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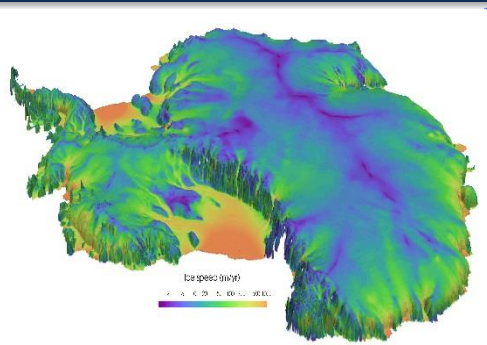

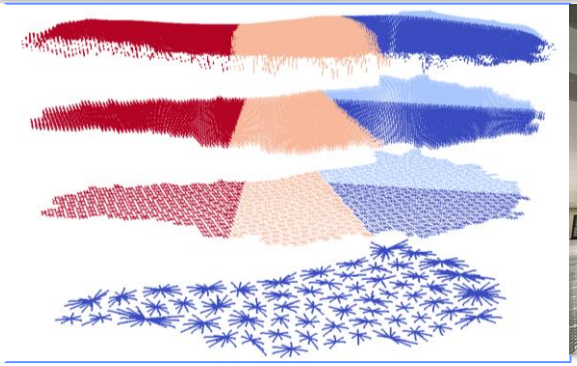

Large-scale Deterministic Inversion and Bayesian Calibration in Land-Ice Modeling

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

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[2] Los Alamos National Laboratory, Los Alamos, NM, USA.

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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SAND2017-6948C

Outline

1. Background.
   - PISCEES project for land-ice modeling.
   - Land-ice model.
2. UQ problem definition.
3. Inversion/calibration.
   - Deterministic inversion.
   - Bayesian inference.
4. Summary & future work.

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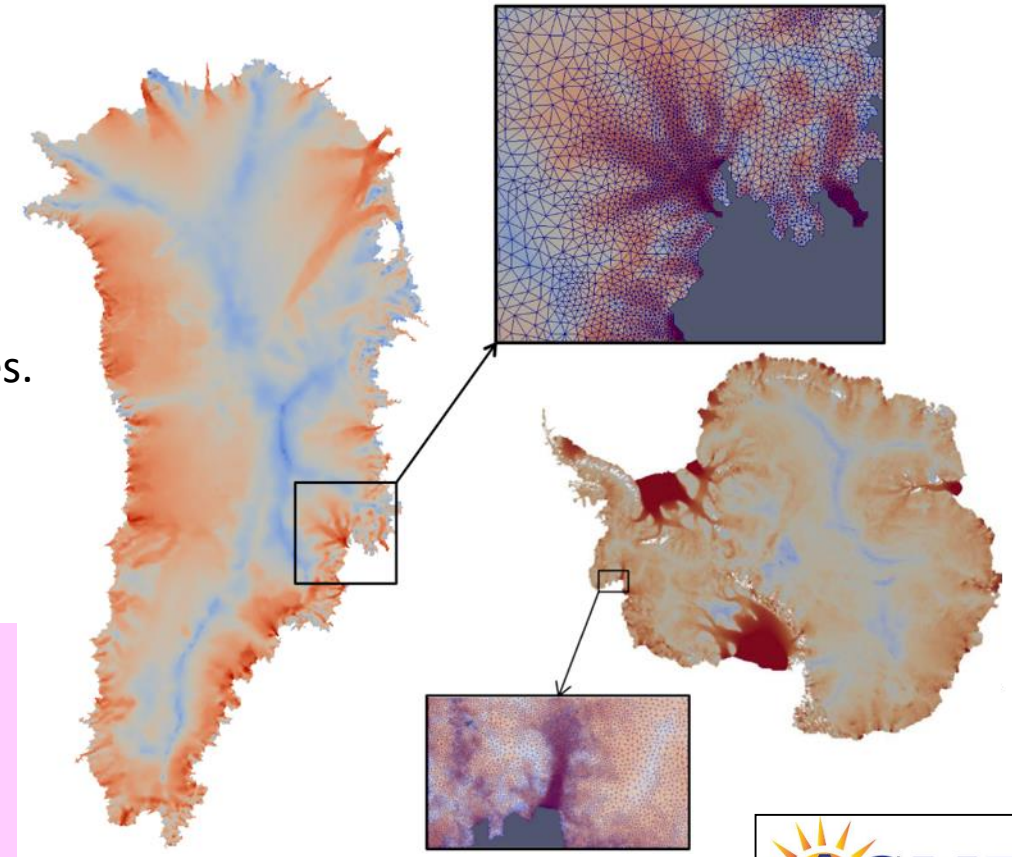
PISCEES Project for Land-Ice Modeling

"PISCEES" = Predicting Ice Sheet Climate Evolution at Extreme Scales
5 year SciDAC3 project began in June 2012; proposal for 5 year continuation project submitted to SciDAC4 call.

<u>Sandia's Role in the PISCEES Project</u>: to **develop** and **support** a robust and scalable land ice solver based on the "First-Order" (FO) Stokes equations → *Albany/FELIX**

<u>Requirements for *Albany/FELIX*:</u>

- ***Unstructured grid*** finite elements.
- ***Scalable, fast*** and ***robust.***
- ***Verified*** and ***validated.***
- ***Portable*** to new architecture machines.
- ***Advanced analysis*** capabilities: deterministic inversion, calibration, uncertainty quantification.



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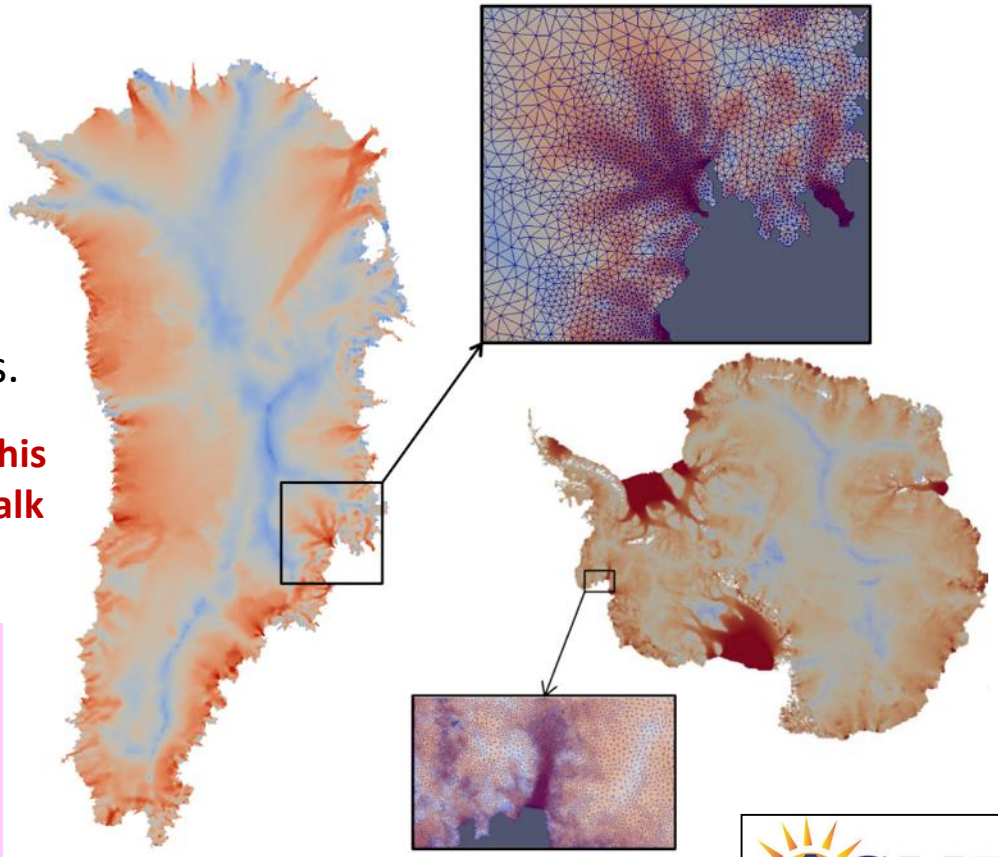

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The First-Order Stokes Model

- Ice behaves like a very ***viscous shear-thinning fluid*** (similar to lava flow).
- ***Quasi-static*** model with ***momentum balance*** given by ***"First-Order" Stokes PDEs***: "nice" elliptic approximation* to Stokes' flow equations.

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

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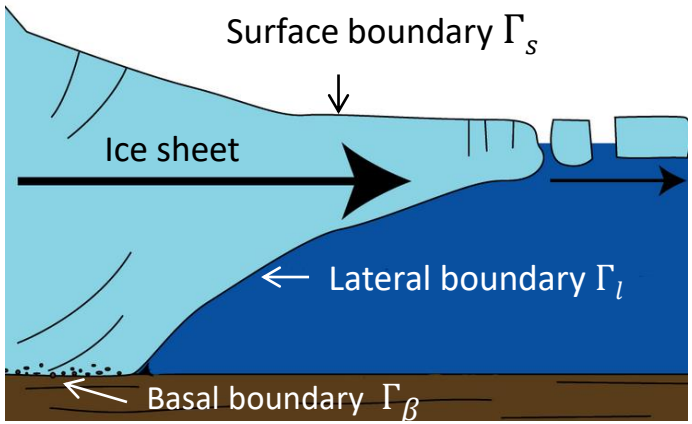
$$\mu = \frac{1}{2} A(T)^{-\frac{1}{n}} \left(\frac{1}{2}\sum_{ij} \dot{\boldsymbol{\epsilon}}_{ij}{}^2\right)^{\left(\frac{1}{2n}-\frac{1}{2}\right)} \qquad (n = 3)$$



- Relevant boundary conditions:
  - ***Stress-free BC:*** $2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} = 0$, on Γ_s
  - ***Floating ice BC:*** $2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} = \begin{cases} \rho g z \boldsymbol{n}, & \text{if } z > 0 \\ 0, & \text{if } z \le 0 \end{cases}$, on Γ_l
  - ***Basal sliding BC:*** $2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} + \beta(x,y)u_i = 0$, on Γ_β

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

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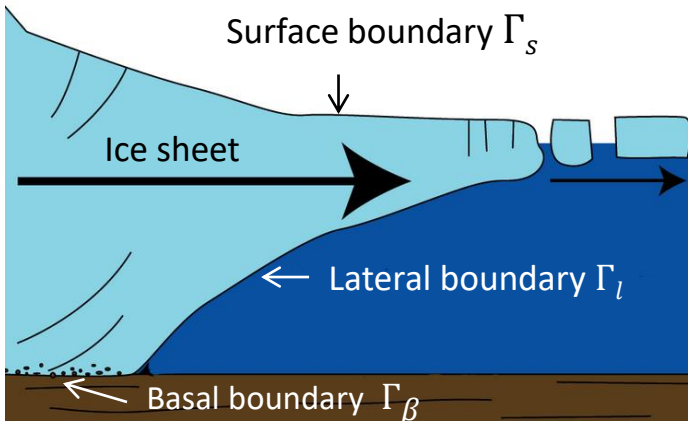

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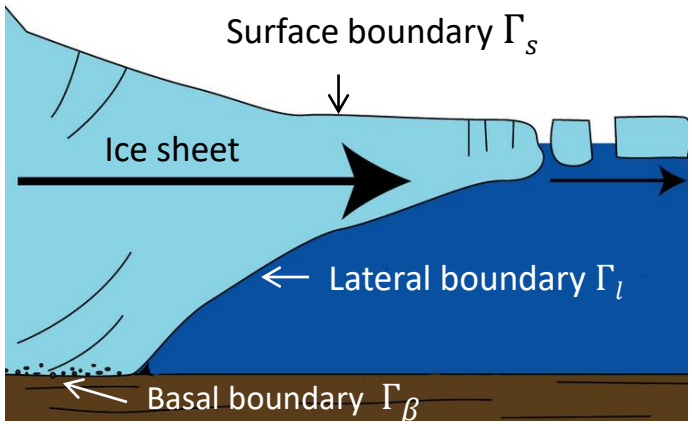

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$\beta(x,y) =$ basal sliding coefficient

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Thickness & Temperature Equations

- 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).

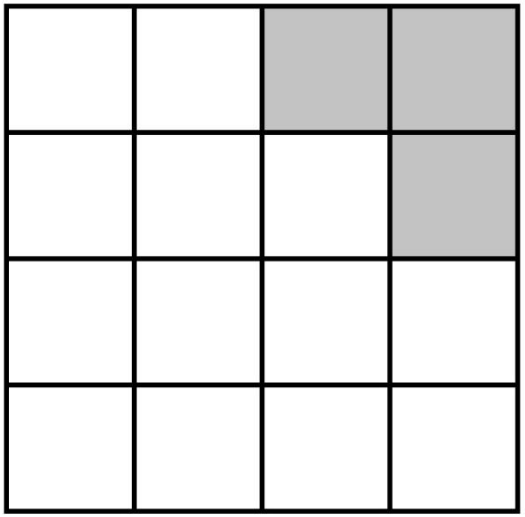
- ***Temperature equation*** (advection-diffusion):

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

(energy balance).

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

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



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

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

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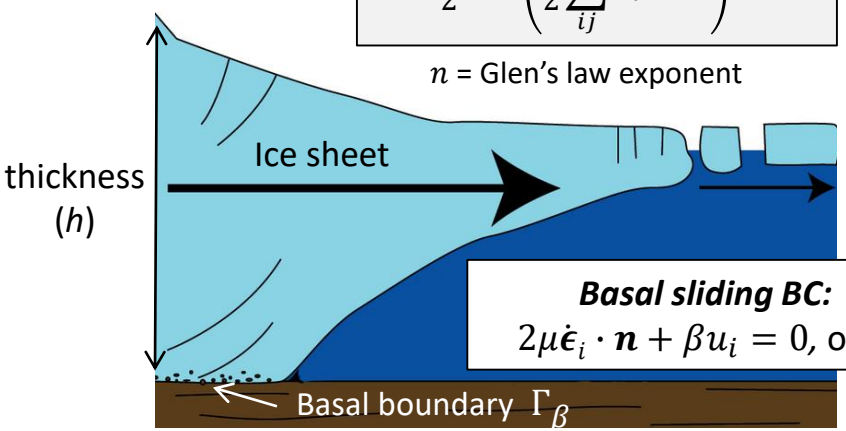

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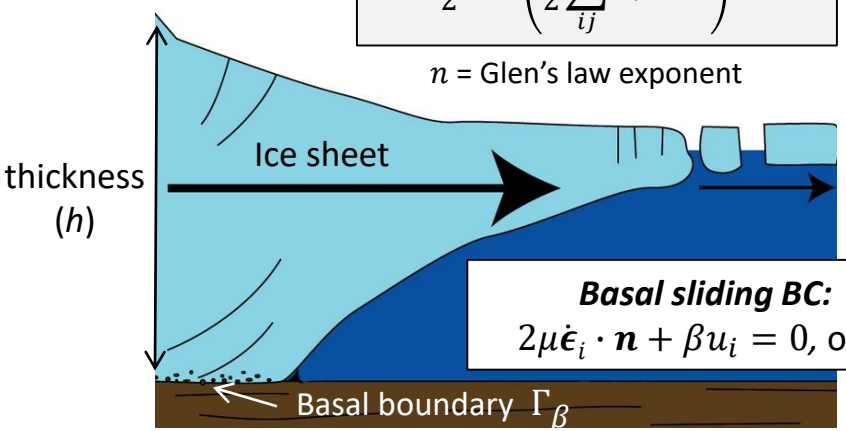

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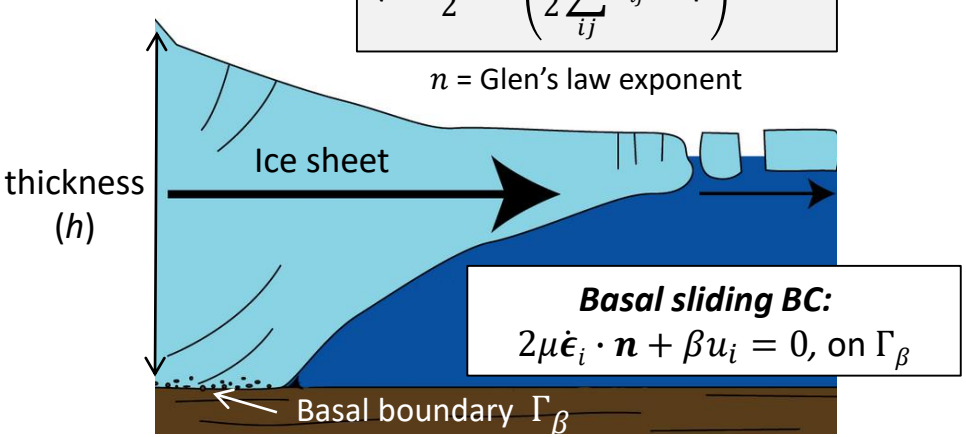

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UQ Workflow

Stage 1:
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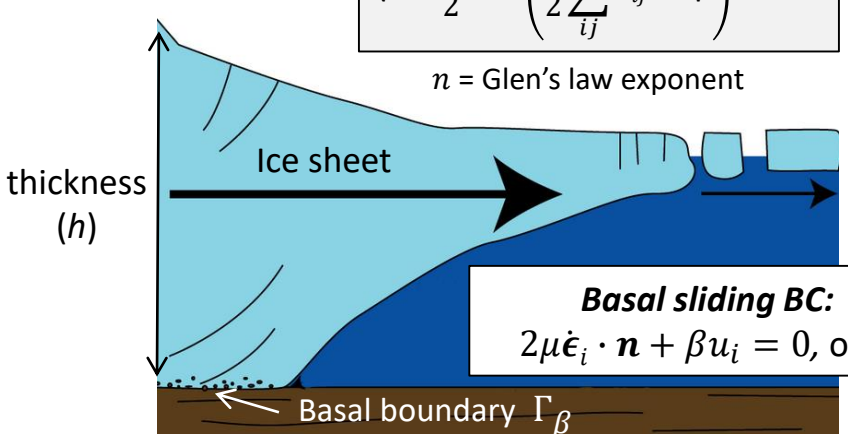

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Deterministic inversion

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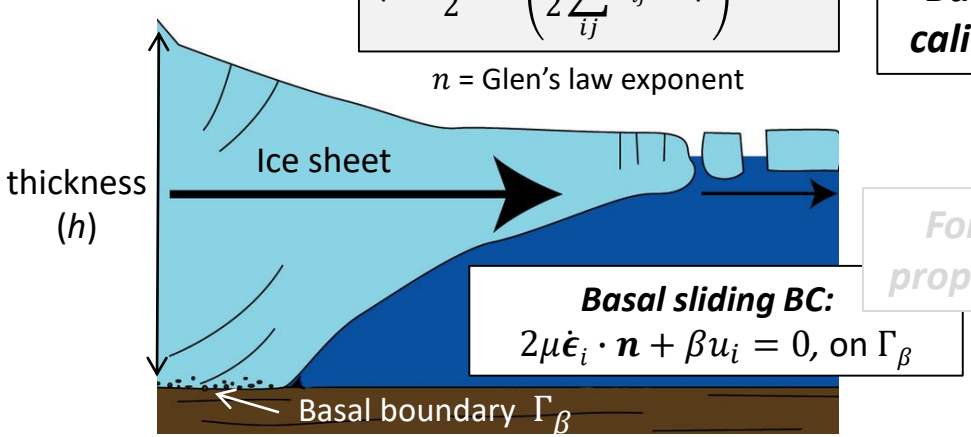

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Estimation of Ice Sheet Initial Condition

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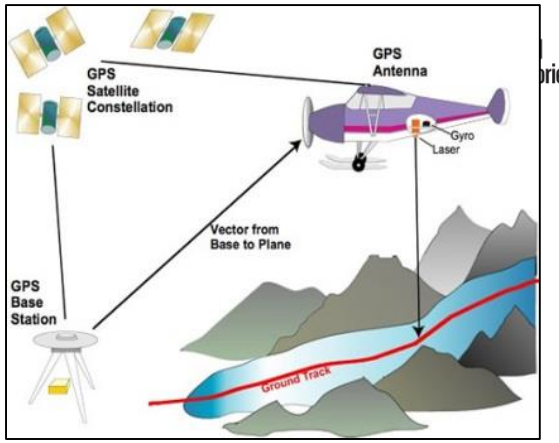
Stage 3:
Propagate uncertain initial condition through ice-sheet evolution model

Goal: 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).

Available Data & Assumptions



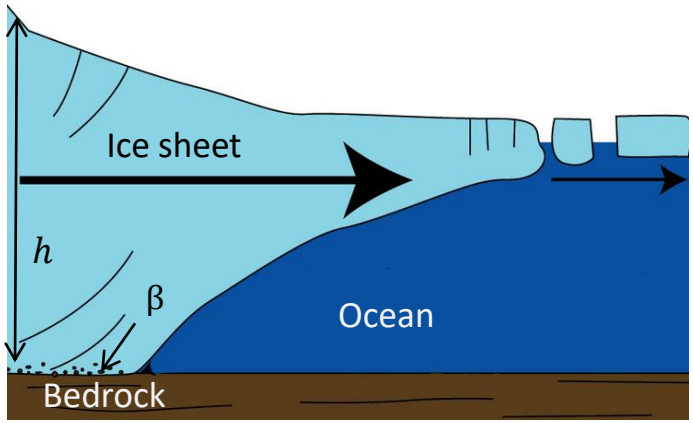
Available data/measurements:

- ice extent and surface topography.
- surface velocity.
- surface mass balance (SMB).
- ice thickness h (sparse measurements).

Sources of data: satellite infrarometry, radar, altimetry, etc.

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 first-order Stokes equations.
- ice close to mechanical equilibrium.

Deterministic Inversion

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First-Order Stokes PDE-Constrained optimization problem for initial condition*:

minimize $_{\beta,h}$ $m(\beta, h)$
s.t. FO Stokes PDEs

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

$$m(\beta, h) = \int_\Gamma \frac{1}{\sigma_u^2} |\boldsymbol{u} - \boldsymbol{u}^{obs}|^2 ds$$ surface velocity mismatch

$$+ \int_\Gamma \frac{1}{\sigma_\tau^2} |div(\boldsymbol{U}h) - \tau_s|^2 ds$$ SMB mismatch

$$+ \int_\Gamma \frac{1}{\sigma_h^2} |h - h^{obs}|^2 ds$$ thickness mismatch

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* Perego, Stadler, Price, *JGR*, 2014.

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Solving FO Stokes PDE-constrained optimization problem for initial condition significantly **reduces non-physical model transients**!

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Deterministic Inversion Algorithm & Software

First-Order Stokes PDE-Constrained optimization problem for initial condition*:

minimize $_{\beta,h}$ $m(\beta, h)$
s.t. FO Stokes PDEs

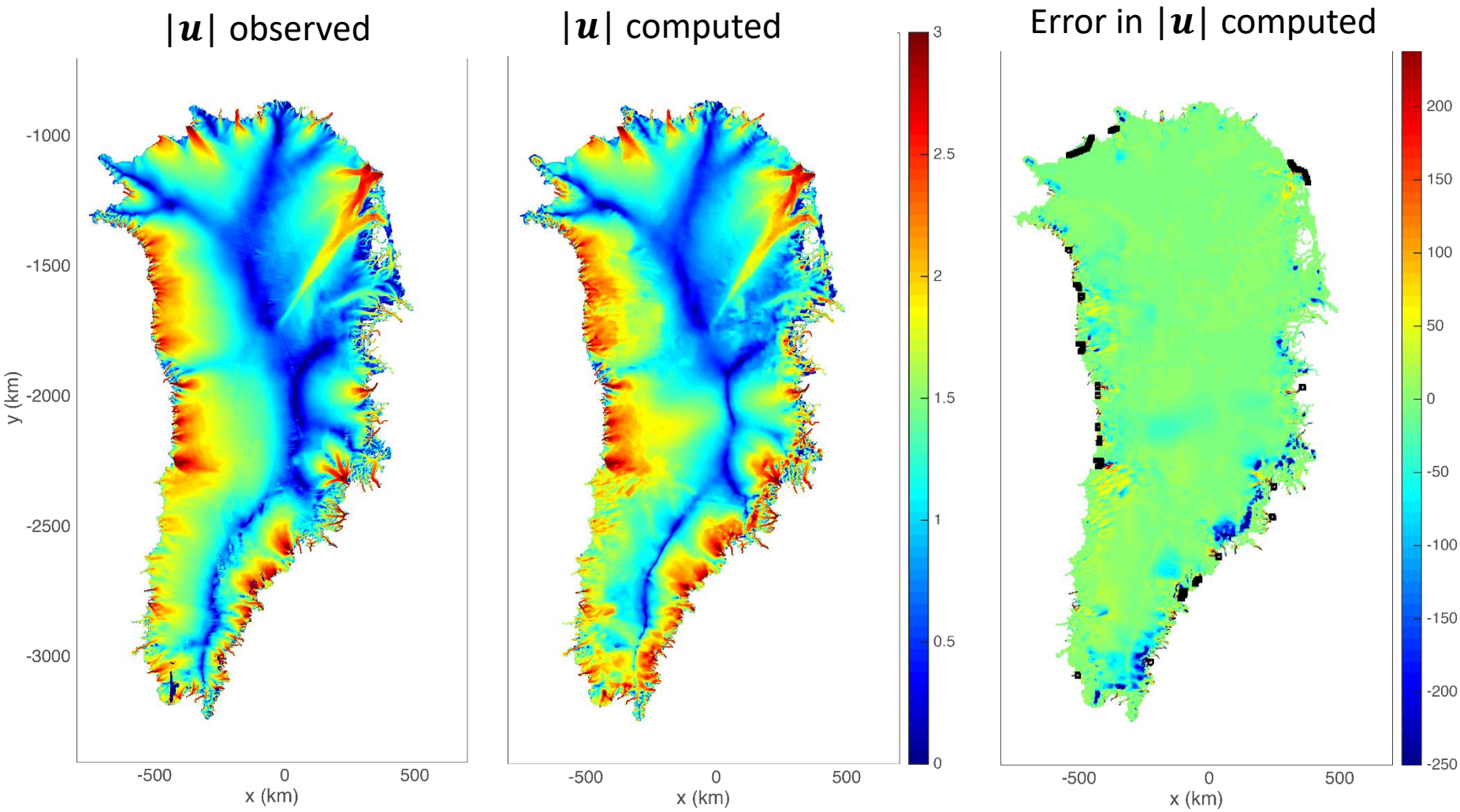
→ Solved via embedded ***adjoint-based PDE-constrained optimization*** algorithm in Albany/FELIX.

Algorithm	Software
Finite Element Method discretization	Albany
Quasi-Newton optimization (L-BFGS)	ROL
Nonlinear solver (Newton)	NOX
Krylov linear solvers	AztecOO+Ifpack/ML

- **<u>Some details:</u>**
  - ***Regularization:*** Tikhonov.
  - Total derivatives of objective functional $m(\beta, h)$ computed using ***adjoints*** and ***automatic differentiation*** (Sacado package of Trilinos).
  - ***Gradient-based optimization***: limited memory BFGS initialized with Hessian of regularization terms (ROL) with backtrack linesearch.

* Perego, Stadler, Price, *JGR*, 2014.

Deterministic Inversion: 1km Greenland Initial Condition



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Goal: solve inverse problem for ice sheet initial state but in ***Bayesian framework***

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- ***Naïve parameterization***: represent each degree of freedom on mesh be an uncertain variable

$$\beta(\boldsymbol{x}) = (z_1, z_2, \dots, z_{n_{\mathrm{dof}}})$$

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Intractable due to **curse of dimensionality**: $n_{\mathrm{dof}} = O(100K)$!

Bayesian Inference

UQ Workflow

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Deterministic inversion is consistent with Bayesian analog: it is used to find the MAP point of posterior.

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Bayesian Inference Assumptions

- Additive ***Gaussian noise*** model: $\boldsymbol{y}^{\text{obs}} = \boldsymbol{f}(\boldsymbol{z}) + \epsilon, \;\; \epsilon \sim N(\boldsymbol{0}, \boldsymbol{\Gamma}_{\text{obs}})$

  ⇒ **Mismatch functional to be minimized:**

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Evaluation of misfit Hessian is **expensive!** $\Rightarrow$ further approximation required.

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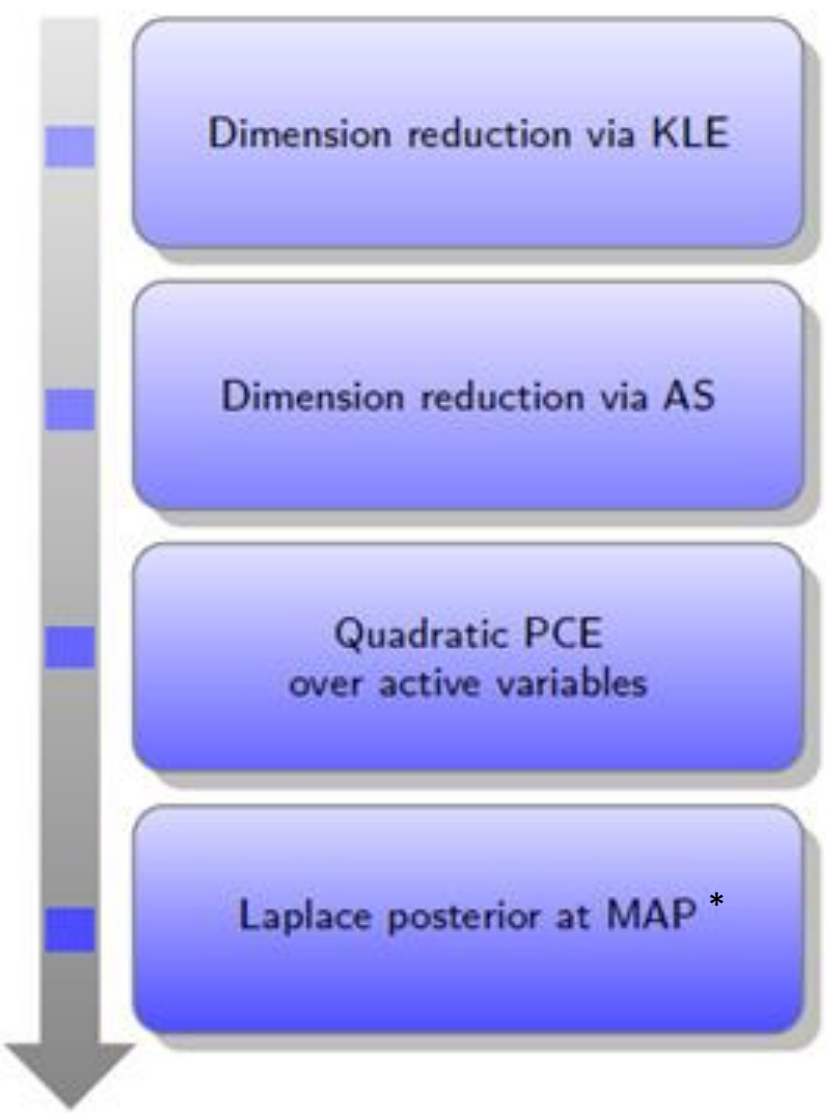
Bayesian Inference Workflow

KLE = Karhunen-Loeve Expansion
AS = Active Subspace
PCE = Polynomial Chaos Expansion
MAP = Maximum a Posteriori

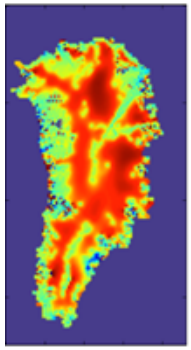


Two-part ***dimension reduction*** procedure to obtain modes $\phi_i(\boldsymbol{x})$

Procedure for computing ***covariance of normal Laplace posterior***, $\boldsymbol{\Gamma}_{\text{post}}$

* Bui-Thanh, Ghattas, Martin, Stadler, *SISC*, 2013.

Karhunen-Loeve Expansion (KLE)

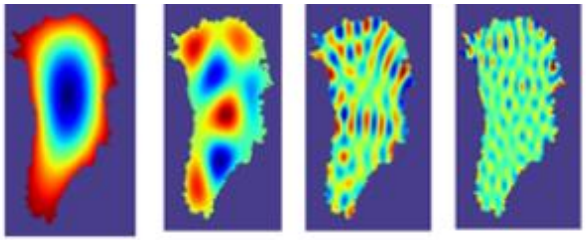


Best fit $\bar{\beta}$

$O(100K)$ dimensional inversion problem can be reduced to smaller dimensional problem using ***Karhunen-Loeve Expansion (KLE)***

$$\log(\beta(\boldsymbol{x})) = \log(\bar{\beta}) + \sum_{i=1}^{d} \sqrt{\lambda_i}\, \phi_i(\boldsymbol{x}) z_i$$

KLE modes ϕ_i



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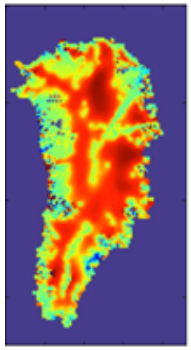

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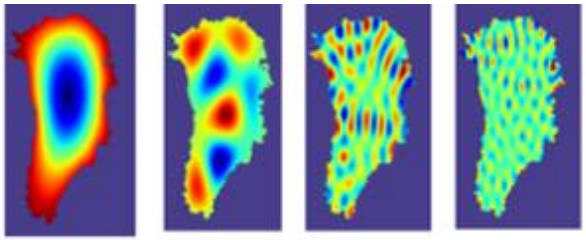

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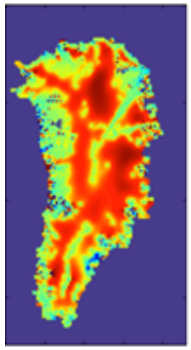

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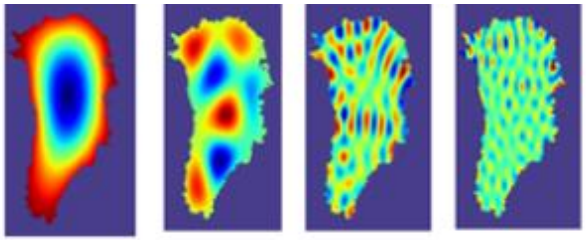

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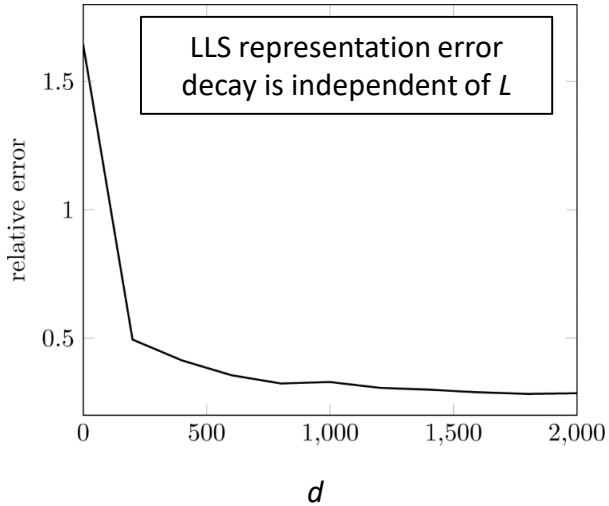

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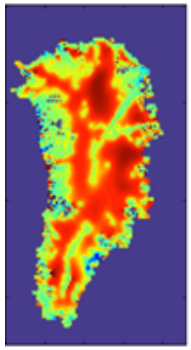

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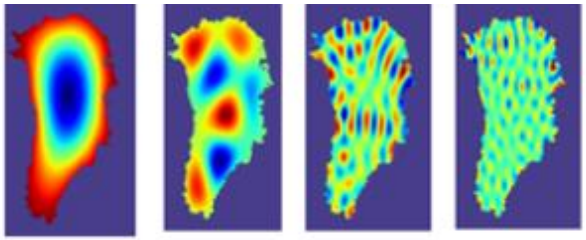

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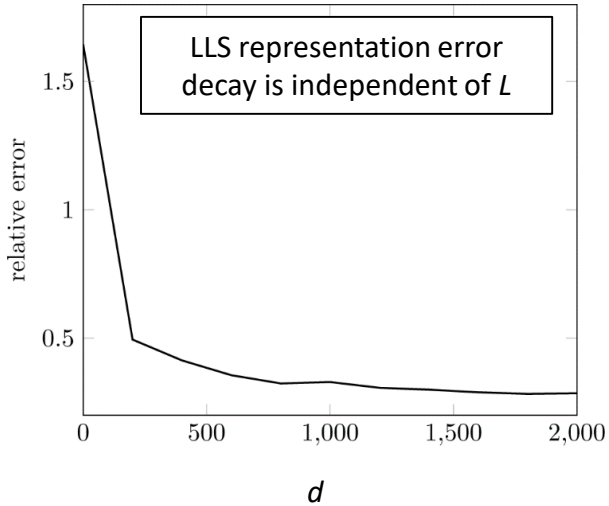
$\Rightarrow$ d should be $O(1000)$



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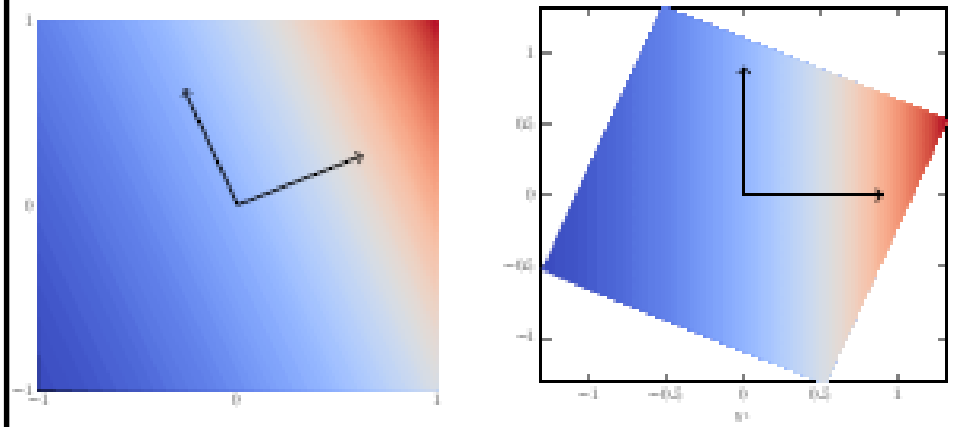
Example*: $m(\boldsymbol{z}) = \exp(0.7z_1 + 0.3z_2)$



<u>Dimension reduction via AS:</u>

(i) Rotate coords s.t. directions of strongest variation are aligned with the rotated coords.

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→ Bivariate function $m(\boldsymbol{z})$ is effectively ***univariate*** in rotated coordinate system

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- AS identified using ***gradients of mismatch function*** ∇m: $\int_{\mathbb{R}^d} \nabla m(z) \nabla m(z)^T d\rho(z) = \boldsymbol{W}\boldsymbol{\Lambda}\boldsymbol{W}^T$

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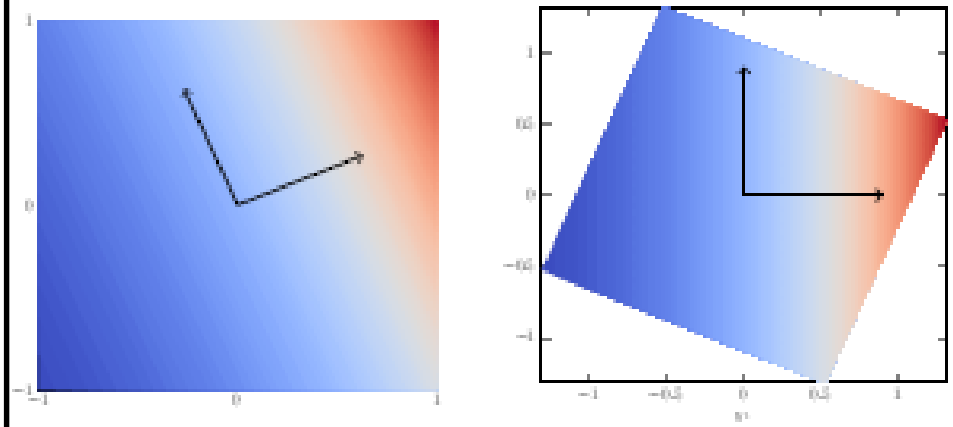

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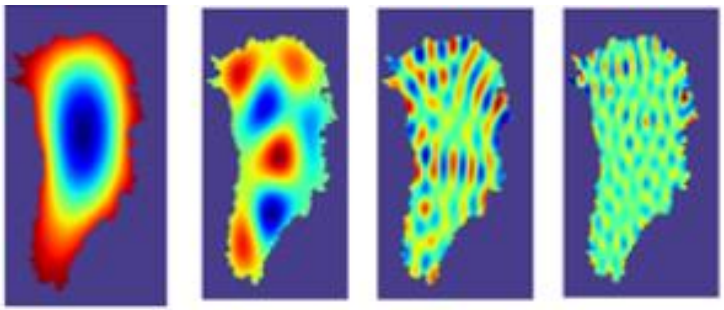
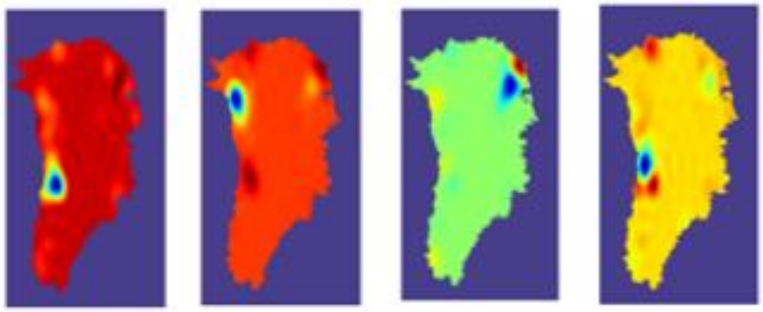
Greenland Bayesian Inference via KLE + AS

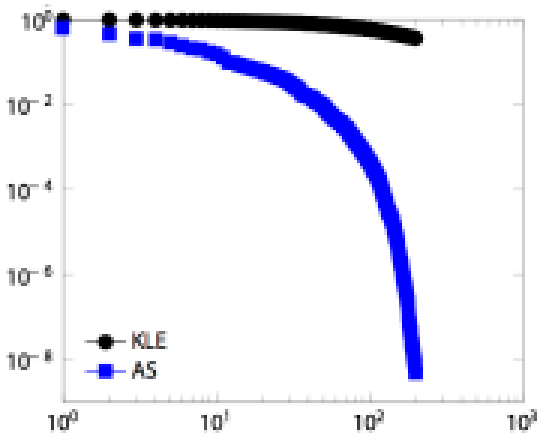
KLE modes



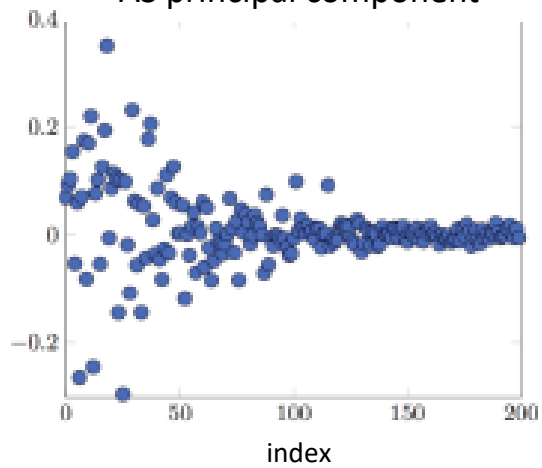
Data-informed (AS) directions (d=73*)



KLE and AS amplitudes



AS principal component



Gradients of mismatch function obtained via ***adjoint solve*** in Albany/FELIX.

- ***Above, left***: fewer modes are needed to build the basal friction parameter map when using KLE + AS methods than when using straight KLE.
- ***Above, right***: relative clustering of large values towards smaller indices implies KLE coefficients corresponding to larger singular values contribute most to variability in $m(\boldsymbol{z})$.

* Value of d was obtained via cross-validation.

Active Subspaces for Inference

Revert to prior in un-informed directions

$$\pi_{\text{pos}}(\mathbf{z}) \approx C_{\text{evid}}^{-1} \underbrace{\exp(-\hat{m}_s(\mathbf{W}_1^T\mathbf{z}))\pi_{\text{pr}}(\mathbf{W}_1^T\mathbf{z})}_{\text{Approximate posterior only in directions informed by data}} \overbrace{\pi_{\text{pr}}(\mathbf{W}_2^T\mathbf{z})}$$

Various levels of approximation can be employed:

- Reduce dimension but no surrogate of misfit
  - Perform MCMC in active subspace to improve mixing
- Surrogate of misfit with rotation but no dimension reduction
  - Leverage increased sparsity induced by rotation
- Surrogate of misfit and dimension reduction
  - **Combine MCMC in active subspaces with surrogates that adaptively target regions of high probability**

Quadratic PCE over Active Variables

Idea: approximate misfit $m(\boldsymbol{z})$ using quadratic PCE for efficient computation of misfit Hessian.

$$m(\boldsymbol{z}) \approx \hat{m}(\boldsymbol{z}) = \text{quadratic PCE function}$$

- Approximate misfit over active variables using a quadratic function obtained via compressed sensing (using M= 733 samples and a PCE with 20,301 terms)*:

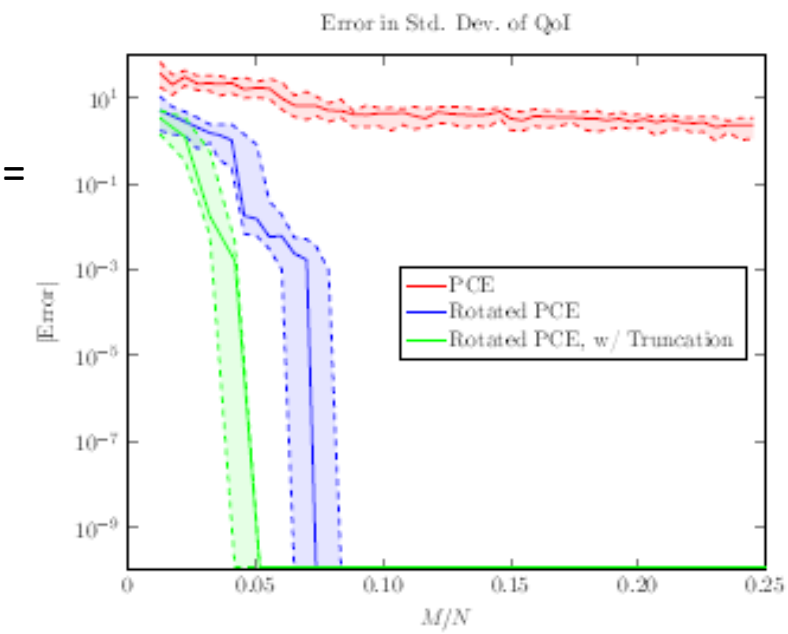
$$\frac{||m(\boldsymbol{z}) - \hat{m}(\boldsymbol{z})||_{l_\rho^2}}{||m(\boldsymbol{z}) - \sum_{i=1}^{M} m(\boldsymbol{z}^{(i)})\,||_{l_\rho^2}} \approx 0.981$$

- Approximate misfit with quadratic PCE in rotated d = 200 space:

$$\frac{||m(\boldsymbol{z}) - \hat{m}(\boldsymbol{W}^T\boldsymbol{z})||_{l_\rho^2}}{||m(\boldsymbol{z}) - \sum_{i=1}^{M} m(\boldsymbol{z}^{(i)})\,||_{l_\rho^2}} \approx 0.190$$

- Approximate misfit with ***quadratic PCE*** in ***rotated and truncated*** d = 73 space:

$$\frac{||m(\boldsymbol{z}) - \hat{m}_{s=73}\,(\boldsymbol{W}_1^T\boldsymbol{z})||_{l_\rho^2}}{||m(\boldsymbol{z}) - \sum_{i=1}^{M} m(\boldsymbol{z}^{(i)})\,||_{l_\rho^2}} \approx 0.136$$



$\text{rank}(A) = 5,\ d = 15,\ z_i \sim N(1/2, 1/5)$

* Ratios are improvements relative to using mean of data; want ratio close to 0.

Low Rank Laplace-Based Covariance*

$$\pi_{\text{pos}}\left(\boldsymbol{z} \mid \boldsymbol{y}^{\text{obs}}\right) = N(\boldsymbol{z}_{\text{MAP}}, \boldsymbol{\Gamma}_{\text{post}})$$

- ***Linearize*** parameter-to-observable map around MAP point:

$$\boldsymbol{y}^{\text{obs}} = \boldsymbol{f}(\boldsymbol{z}) + \epsilon \approx \boldsymbol{f}(\boldsymbol{z}_{\text{MAP}}) + \boldsymbol{F}(\boldsymbol{z} - \boldsymbol{z}_{\text{MAP}}) + \epsilon$$

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- ***Covariance*** of Gaussian Laplace ***posterior*** given by:

$$\boxed{\boldsymbol{\Gamma}_{\text{post}} = \left(\boldsymbol{H}_{\text{misfit}}^{\text{PCE}} + \boldsymbol{\Gamma}_{\text{prior}}^{-1}\right)^{-1}}$$

* Bui-Thanh, Ghattas, Martin, Stadler, *SISC*, 2013.

Low Rank Laplace-Based Covariance*

$$\pi_{\text{pos}}(\boldsymbol{z} \mid \boldsymbol{y}^{\text{obs}}) = N(\boldsymbol{z}_{\text{MAP}}, \boldsymbol{\Gamma}_{\text{post}})$$

$\boldsymbol{\Gamma}_{\text{post}}$ is dense!
$\Rightarrow$ ***prohibitively expensive*** to store & construct.

- ***Linearize*** parameter-to-observable map around MAP point:

$$\boldsymbol{y}^{\text{obs}} = \boldsymbol{f}(\boldsymbol{z}) + \epsilon \approx \boldsymbol{f}(\boldsymbol{z}_{\text{MAP}}) + \boldsymbol{F}(\boldsymbol{z} - \boldsymbol{z}_{\text{MAP}}) + \epsilon$$

where $\boldsymbol{F}$ = Frechet derivative of $\boldsymbol{f}$.

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- ***Low-rank approximation*** of $\boldsymbol{\Gamma}_{\text{post}}$ obtained using Sherman-Morrison-Woodbury formula:

$$\boldsymbol{\Gamma}_{\text{post}} \approx \boldsymbol{\Gamma}_{\text{prior}} - \widetilde{\boldsymbol{V}}_r \boldsymbol{D}_r \widetilde{\boldsymbol{V}}_r^{\Diamond}$$

Symbols*:

$\boldsymbol{V}_r, \boldsymbol{D}_r$: eigenvecs, eigenvals of $\widetilde{\boldsymbol{H}}_{\text{misfit}}$

$\widetilde{\boldsymbol{H}}_{\text{misfit}}$ = prior-preconditioned Hessian of data misfit = $\boldsymbol{\Gamma}_{\text{prior}}^{1/2} \boldsymbol{H}_{\text{misfit}} \boldsymbol{\Gamma}_{\text{prior}}^{1/2}$

$\boldsymbol{H}_{\text{misfit}}$ = Gauss-Newton portion of Hessian misfit = $\boldsymbol{F}^{\natural} \boldsymbol{\Gamma}_{\text{obs}}^{-1} \boldsymbol{F}$

$\widetilde{\boldsymbol{V}}_r$ = $\boldsymbol{\Gamma}_{\text{prior}}^{1/2} \boldsymbol{V}_r$, $\widetilde{\boldsymbol{V}}_r^{\Diamond}$ = adjoint of $\widetilde{\boldsymbol{V}}_r$

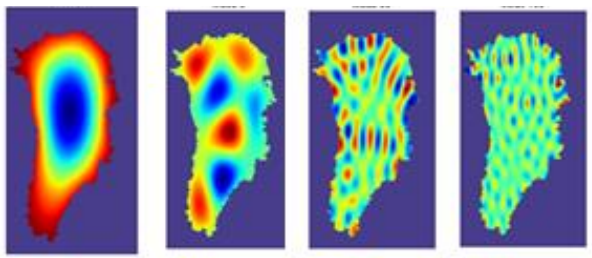
$\boldsymbol{\Gamma}_{\text{prior}}^{-1}$ = $\boldsymbol{M}^{-1}\boldsymbol{K}$, $\boldsymbol{K}$= Laplace stiffness.

- $\widetilde{\boldsymbol{H}}_{\text{misfit}}$ and its EV decomposition can be computed efficiently using a parallel ***matrix-free Lanczos method***.
- ***Rank of*** $\boldsymbol{\Gamma}_{\text{post}}$ = # of modes that informed directions of posterior (AS vectors).

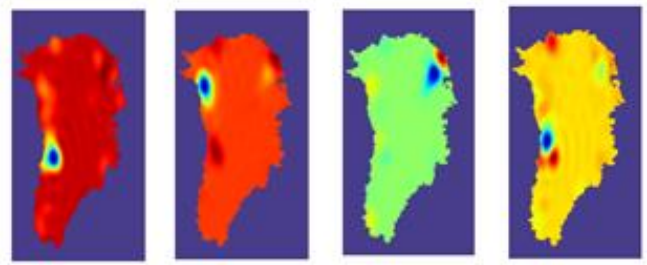
* Bui-Thanh, Ghattas, Martin, Stadler, *SISC*, 2013.

Greenland Bayesian Inference via KLE + AS

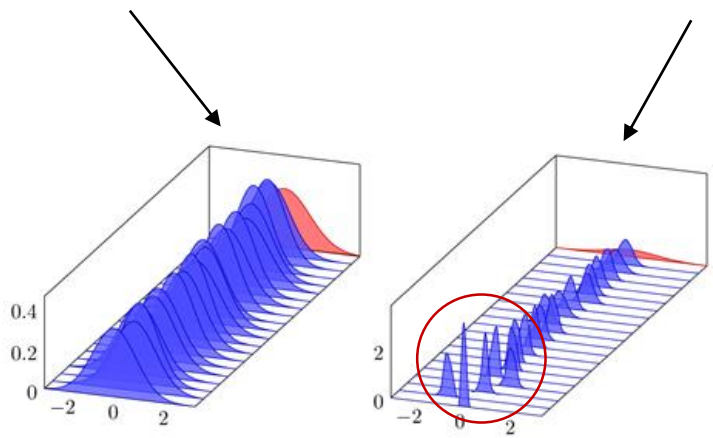
KLE modes



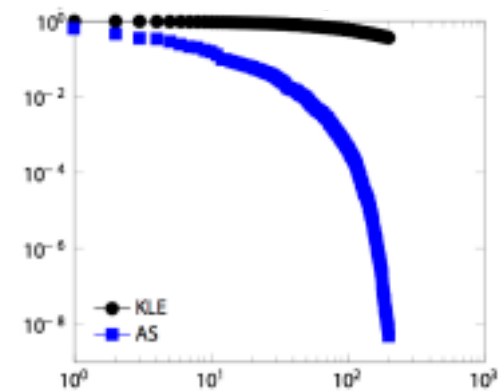
Data-informed (AS) directions (d=73*)



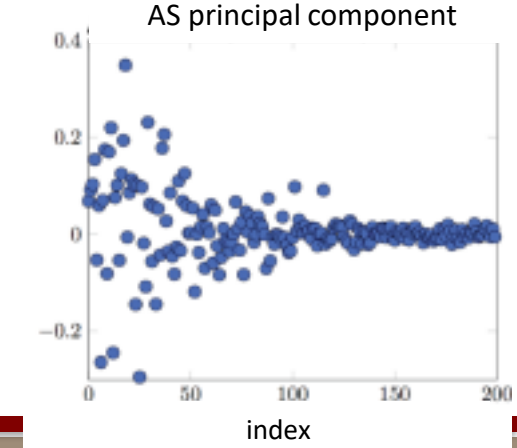
Gradients of mismatch function obtained via ***adjoint solve*** in Albany/FELIX.



KLE and AS amplitudes



AS principal component



- ***Above:*** marginal distributions of Gaussian posterior computed using KLE vs. KLE+AS; ***any shift from mean of 0 is due to observations***.
  - KLE eigenvectors have variance and mean close to prior.
  - Data-informed eigenvectors have smaller variance and are most shifted w.r.t. prior distribution (as expected).

* Value of d was obtained via cross-validation.

Outline

1. Background.
   - PISCEES project for land-ice modeling.
   - Land-ice model.
2. UQ problem definition.
3. Inversion/calibration.
   - Deterministic inversion.
   - Bayesian inference.
4. **Summary & future work.**

Summary & future work

This talk described our ***workflow*** for quantifying uncertainties in expected aggregate ice sheet mass change and its ***demonstration*** on a Greenland ice sheet problem, focusing on ***inversion***.

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- **<u>Future work:</u>**
  - Execute ***full UQ workflow*** (inversion + forward propagation) on realistic Greenland/Antarctic ice sheet problems.
  - ***Squared Laplace covariance operator approach**** (no KLE)
    - Less expensive than building PCE.
    - Allows higher dimensional parameter spaces.
  - Incorporate effects of ***other sources of uncertainty***, e.g., surface height, surface mass balance.

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Summary & future work

This talk described our ***workflow*** for quantifying uncertainties in expected aggregate ice sheet mass change and its ***demonstration*** on a Greenland ice sheet problem, focusing on ***inversion***.

- **<u>Future work:</u>**

We are well-positioned to **do these efforts in parallel!**

  - Execute ***full UQ workflow*** (inversion + forward propagation) on realistic Greenland/Antarctic ice sheet problems.
  - ***Squared Laplace covariance operator approach**** (no KLE)
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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.*

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Multiphysics Code

The ***Albany/FELIX land-ice solver*** is implemented within the ***Albany multi-physics code***.

Albany = Sandia open-source* parallel, C++, multi-physics finite element code.

- ***Component-based*** design for rapid development of new physics & capabilities.
- Extensive use of libraries from the open-source ***Trilinos*** project:
  - Automatic differentiation.
  - Discretizations/meshes, mesh adaptivity.
  - Solvers, time-integration schemes.
  - Performance-portable kernels.
- ***Advanced analysis*** capabilities:
  - Parameter estimation.
  - Uncertainty quantification (DAKOTA).
  - Optimization (DAKOTA, ROL).
  - Sensitivity analysis.

40+ packages; 120+ libraries

Analysis Tools (*black-box*)
- Optimization
- UQ (sampling)
- Parameter Studies
- Calibration
- Reliability

Composite Physics
- MultiPhysics Coupling
- System UQ

Analysis Tools (*embedded*)
- Nonlinear Solver
- Time Integration
- Continuation
- Sensitivity Analysis
- Stability Analysis
- Constrained Solves
- Optimization
- UQ Solver

Linear Algebra
- Data Structures
- Iterative Solvers
- Direct Solvers
- Eigen Solver
- Preconditioners
- Multi-Level Methods

Mesh Tools
- Mesh I/O
- Inline Meshing
- Partitioning
- Load Balancing
- Adaptivity
- Grid Transfers
- Quality Improvement
- Search
- DOF map

Mesh Database
- Mesh Database
- Geometry Database
- Solution Database
- Checkpoint/Restart

Utilities
- Input File Parser
- Parameter List
- Memory Management
- I/O Management
- Communicators
- Runtime Compiler

Architecture-Dependent Kernels
- Multi-Core
- Accelerators

Post Processing
- In-situ Visualization
- Verification
- QOI Computation
- Model Reduction

Local Fill

Discretizations
- Discretization Library
- Field Manager

Derivative Tools
- Sensitivities
- Derivatives
- Adjoints
- UQ / PCE Propagation

Physics Fill
- PDE Terms
- Source Terms
- BCs
- Material Models
- Responses
- Parameters

* https://github.com/gahansen/Albany.

Computing the Active Subspace

Gradients of mismatch $\nabla_\beta m$ can be used to identify subspace that controls variation in likelihood function (active subspace)

- Mismatch ***approximated*** by related function of fewer variables g:

$$m(\boldsymbol{z}) = \frac{1}{2}(\boldsymbol{d} - \boldsymbol{f}(\boldsymbol{z}))^T \boldsymbol{\Gamma}_{\text{obs}}^{-1}(\boldsymbol{d} - \boldsymbol{f}(\boldsymbol{z})) \approx g(\underbrace{\boldsymbol{W}_1^T \boldsymbol{z}}_{\text{Linear transformation (rotation) of coords}})$$

$\boldsymbol{W}_1^T \boldsymbol{z}$ = "active variables"

- Active subspace computed using $\int_{\mathbb{R}^d} \nabla m(z) \nabla m(z)^T d\rho(z) = \boldsymbol{W}\boldsymbol{\Lambda}\boldsymbol{W}^T$
  - Sample gradient using MC: $\left[\nabla m\left(z^{(1)}\right), \ldots, \nabla m\left(z^{(M)}\right)\right]$.
  - Form Gauss-Newton approx. of Hessian averaged over prior:

$$\boldsymbol{C} = \frac{1}{M}\sum_{i=1}^{M} \nabla m\left(z^{(i)}\right) \nabla m\left(z^{(i)}\right)^T$$

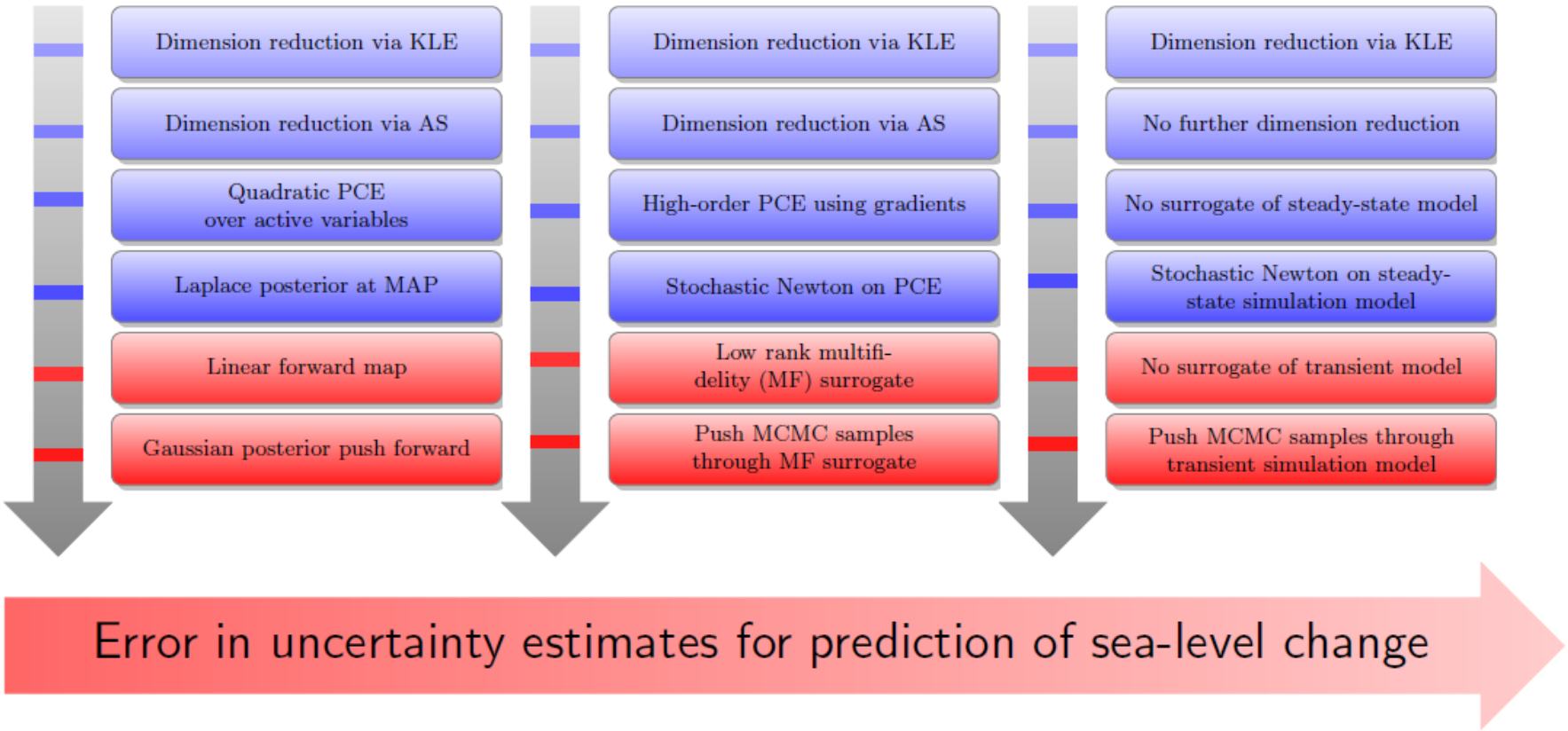
  - Compute eigenvalue decomposition: $\boldsymbol{C} = \boldsymbol{W}\boldsymbol{\Lambda}\boldsymbol{W}^T$
    $\rightarrow$ eigenvectors $\boldsymbol{W}$ define rotation of $\mathbb{R}^M$.

Perturbing $m(\boldsymbol{z})$ along columns of $\boldsymbol{W}_1$ changes $m(\boldsymbol{z})$ more.

- Partition $\boldsymbol{z}$ into ***active*** and ***inactive*** variables:

$$\boldsymbol{z} = \boldsymbol{W}_1^T \boldsymbol{z} + \boldsymbol{W}_2^T \boldsymbol{z}, \quad \boldsymbol{W} = [\boldsymbol{W}_1 \quad \boldsymbol{W}_2]$$

Full UQ Workflow: Varying Levels of Approx.



As with Bayesian inference:

- ***Future work:*** compare errors as accuracy of approximation is increased to gain insight into viability of lower-dimensional approximations.
- Lessons can be learned by avoiding use of highest fidelity model.