Computational Challenges in Ice Sheet Modeling

Mauro Perego[1]

joint collaboration with

J. D. Jakeman[1], S. Price[2], A. Salinger[1], G. Stadler[3] and I. K. Tezaur[1]

[1]Sandia National Laboratories, NM, USA

[2]Los Alamos National Laboratory, NM, USA

[3]Courant Institute, NY, USA

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Center for Computing Research

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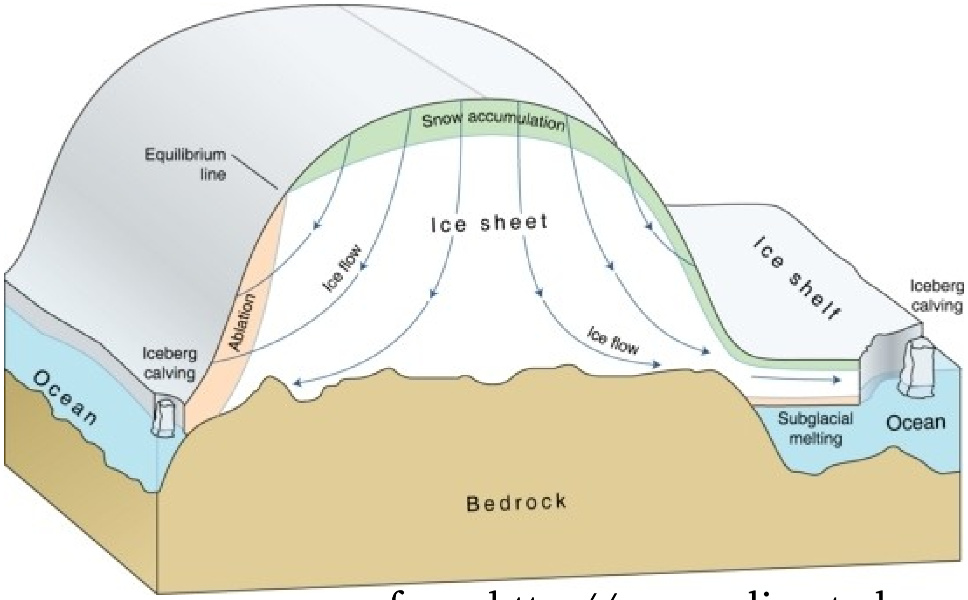
Brief introduction and motivation

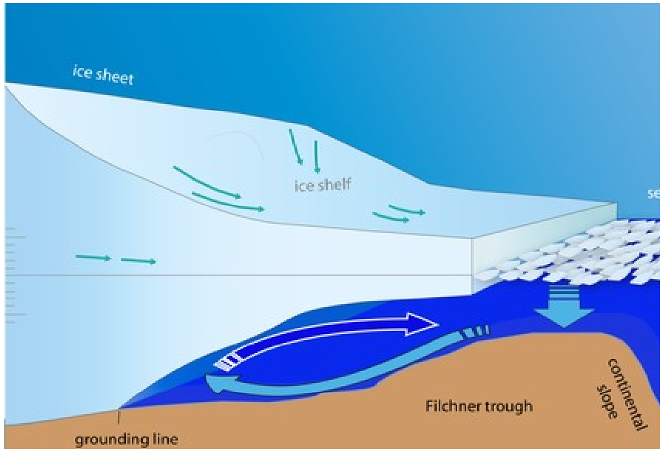
- Modeling ice sheets (Greenland and Antarctica) dynamics is essential to provide estimates for sea level rise in next decades to centuries.
- Ice behaves like a very viscous shear-thinning fluid (similar to lava flow) and can be modeled with nonlinear Stokes equation.
- Greenland and Antarctica ice sheets store most of the fresh water on hearth.
  They have a shallow geometry (thickness up to 3km, horizontal extensions of thousands of km).



from http://www.climate.be

(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

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

Ice Sheet Modeling

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Ice Sheet Modeling

Main components of an ice model:

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

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

- **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)**

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

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

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

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

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

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

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

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

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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

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

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

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

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

First Order* or Blatter-Pattyn model

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

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

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.

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

Estimation of ice sheet initial state

Steady state equations and basal sliding conditions

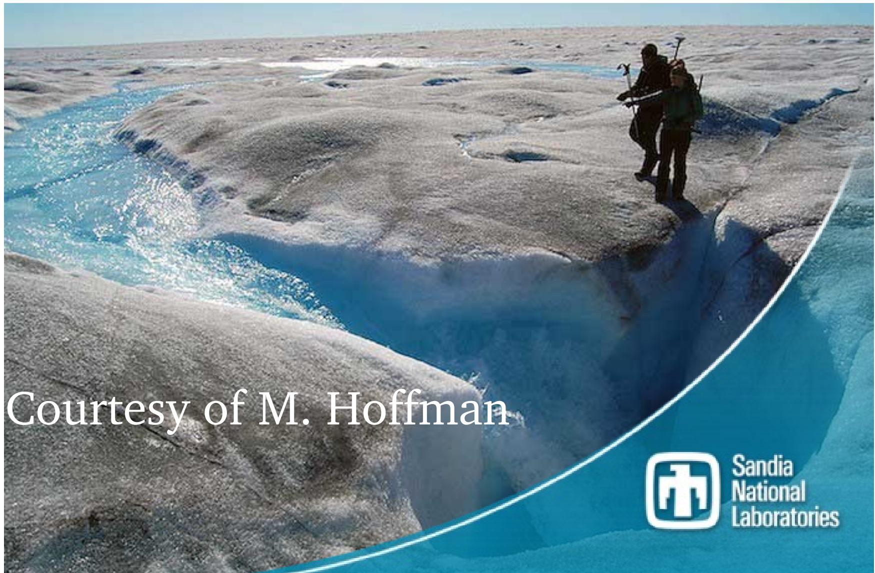
How to prescribe ice sheet mechanical equilibrium:

$$\frac{\partial H}{\partial t} = -\overbrace{\mathrm{div}\,(\mathbf{U}H)}^{\textit{flux divergence}} + \underbrace{\tau_{\mathrm{smb}}}_{\textit{Surface Mass Balance}}, \qquad \mathbf{U} = \frac{1}{H}\int_z \mathbf{u}\,dz.$$

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

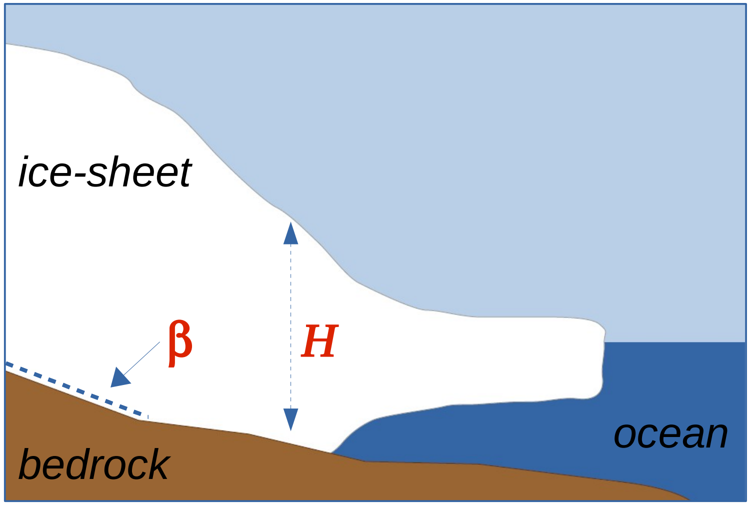
Boundary condition at ice-bedrock interface :

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



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 (or FO) equation***

Additional Assumption (for now)

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

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

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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 $\mathcal{J}$

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

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

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

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

Solve State System	$\mathcal{F}(\mathbf{u}, \beta, H) = 0$
Solve Adjoint System	$\langle \mathcal{F}^*_{\mathbf{u}}(\mathbf{u};\, \boldsymbol{\lambda}),\, \boldsymbol{\delta}_{\mathbf{u}} \rangle = \mathcal{J}_{\mathbf{u}}(\mathbf{u};\, \boldsymbol{\delta}_{\mathbf{u}}), \quad \forall \boldsymbol{\delta}_{\mathbf{u}}$
Total derivatives	$\mathcal{G}(\delta_\beta, \delta_H) = \mathcal{J}_{(\beta,H)}(\delta_\beta, \delta_H) - \langle \boldsymbol{\lambda}, \mathcal{F}_{(\beta,H)}(\delta_\beta, \delta_H) \rangle$
Derivative w.r.t. β	$\mathcal{G}_1(\delta_\beta) = \alpha_\beta \int_\Sigma \nabla\beta \cdot \nabla\delta_\beta \, ds - \int_\Sigma \delta_\beta \, \mathbf{u} \cdot \boldsymbol{\lambda} \, ds$

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)

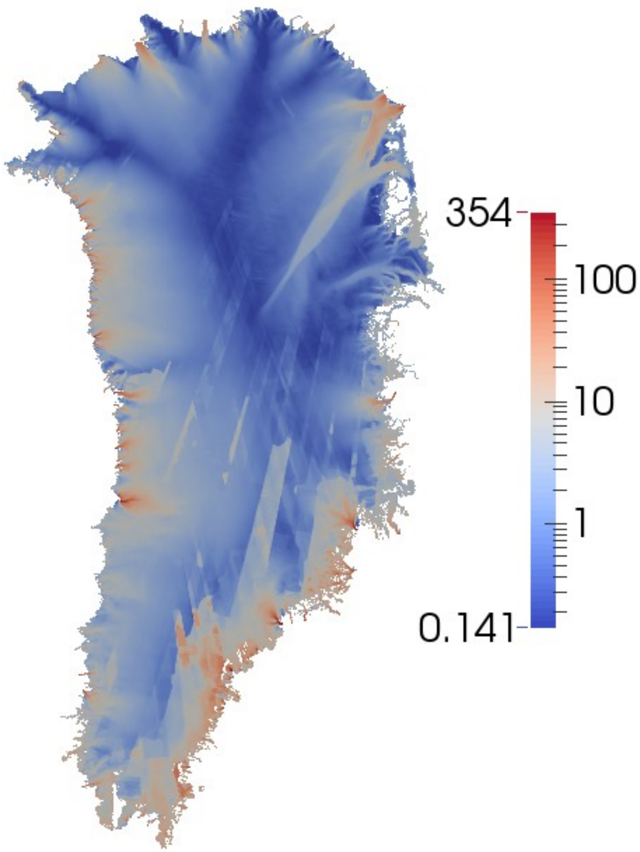
Optimization algorithm:

Reduce Gradient optimization, using L-BFGS.
Storage: 50-200, Linesearch: backtrack

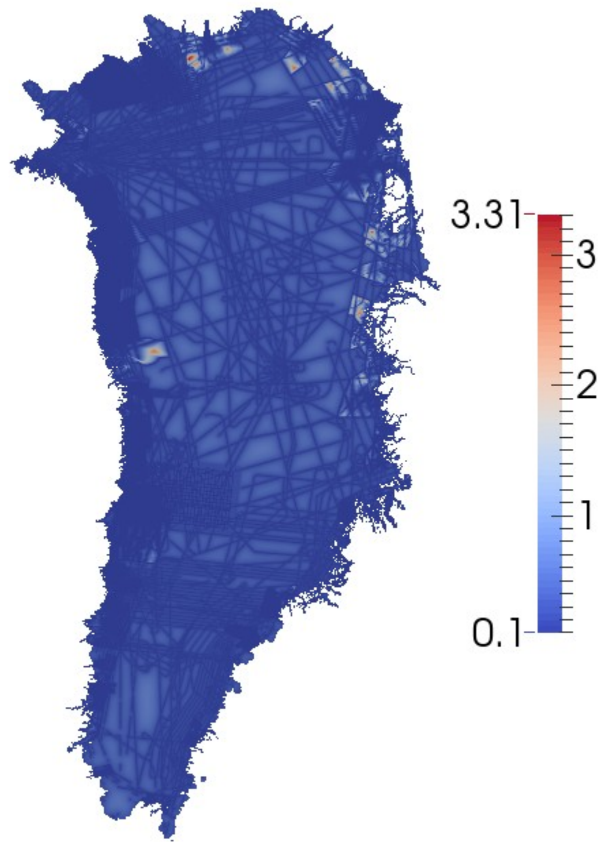
Deterministic Inversion for Greenland ice sheet

Errors associated with velocity and thickness observations

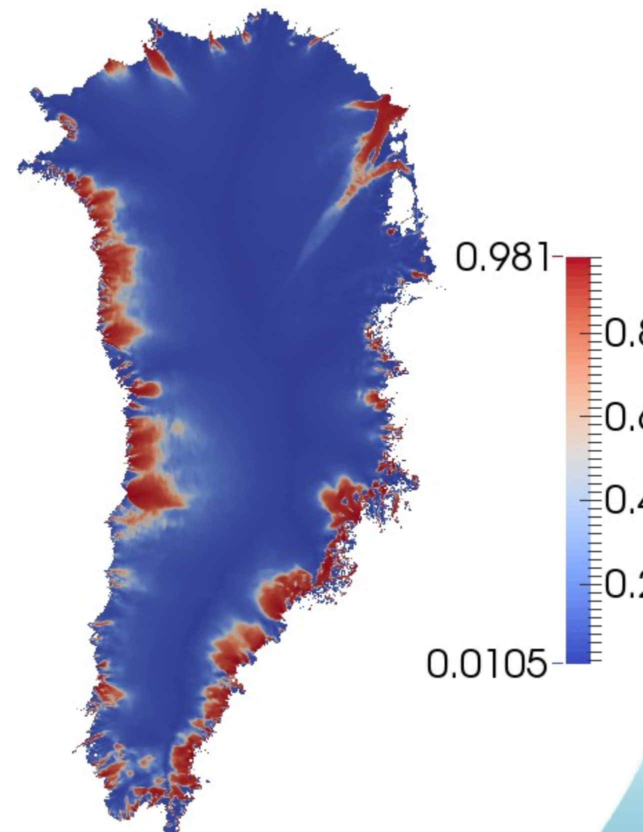
$\sigma_{\mathbf{u}}$: surf. velocity err. in m/yr



σ_H: thickness err. in km



σ_τ: $\dfrac{dH}{dt}$ err. in m/yr

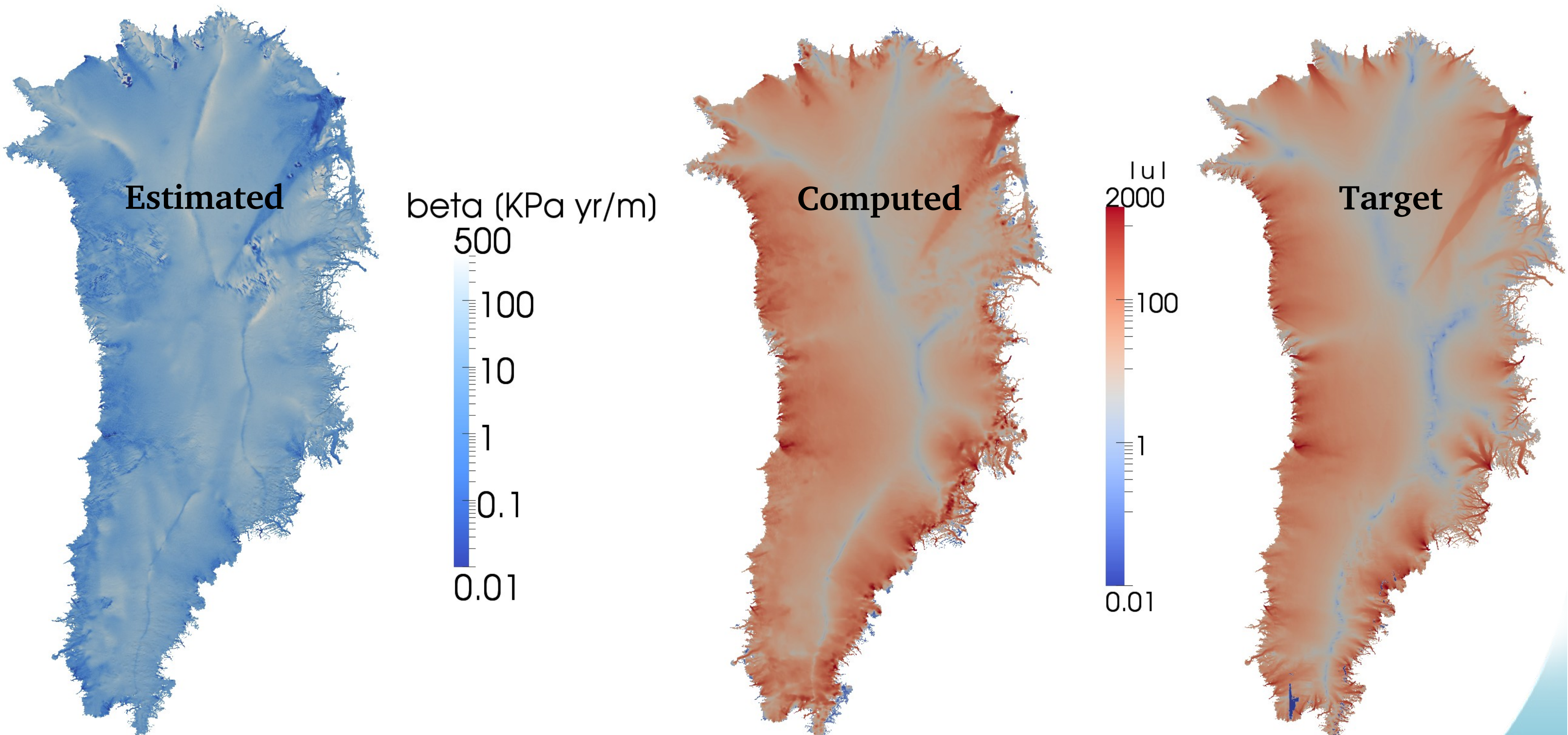


Geometry and fields Bamber et al.[2013], temperature computed with CISM (Shannon et al. [2013])

Greenland Inversion

velocity mismatch only, tuning basal friction

Inversion with 1.6M parameters



Basal friction coefficient (m/yr)

surface velocity magnitude (m/yr)

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

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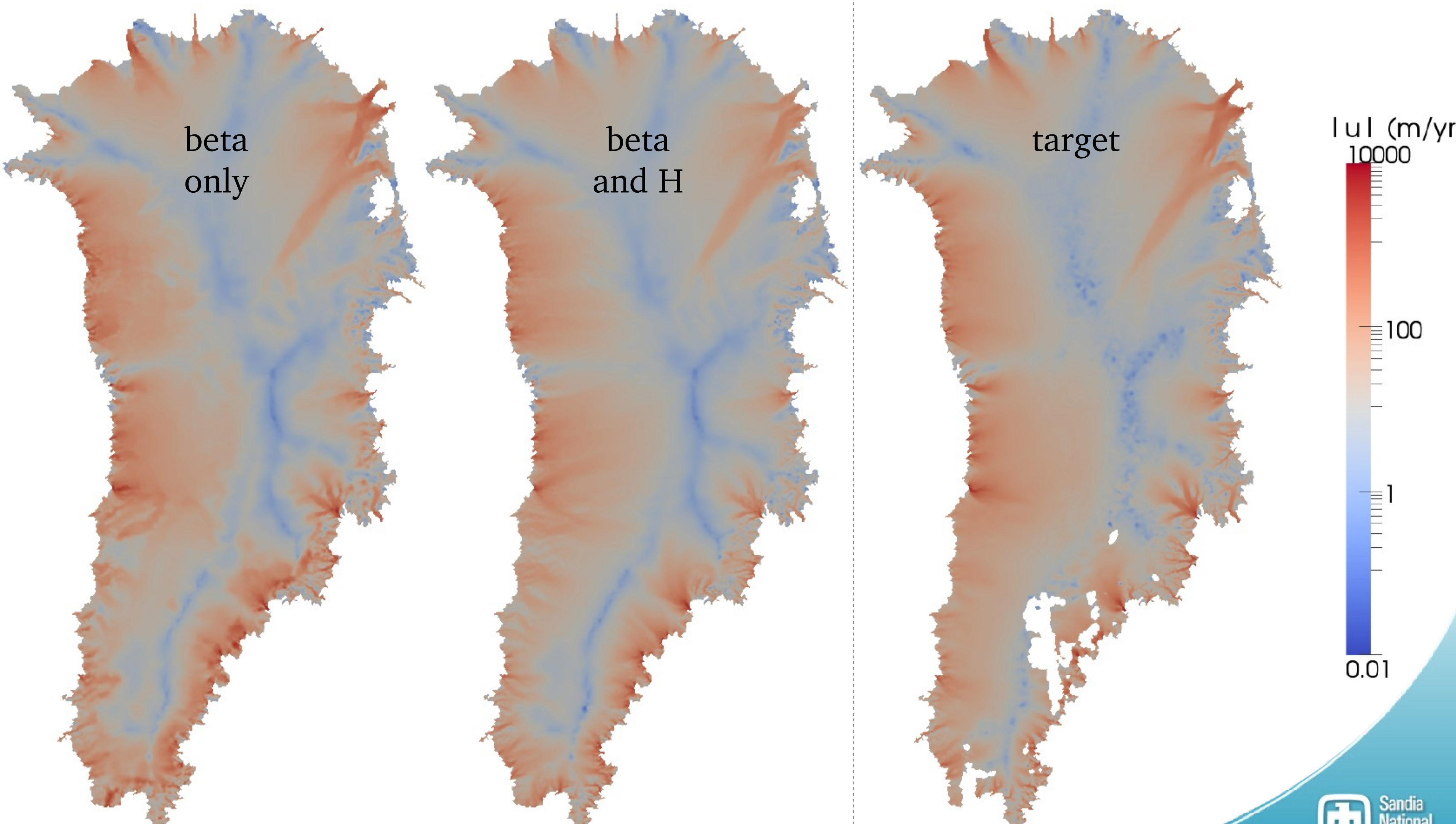
Deterministic Inversion for Greenland ice sheet

Inversion results: surface velocities

computed surface velocity

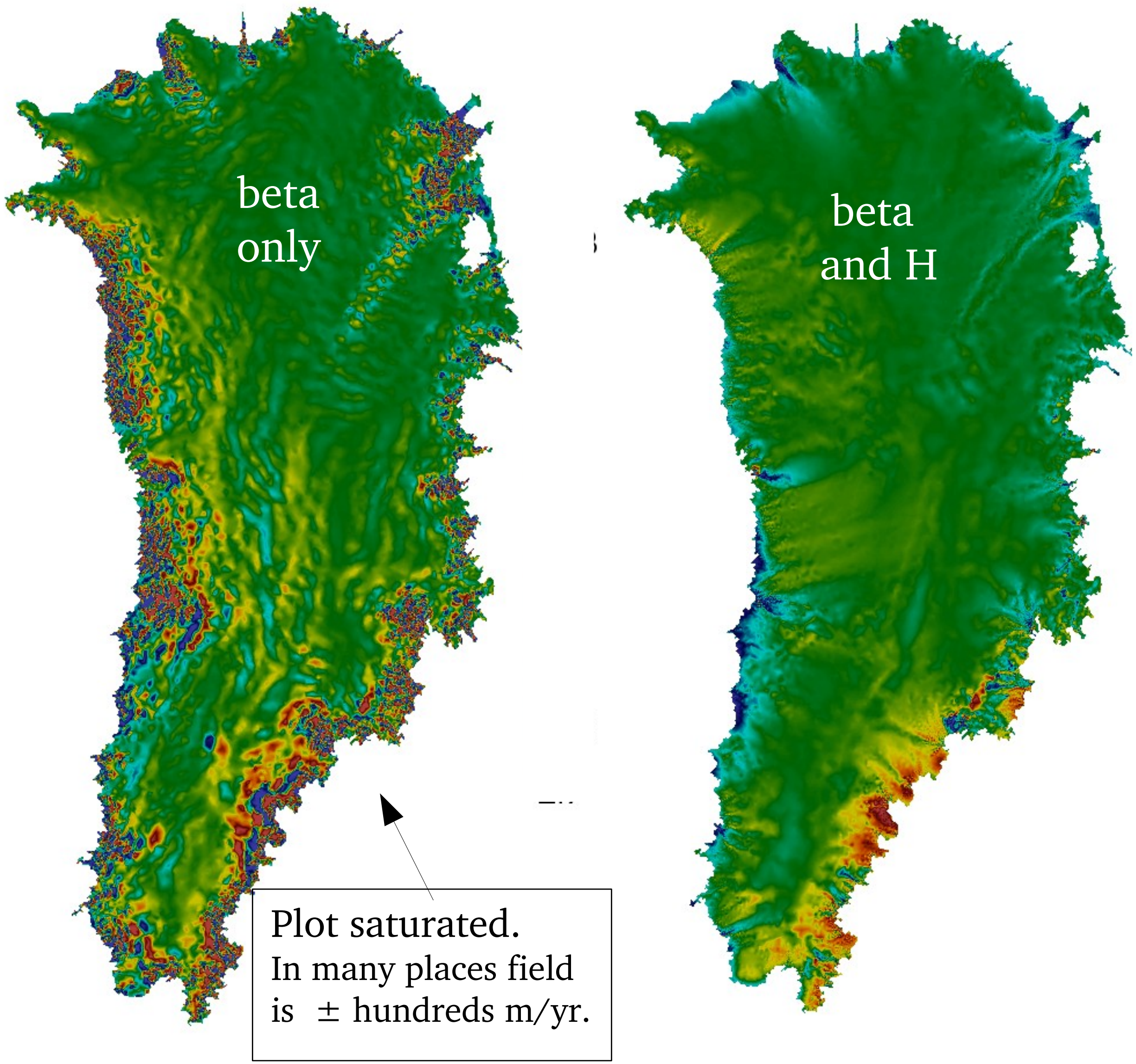
observed surface velocity



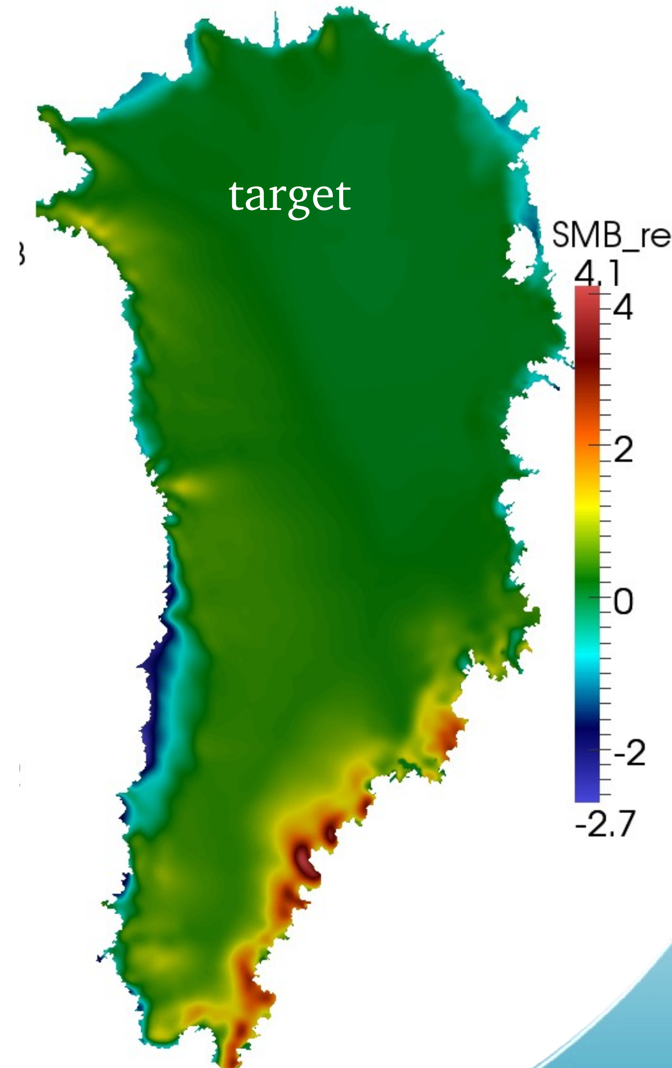
Deterministic Inversion for Greenland ice sheet

Inversion results: surface mass balance (SMB)

SMB (m/yr) needed for equilibrium



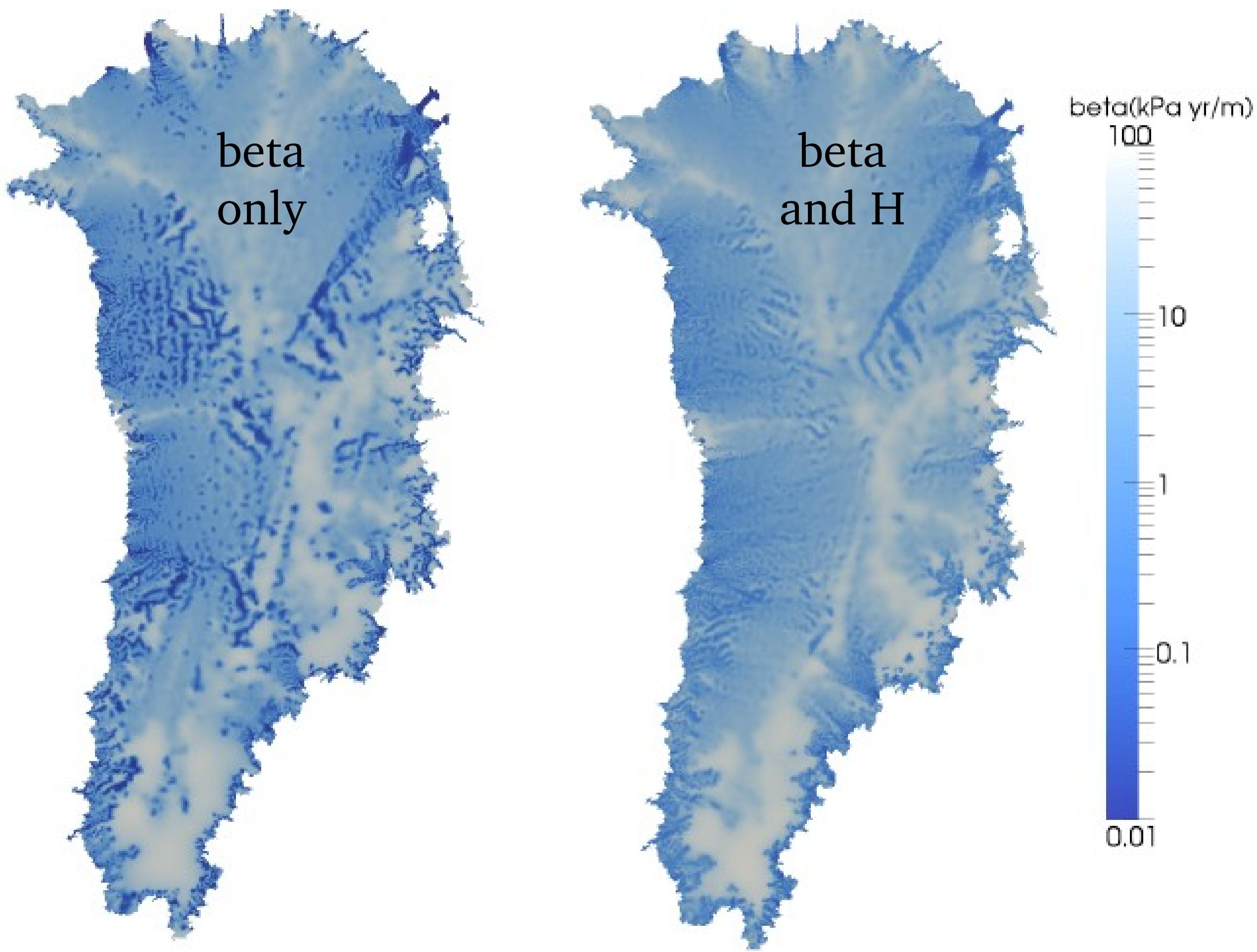
SMB from climate model
(Ettema et al. 2009, RACMO2/GR)



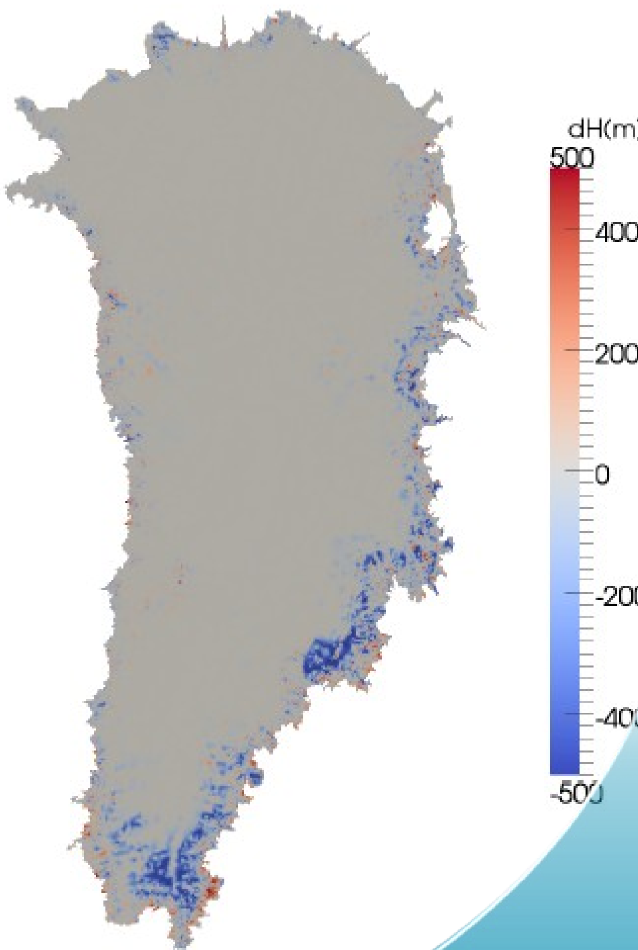
Deterministic Inversion for Greenland ice sheet

Estimated beta and change in topography

recovered basal friction



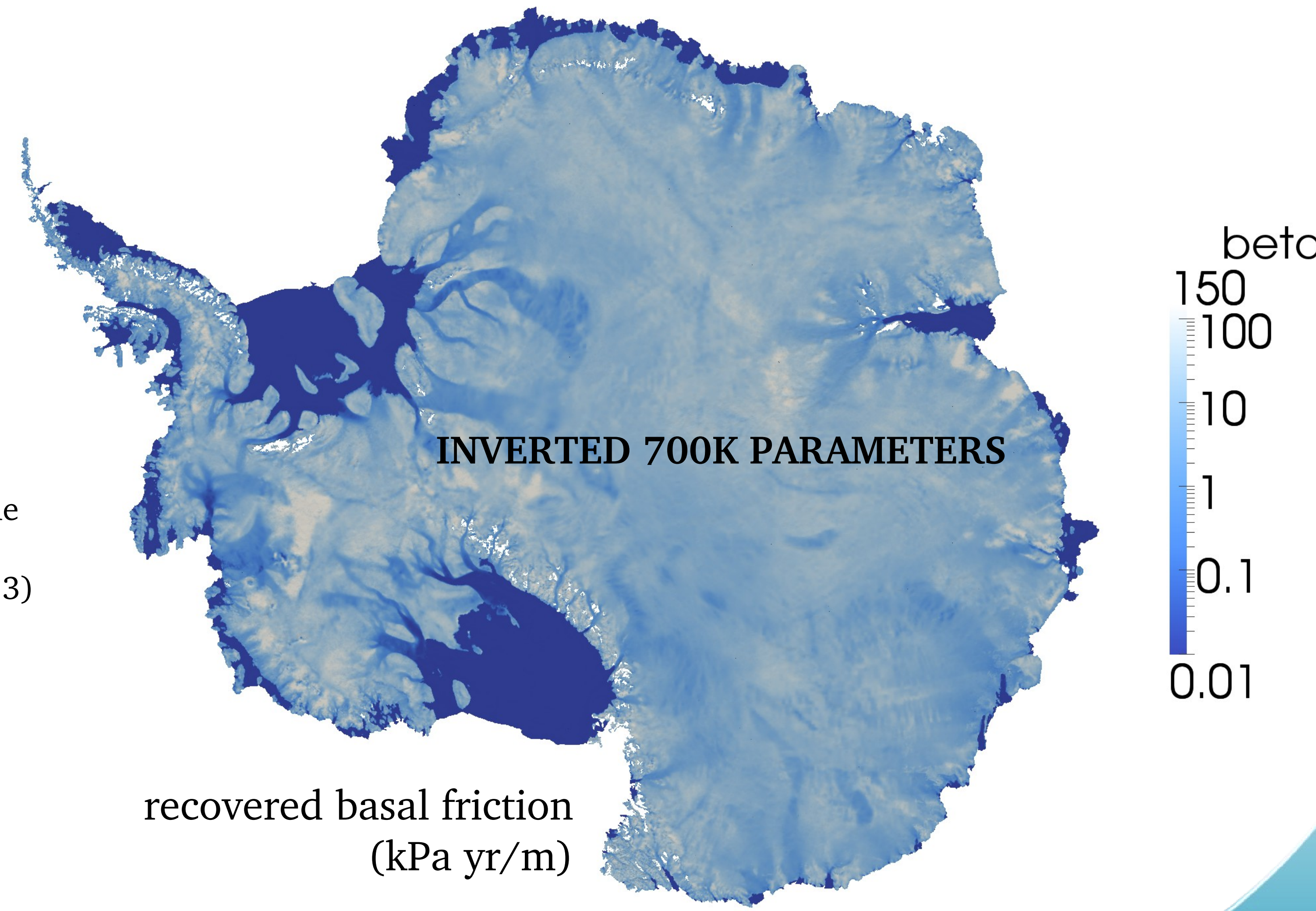
difference between recovered and observed thickness



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

Antarctica Inversion

velocity mismatch only, tuning basal friction

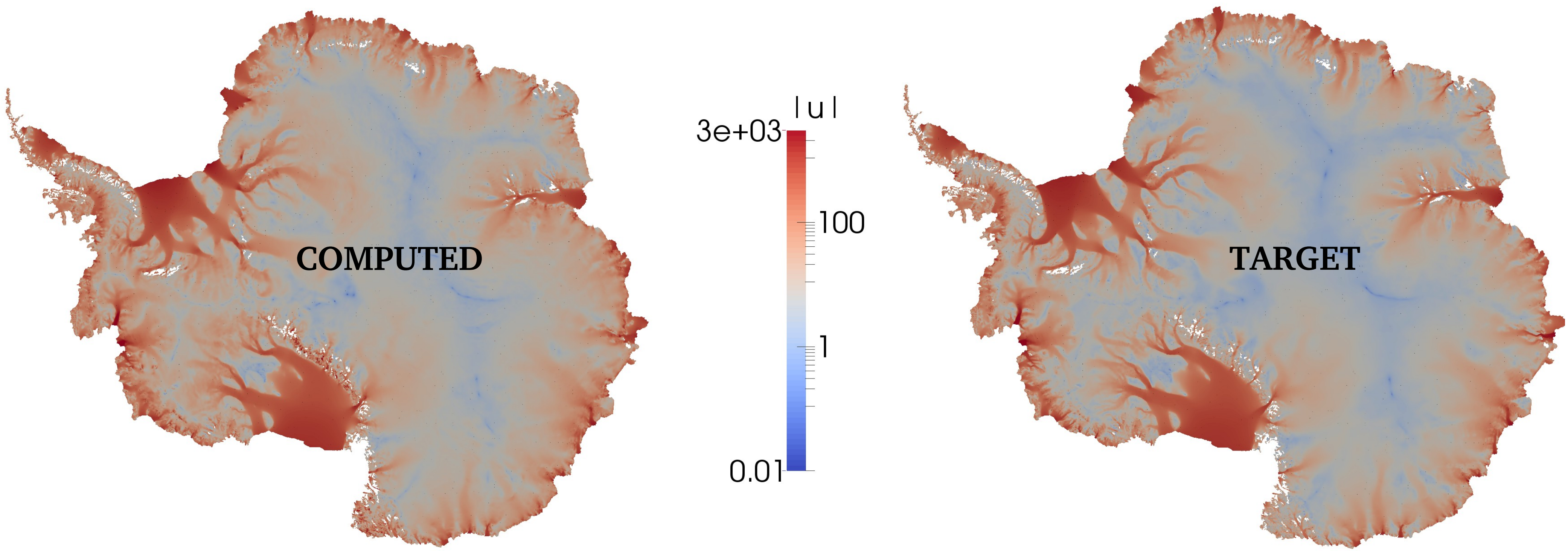


recovered basal friction
(kPa yr/m)

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)

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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.. but not that small!

Study on Antarctica ice-sheet by Omar Ghattas group:

$$\begin{aligned}\mathcal{J}(\beta) &= \int_\Sigma \frac{1}{\sigma_u^2} |\mathbf{u}(\beta) - \mathbf{u}^{obs}|^2 \, ds + \alpha \int_\Sigma |\nabla \beta|^2 \, ds \\ &= \mathcal{J}_{\text{misfit}}(\beta) + \mathcal{R}(\beta)\end{aligned}$$

$$\pi_{\text{prior}} \propto \exp\left[-\mathcal{R}(\beta)\right], \qquad \pi_{\text{like}} \propto \exp\left[-\mathcal{J}_{\text{misfit}}(\beta)\right], \qquad \pi_{\text{post}} \propto \exp\left[-\mathcal{J}(\beta)\right]$$

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

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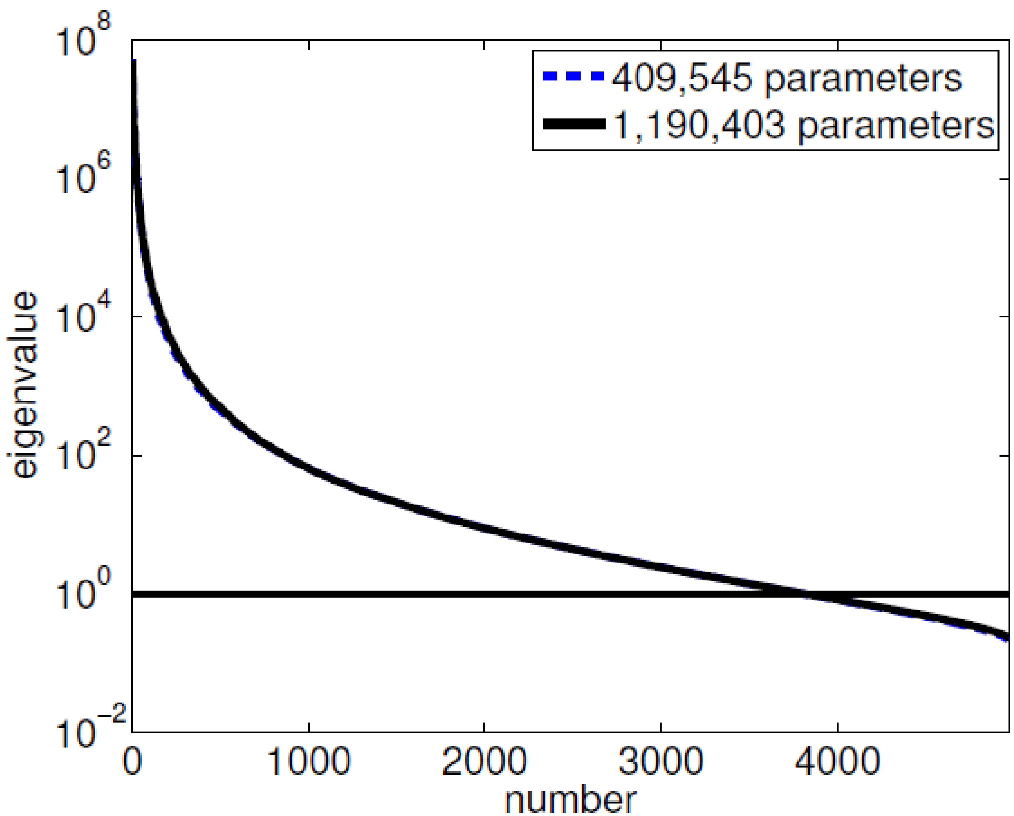
Building the Gaussian posterior approximation using Hessian from deterministic inversion

The Hessian provides a way to compute the Covariance of a Gaussian approx. of the posterior.

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

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

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

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***.

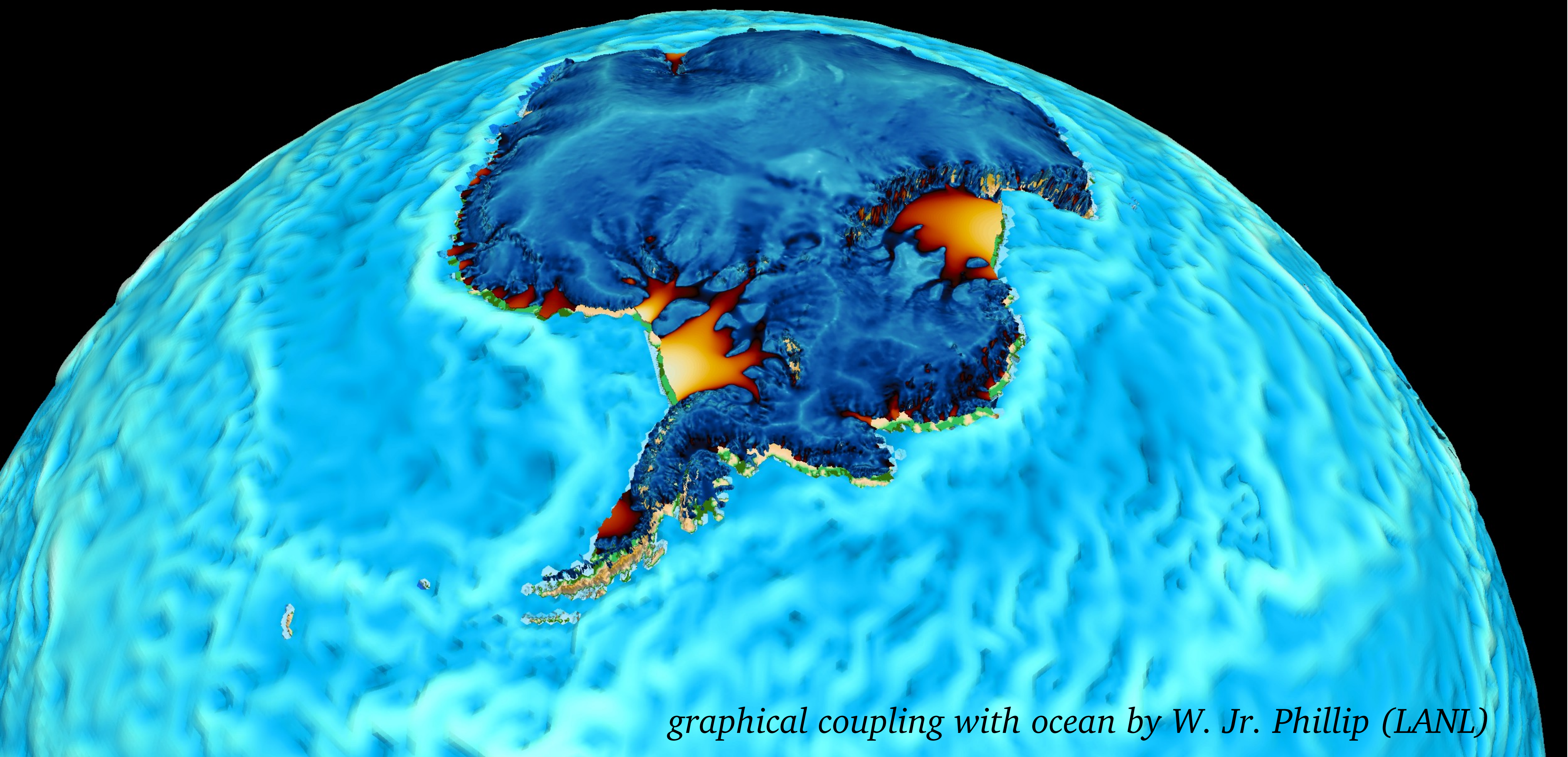
Considerations on Bayesian Calibration and Uncertainty Propagation

- High dimensional parameter space. Even if we accept the Gaussian approximation for the posterior, forward propagation is still unfeasible. Performing the Bayesian calibration to recover the true distribution for the parameters is also unfeasible.

- Strategies for forward propagations:
  - build emulator (polynomial chaos) of the forward model and sample emulator (issue: it's very expensive to build emulator)
  - use cheap physical models (e.g. SIA) or low resolution solves to reduce the cost of building the emulator.
  - use sensitivitive and active subspace methods to reduce parameter space.
  - use techniques such as the **compressed sensing technique*** to adaptively select significant modes and the basis for the parameter space.
  - Improve fidelity of the model (e.g. physical-based model for sliding considering subglacial hydrology) to reduce the parameter space.

*Jakeman, Eldred, Sargsyan, JCP, 2015

Thank you for your attention



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