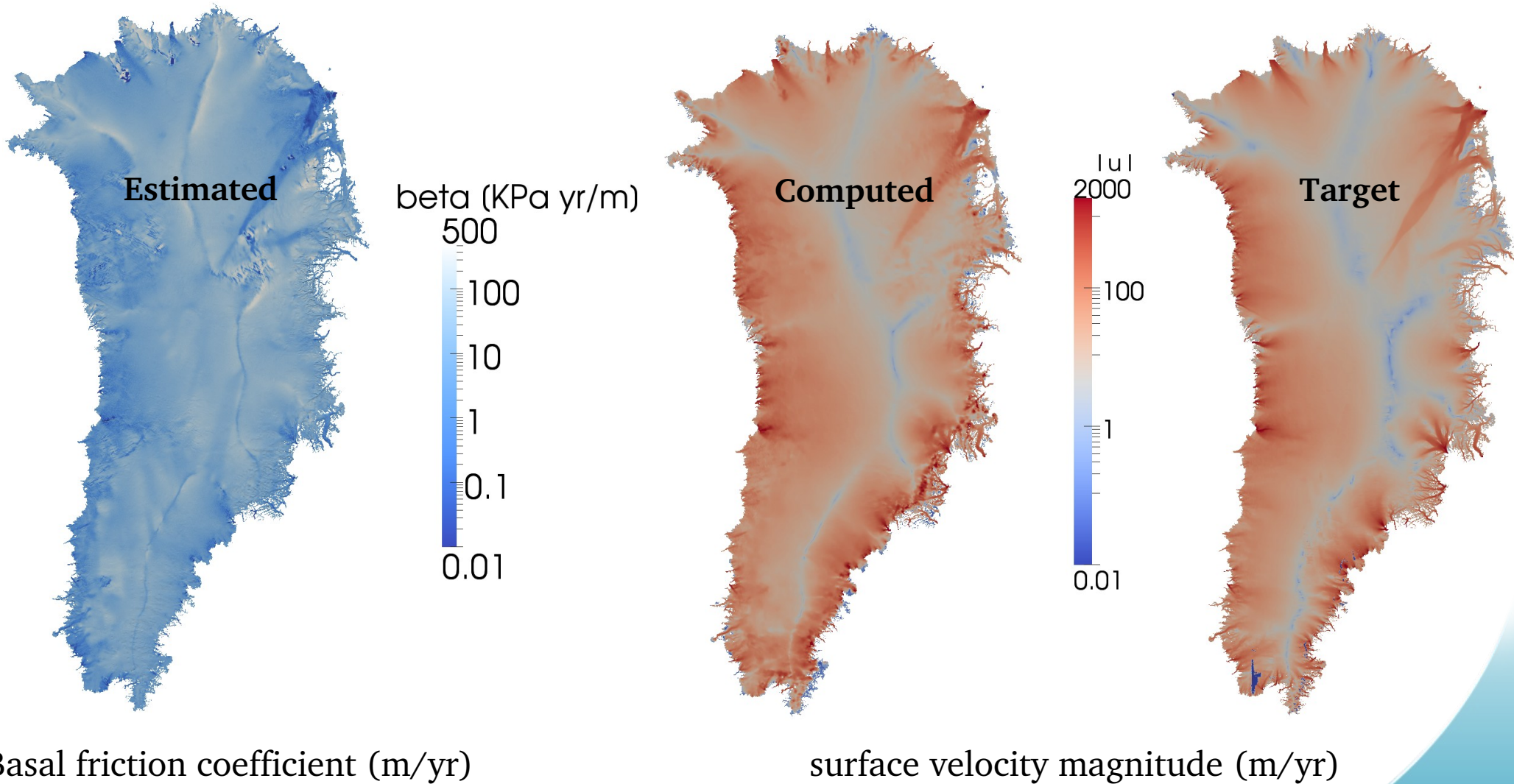


difference between recovered and observed thickness



# Greenland Inversion using Albany-Piro-ROL

Inversion with 1.6M parameters





# Discussion

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 than ideal (computed quantities on average 3-4 sigmas away from observations). Possible causes are:

1. Temperature is assumed as given, with no uncertainty associated with it.
2. 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.
3. 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.