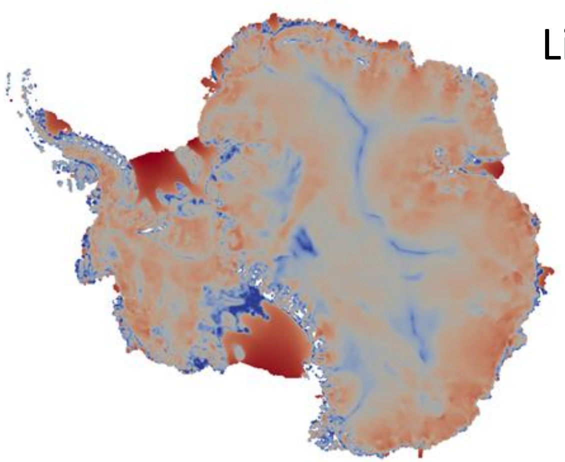
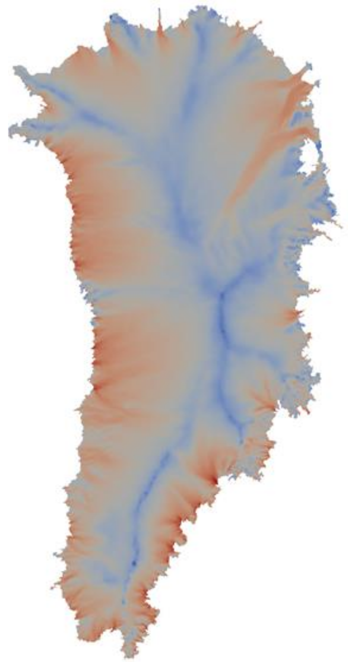
Towards Uncertainty Quantification in 21st Century Sea-Level Rise Predictions: Efficient Methods for Bayesian Calibration and Forward Propagation of Uncertainty for Land-Ice Models

I. Tezaur[1], J. Jakeman[1], M. Eldred[1], M. Perego[1], A. Salinger[1], S. Price[2]

[1] Sandia National Laboratories
Livermore, CA and Albuquerque, NM, USA
[2] Los Alamos National Laboratory
Los Alamos, NM, USA





SIAM Conference on Uncertainty Quantification (SIAM UQ16)
April 5-8, 2016
Lausanne, Switzerland

SAND2016-2717C

Sandia National Laboratories

Outline

- The PISCEES project, land-ice equations and relevant codes (*Albany/FELIX*, *CISM-Albany*, *MPAS-Alban*y).
- Uncertainty Quantification Problem Definition.
- Bayesian Calibration.
  - Methodology.
  - Demonstrations.
- Forward Propagation of Uncertainty.
  - Methodology.
  - Demonstrations.
- Summary and Future Work.

Outline

- **The PISCEES project, land-ice equations and relevant codes (*Albany/FELIX*, *CISM-Albany*, *MPAS-Albany*).**
- Uncertainty Quantification Problem Definition.
- Bayesian Calibration.
  - Methodology.
  - Demonstrations.
- Forward Propagation of Uncertainty.
  - Methodology.
  - Demonstrations.
- Summary and Future Work.

PISCEES Project and Relevant Solvers (*Albany-FELIX, CISM/MPAS-Albany*)

"PISCEES" = Predicting Ice Sheet Climate Evolution at Extreme Scales
5 year project funded by SciDAC, which began in June 2012

Sandia's Role in the PISCEES Project: to **develop** and **support** a robust and scalable land ice solver based on the "First-Order" (FO) Stokes approximation

Dycore will provide actionable predictions of 21st century sea-level rise (including uncertainty).

- **Requirements for our land-ice solver:**
  - Scalable, fast, robust.
  - Dynamical core (dycore) when coupled to codes that solve thickness and temperature evolution equations (*CISM/MPAS LI* codes).
  - Performance-portability.
  - Advanced analysis capabilities (adjoint-based deterministic inversion, Bayesian calibration, UQ, sensitivity analysis).

***Albany/FELIX* Solver (steady):**
Ice Sheet PDEs (First Order Stokes)
(stress-velocity solve)

⇄

***CISM/MPAS* Land Ice Codes (dynamic):**
Ice Sheet Evolution PDEs
(thickness, temperature evolution)

PISCEES Project and Relevant Solvers (*Albany-FELIX, CISM/MPAS-Albany*)

SciDAC Scientific Discovery through Advanced Computing

"PISCEES" = Predicting Ice Sheet Climate Evolution at Extreme Scales
5 year project funded by SciDAC, which began in June 2012

Sandia's Role in the PISCEES Project: to **develop** and **support** a robust and scalable land ice solver based on the "First-Order" (FO) Stokes approximation

Dycore will provide actionable predictions of 21st century sea-level rise (including uncertainty).

- **Requirements for our land-ice solver:**
  - Scalable, fast, robust.
  - Dynamical core (dycore) when coupled to codes that solve thickness and temperature evolution equations (*CISM/MPAS LI* codes).
  - Performance-portability.
  - Advanced analysis capabilities (adjoint-based deterministic inversion, **Bayesian calibration, UQ,** sensitivity analysis).

This talk

Albany/FELIX Solver (steady):
Ice Sheet PDEs (First Order Stokes)
(stress-velocity solve)

⇄

CISM/MPAS Land Ice Codes (dynamic):
Ice Sheet Evolution PDEs
(thickness, temperature evolution)

Laboratories

The First-Order Stokes Model for Ice Sheets & Glaciers

- Ice sheet dynamics are given by the ***"First-Order" Stokes PDEs***: approximation* to viscous incompressible ***quasi-static*** Stokes flow with power-law viscosity.

$$\begin{cases} -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_1) = -\rho g \dfrac{\partial s}{\partial x} \\ -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_2) = -\rho g \dfrac{\partial s}{\partial y} \end{cases}, \quad \text{in } \Omega$$

$$\dot{\boldsymbol{\epsilon}}_1{}^T = (2\dot{\epsilon}_{11} + \dot{\epsilon}_{22}, \dot{\epsilon}_{12}, \dot{\epsilon}_{13})$$
$$\dot{\boldsymbol{\epsilon}}_2{}^T = (2\dot{\epsilon}_{12}, \dot{\epsilon}_{11} + 2\dot{\epsilon}_{22}, \dot{\epsilon}_{23})$$
$$\dot{\epsilon}_{\mathrm{ij}} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

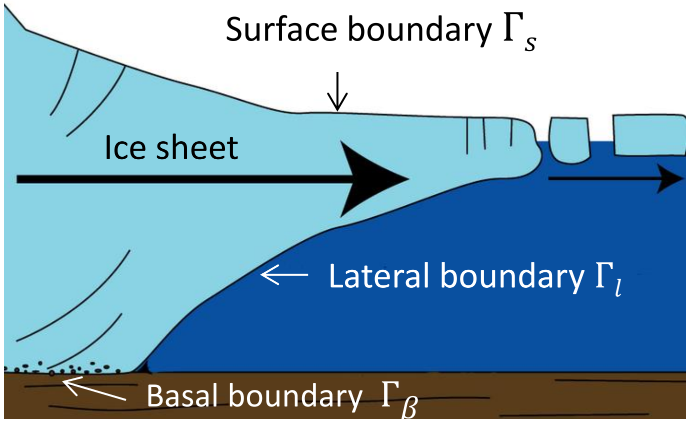
- Viscosity μ is nonlinear function given by "***Glen's law***":

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2}\sum_{ij} \dot{\boldsymbol{\epsilon}}_{ij}{}^2\right)^{\left(\frac{1}{2n}-\frac{1}{2}\right)} \qquad (n = 3)$$

- Relevant boundary conditions:
  - ***Stress-free BC:*** $2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} = 0$, on Γ_s
  - ***Floating ice BC:***

$$2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} = \begin{cases} \rho g z \boldsymbol{n}, & \text{if } z > 0 \\ 0, & \text{if } z \le 0 \end{cases}, \quad \text{on } \Gamma_l$$

  - ***Basal sliding BC:*** $2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} + \beta u_i = 0$, on Γ_β



β = sliding coefficient ≥ 0

***Assumption:** aspect ratio δ is small and normals to upper/lower surfaces are almost vertical.

Implementation of *Albany/FELIX* using *Trilinos*

The ***Albany/FELIX**** First Order Stokes solver is implemented in a Sandia parallel C++ finite element code called…

Started by A. Salinger

Land Ice Physics Set (***Albany/FELIX code***)

Other Albany Physics Sets

"Agile Components"

- Discretizations/meshes
- Solver libraries
- Preconditioners
- Automatic differentiation
- Many others!

- Parameter estimation
- Uncertainty quantification
- Optimization
- Bayesian inference

- Configure/build/test/documentation

*Use of **Trilinos** components has enabled the **rapid** development of the **Albany/FELIX** First Order Stokes dycore!*

*FELIX = "Finite Elements for Land Ice eXperiments".

Ice Sheet Evolution Models

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

$$\frac{\partial h}{\partial t} = -\nabla \cdot (\bar{\boldsymbol{u}} h) + \dot{b}$$

where $\bar{\boldsymbol{u}}$ = vertically averaged velocity, $\dot{b}$ = surface mass balance (conservation of mass).

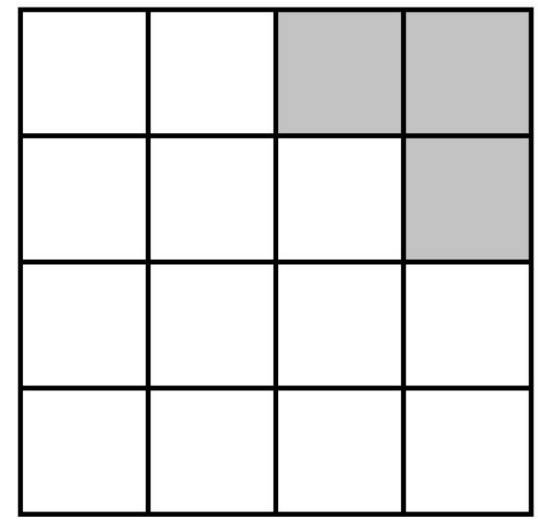
- ***Temperature equation*** (advection-diffusion):

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) - \rho c \boldsymbol{u} \cdot \nabla T + 2 \dot{\boldsymbol{\epsilon}} \boldsymbol{\sigma}$$

(energy balance).

- ***Flow factor*** A in Glen's law depends on temperature T: $A = A(T)$.

- Ice sheet ***grows/retreats*** depending on thickness h.



time t_0

Ice-covered ("active") cells shaded in white ($h > h_{min}$)

Ice Sheet Evolution Models

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

$$\frac{\partial h}{\partial t} = -\nabla \cdot (\bar{\boldsymbol{u}} h) + \dot{b}$$

where $\bar{\boldsymbol{u}}$ = vertically averaged velocity, $\dot{b}$ = surface mass balance (conservation of mass).

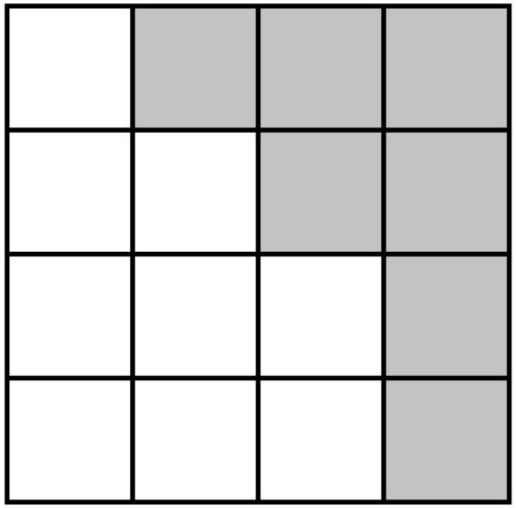
- ***Temperature equation*** (advection-diffusion):

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) - \rho c \boldsymbol{u} \cdot \nabla T + 2 \dot{\boldsymbol{\epsilon}} \boldsymbol{\sigma}$$

(energy balance).

- ***Flow factor*** A in Glen's law depends on temperature T: $A = A(T)$.

- Ice sheet ***grows/retreats*** depending on thickness h.



time t_1

Ice-covered ("active") cells shaded in white ($h > h_{min}$)

Ice Sheet Evolution Models

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

$$\frac{\partial h}{\partial t} = -\nabla \cdot (\overline{\boldsymbol{u}}h) + \dot{b}$$

where $\overline{\boldsymbol{u}}$ = vertically averaged velocity, $\dot{b}$ = surface mass balance (conservation of mass).

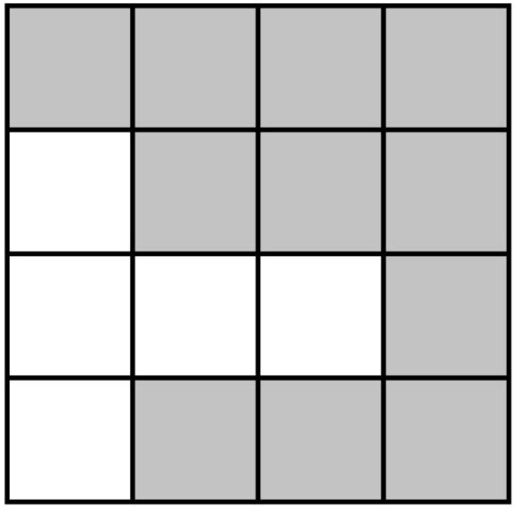
- ***Temperature equation*** (advection-diffusion):

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) - \rho c \boldsymbol{u} \cdot \nabla T + 2\dot{\boldsymbol{\epsilon}}\boldsymbol{\sigma}$$

(energy balance).

- ***Flow factor*** A in Glen's law depends on temperature T: $A = A(T)$.

- Ice sheet ***grows/retreats*** depending on thickness h.



time t_2

Ice-covered ("active") cells shaded in white ($h > h_{min}$)

Sandia National Laboratories

Interfaces to *CISM* and *MPAS LI* for Transient Simulations

CISM-Albany

cism_driver

CISM (Fortran)
Thickness evolution, temperature solve, coupling to CESM

C++/Fortran Interface, Mesh Conversion

output file

Albany/FELIX (C++)
velocity solve

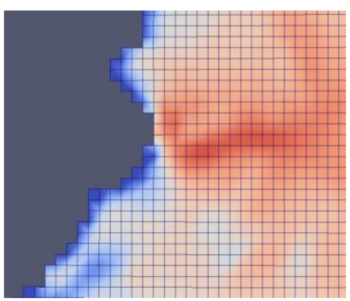
MPAS LI-Albany

LandIce_model

MPAS Land-Ice (Fortran)
Thickness evolution, temperature solve, coupling to DOE-ESM

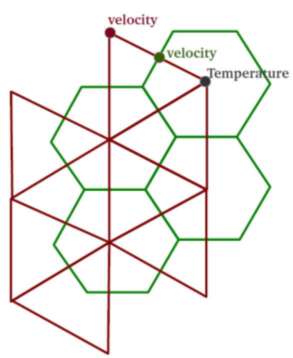
C++/Fortran Interface, Mesh Conversion

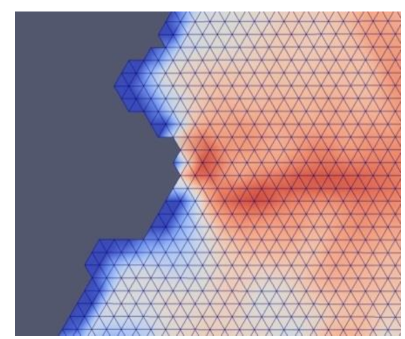
output file



- Structured hexahedral meshes (rectangles extruded to hexes).

- Tetrahedral meshes (dual of hexaganonal mesh, extruded to tets).





Albany/FELIX has been coupled to two land ice dycores: **C**ommunity **I**ce **S**heet **M**odel (***CISM***) and **M**odel for **P**rediction **A**cross **S**cales for **L**and **I**ce (***MPAS LI***)

Sandia National Laboratories

Outline

- The PISCEES project, land-ice equations and relevant codes (*Albany/FELIX*, *CISM-Albany*, *MPAS-Alban*y).
- **Uncertainty Quantification Problem Definition.**
- Bayesian Calibration.
  - Methodology.
  - Demonstrations.
- Forward Propagation of Uncertainty.
  - Methodology.
  - Demonstrations.
- Summary and Future Work.

Uncertainty Quantification (UQ) Problem Definition

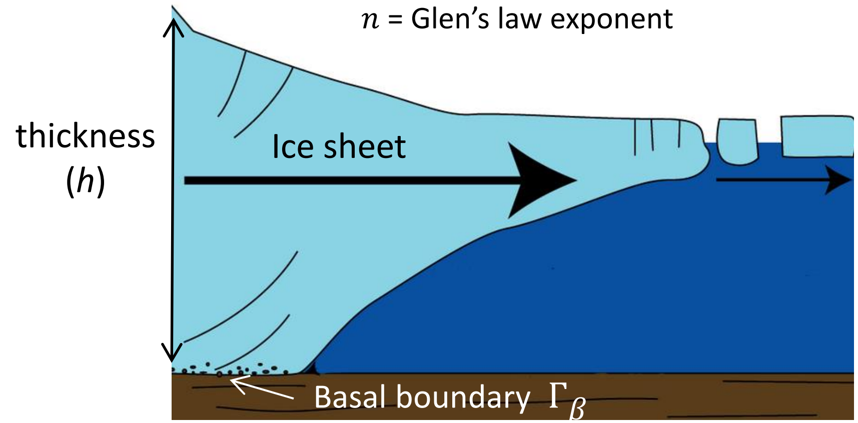
Quantity of Interest (QoI) in Ice Sheet Modeling:
total ice mass loss/gain during 21st century
→ ***sea level rise prediction.***

There are several sources of uncertainty, most notably:

- Climate forcings (e.g., surface mass balance).
- Basal friction (β).
- Ice sheet thickness (h).
- Geothermal heat flux.
- Model parameters (e.g., Glen's flow law exponent).

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2} \sum_{ij} \dot{\epsilon}_{ij}^{\,2} + \gamma \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

n = Glen's law exponent



Basal sliding BC:
$2\mu\dot{\epsilon}_i \cdot \boldsymbol{n} + \beta u_i = 0$, on Γ_β

Uncertainty Quantification (UQ) Problem Definition

Quantity of Interest (QoI) in Ice Sheet Modeling:
total ice mass loss/gain during 21st century
→ ***sea level rise prediction.***

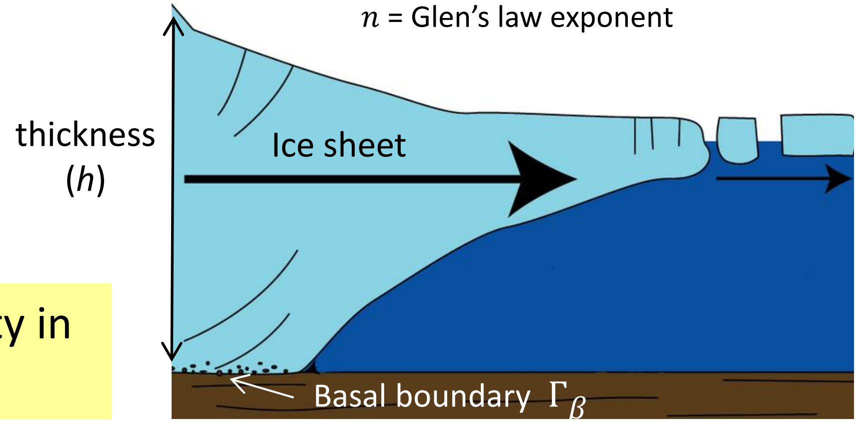
There are several sources of uncertainty, most notably:

- Climate forcings (e.g., surface mass balance).
- **Basal friction ($\boldsymbol{\beta}$).**
- Ice sheet thickness (h).
- Geothermal heat flux.
- Model parameters (e.g., Glen's flow law exponent).

As a first step, we focus on effect of uncertainty in **basal friction ($\boldsymbol{\beta}$)** only.

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2} \sum_{ij} \dot{\epsilon}_{ij}^{\,2} + \gamma \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

n = Glen's law exponent



Basal sliding BC:
$2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} + \beta u_i = 0$, on Γ_β

Uncertainty Quantification (UQ) Problem Definition

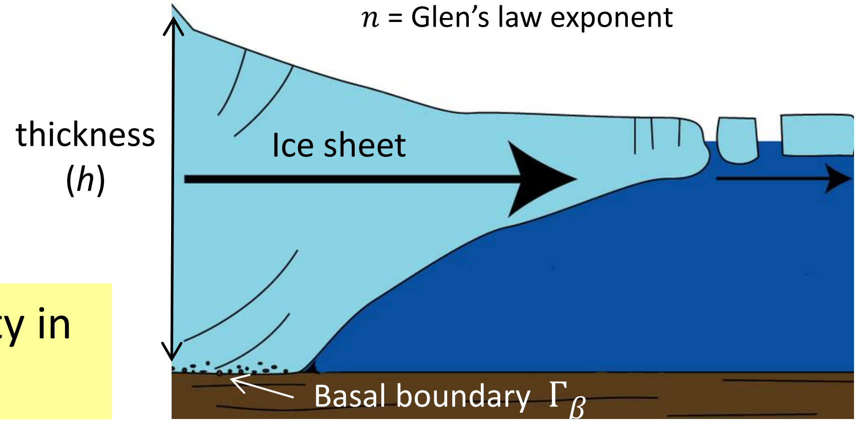
Quantity of Interest (QoI) in Ice Sheet Modeling:
total ice mass loss/gain during 21st century
→ ***sea level rise prediction.***

There are several sources of uncertainty, most notably:

- Climate forcings (e.g., surface mass balance).
- **Basal friction ($\boldsymbol{\beta}$).**
- Ice sheet thickness (h).
- Geothermal heat flux.
- Model parameters (e.g., Glen's flow law exponent).

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2} \sum_{ij} \dot{\boldsymbol{\epsilon}}_{ij}^{\,2} + \gamma \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

n = Glen's law exponent



As a first step, we focus on effect of uncertainty in **basal friction ($\boldsymbol{\beta}$)** only.

This is a ***real*** application where standard UQ methods ***do not work*** out of the box!

Basal sliding BC:
$2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} + \beta u_i = 0$, on Γ_β

Uncertainty Quantification (UQ) Problem Definition

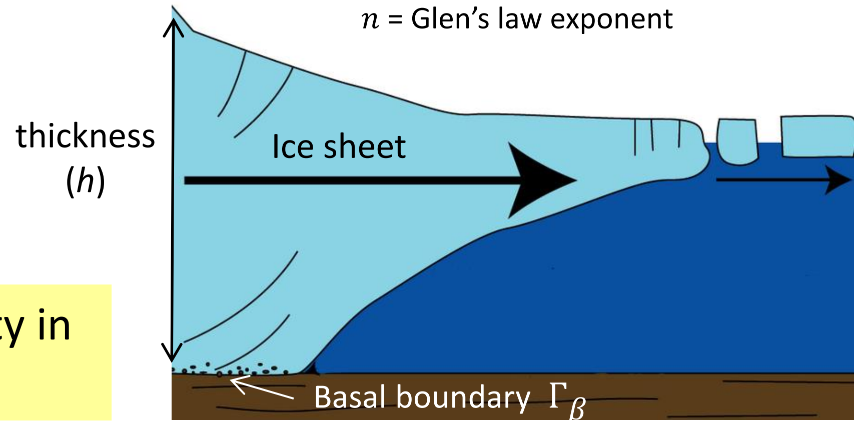
Quantity of Interest (QoI) in Ice Sheet Modeling:
total ice mass loss/gain during 21st century
→ ***sea level rise prediction.***

There are several sources of uncertainty, most notably:

- Climate forcings (e.g., surface mass balance).
- **Basal friction ($\boldsymbol{\beta}$).**
- Ice sheet thickness (h).
- Geothermal heat flux.
- Model parameters (e.g., Glen's flow law exponent).

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2} \sum_{ij} \dot{\epsilon}_{ij}{}^{2} + \gamma \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

n = Glen's law exponent



As a first step, we focus on effect of uncertainty in **basal friction ($\boldsymbol{\beta}$)** only.

This is a ***real*** application where standard UQ methods ***do not work*** out of the box!

Basal sliding BC:
$2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} + \beta u_i = 0$, on Γ_β

→ This talk tells the story of what we have tried and learned.

Uncertainty Quantification Workflow

Goal: UQ in 21st century aggregate ice sheet mass loss (QoI)

- **Deterministic inversion:** perform adjoint-based deterministic inversion to estimate initial ice sheet state (i.e., characterize the present state of the ice sheet to be used for performing prediction runs).

- **Bayesian calibration:** construct the posterior distribution using Markov Chain Monte Carlo (MCMC) run on an emulator of the forward model → *Bayes' Theorem:* assume prior distribution; update using data:

$$\underbrace{\pi(\theta|d)}_{\text{posterior}} = \frac{\overbrace{\pi(d|\theta)}^{\text{likelihood}}\ \overbrace{\pi(\theta)}^{\text{prior}}}{\pi(d)} = \frac{\pi(d|\theta)\ \pi(\theta)}{\int \pi(d|\theta)\ \pi(\theta)\ d\theta}$$

What are the parameters that render a given set of observations?

- **Forward propagation:** sample the obtained distribution and perform ensemble of forward propagation runs to compute the uncertainty in the QoI.

What is the impact of uncertain parameters in the model on quantities of interest (QoI)?

Laboratories

Uncertainty Quantification Workflow

Goal: UQ in 21st century aggregate ice sheet mass loss (QoI)

- **Deterministic inversion:** perform adjoint-based deterministic inversion to estimate initial ice sheet state (i.e., characterize the present state of the ice sheet to be used for performing prediction runs).

What are the parameters that render a given set of observations?

This talk

- **Bayesian calibration:** construct the posterior distribution using Markov Chain Monte Carlo (MCMC) run on an emulator of the forward model → *Bayes' Theorem:* assume prior distribution; update using data:

$$\underbrace{\pi(\theta|d)}_{\text{posterior}} = \frac{\overbrace{\pi(d|\theta)}^{\text{likelihood}}\ \overbrace{\pi(\theta)}^{\text{prior}}}{\pi(d)} = \frac{\pi(d|\theta)\ \pi(\theta)}{\int \pi(d|\theta)\ \pi(\theta)\ d\theta}$$

- **Forward propagation:** sample the obtained distribution and perform ensemble of forward propagation runs to compute the uncertainty in the QoI.

What is the impact of uncertain parameters in the model on quantities of interest (QoI)?

Outline

- The PISCEES project, land-ice equations and relevant codes (*Albany/FELIX*, *CISM-Albany*, *MPAS-Alban*y).
- Uncertainty Quantification Problem Definition.
- **Bayesian Calibration.**
    - **Methodology.**
    - **Demonstrations.**
- Forward Propagation of Uncertainty.
    - Methodology.
    - Demonstrations.
- Summary and Future Work.

Bayesian Calibration: Demonstration of Workflow using KLE

Albany/FELIX has been hooked up to ***DAKOTA*** (in "black-box" mode) for ***UQ/ Bayesian calibration.***

Difficulty in UQ: "Curse of Dimensionality"
The β field inversion problems has $O(100K)$ dimensions!

Bayesian Calibration: Demonstration of Workflow using KLE

Albany/FELIX has been hooked up to ***DAKOTA*** (in "black-box" mode) for ***UQ/ Bayesian calibration.***

Difficulty in UQ: "Curse of Dimensionality"
The β field inversion problems has $O(100K)$ dimensions!

Approach: Reduce $O(100K)$ dimensional problem to $O(10)$ dimensional problem.

Bayesian Calibration: Demonstration of Workflow using KLE

Albany/FELIX has been hooked up to ***DAKOTA*** (in "black-box" mode) for ***UQ/ Bayesian calibration.***

Difficulty in UQ: "Curse of Dimensionality"
The β field inversion problems has $O(100K)$ dimensions!

Approach: Reduce $O(100K)$ dimensional problem to $O(10)$ dimensional problem.

- For initial demonstration of workflow, we use the ***Karhunen-Loeve Expansion (KLE)***:

Bayesian Calibration: Demonstration of Workflow using KLE

Albany/FELIX has been hooked up to ***DAKOTA*** (in "black-box" mode) for ***UQ/ Bayesian calibration.***

Difficulty in UQ: "Curse of Dimensionality"
The β field inversion problems has $O(100K)$ dimensions!

Approach: Reduce $O(100K)$ dimensional problem to $O(10)$ dimensional problem.

- For initial demonstration of workflow, we use the ***Karhunen-Loeve Expansion (KLE)***:

  1. Assume analytic covariance kernel $C(r_1, r_2) = exp\left(-\frac{(r_1 - r_2)^2}{L^2}\right)$.

Bayesian Calibration: Demonstration of Workflow using KLE

Albany/FELIX has been hooked up to ***DAKOTA*** (in "black-box" mode) for ***UQ/ Bayesian calibration.***

Difficulty in UQ: "Curse of Dimensionality"
The β field inversion problems has $O(100K)$ dimensions!

Approach: Reduce $O(100K)$ dimensional problem to $O(10)$ dimensional problem.

- For initial demonstration of workflow, we use the ***Karhunen-Loeve Expansion (KLE)***:

  1. Assume analytic covariance kernel $C(r_1, r_2) = exp\left(-\frac{(r_1 - r_2)^2}{L^2}\right)$.
  2. Perform eigenvalue decomposition of C.

Bayesian Calibration: Demonstration of Workflow using KLE

Albany/FELIX has been hooked up to ***DAKOTA*** (in "black-box" mode) for ***UQ/ Bayesian calibration.***

Difficulty in UQ: "Curse of Dimensionality"
The β field inversion problems has $O(100K)$ dimensions!

Approach: Reduce $O(100K)$ dimensional problem to $O(10)$ dimensional problem.

- For initial demonstration of workflow, we use the ***Karhunen-Loeve Expansion (KLE)***:

  1. Assume analytic covariance kernel $C(r_1, r_2) = exp\left(-\frac{(r_1-r_2)^2}{L^2}\right)$.
  2. Perform eigenvalue decomposition of C.
  3. Expand* $\beta - \bar{\beta}$ in basis of eigenvectors $\{\boldsymbol{\phi}_k\}$ of C, with random variables $\{{\xi_k}^{\beta}\}$:

$$\boxed{\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{{\lambda_k}^{\beta}}\boldsymbol{\phi}_k \, {\xi_k}^{\beta}(\omega)}$$

$\bar{\beta}$ = initial condition for β (from deterministic inversion or spin-up)

*In practice, expansion is done on $\log(\beta)$ to avoid negative values of β.

Bayesian Calibration: Demonstration of Workflow using KLE

Albany/FELIX has been hooked up to ***DAKOTA*** (in "black-box" mode) for ***UQ/ Bayesian calibration.***

Difficulty in UQ: "Curse of Dimensionality"
The β field inversion problems has $O(100K)$ dimensions!

Approach: Reduce $O(100K)$ dimensional problem to $O(10)$ dimensional problem.

- For initial demonstration of workflow, we use the ***Karhunen-Loeve Expansion (KLE)***:

Offline

1. Assume analytic covariance kernel $C(r_1, r_2) = exp\left(-\frac{(r_1 - r_2)^2}{L^2}\right)$.
2. Perform eigenvalue decomposition of C.

Online

3. Expand* $\beta - \bar{\beta}$ in basis of eigenvectors $\{\boldsymbol{\phi}_k\}$ of C, with random variables $\{{\xi_k}^{\beta}\}$:

$$\boxed{\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{{\lambda_k}^{\beta}} \boldsymbol{\phi}_k \, {\xi_k}^{\beta}(\omega)}$$

$\bar{\beta}$ = initial condition for β (from deterministic inversion or spin-up)

Inference/calibration is for coefficients of KLE
$\Rightarrow$ ***significant dimension reduction***.

*In practice, expansion is done on $\log(\beta)$ to avoid negative values of β.

Sandia National Laboratories

Bayesian Calibration: Demonstration of Workflow using KLE (cont'd)

- **<u>Step 1 (*Trilinos*):</u>** Reduce $O(100K)$ dimensional problem to $O(10)$ dimensional problem using ***Karhunen-Loeve Expansion (KLE)***:

Offline

1. Assume analytic covariance kernel $C(r_1, r_2) = exp\left(-\frac{(r_1 - r_2)^2}{L^2}\right)$.
2. Perform eigenvalue decomposition of C.

Online

3. Expand* $\beta - \bar{\beta}$ in basis of eigenvectors $\{\boldsymbol{\phi}_k\}$ of C, with random variables $\{\xi_k{}^{\beta}\}$:

$$\boxed{\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{\lambda_k{}^{\beta}}\boldsymbol{\phi}_k \xi_k{}^{\beta}(\omega)}$$

$\bar{\beta}$= initial condition for β (from deterministic inversion or spin-up)

*In practice, expansion is done on $\log(\beta)$ to avoid negative values of β.

Trilinos

Sandia National Laboratories

Bayesian Calibration: Demonstration of Workflow using KLE (cont'd)

- **<u>Step 1 (*Trilinos*):</u>** Reduce $O(100K)$ dimensional problem to $O(10)$ dimensional problem using ***Karhunen-Loeve Expansion (KLE)***:

Offline

1. Assume analytic covariance kernel $C(r_1, r_2) = exp\left(-\frac{(r_1 - r_2)^2}{L^2}\right)$.
2. Perform eigenvalue decomposition of C.

Online

3. Expand* $\beta - \bar{\beta}$ in basis of eigenvectors $\{\boldsymbol{\phi}_k\}$ of C, with random variables $\{\xi_k{}^{\beta}\}$:

$$\boxed{\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{\lambda_k{}^{\beta}}\, \boldsymbol{\phi}_k\, \xi_k{}^{\beta}(\omega)}$$

$\bar{\beta}$= initial condition for β (from deterministic inversion or spin-up)

- **<u>Step 2 *(DAKOTA)*:</u>** ***Polynomial Chaos Expansion (PCE)*** emulator for mismatch (over surface velocity, SMB, thickness) discrepancy.

*In practice, expansion is done on $\log(\beta)$ to avoid negative values of β.

Trilinos DAKOTA Sandia National Laboratories

Bayesian Calibration: Demonstration of Workflow using KLE (cont'd)

- **Step 1 (*Trilinos*):** Reduce $O(100K)$ dimensional problem to $O(10)$ dimensional problem using ***Karhunen-Loeve Expansion (KLE)***:

Offline

1. Assume analytic covariance kernel $C(r_1, r_2) = exp\left(-\frac{(r_1-r_2)^2}{L^2}\right)$.
2. Perform eigenvalue decomposition of C.

Online

3. Expand* $\beta - \bar{\beta}$ in basis of eigenvectors $\{\boldsymbol{\phi}_k\}$ of C, with random variables $\{{\xi_k}^\beta\}$:

$$\boxed{\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{{\lambda_k}^\beta}\boldsymbol{\phi}_k\, {\xi_k}^\beta(\omega)}$$

$\bar{\beta}$= initial condition for β (from deterministic inversion or spin-up)

- **Step 2 (*DAKOTA*):** ***Polynomial Chaos Expansion (PCE)*** emulator for mismatch (over surface velocity, SMB, thickness) discrepancy.

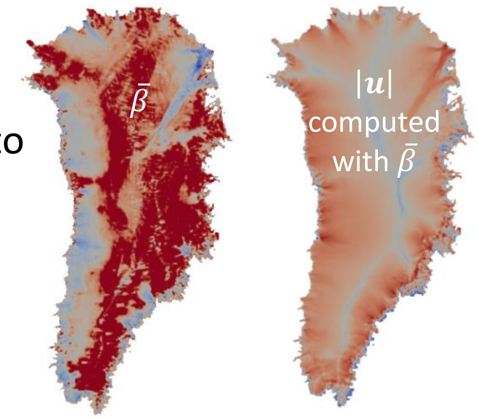
- **Step 3 (*QUESO*):** ***Markov Chain Monte Carlo (MCMC)*** calibration using PCE emulator.

  →can obtain MAP point and posterior distributions on KLE coefficients.

*In practice, expansion is done on $\log(\beta)$ to avoid negative values of β.

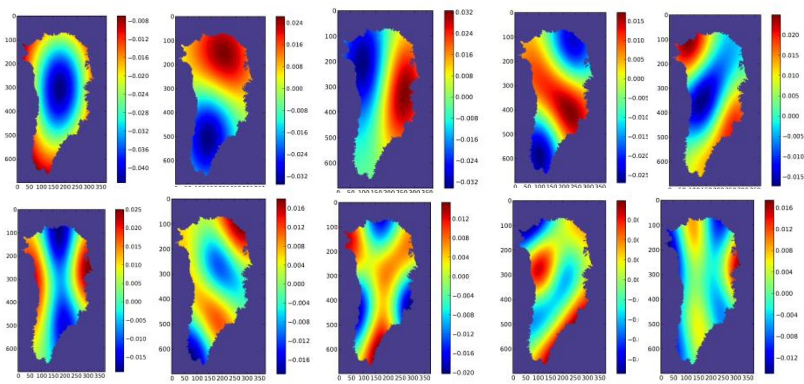
Initial Demonstration: Bayesian Calibration for 4km GIS Problem

- Mean $\bar{\beta}$ field obtained through spin-up over 100 years (cheaper than inversion, gives reasonable agreement with present-day velocity field).
- Correlation length L (L^2=*0.05*) selected s.t. slow decay of KLE eigenvalues to enable refinement *(left):* 10 KLE modes capture 27.3% of covariance energy.

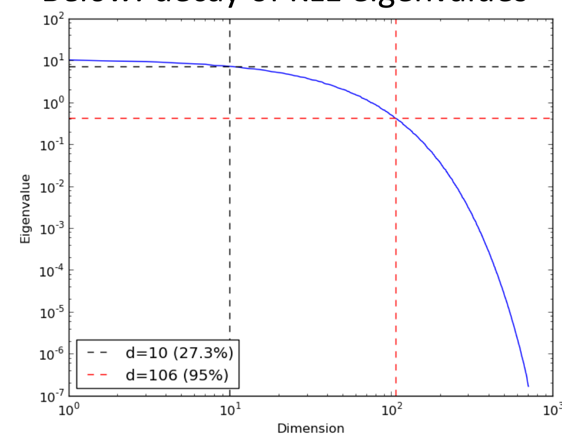


Modes 1-5:

Modes 6-10:



Below: decay of KLE eigenvalues



- Mismatch function (calculated in *Albany/FELIX*):

$$J(\beta) = \int_{\Gamma_{top}} \frac{1}{{\sigma_u}^2} |\boldsymbol{u} - \boldsymbol{u}^{obs}|^2 ds$$

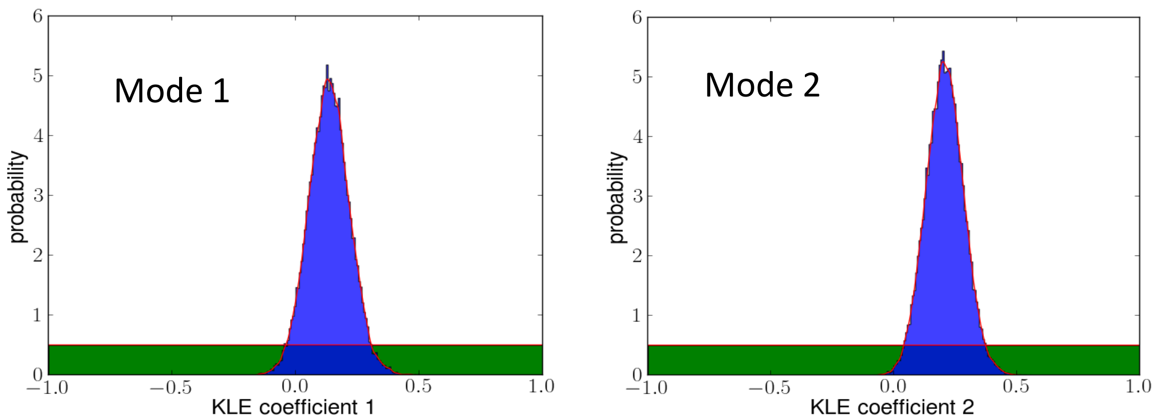
- PCE emulator was formed for the mismatch $J(\beta)$ using uniform $[-1,1]$ prior distributions and 286 high-fidelity runs on Hopper (286 points = 3rd degree polynomial in 10D).

Sandia National Laboratories

Initial Demonstration: Bayesian Calibration for 4km GIS Problem

- For calibration, MCMC (Delayed Rejection Adaptive Metropolis – DRAM) was performed on the PCE with 2K samples.

- ***Posterior distributions*** for 10 KLE coefficients:



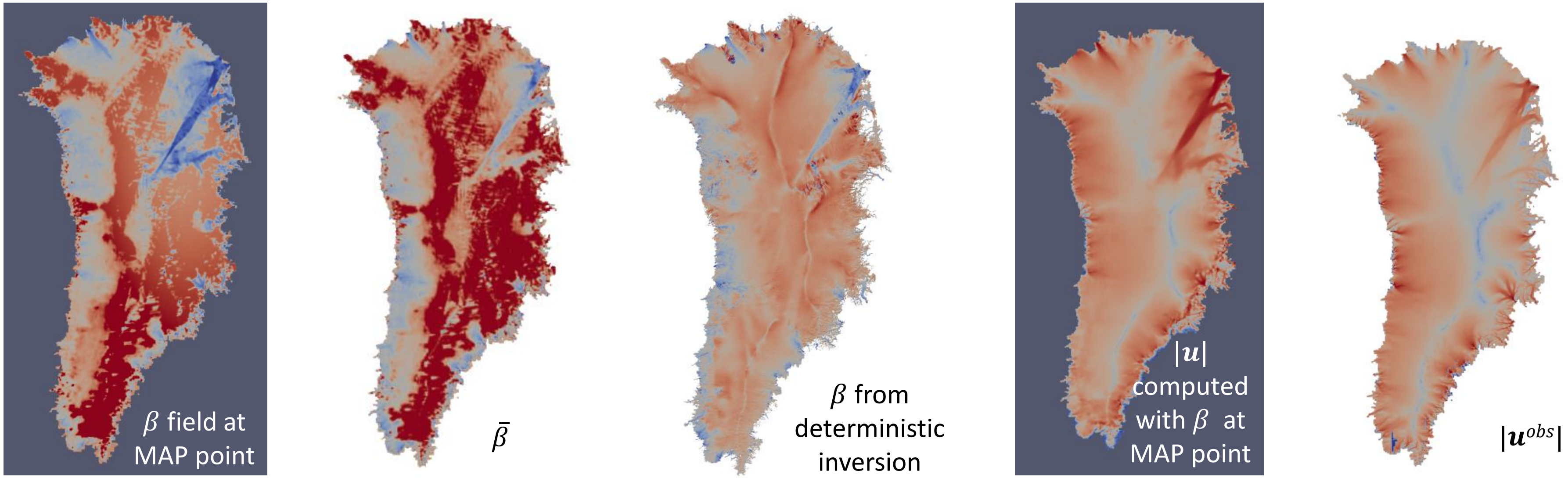
…

Green = prior (uniform [-1,1])
Blue = posterior

- Distributions are peaked rather than uniform ⇒ data informed the posteriors.

- ***MAP point***: $\boldsymbol{\xi} = (0.372, -0.679, -0.420, -0.189, -7.38\text{e}{-2}, -0.255, 0.449, -0.757, 0.847, -0.447)$

Initial Demonstration: Bayesian Calibration for 4km GIS Problem



- Ice is too fast at MAP point. Possible explanations:
  - Surrogate error (based on cross-validation).
  - Mean field error.
  - Bad modes (modes lack fine scale features).

Mismatch $J(\beta)$ at MAP point: $1.87 \times$ mismatch at $\bar{\beta}$

Next Step: Bayesian Calibration of β, h for 8km, 16km GIS Problems

- Mean $\bar{\beta}$, $\bar{h}$ fields obtained deterministic inversion minimizing

$$J(\beta, h) = \alpha_v \int_{\Gamma_{top}} |\boldsymbol{u} - \boldsymbol{u}^{obs}|^2 ds + \alpha \int_{\Gamma} |div(\boldsymbol{u}H) - SMB|^2 ds + \alpha_H \int_{\Gamma_{top}} |h - h^{obs}|^2 ds$$

Next Step: Bayesian Calibration of β, h for 8km, 16km GIS Problems

- Mean $\bar{\beta}$, $\bar{h}$ fields obtained deterministic inversion minimizing

$$J(\beta, h) = \alpha_v \int_{\Gamma_{top}} |\boldsymbol{u} - \boldsymbol{u}^{obs}|^2 ds + \alpha \int_{\Gamma} |div(\boldsymbol{u}H) - SMB|^2 ds + \alpha_H \int_{\Gamma_{top}} |h - h^{obs}|^2 ds$$

- Prior and expected variation in β, h is unknown…

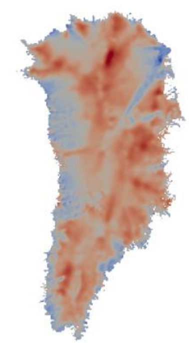
Next Step: Bayesian Calibration of β, h for 8km, 16km GIS Problems

- Mean $\bar{\beta}$, $\bar{h}$ fields obtained deterministic inversion minimizing

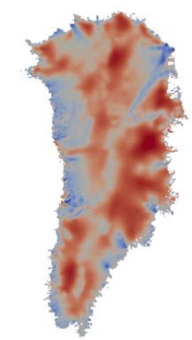
$$J(\beta, h) = \alpha_v \int_{\Gamma_{top}} |\boldsymbol{u} - \boldsymbol{u}^{obs}|^2 ds + \alpha \int_{\Gamma} |div(\boldsymbol{u}H) - SMB|^2 ds + \alpha_H \int_{\Gamma_{top}} |h - h^{obs}|^2 ds$$

- Prior and expected variation in β, h is unknown…
- <u>*Idea to estimate K and L:*</u> solve LLS problem

$$min_{L,K} \left\| \exp\left(\bar{\beta}^{opt}(\min J(\beta)) - \bar{\beta}^{opt}(\min J(\beta, h)) - \sum_{k=1}^{K} \sqrt{\lambda_k{}^{\beta}} \boldsymbol{\phi}_k \, \xi_k{}^{\beta}(\omega) \right) \right\|$$



$\bar{\beta}^{opt}$ (min $J(\beta, h)$)



$\bar{\beta}^{opt}(\min J(\beta))$

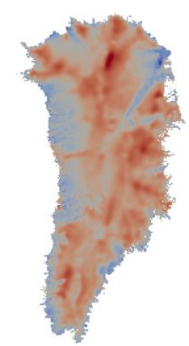
Next Step: Bayesian Calibration of β, h for 8km, 16km GIS Problems

- Mean $\bar{\beta}$, $\bar{h}$ fields obtained deterministic inversion minimizing

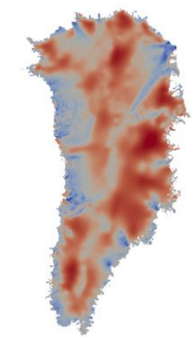
$$J(\beta,h) = \alpha_v \int_{\Gamma_{top}} |\boldsymbol{u} - \boldsymbol{u}^{obs}|^2 ds + \alpha \int_{\Gamma} |div(\boldsymbol{u}H) - SMB|^2 ds + \alpha_H \int_{\Gamma_{top}} |h - h^{obs}|^2 ds$$

- Prior and expected variation in β, h is unknown…
- <u>*Idea to estimate K and L:*</u> solve LLS problem

$$min_{L,K} \left\| \exp\left(\bar{\beta}^{opt}(\min J(\beta)) - \bar{\beta}^{opt}(\min J(\beta,h)) - \sum_{k=1}^{K} \sqrt{\lambda_k{}^{\beta}}\boldsymbol{\phi}_k \, \xi_k{}^{\beta}(\omega) \right) \right\|$$

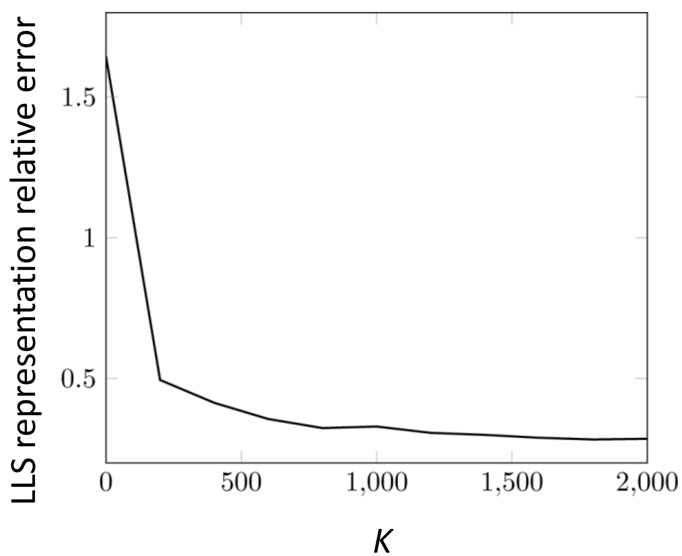


$\bar{\beta}^{opt}$ (min $J(\beta,h)$)



$\bar{\beta}^{opt}(\min J(\beta))$

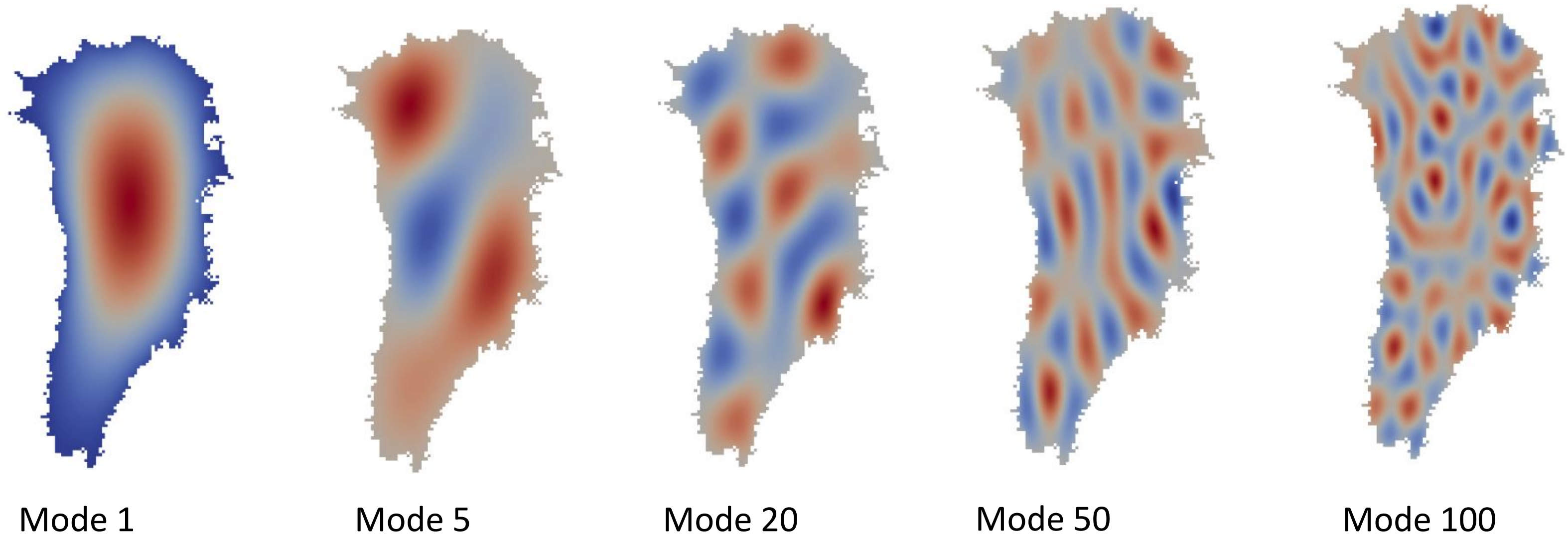
$\Rightarrow$



LLS representation error decay is independent of *L*

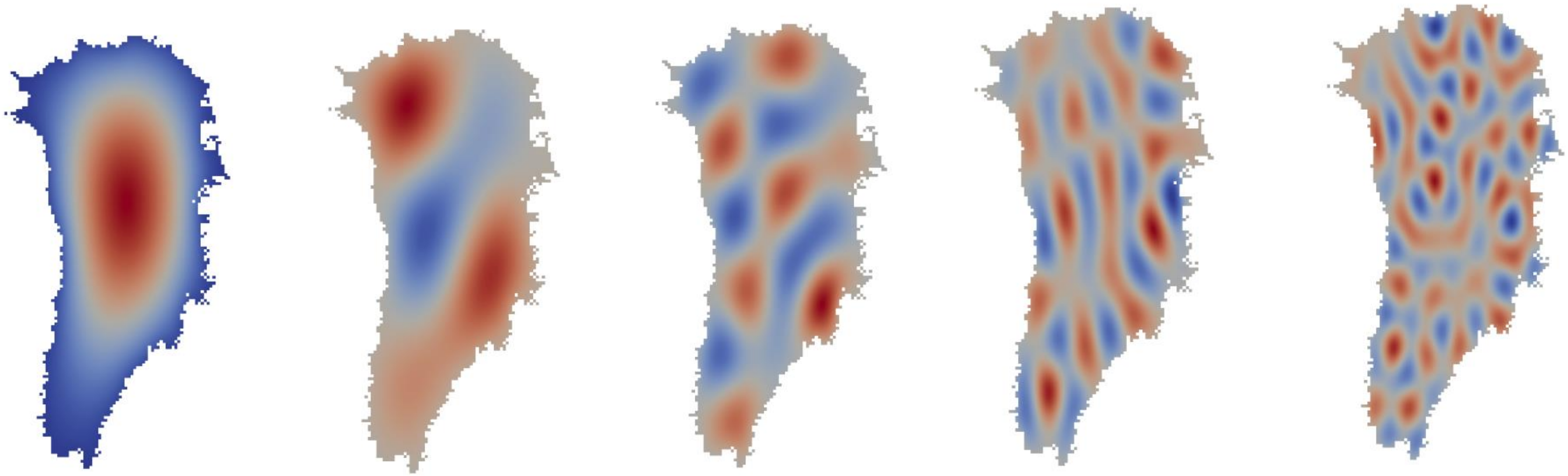
Next Step: Bayesian Calibration of β, h for 8km, 16km GIS Problems

- **Conclusion 1:** use more modes (*O(100)*, *O(1000)*).



Next Step: Bayesian Calibration of β, h for 8km, 16km GIS Problems

- **<u>Conclusion 1:</u>** use more modes (*O(100), O(1000)*).



Mode 1 Mode 5 Mode 20 Mode 50 Mode 100

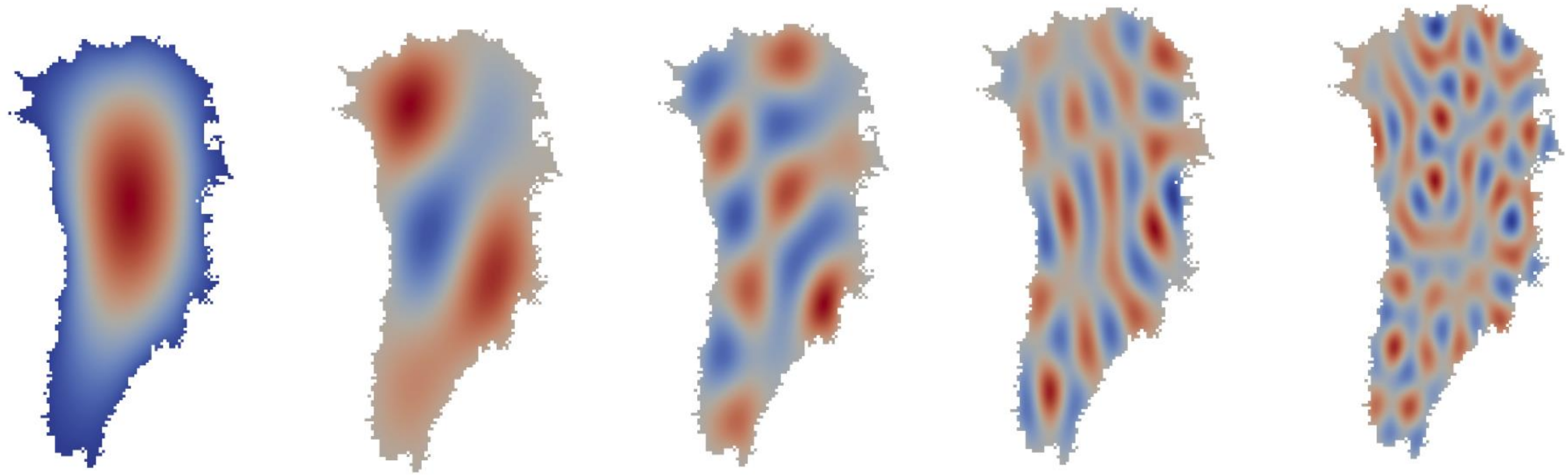
- **<u>Conclusion 2:</u>** *L* does not affect LLS reconstruction because representation error decay is independent of *L*.
  - Coefficients in LLS fitting were of the same order.

  $\Longrightarrow$ We can assume every random variable has the same variance:

$$\boxed{\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \cancel{\sqrt{\lambda_k{}^{\beta}}}\, \boldsymbol{\phi}_k\, \xi_k{}^{\beta}(\omega), \quad h(\omega) = \bar{h} + \sum_{k=1}^{K} \cancel{\sqrt{\lambda_k{}^{h}}}\, \boldsymbol{\phi}_k \xi_k{}^{h}(\omega)}$$

Next Step: Bayesian Calibration of β, h for 8km, 16km GIS Problems

- **<u>Conclusion 1:</u>** use more modes (*O(100), O(1000)*).



Mode 1 Mode 5 Mode 20 Mode 50 Mode 100

- **<u>Conclusion 2:</u>** *L* does not affect LLS reconstruction because representation error decay is independent of *L*.
  - Coefficients in LLS fitting were of the same order.

  $\Longrightarrow$ We can assume every random variable has the same variance:

$$\boxed{\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \boldsymbol{\phi}_k \, \xi_k{}^{\beta}(\omega), \quad h(\omega) = \bar{h} + \sum_{k=1}^{K} \boldsymbol{\phi}_k \xi_k{}^{h}(\omega)}$$

Next Step: Improve Efficiency of MCMC Using Gradient/Hessian Information

MCMC with active subspaces using gradient information

- Gradients ($^{d(mismatch)}/_{d\beta}$, $^{d(mismatch)}/_{dh}$) can be used to identify subspace that controls variation in likelihood function → this info can improve MCMC performance by reducing correlation between samples.
- Surrogates (to reduce sampling cost) are feasible for high-dimensional parameter spaces with active subspaces.
- Plan: combine MCMC in active subspaces with surrogates that adaptively target regions of high probability.

Exploit Hessian structure

- Improve MCMC by informing proposal covariance by structure of Hessian → posterior Hessian-based proposal distribution properly balances likelihood and prior, performing better than either alone.
- Leverage analytic emulator gradients for QOI → full or Gauss-Newton misfit Hessian.
- Stochastic Newton: low rank approximation for prior-preconditioned misfit Hessian → multivariate normal proposal covariance for MCMC.

$$\boxed{\nabla^2_\xi M(\xi) = \underbrace{\nabla_\xi f(\xi)^T \Gamma_{\mathbf{d}}^{-1} \nabla_\xi f(\xi)}_{\text{Gauss-Newton approx}} + \nabla^2_\xi f(\xi) \cdot \left[\Gamma_{\mathbf{d}}^{-1}(f(\xi) - \mathbf{d})\right]}$$

$$\boxed{L_0^T H_M L_0 \approx V_r \Lambda_r V_r^T}$$

$$\boxed{\Sigma_{MVN} = H_{\text{nlpost}}^{-1} \approx L_0 \left[I - V_r D_r V_r^T\right] L_0^T}$$

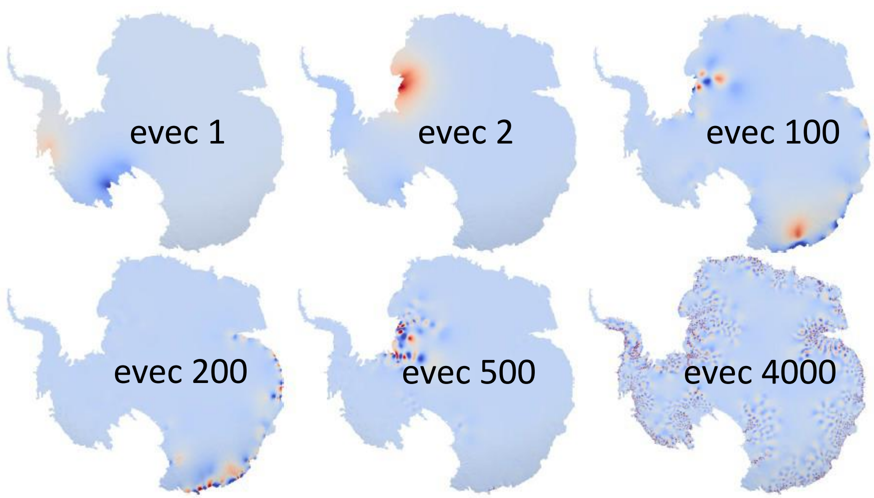
Sandia National Laboratories

Next Step: Better Reduced Bases for Bayesian Calibration using Hessian Info

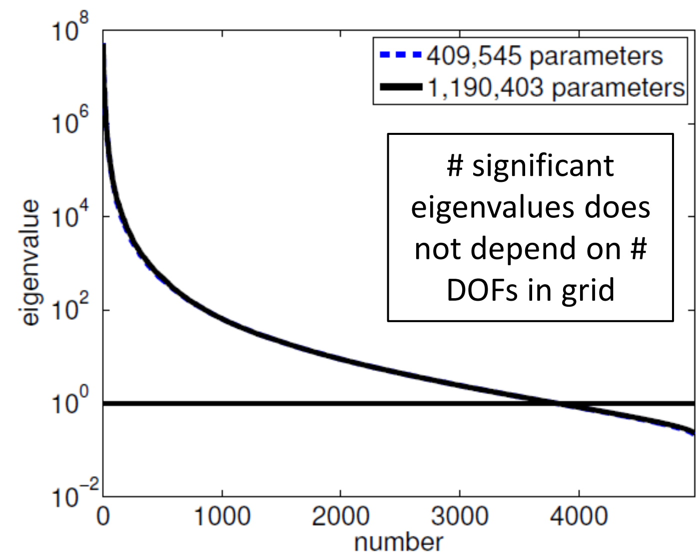
- Hessian of the merit (mismatch) functional can provide a way to compute the covariance of a Gaussian posterior:

$$\boldsymbol{C}_{post} = (\boldsymbol{C}_{prior}\boldsymbol{H}_{misfit} + \boldsymbol{I})^{-1}\boldsymbol{C}_{prior}$$

- We want to limit only the most important directions (eigenvectors) of $\boldsymbol{C}_{post}$.



Figures courtesy of O. Ghattas' group (Isaac et al., 2004)



Right: log-linear plot of the spectra of a prior-preconditioned data misfit Hessian at the MAP point for two successively finer parameter/state meshes of the inverse ice sheet problem.

Outline

- The PISCEES project, land-ice equations and relevant codes (*Albany/FELIX*, *CISM-Albany*, *MPAS-Alban*y).
- Uncertainty Quantification Problem Definition.
- Bayesian Calibration.
    - Methodology.
    - Demonstrations.
- **Forward Propagation of Uncertainty.**
    - **Methodology.**
    - **Demonstrations.**
- Summary and Future Work.

Forward Propagation

PCE Emulator

$$\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{{\lambda_k}^{\beta}}\,\boldsymbol{\phi}_k\,{\xi_k}^{\beta}(\omega)$$

Model realizations
Forward propagation
(e.g., 2000-2050)

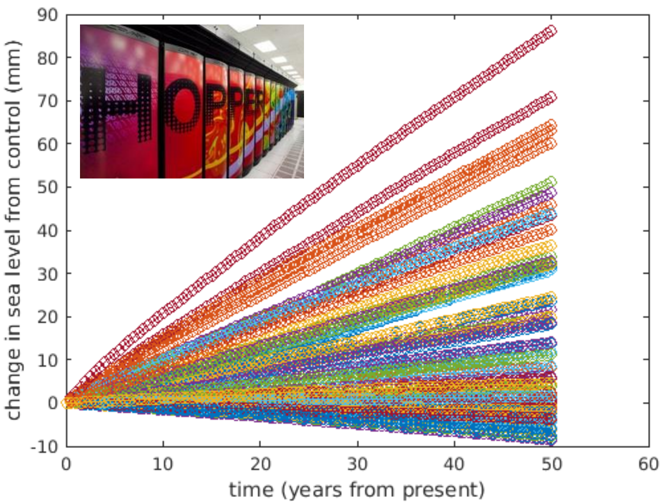
DAKOTA, Albany/FELIX
QoI(β)
(total ice mass loss)

- Parameter (β) distribution can either be assumed to be Gaussian (based on Hessian information) or can be the result of Bayesian calibration.
- Emulator is built using *DAKOTA* coupled with *CISM-Albany* for forward runs.
- MCMC (Delayed Rejection Adaptive Metropolis – DRAM) was used to perform uncertainty propagation (*QUESO*).

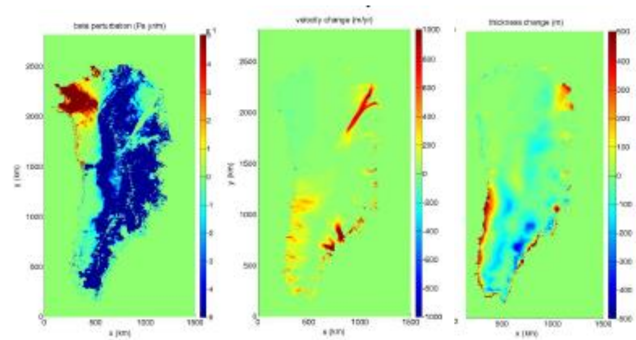
Initial Demonstration: Forward Propagation for 4km GIS Problem

Procedure:

- We first ran 66* *CISM-Albany* high-fidelity simulations on Hopper with β sampled from a uniform $[-1,1]$ distribution and ***no forcing*** for 50 years.



Left: SLR distribution from ensemble of 66 high-fidelity simulations (differenced against control run using the $\bar{\beta}$ distribution). ***All 66 runs ran to completion out-of-the-box on Hopper!***



Above: β, velocity and thickness perturbations. Ice thickness changed > 500m in some places.

- We then used the results of these runs to create a PCE emulator for the SLR.
- Using emulator, propagated posterior distributions computed in Bayesian calibration (using KLE) through the model to get posteriors on SLR (MCMC on PCE emulator with 2K samples).

*66 points = 2D polynomial in 10D.

Initial Demonstration: Forward Propagation for 4km GIS Problem

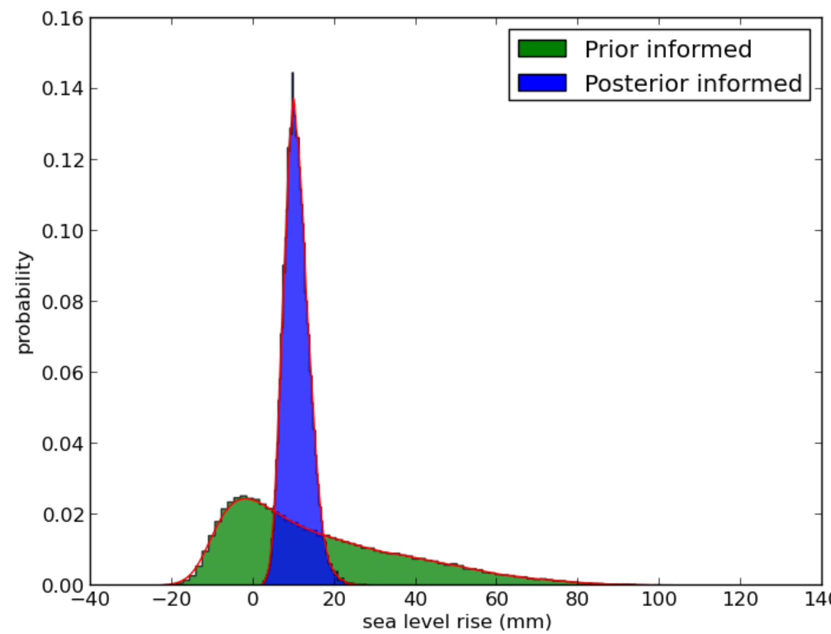
Disclaimer: these results illustrate that we have in place all steps of our UQ workflow. *They are NOT yet actual uncertainty bounds for sea-level rise.*

Expected PDF of SLR: normal distribution centered around 0 SLR since no forcing.

Prior informed (green): uniform distribution translates to distribution skewed w.r.t. model outputs.

- Larger fraction of the ice sheet currently has a β value that forces no (or slow) basal sliding.
- Areas with little sliding: not affected by increase in β, but greatly affected by decrease in β (velocity in these regions will change significantly from initial condition).
- Since we sample from a uniform distribution when perturbing β, we expect to see a disproportionately large signal when reducing β vs. increasing it.

PDF of SLR



Posterior informed (blue): centered on positive tail of prior – not consistent with observations.

- Could be due to "ad hoc" β used as mean field (spin-up over 100 years).
- May be that emulator was been built with a (non-physical) positive mass balance while calibration was done on present-day observations (consistent with ice losing mass).

Outline

- The PISCEES project, land-ice equations and relevant codes (*Albany/FELIX*, *CISM-Albany*, *MPAS-Alban*y).
- Uncertainty Quantification Problem Definition.
- Bayesian Calibration.
    - Methodology.
    - Demonstrations.
- Forward Propagation of Uncertainty.
    - Methodology.
    - Demonstrations.
- **Summary and Future Work.**

Summary and Ongoing Work

- This talk described our ***workflow*** for quantifying uncertainties in expected aggregate ice sheet mass loss and its ***demonstration*** on some Greenland ice sheet problems.
- Our choice of prior is somewhat arbitrary; however it is possible to build an informed Gaussian distribution using the ***Hessian of the deterministic inversion*.**
- We plan to use ***gradient information*** to combine MCMC in ***active subspaces*** with surrogates.
- 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., the shallow ice model or SIA) or ***low resolution solves*** to reduce the cost of building the emulator.
- In future work, we plan to look at effects of ***other sources of uncertainty***, e.g., surface mass balance.

Albany Trilinos DAKOTA QUEST

Sandia National Laboratories

Funding/Acknowledgements

Support for this work was provided through Scientific Discovery through Advanced Computing (**SciDAC**) projects funded by the U.S. Department of Energy, Office of Science (**OSCR**), Advanced Scientific Computing Research and Biological and Environmental Research (**BER**) → **PISCEES SciDAC Application Partnership.**

PISCEES team members: *K. Evans, M. Gunzburger, M. Hoffman, C. Jackson, P. Jones, W. Lipscomb, M. Perego, S. Price, A. Salinger, I. Tezaur, R. Tuminaro, P. Worley.*

Trilinos/DAKOTA collaborators*: M. Eldred, J. Jakeman, E. Phipps, L. Swiler.*

Computing resources: *NERSC, OLCF.*

Thank you! Questions?

References

[1] M.A. Heroux *et al.* “An overview of the Trilinos project.” *ACM Trans. Math. Softw.* **31**(3) (2005).

[2] A.G. Salinger *et al*. "Albany: Using Agile Components to Develop a Flexible, Generic Multiphysics Analysis Code", *Comput. Sci. Disc.* (submitted, 2015).

[3] **I. Tezaur**, M. Perego, A. Salinger, R. Tuminaro, S. Price. "*Albany/FELIX*: A Parallel, Scalable and Robust Finite Element Higher-Order Stokes Ice Sheet Solver Built for Advanced Analysis", *Geosci. Model Develop.* 8 (2015) 1-24.

[4] **I. Tezaur**, R. Tuminaro, M. Perego, A. Salinger, S. Price. "On the scalability of the *Albany/FELIX* first-order Stokes approximation ice sheet solver for large-scale simulations of the Greenland and Antarctic ice sheets", *MSESM/ICCS15*, Reykjavik, Iceland (June 2014).

[5] R.S. Tuminaro, **I. Tezaur**, M. Perego, A.G. Salinger. "A Hybrid Operator Dependent Multi-Grid/Algebraic Multi-Grid Approach: Application to Ice Sheet Modeling", *SIAM J. Sci. Comput.* (in prep).

[6] R. Tuminaro. “ML’s SemiCoarsening Feature, Addition to ML 5.0 Smoothed Aggregation User’s Guide” , Sandia National Laboratories Report, SAND2006-2649, Sandia National Laboratories, Albuquerque, NM, 2014.

References (cont'd)

[7] S. Shannon, *et al.* "Enhanced basal lubrication and the contribution of the Greenland ice sheet to future sea-level rise", *P. Natl. Acad. Sci.,* 110 (2013) 14156-14161.

[8] P. Fretwell, *et al.* "BEDMAP2: Improved ice bed, surface, and thickness datasets for Antarctica", *The Cryosphere* 7(1) (2013) 375-393.

[9] F. Pattyn. "Antarctic subglacial conditions inferred from a hybrid ice sheet/ice stream model", *Earth and Planetary Science Letters 295 (2010).*

[10] M. Perego, S. Price, G. Stadler. "Optimal Initial Conditions for Coupling Ice Sheet Models to Earth System Models", *J. Geophys. Res.* 119 (2014) 1894-1917.

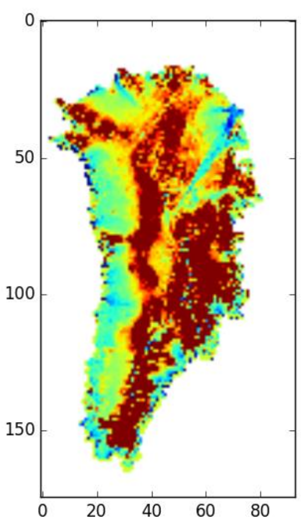
[11] J. Jakeman, M. Eldred, K. Sargsyan. "Enhancing l1-minimization estimates of polynomial chaos expansions using basis selection", *J. Comp. Phys.* 289 (2015) 18-34.

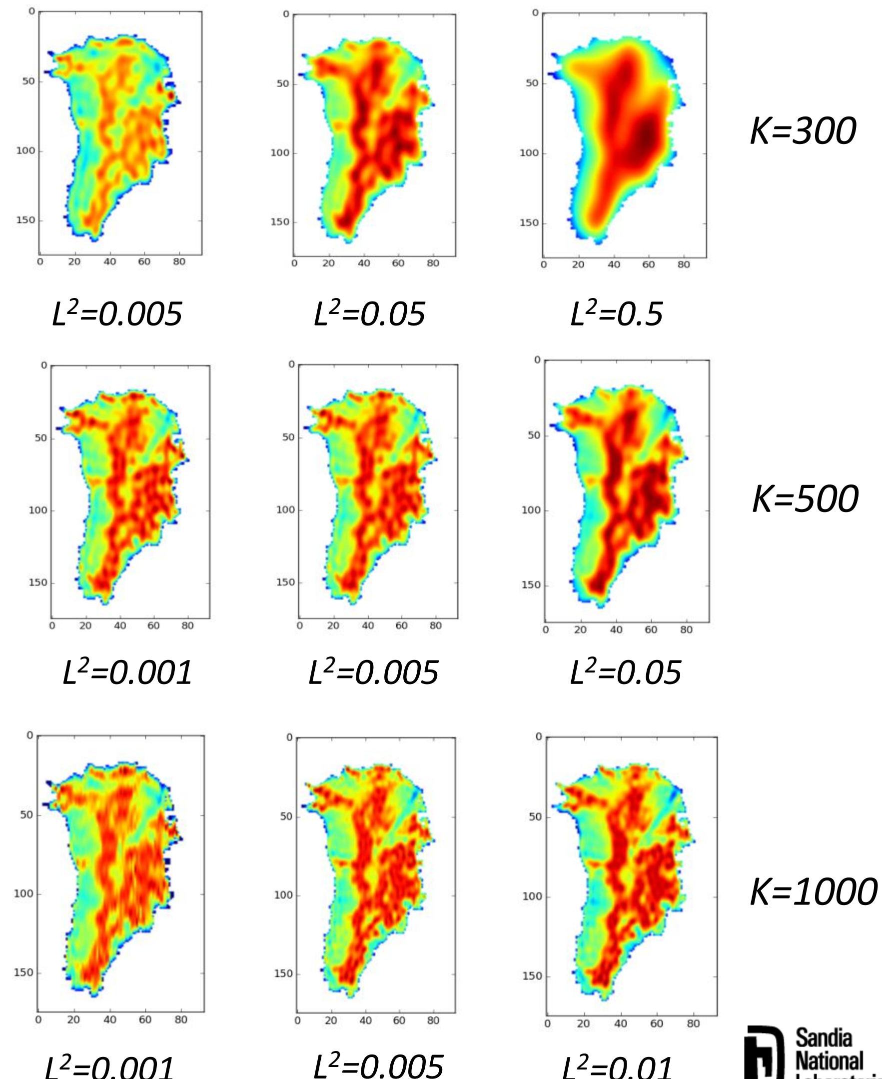
Sandia National Laboratories

Appendix: Bayesian Calibration of β, h for 8km, 16km GIS Problems

- Length scale L and dimension size K can be fine-tuned by looking at reconstruction of β using the KLE modes.
- Larger $L \Rightarrow$ smoother (too diffusive) reconstruction.
- High dimension K in plots due to omitting $\bar{\beta}$ from reconstruction:

$$\beta = \sum_{k=1}^{K} a_k \phi_k$$





Left: $\bar{\beta}$ for 16km GIS

Right: $\bar{\beta}$ reconstructed with K KLE modes as a function of length scale L for 16km GIS