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Predicting Ice Sheet and Climate Evolution at Extreme Scales (PISCEES)

MIT Final Report
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1 Outline of Activities

A main research objectives of PISCEES is the development of formal methods for quantifying uncertainties in ice sheet modeling. Uncertainties in simulating and projecting mass loss from the polar ice sheets arise primarily from initial conditions, surface and basal boundary conditions, and model parameters. In general terms, two main chains of uncertainty propagation may be identified:

1. inverse propagation of observation and/or prior onto posterior control variable uncertainties;
2. forward propagation of prior or posterior control variable uncertainties onto those of target output quantities of interest (e.g., climate indices or ice sheet mass loss).

A related goal is the development of computationally efficient methods for producing initial conditions for an ice sheet that are close to available present-day observations and essentially free of artificial model drift, which is required in order to be useful for model projections ("initialization problem"). To be of maximum value, such optimal initial states should be accompanied by "useful" uncertainty estimates that account for the different sources of uncerainties, as well as the degree to which the optimum state is constrained by available observations.

The PISCEES proposal outlined two approaches for quantifying uncertainties. The first targets the full exploration of the uncertainty in model projections with sampling-based methods and a workflow managed by DAKOTA (the main delivery vehicle for software developed under QUEST). This is feasible for low-dimensional problems, e.g., those with a handful of global parameters to be inferred. This approach can benefit from derivative/adjoint information, but it is not necessary, which is why it often referred to as "non-intrusive". The second approach makes heavy use of derivative information from model adjoints to address quantifying uncertainty in high-dimensions (e.g., basal boundary conditions in ice sheet models). The use of local gradient, or Hessian information (i.e., second derivatives of the cost function), requires additional code development and implementation, and is thus often referred to as an "intrusive" approach.

Within PISCEES, MIT has been tasked to develop methods for derivative-based UQ, the "intrusive" approach discussed above. These methods rely on the availability of first (adjoint) and second (Hessian) derivative code, developed through intrusive methods such as algorithmic differentiation (AD). While representing a significant burden in terms of code development, derivative-baesd UQ is able to cope with very high-dimensional uncertainty spaces. That is, unlike sampling methods (all variations of Monte Carlo), calculational burden is independent of the dimension of the uncertainty space. This is a significant advantage for spatially distributed uncertainty fields, such as three-dimensional initial conditions, three-dimensional parameter fields, or two-dimensional surface and basal boundary conditions. Importantly, uncertainty fields for ice sheet models generally fall into this category.

2 Initialization via ice sheet/stream/shelf state and parameter estimation for prediction

The MIT team (Heimbach) has been pursuing intrusive strategies for initialization of ice flow models, but with no implicit assumption that observed ice sheets are in equilibrium with their environment. The approach uses adjoints to assimilate time-dependent observations into large-scale models and produces initial states with minimum artificial drift in the model state. These methods, which make a best attempt at capturing realistic transients, would be ideal for model initialization prior to forward time integrations. In a recent publication [Goldberg and Heimbach, 2013], the adjoint is generated by a combination of analytic methods and the use of algorithmic differentiation (AD) software. Several experiments are carried out with idealized geometries and synthetic surface observations, including inversion of time-dependent surface elevations for past ice thickness distributions, the simultaneous retrieval of basal traction and topography, and a demonstration of using adjoints to explore model sensitivities (Figure 1).

A general outline of the transient state and parameter estimation problem in the context of ocean and ice sheet models is provided in Wunsch and Heimbach [2013].

3 Ice flow model calibration via adjoint methods

Our ice flow model calibration approach borrows ideas from ocean state and parameter estimation (see Stammer et al. [2015] for a recent review). MIT's focus is on extending the current practice of performing steady-state (or shnapshot) ice flow inversions (e.g., Perego et al. [2014]) to those based

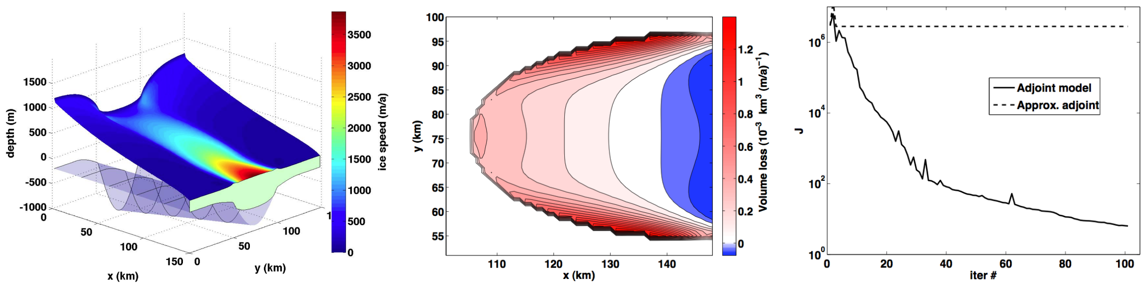

Figure 1: Idealized, coupled ice sheet/ocean model test case (left panel) for exploring adjoint-based sensitivities and data assimilation (after Goldberg and Heimbach [2013]). The middle panel shows deduced sensitivities of volume loss from the coupled system to submarine melt rates. The right panel shows convergence of the adjoint-based optimization algorithm, which includes time dependent assimilation of synthetic surface elevation change data. Convergence is robust only when the adjoint takes full account of system nonlinearities. From Goldberg and Heimbach [2013].

upon transient models and the use of time-resolved observations of diverse variables. To this end, we apply a mix of "intrusive" – based on algorithmic differentiation – and non-intrusive methods to develop an efficient adjoint of a transient ice flow model. The power of AD is documented in previous reports and has been summarized at a 2014 Dagstuhl workshop [Heimbach 2015]. The ability to mix such approaches offers the prospect of smooth integration of high-end steady state ice flow solvers currently developed within PISCEES into the transient framework.

The prototype framework developed has been applied to calibrate model simulations of the ice flow behavior of Smith, Pope, and Kohler Glaciers in the western Amundsen Sea Embayment, West Antarctica [Goldberg et al. 2015]. The study showcases the use of time-resolved velocity and ice height observations from satellite interferometric synthetic aperture radar (InSAR) and laser altimetry, respectively, to constrain an ice flow model over the period 2000 to 2011. To our knowledge, this is one of the first examples of time-dependent data assimilation for use in the calibration and optimization of a next-generation ice flow model. The transient state for 2011 is then used as initial condition for a 30-year forecast. Because no additional forcing is applied, the resulting change in ice volume above floatation (VAF), i.e. the portion of mass loss contributing to sea level, is considered as committed sea level rise.

By way of example, Fig. 2 shows the residual misfit between simulated and observed ice surface elevation in 2011 after snapshot (or steady-state) calibration (left panel) versus transient calibration (right panel). The transient nature of the problem shows a marked benefit on the fidelity of the 2011 state, and which is used as initial condition used for projecting 30-year mass changes

4 Intrusive, Hessian-based inverse-predictive UQ

Extending the use of derivative information for UQ, the MIT team has also begun to explore the systematic use of Hessian information to produce posterior uncertainty estimates of forcing and

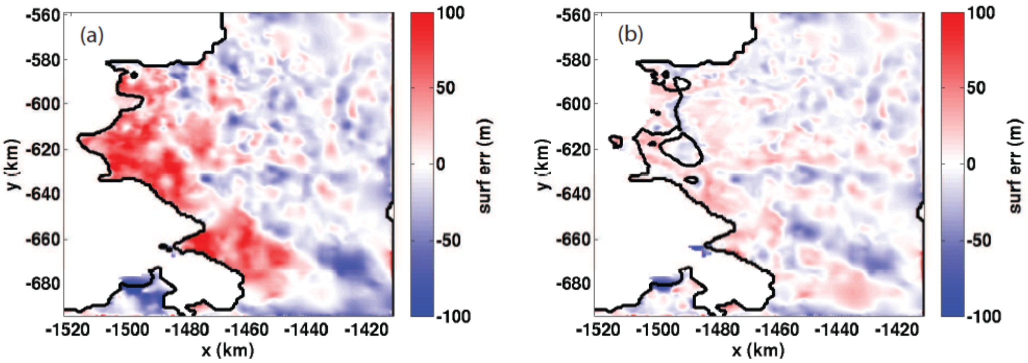

Figure 2: Difference between modeled and observed 2011 surface elevation using snapshot (a) and transient (b) adjoint-based model calibration. From Godlberg et al. [2015].

parameter fields of a dynamic model (initially a barotropic ocean model, the underlying code of which is being used to study ice shelf-ocean interactions). The concept of Hessian-based inverse-predictive UQ has been developed by PI Heimbach and graduate student Alex Kalmikov. Kalmikov successfully completed his Ph.D. thesis in January 2013 in the MIT-WHOI Joint Program in Ocean Engineering, and concluded his post-doc at MIT in October 2013.

To accelerate the breakthrough of a proof-of-concept study we implemented the machinery in the context of an ocean model for three reasons: (1) derivative code of the model were available through well-developed intrusive methods; (2) the problem at hand provided an example of highly non-trivial second-derivative generation for a high-dimensional (10^5) control space; and (3) we were very familiar with the code, enabling rapid implementation of the method. The concepts developed are sufficiently general to be implemented in an ice sheet model once derivative components of the ice sheet model become available. For the FELIX-FO and FELIX-Stokes dycores being developed under PISCEES, we anticipate such derivative information to be available within the next year of the project.

The Hessian information is used to infer which elements (spatial patterns) of a high dimensional uncertainty space are well constrained by observations and which elements remain poorly constrained despite observations (Kalmikov and Heimbach, 2013). A UQ chain is explored (Fig. 3), in which the inverse uncertainty propagation to obtain posterior error estimates is followed by a forward uncertainty step, in which the posterior uncertainties are propagated via the dynamical model onto target quantities of interests (such as heat or mass transports in oceanography, or ice volume above floatation in ice sheet modeling).

5 Use of simplified ice models for concept studies and education

While awaiting the availability of a working adjoint model within the PISCEES modeling infrastructure, work at MIT has focussed on concept studies and education. Since completion of his Master's thesis and an internship at Sandia National Lab, working with Bart van Bloemen Waan-

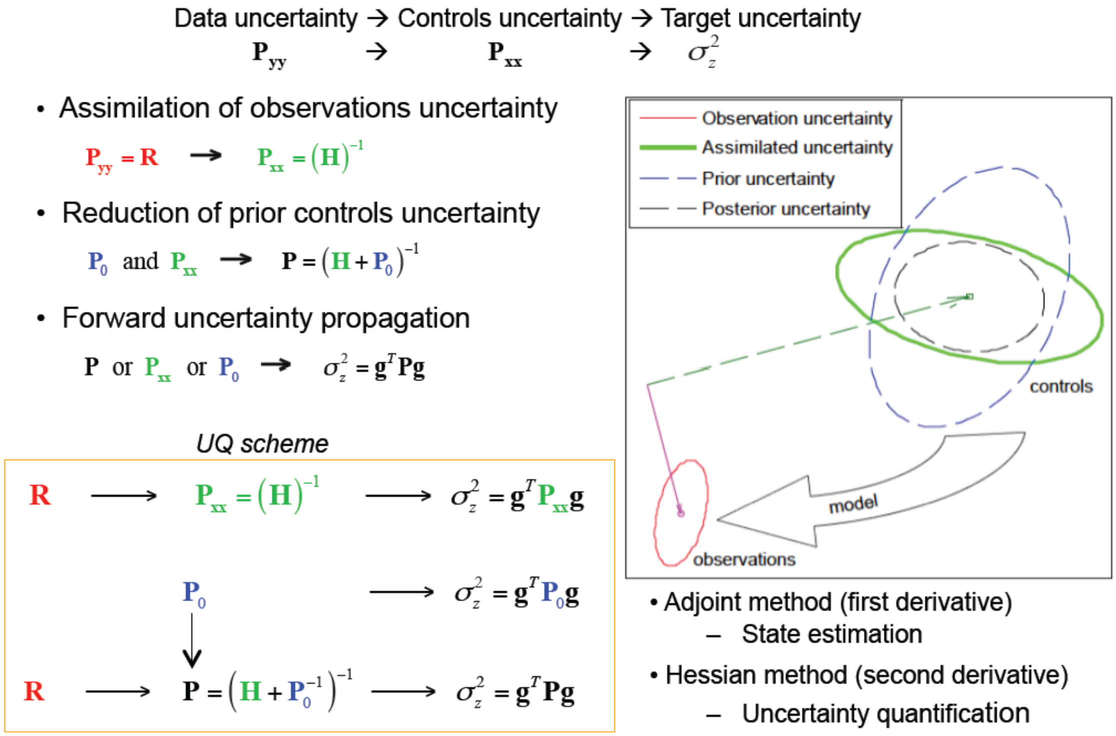

Figure 3: UQ propagation chain, in derivative-based UQ (from Kalmikov and Heimbach, 2013). Observation (red) and prior (blue) parameter, forcing, or initial state uncertainties are used in a derivative-based (adjoint) inversion scheme to infer posterior uncertainty estimates (black) via the inverse Hessian. Where observations have a strong impact, posterior uncertainties are significantly reduced; where observation impact is small, posterior estimates deviate little from their priors. Posterior uncertainties are then propagated via the dynamical model's tangent linear and adjoint operators ($\mathbf{g}$, $\mathbf{g}^T$) to produce error estimates σ_z for the target quantity of interest, z. From Kalmikov and Heimbach [2014].

ders on uncertainty quantification methods Andrew Davis has been accepted in MIT's Aero/Astro doctoral program, where he is now continuing work on uncertainty quantification in glacier models using deterministic (i.e., adjoint) and stochastic methods. His co-advisor in Aero/Astro is Youssef Marzouk who is also MIT's PI on the SciDAC Institute "Quantification of Uncertainty in Extreme Scale Computations" (QUEST).

6 Community service

PI Heimbach serves as co-chair on the US CLIVAR Working Group on Greenland Ice Sheet-Ocean interactions (GRISO WG). He co-authored several reviews of the state of knowledge of the subject, including the review in Bull. Amer. Met. Soc. [Straneo et al., 2013], the review in Nature [Straneo and Heimbach, 2013], and the US CLIVAR GRISO workshop summary [Heimbach et al., 2014].

Heimbach was one of the lead organizers of an international US CLIVAR-sponsored Workshop on "Understanding the Response of Greenland's Marine Terminating Glaciers to Oceanic and Atmospheric Forcing", held near Boston, MA, from June 4 to 7, 2013, see `http://www.usclivar.org/meetings/griso-workshop`. A workshop report bei Heimbach et al. [2014] contains key recommendations and requirements to advance the science in the coming 5 to 10 years.

7 Publications, theses, conference proceedings

2015

• Goldberg, D., P. Heimbach, I. Joughin, and B. Smith, 2015: Committed retreat of Smith, Pope, and Kohler Glaciers over the next 30 years inferred by transient model calibration. *The Cryosphere*, 9, 2429-2446, doi:10.5194/tc-9-2429-2015

• Heimbach, P., 2015: Application of derivative code in climate modeling. in: N. Gauger, M. Giles, M. Gunzburger, and U. Naumann (eds.): Adjoint Methods in Computational Science, Engineering, and Finance. *Dagstuhl Reports*, 4(9), 14-16, doi:10.4230/DagRep.4.9.1.

2014

• Heimbach, P., F. Straneo, O. Sergienko, and G. Hamilton, 2014: International workshop on understanding the response of Greenlands marine-terminating glaciers to oceanic and atmospheric forcing: Challenges to improving observations, process understanding and modeling. June 4-7, 2013, Beverly, MA, USA. US CLIVAR Report 2014-1, US CLIVAR Project Office, Washington DC, 20006.

• Heimbach, P., F. Straneo, and O. Sergienko, 2014: Understanding the response of Greenland's marine terminating glaciers to oceanic and atmospheric forcing (Guest Editorial). *US CLIVAR Variations*, 12(2), pp. 1–2.

• Kalmikov, A. and P. Heimbach, 2014: A Hessian-based method for Uncertainty Quantification in Global Ocean State Estimation. *SIAM J. Scientific Computing* (Special Section on Planet Earth and Big Data), 36(5), S267S295, doi:10.1137/130925311.

2013

• Goldberg, D. and P. Heimbach, 2013: Parameter and state estimation with a time-dependent adjoint marine ice sheet model. *The Cryosphere*, 7, 1659-1678, doi:10.5194/tc-7-1659-2013.

• Heimbach, P., F. Straneo, O. Sergienko, and G. Hamilton, 2014: Understanding the Response of Greenlands Marine-Terminating Glaciers to Oceanic and Atmospheric Forcing. Challenges to improving observations, process understanding and modeling. Report from a US CLIVAR-sponsored International Workshop, June 4-7, 2013, Beverly, MA, USA. US CLIVAR Report 2014-1, US CLIVAR Project Office, Washington DC, 20006.

• Kalmikov, A., 2013: Uncertainty Quantification in Ocean State Estimation. Ph.D. thesis, MIT-

WHOI Joint Program in Ocean Engineering, February 2013, Cambridge, MA.

• Straneo, F. and P. Heimbach, 2013: North Atlantic warming and the retreat of Greenland's outlet glaciers. *Nature*, 504, 36-43, doi:10.1038/nature12854.

• Straneo, F., P. Heimbach, O. Sergienko, and 15 others, 2013: Challenges to Understand the Dynamic Response of Greenlands Marine Terminating Glaciers to Oceanic and Atmospheric Forcing. *Bull. Amer. Met. Soc.*, 94(8), 1131-1144, doi:10.1175/BAMS-D-12-00100.

• Wunsch, C. and P. Heimbach, 2013: Dynamically and kinematically consistent global ocean circulation and ice state estimates. In: *Ocean Circulation and Climate: A 21st Century Perspective*, (G.Siedler, J.Church, J.Gould and S.Griffies, eds.), Chapter 21, pp. 553-579, Elsevier, doi:10.1016/B978-0-12-391851-2.00021-0.

8 Conference/workshop presentations

2015

2015/08: IGS 2015, International Glaciology Society Symposium 2015 on "Contemporary ice-sheet dynamics: ocean interaction, meltwater, and non-linear effects", Churchill College, Cambridge, UK.

2015/06: SIAM Conference on Mathematical and Computational Issues in the Geosciences 2015, Stanford University, Stanford, CA (mini-symposium on "Bayesian methods for large-scale geophysical inverse problems")

2014

2014/09: Dagstuhl Seminar on "Adjoint Methods in Computational Science, Engineering, and Finance" (14371), Schloss Dagstuhl (Leibniz-Zentrum für Informatik), Germany

2014/07: SIAM Annual Meeting, Minisymposium on "Mathematical Challenges in the Geosciences", Chicago, IL

2014/07: "Ice Sheet MIP for CMIP6" Workshop, NASA/GSFC, Greenbelt, MD

2014/06: "Atmospheric, Oceanic, and Ice Flow Adjoint Modelling in the UK", Centre for Mathematical Sciences (CMS), University of Cambridge, and British Antarctic Survey (BAS), UK.

2014/05: IGS Symposium on the Contribution of Glaciers and Ice Sheets to Sea Level Change, Chamonix, France

2014/05: DOE ACME Integrated Climate Modeling PI Meeting, Bolger Center, Washington, D.C.

2013

2013/02: CLIVAR/WGOMD/SOP Workshop on Sea Level Rise, Ocean/Ice Shelf Interactions and

Ice Sheets, Hobart, Australia. *"Understanding the Dynamic Response of Greenlands Marine Terminating Glaciers to Oceanic and Atmospheric Forcings"*.

2013/02: SIAM Conference on Computational Science and Engineering (CSE'13), Boston, MA.
– *"State and parameter sensitivities and estimation in coupled ocean/ice shelf/ice stream evolution"*.
– *"Dynamically and kinematically consistent global ocean-ice state and parameter estimation with a general circulation model and its adjoint"*.

2013/04: EGU 2013, Vienna.
– *"Deterministic versus stochastic trends in global sea level reconstructions"*.
– *"Adjoint-based sensitivities and data assimilation with a time-dependent marine ice sheet model"*.

2013/04: ICES & Jackson School of Geosciences, U. Texas, Austin.
– *"Uncertainty Quantification in Ocean State Estimation, with application to Drake Passage transport"*.
– *"Forward and inverse modeling of ice shelf-ocean interactions of the Pine Island Glacier and sub-ice shelf cavity system"*.

2013/05: Workshop on Large-Scale Inverse Problems and Quantification of Uncertainty: Big Data Meets Big Models, Bishops Lodge, Santa Fe, NM
– *Uncertainty Quantification in Global Ocean State Estimation*

2013/06: U.S. CLIVAR-sponsored International Workshop on "Understanding the Response of Greenlands Marine Terminating Glaciers to Oceanic and Atmospheric Forcing", Beverly, MA
– *Organizing and Scientific Steering Committee*

2013/07: Davos Atmosphere and Cryosphere Assembly DACA-13, Davos, Switzerland.
– *Sensitivity of sub-ice shelf melt rate parameterizations in a general circulation model: thermodynamic versus dynamic forcing*
– *Adjoint-based sensitivities and data assimilation with a time-dependent marine ice sheet model*

2013/07: SIAM Annual Meeting, San Diego, CA: Mini-Symposium Title: Uncertainty Quantification in Climate Modeling and Prediction.
– *Uncertainty Quantification in Global Ocean State Estimation*

2013/12: AGU Fall Meeting, San Francisco, CA
– *IARPC Glacier-Fjord Implementation Team Open Meeting*
– *Uncertainty Quantification in Global Ocean State Estimation*