SIAMUQ — UQ Challenge Benchmarks

UQ Benchmark Problems for Multiphysics Modeling

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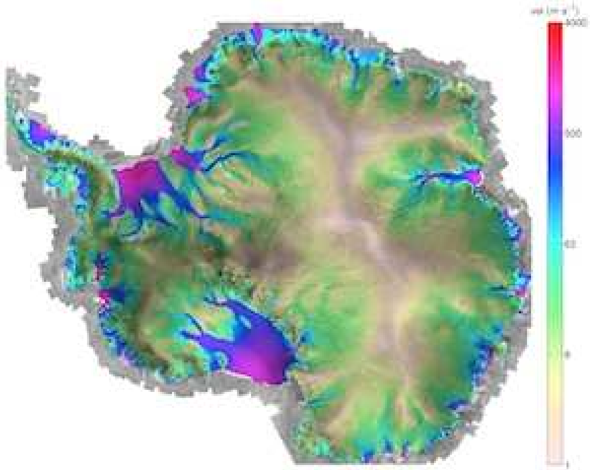
Motivation

- Previous presentation at **USNCCM2013 — UQ Challenge Benchmarks:**
  - General discussion of challenges in UQ for multiphysics modeling.
  - Identification of thermomechanics as a general context to articulate benchmark problems in.

- This presentation at **SIAMUQ2014 — UQ Challenge Benchmarks:**
  - Articulation of benchmark problems in the specific context of ice sheet modeling.



  - Feedback from, and iteration with, the UQ and USACM communities is still required.

Plan

- Motivation.
- Plan.
- Challenges in UQ for multiphysics modeling.
- Ice sheet modeling.
- Ice sheet benchmarks problems.
- Conclusion.
- References.

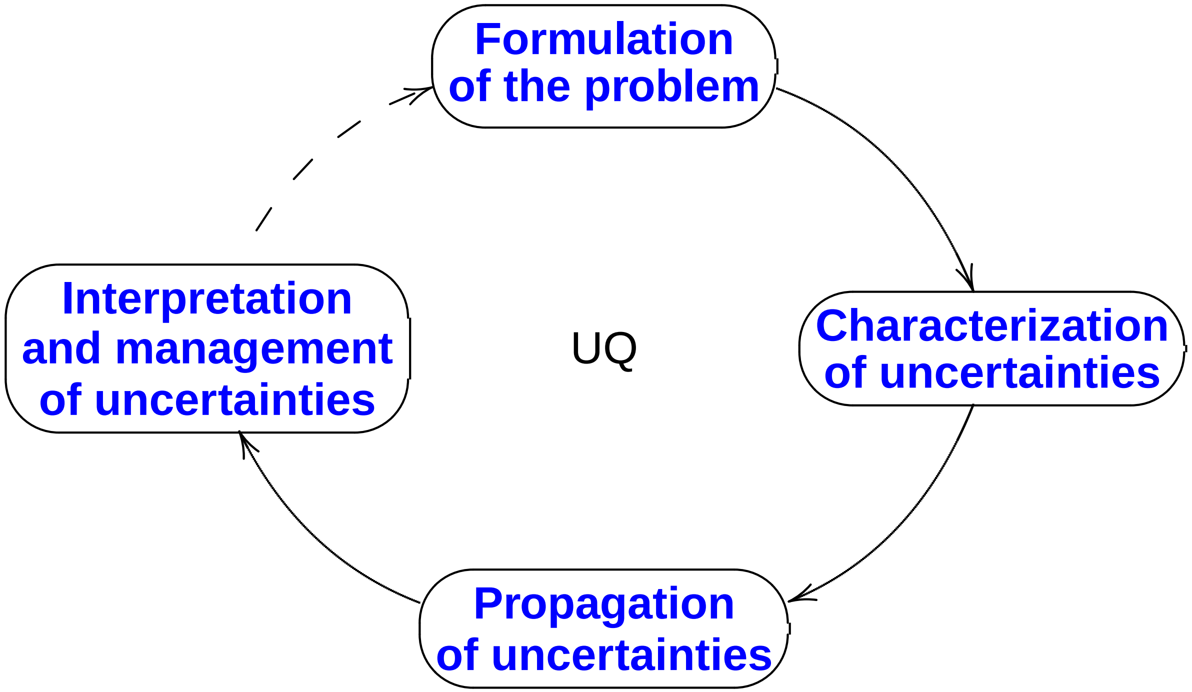
Challenges in UQ for multiphysics modeling

Challenges in UQ for multiphysics modeling

- **Coupling of physics can take a variety of forms**:
  - single equation with multiple terms that represent different physical phenomena,
  - system of multiple components coupled through bulk parameters or loadings or both,
  - system of multiple components coupled across shared interfaces,
  - system of multiple components with different types of physical description,
  - system of multiple components with different rates or resolutions or both,
  - . . .

- Various **challenges** follow from there being **two or more distinguishable components** with **some form of coupling** between them.

Challenges in UQ for multiphysics modeling



- This is just one way of decomposing a UQ analysis into subanalyses to help us make an inventory of some of the challenges that are presented to us in UQ for multiphysics modeling.

Challenges in UQ for multiphysics modeling

- **Characterization of uncertainties** involves inferring from available information a representation of parametric uncertainties and modeling errors associated with a model.

- Various challenges follow from there being two or more components with some form of coupling:
  - **Issue of dependence of parametric uncertainties**:

    Parameters of different components of a multiphysics problem can depend on one another.
  - **Issue of dimensionality of parametric uncertainties**:

    The amount of data and the work required for characterizing parametric uncertainties increases quickly with the number of parameters.
  - **Issue of modeling errors stemming from the coupling**:

    Uncertainties can stem not only from the components themselves but also from their coupling.
  - . . .

- For example, when characterizing uncertainties involved in **multiphysics constitutive models and equations of state**, there can be issues of jointly characterizing uncertainties in parameters involved in these multiphysics constitutive models and equations of state, as well as issues of characterizing modeling errors that may exist in their functional forms themselves.

Challenges in UQ for multiphysics modeling

- **Propagation of uncertainties** involves mapping the characterization of the parametric uncertainties and modeling errors into a characterization of the induced uncertainty in predictions.

- Various challenges follow from there being two or more components with some form of coupling:
  - **Issues of mathematical analysis**:

    Local versus global well-posedness and regularity results. Nonlinearities. Bifurcations. ...
  - **Issues of numerical solution**:

    Tightly coupled vs. partitioned. Preconditioning. Convergence. Stability. Scalability. ...

- How do merits and limitations of intrusive versus nonintrusive methods evolve in the presence of these issues of mathematical analysis and numerical solution?

- How do recent improvements, such as preconditioned intrusive methods and multilevel Monte Carlo methods, carry over to UQ for multiphysics modeling?

- Software (Dakota, Stokhos, UQTk, QUESO, GPMSA,...) for rapid application development.

- ...

Challenges in UQ for multiphysics modeling

- **Analysis and management of uncertainties** involves exploiting uncertainty quantification to gain insight useful for optimal reduction of uncertainties, model validation, design optimization, . . .

- Various challenges follow from there being two or more components with some form of coupling:
  - **New types of quantity of interest**:

    Predicting decay rates, bifurcations, . . . versus predicting states at specific times and locations.

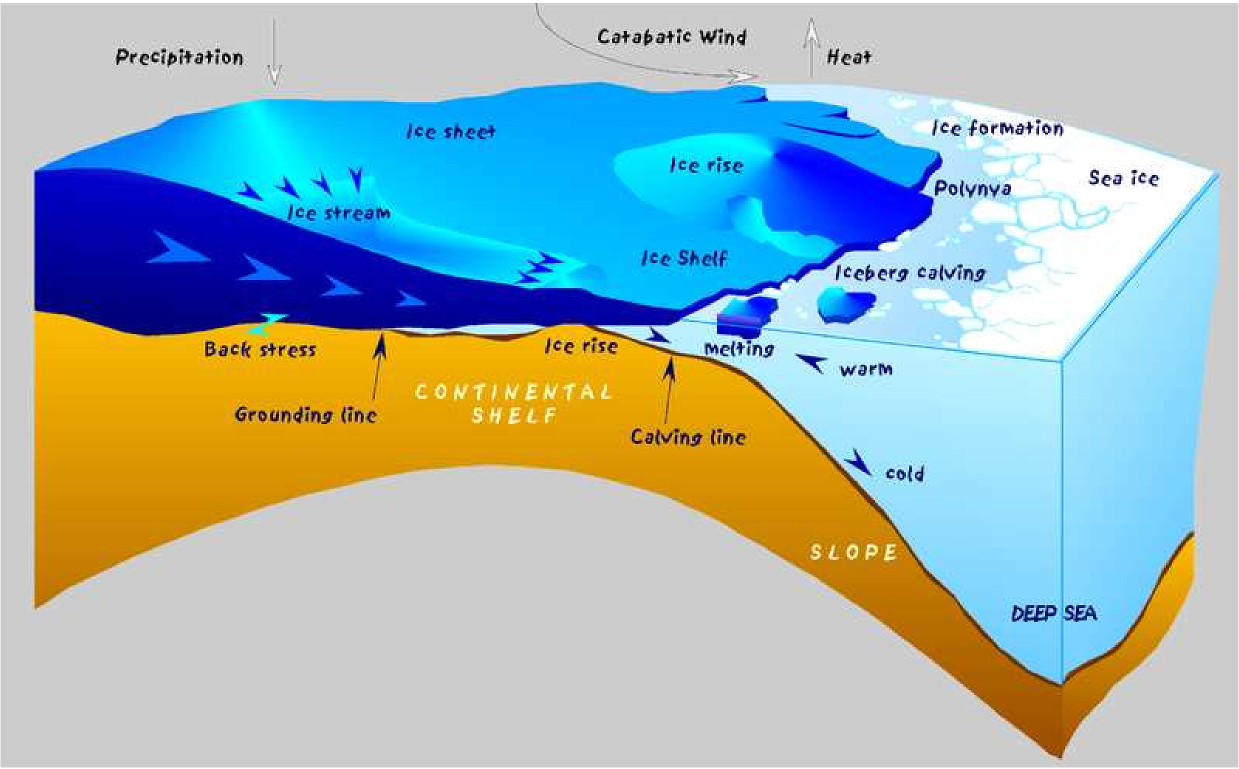
  - **New types of question**:

    Dependence between quantities of interest relevant to different components. Apportioning uncertainties in quantities of interest to different components. Missing physics. . . .

- For example, in the electromechanical modeling of an AFM tip, interest could be in predicting the pull-in voltage (instability) rather than in predicting the displacement for a specific voltage.

Ice sheet modeling

Ice sheet modeling



- Ice sheets are ice masses of continental size which rest on solid land (lithosphere).
- Ice sheets show gravity-driven creep flow. This leads to thinning and horizontal spreading, which is counterbalanced by snow accumulation in the higher areas and melting and calving in the lower areas. Any imbalance leads to either growing or shrinking ice sheets.

Constitutive model for ice

- Ice is usually assumed **incompressible** and to obey a **nonlinearly viscous constitutive model**, which relates the deviatoric stress tensor to the strain rate tensor as follows:

$$\boldsymbol{\sigma}_{\mathrm{D}} = 2\,\eta\big(T, i_{\boldsymbol{D}}^{(2)}\big)\ \boldsymbol{D},$$

  in which the viscosity depends on the temperature and the second invariant of the strain rate tensor:

$$\eta\big(T, i_{\boldsymbol{D}}^{(2)}\big) = \frac{1}{2}\, b(T)\ \big(i_{\boldsymbol{D}}^{(2)}\big)^{-\frac{1}{2}(1-1/n)}, \quad b(T) = \big(a(T)\big)^{-1/n}, \quad a(T) = a_0 \exp\left(-\frac{q}{r(T+\beta p)}\right).$$

- **Issues relevant to uncertainty quantification**:
  - **Parametric uncertainties**: The value of the exponent n has been a matter of debate. Values of n deduced from experiments range from 1.5 to 4.2 with a mean of about 3.
  - **Modeling errors**: The model form has also been a matter of debate. As compared to a general Rivlin-Ericksen representation, this constitutive model lacks dependence on the third invariant of the strain rate tensor and ignores a term quadratic in this strain rate tensor.

Ice sheet modeling

Dynamics of ice sheets — governing equations

- **Conservation of mass:**

$$\text{div}(\boldsymbol{v}) = 0.$$

- **Conservation of momentum:**

$$\textbf{div}(-p\boldsymbol{I} + 2\eta\boldsymbol{D}) + (\rho\boldsymbol{g} - 2\boldsymbol{\omega} \times \boldsymbol{v}) = \rho\frac{d\boldsymbol{v}}{dt};$$

neglecting the acceleration and Coriolis terms based on dimensional analysis, we obtain

$$-\boldsymbol{\nabla} p + \eta\textbf{divD}\boldsymbol{v} + 2\boldsymbol{D}(\boldsymbol{\nabla}\eta) + \rho\boldsymbol{g} = \boldsymbol{0}.$$

- **Conservation of energy:**

$$\rho\frac{de}{dt} = \text{tr}(\boldsymbol{\sigma}\boldsymbol{D}) - \text{div}(\boldsymbol{q});$$

assuming $\boldsymbol{q} = -\boldsymbol{K}(\boldsymbol{\nabla}T)$ and $e = cT$ and using $\text{tr}(\boldsymbol{\sigma}\boldsymbol{D}) = 4\eta i_{\boldsymbol{D}}^{(2)}$, we obtain

$$\rho c\frac{dT}{dt} = 4\eta i_{\boldsymbol{D}}^{(2)} + \text{div}\big(\boldsymbol{K}(\boldsymbol{\nabla}T)\big).$$

Dynamics of ice sheets — boundary conditions

- **Free-surface boundary conditions:**

$$\frac{\partial h}{\partial t} + v_x \frac{\partial h}{\partial x} + v_y \frac{\partial h}{\partial y} - v_z = n_\mathrm{s} a_\mathrm{s} \qquad \text{(free-surface mass balance)},$$

$$\boldsymbol{\sigma}(\boldsymbol{n}) = \mathbf{0} \qquad \text{(stress-free b.c.)},$$

$$T = T_\mathrm{s} \qquad \text{(thermodynamic b.c.)}.$$

- **Ice-base boundary conditions:**

$$\frac{\partial b}{\partial t} + v_x \frac{\partial b}{\partial x} + v_y \frac{\partial b}{\partial y} - v_z = n_\mathrm{b} a_\mathrm{b} \qquad \text{(basal mass balance)},$$

$$\boldsymbol{v}_\mathrm{b} = \begin{cases} 0 & \text{if } T_\mathrm{b} < T_\mathrm{m}, \\ -\, c_\mathrm{b} \dfrac{\tau_\mathrm{b}^p}{n_\mathrm{b}^q} \boldsymbol{e}_\mathrm{t} & \text{if } T_\mathrm{b} = T_\mathrm{m}, \end{cases} \qquad \text{(basal-sliding b.c.)},$$

$$\begin{cases} \boldsymbol{K}(\boldsymbol{\nabla})T \cdot \boldsymbol{n} = q_\mathrm{geo} & \text{if } T_\mathrm{b} < T_\mathrm{m} \text{ (cold base)}, \\ T = T_\mathrm{m} & \text{(temperate base)}, \end{cases} \qquad \text{(thermodynamic b.c.)}.$$

- **Issues relevant to uncertainty quantification**:
  - **Parametric uncertainties**: The values of the exponents p and q have been a matter of debate. Values of $(p, q) = (3, 1)$ and $(p, q) = (3, 2)$ are commonly used for sliding on hard rock.

Numerical implementation

- FE and FD implementations have been considered. Challenges in FE-type implementation:

conservation of mass }	$\longrightarrow$ mixed FE + stabilization
conservation of momentum }	$\longrightarrow$ iteration for nonlinear constitutive model
conservation of energy	$\longrightarrow$ inequality associated with melting condition
	$\longrightarrow$ stabilization
time stepping	
preconditioning	

- Implementations are available in open-source codes:
  - CISM Community Ice Sheet Model (http://oceans11.lanl.gov/trac/CISM).
  - ISSM Ice Sheet System Model (http://issm.jpl.nasa.gov/).
  - ...

- **Issues relevant to uncertainty quantification**:
  Presence of some of the challenges that we can expect to be present in multiphysics models, such as stabilization, iteration, inequalities, time stepping, preconditioning,. . .

Ice sheet benchmarks problems

Ice sheet benchmarks problems

- There already exist benchmark problems in the ice-sheet modeling community:

The Cryosphere, 2, 95–108, 2008
www.the-cryosphere.net/2/95/2008/
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The Cryosphere

Benchmark experiments for higher-order and full-Stokes ice sheet models (ISMIP–HOM)*

F. Pattyn[1], L. Perichon[1], A. Aschwanden[2], B. Breuer[3], B. de Smedt[4], O. Gagliardini[5], G. H. Gudmundsson[6], R. C. A. Hindmarsh[6], A. Hubbard[7], J. V. Johnson[8], T. Kleiner[3], Y. Konovalov[9], C. Martin[6], A. J. Payne[10], D. Pollard[11], S. Price[10], M. Rückamp[3], F. Saito[12], O. Souček[13], S. Sugiyama[14], and T. Zwinger[15]

A detailed description of, and results obtained for, these benchmark problems can be found in

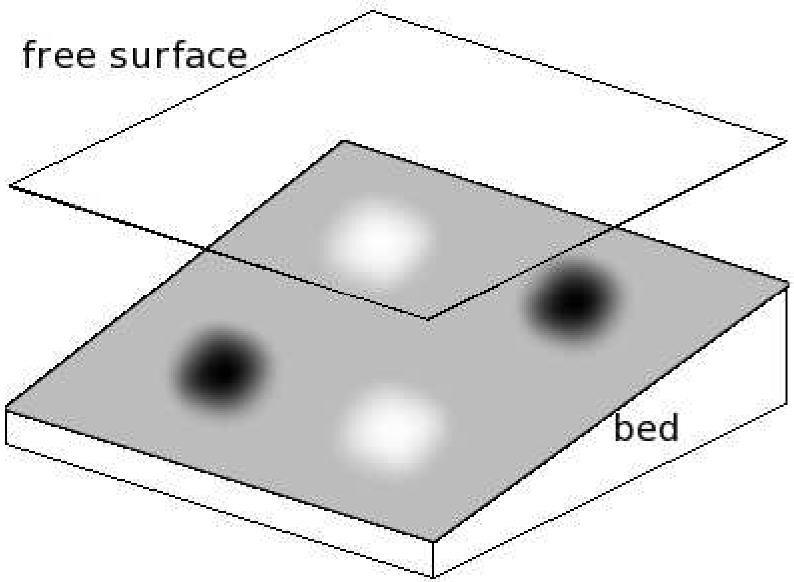
- F. Pattyn and T. Payne. Benchmark experiments for numerical higher-order ice-sheet models, Technical report, Université Libre de Bruxelles, Belgium, 2006.
- F. Pattyn et al. Benchmark experiments for higher-order and full-Stokes ice sheet models (ISMIP-HOM). The Cryosphere, 2:95–108, 2008.

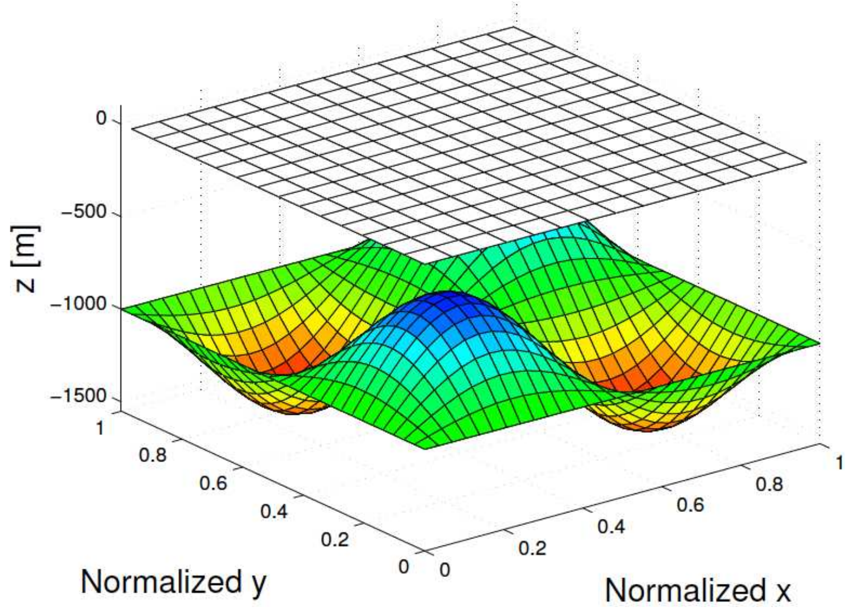
- These existing benchmark problems could serve as a **starting point to define a progression of benchmark problems** in UQ for multiphysics modeling.

Ice sheet benchmarks problems

- The ISMIP-HOM benchmark problems are a collection (A to F) of problems on simple geometries, including both steady-state and time-dependent problems.

- For example, ISMIP-HOM problem A concerns the computation of the steady-state velocity of an ice flow over a bumpy bed on a rectangular domain with periodic boundary conditions along the sides:





- The ISMIP-HOM benchmark problems are isothermal; hence, they need to be extended with a conservation-of-energy component to suit our purpose.

ISMIP-HOM problem A

- **Governing equations and boundary conditions**:

$$
\begin{aligned}
&\mathrm{div}(\boldsymbol{v}) = 0 && \text{(conservation of mass)},\\
&-\boldsymbol{\nabla} p + \eta\,\mathbf{div}\mathbf{D}\boldsymbol{v} + 2\boldsymbol{D}(\boldsymbol{\nabla}\eta) + \rho\boldsymbol{g} = \mathbf{0} && \text{(conservation of momentum)},\\
&\eta\big(i_{\boldsymbol{D}}^{(2)}\big) = \frac{1}{2}\, a^{-1/n}\, \big(i_{\boldsymbol{D}}^{(2)}\big)^{-\frac{1}{2}(1-1/n)}, && \\
&v_x \frac{\partial h}{\partial x} + v_y \frac{\partial h}{\partial y} - v_z = 0 && \text{(free-surface mass balance)},\\
&\boldsymbol{\sigma}(\boldsymbol{n}) = \mathbf{0} && \text{(free-surface stress-free b.c.)},\\
&v_x \frac{\partial b}{\partial x} + v_y \frac{\partial b}{\partial y} - v_z = 0 && \text{(basal mass balance)},\\
&\boldsymbol{v}_b = \mathbf{0} && \text{(cold-base sliding b.c.)}.
\end{aligned}
$$

- **Parameter values**: Domain size $\ell = 20\,000$ m, free-surface position $h = -x\tan(\alpha)$ with $\alpha = 0.5^\circ$, bed position $b(x,y) = -x\tan(\alpha) - 1000 + 500\sin(2\pi/\ell x)\sin(2\pi/\ell y)$, $a = 3.16 \times 10^{-24}$ Pa^{-n} s^{-1}, $\rho = 910$ kg m^{-3}, $g = 9.81$ m s^{-2}, and $n = 3$.

- **Quantity of interest**: steady-state velocity at the free surface.

Ice sheet benchmarks problems

ISMIP-HOM problem A extended with a conservation-of-energy component

- **Governing equations and boundary conditions**:

$$\mathrm{div}(\boldsymbol{v}) = 0 \qquad \text{(conservation of mass)},$$

$$-\boldsymbol{\nabla} p + \eta \,\mathbf{div}\mathbf{D}\boldsymbol{v} + 2\boldsymbol{D}(\boldsymbol{\nabla}\eta) + \rho \boldsymbol{g} = \boldsymbol{0} \qquad \text{(conservation of momentum)},$$

$$\eta(T, i_{\boldsymbol{D}}^{(2)}) = \frac{1}{2}\left(a_0 \exp\left(-\frac{q}{r(T+\beta p)}\right)\right)^{-1/n} \left(i_{\boldsymbol{D}}^{(2)}\right)^{-\frac{1}{2}(1-1/n)},$$

$$4\eta i_{\boldsymbol{D}}^{(2)} + \mathrm{div}(k\boldsymbol{\nabla} T) = 0 \qquad \text{(conservation of energy)},$$

$$v_x \frac{\partial h}{\partial x} + v_y \frac{\partial h}{\partial y} - v_z = 0 \qquad \text{(free-surface mass balance)},$$

$$\boldsymbol{\sigma}(\boldsymbol{n}) = \boldsymbol{0} \qquad \text{(free-surface stress-free b.c.)},$$

$$T = T_{\mathrm{s}} \qquad \text{(free-surface thermodynamic b.c.)}.$$

$$v_x \frac{\partial b}{\partial x} + v_y \frac{\partial b}{\partial y} - v_z = 0 \qquad \text{(basal mass balance)},$$

$$\boldsymbol{v}_b = \boldsymbol{0} \qquad \text{(cold-base sliding b.c.)},$$

$$k\boldsymbol{\nabla} T \cdot \boldsymbol{n} = q_{\mathrm{geo}} \qquad \text{(cold-base thermodynamic b.c.)}.$$

- **Parameter values**: Domain size $\ell = 20\,000$ m, free-surface position $h = -x\tan(\alpha)$ with $\alpha = 0.5^\circ$, bed position $b(x,y) = -x\tan(\alpha) - 1000 + 500\sin(2\pi/\ell x)\sin(2\pi/\ell y)$, $a_0 = 3.985 \times 10^{-13}$ Pa^{-n} s^{-1}, q=60×10^3 J mol^{-1}, r=8.314 J K^{-1} mol^{-1}, β=9.8×10^{-8} K Pa^{-1}, ρ=910 kg m^{-3}, g=9.81 m s^{-2}, $n = 3$, $k = 2.07$ W m^{-1} K^{-1}, $T_{\mathrm{s}} = -57^\circ$, and $q_{\mathrm{geo}} = 42 \times 10^{-3}$ W m^{-2}.
- **Quantity of interest**: steady-state velocity at the free surface.

Ice sheet benchmarks problems

A first UQ benchmark problem:

- As a starting point, uncertainty could be introduced in the exponent n of the constitutive model (value ranges from 1.5 to 4.2 with a mean of 3), and the benchmark problem could involve the propagation of this uncertainty to the steady-state velocity at the free surface.

Which studies could be carried out in the context of this benchmark problem?

- Implementation of this benchmark problem using different computational packages developed by the community, such as Dakota, Stokhos, UQTk, QUESO, GPMSA,. . .
- Comparison of nonintrusive and intrusive methods in terms of the level of difficulty of their coding and in terms of their computational efficiency.
- Study of applicability of recent improvements, such as preconditioned intrusive methods, multilevel Monte Carlo methods,. . .
- . . .

What could we get out of this?

- Illustrations of implementations in Dakota, Stokhos, UQTk, QUESO, GPMSA,. . . could serve as very useful references to foster further adoption of these computational packages in the community.
- Guidance for appropriate directions for future research and development of uncertainty propagation methods for multiphysics applications.
- . . .

A first progression: high-dimensionality:

- Uncertainty could be introduced in some of the other parameters (a_0, q, β, ρ, k, T_s, and q_geo). Alternatively, the parameter n and/or other parameters could be represented as a random field.

A second progression: UQ of constitutive model:

- Different experiments have indicated not only disparate optimal values for the parameters involved in this constitutive model but also disparate optimal model forms, thus suggesting that there are not only parametric uncertainties but also modeling errors in the constitutive model of ice.

- A benchmark problem could be focused on accounting not only for parametric uncertainties but also for modeling errors in the constitutive model of ice.

Ice sheet benchmarks problems

Outlook: many interesting challenges could be studied at a later stage:

- Multiphyiscs flow over uncertain rough surfaces.
- Domain decomposition methods for UQ for large-scale multiphysics problems.
- Coupling of mulifidelity models (full Stokes vs. first-order and shallow-ice approximations).
- Model-form uncertainty of multiphysics constitutive models.
- Inversion of multiphysics models under uncertainty.
- . . .

Conclusion

- General discussion of some of the challenges in UQ for multiphysics modeling.
- General discussion of numerical modeling of ice-sheet flows.
- As a starting point, UQ benchmark problems for multiphysics modeling could be obtained by extending existing benchmark problems for numerical modeling of ice-sheet flows.
- Illustrations of implementations in Dakota, Stokhos, UQTk, QUESO, GPMSA,. . . could serve as useful references to foster their further adoption, and insight could be gained into appropriate directions for future research of uncertainty propagation methods for multiphysics applications.
- This starting point could serve as a platform on the basis of which at a later stage, numerous very interesting challenges could be studied.

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