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

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• 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.
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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

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).

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

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)
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This talk

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CISM/MPAS Land Ice Codes (dynamic):
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The First-Order Stokes Model for Ice Sheets & Glaciers

- Ice sheet dynamics are given by the “First-Order” Stokes PDEs: approximation* to viscous incompressible \textit{quasi-static} Stokes flow with power-law viscosity.

\[
\begin{aligned}
- \nabla \cdot (2\mu \dot{\varepsilon}_1) &= -\rho g \frac{\partial s}{\partial x} , \text{ in } \Omega \\
- \nabla \cdot (2\mu \dot{\varepsilon}_2) &= -\rho g \frac{\partial s}{\partial y}
\end{aligned}
\]

- Viscosity $\mu$ is nonlinear function given by “Glen’s law”:

\[
\mu = \frac{1}{2} A \left( \frac{1}{2} \sum_{ij} \dot{\varepsilon}_{ij}^2 \right)^{\frac{1}{2n-1}} (n = 3)
\]

- Relevant boundary conditions:
  - \textit{Stress-free BC}: \(2\mu \dot{\varepsilon}_i \cdot \mathbf{n} = 0\), on $\Gamma_s$
  - \textit{Floating ice BC}:
    \[
    2\mu \dot{\varepsilon}_i \cdot \mathbf{n} = \begin{cases} 
    \rho g z \mathbf{n}, & \text{if } z > 0 \\
    0, & \text{if } z \leq 0
    \end{cases} , \text{ on } \Gamma_l
    \]
  - \textit{Basal sliding BC}: \(2\mu \dot{\varepsilon}_i \cdot \mathbf{n} + \beta u_i = 0\), on $\Gamma_\beta$

*Assumption: aspect ratio $\delta$ 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...

“Agile Components”
- Discretizations/meshes
- Solver libraries
- Preconditioners
- Automatic differentiation
- Many others!

- Parameter estimation
- Uncertainty quantification
- Optimization
- Bayesian inference
- Configure/build/test/documentation

Land Ice Physics Set (Albany/FELIX code)  Other Albany Physics Sets

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

*FELIX = “Finite Elements for Land Ice eXperiments”.

Started by A. Salinger
Ice Sheet Evolution Models

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

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

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

• *Temperature equation* (advection-diffusion):

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

(energy balance).

• *Flow factor* \(A\) in Glen’s law depends on temperature \(T\):

\(A = A(T)\).

• Ice sheet *grows/retreats* depending on thickness \(h\).
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Ice-covered (“active”) cells shaded in white ($h > h_{\text{min}}$)

Time $t_2$
Interfaces to \textit{CISM} and \textit{MPAS LI} for Transient Simulations

- \textit{CISM-Albany}:
  - \textit{CISM} (Fortran): Thickness evolution, temperature solve, coupling to CESM
  - \textit{C++/Fortran Interface, Mesh Conversion}
  - \textit{cism_driver}
  - \textit{output file}

- \textit{Albany/FELIX (C++) velocity solve}:
  - \textit{LandIce_model}
  - \textit{output file}

- \textit{MPAS LI-Albany}:
  - \textit{MPAS Land-Ice (Fortran)}: Thickness evolution, temperature solve, coupling to DOE-ESM
  - \textit{LandIce_model}
  - \textit{output file}

- \textit{Albany/FELIX} has been coupled to two land ice dycores: Community Ice Sheet Model (\textit{CISM}) and Model for Prediction Across Scales for Land Ice (\textit{MPAS LI}).

- • Structured hexahedral meshes (rectangles extruded to hexes).
- • Tetrahedral meshes (dual of hexagonal mesh, extruded to tets).
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Uncertainty Quantification (UQ) Problem Definition

Quantity of Interest (QoI) in Ice Sheet Modeling:

- total ice mass loss/gain during 21\textsuperscript{st} century
- \textit{sea level rise prediction.}

There are several sources of uncertainty, most notably:

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

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

\( n \) = Glen’s law exponent

Baseline sliding BC:

\[ 2\mu \dot{e}_i \cdot n + \beta u_i = 0, \text{ on } \Gamma_{\beta} \]
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As a first step, we focus on effect of uncertainty in **basal friction** ($\beta$) only.

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

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

→ 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 \( \rightarrow \textit{Bayes' Theorem}: \) assume prior distribution; update using data:

\[
\pi(\theta|d) = \left(\frac{\pi(d|\theta)}{\pi(d)}\right) \pi(\theta) = \frac{\pi(d|\theta) \pi(\theta)}{\int \pi(d|\theta) \pi(\theta) d\theta}
\]

- **Forward propagation:** sample the obtained distribution and perform ensemble of forward propagation runs to compute the uncertainty in the QoI.
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What are the parameters that render a given set of observations?

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

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- 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 $\beta$ field inversion problems has $O(100K)$ dimensions!
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  2. Perform eigenvalue decomposition of $C$.
  3. Expand* $\beta - \bar{\beta}$ in basis of eigenvectors $\{\phi_k\}$ of $C$, with random variables $\{\xi_k \beta\}$:

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

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

$\bar{\beta} = \text{initial condition for } \beta$ (from deterministic inversion or spin-up)
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Inference/calibration is for coefficients of KLE $\Rightarrow$ **significant dimension reduction.**
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):**

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

- **Step 3 (QUEST):** **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 $\beta$. 
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.

- Mismatch function (calculated in Albany/FELIX):

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

- 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).
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:

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

  - **MAP point**: $\xi = (0.372, -0.679, -0.420, -0.189, -7.38 \times 10^{-2}, -0.255, 0.449, -0.757, 0.847, -0.447)$
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 $J(\bar{\beta})$ at MAP point: $1.87 \times$ mismatch at $\bar{\beta}$
Next Step: Bayesian Calibration of $\beta, h$ for 8km, 16km GIS Problems

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

$$J(\beta, h) = \alpha_v \int_{\Gamma_{top}} |u - u^{obs}|^2 ds + \alpha \int_{\Gamma} |\text{div}(uH) - SMB|^2 ds + \alpha_H \int_{\Gamma_{top}} |h - h^{obs}|^2 ds$$
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- **Idea to estimate $K$ and $L$:** solve LLS problem

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

\[\bar{\beta}_{opt}(\min J(\beta)) \quad \bar{\beta}_{opt}(\min J(\beta))\]
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  \(\Rightarrow\)

  LLS representation relative error decay is independent of $L$
Next Step: Bayesian Calibration of $\beta, h$ for 8km, 16km GIS Problems

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

---

Mode 1

Mode 5

Mode 20

Mode 50

Mode 100
Next Step: Bayesian Calibration of $\beta, h$ for 8km, 16km GIS Problems

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

- **Conclusion 2:** $L$ does not affect LLS reconstruction because representation error decay is independent of $L$.
  - Coefficients in LLS fitting were of the same order.
  - We can assume every random variable has the same variance:

$$\beta(\omega) = \tilde{\beta} + \sum_{k=1}^{K} \sqrt{\lambda_k} \phi_k \xi_k \beta(\omega), \quad h(\omega) = \tilde{h} + \sum_{k=1}^{K} \sqrt{\lambda_k} h \phi_k \xi_k h(\omega)$$
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Next Step: Improve Efficiency of MCMC Using Gradient/Hessian Information

MCMC with active subspaces using gradient information

- Gradients \( \frac{d(mismatch)}{d\beta}, \frac{d(mismatch)}{dh} \) can be used to identify subspace that controls variation in likelihood function \( \rightarrow \) 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 \( \rightarrow \) posterior Hessian-based proposal distribution properly balances likelihood and prior, performing better than either alone.
- Leverage analytic emulator gradients for QOI \( \rightarrow \) full or Gauss-Newton misfit Hessian.
- Stochastic Newton: low rank approximation for prior-preconditioned misfit Hessian \( \rightarrow \) multivariate normal proposal covariance for MCMC.

\[
\nabla^2_{\xi} M(\xi) = \nabla_{\xi} f(\xi)^T \Gamma_d^{-1} \nabla_{\xi} f(\xi) + \nabla^2_{\xi} f(\xi) \cdot \left[ \Gamma_d^{-1} (f(\xi) - d) \right]
\]

Gauss-Newton approx
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:

\[
C_{\text{post}} = (C_{\text{prior}}H_{\text{misfit}} + I)^{-1}C_{\text{prior}}
\]

- We want to limit only the most important directions (eigenvectors) of \(C_{\text{post}}\).

*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.

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

# significant eigenvalues does not depend on # DOFs in grid
• 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.
Forward Propagation

PCE Emulator

\[
\beta(\omega) = \tilde{\beta} + \sum_{k=1}^{K} \sqrt{\lambda_k} \phi_k \xi_k^\beta(\omega)
\]

Model realizations

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

DAKOTA, Albany/FELIX

QoI(\beta)

(total ice mass loss)

• Parameter (\beta) 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 $\beta$ 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 $\beta$ distribution). **All 66 runs ran to completion out-of-the-box on Hopper!**

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

**Posterior informed (blue):** centered on positive tail of prior – not consistent with observations.
- Could be due to “ad hoc” $\beta$ 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).
• The PISCEES project, land-ice equations and relevant codes (Albany/FELIX, CISM-Albany, MPAS-Albany).

• Uncertainty Quantification Problem Definition.

• Bayesian Calibration.
  • Methodology.
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• 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.
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**Computing resources:** NERSC, OLCF.

Thank you! Questions?
References


References (cont’d)


Appendix: Bayesian Calibration of $\beta, h$ for 8km, 16km GIS Problems

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

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

**Left:** $\tilde{\beta}$ for 16km GIS

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