## Introduction to Computational and Variational Methods for Inverse Problems CSE 397/GEO 391/ME 397/ORI 397 Fall 2015

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slides downloadable from:

http://users.ices.utexas.edu/~omar/inverse\_problems/intro.pdf

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## The inverse problem: Determining cause from effect

- Integrating data and models to infer uncertain parameters is an inverse problem (also called data assimilation, history-matching, parameter estimation, model calibration, system identification, etc.)
- Applications across a broad spectrum of natural and engineered systems (seismic inversion, medical imaging, weather forecasting, non-destructive testing, inverse scattering, reservoir parameter estimation, remote sensing, source localization, ...)
- Some key milestones in regularization-based inversion
  - 1920s: Hadamard lays down theoretical foundations for ill-posed problems
  - 1950s-60s: Marchuk introduces idea of adjoint method
  - 1960s-70s: Tikhonov's work on regularization provides a systematic means for computing inverse solutions
  - 2000s: Advent of terascale supercomputers and advanced algorithms permits solution of some large-scale regularized inverse problems

# The inverse problem: Determining cause from effect

- Integrating data and models to infer uncertain parameters is an inverse problem (also called data assimilation, history-matching, parameter estimation, model calibration, system identification, etc.)
- Applications across a broad spectrum of natural and engineered systems (seismic inversion, medical imaging, weather forecasting, non-destructive testing, inverse scattering, reservoir parameter estimation, remote sensing, source localization, ...)
- Some key milestones in Bayesian inversion
  - 1763: Bayes' theorem
  - Metropolis (1953) and Hastings (1970) lay groundwork for Markov chain Monte Carlo Method, providing a method for computing solutions to Bayesian inverse problems
  - 2010s: Advent of petascale supercomputers and advanced algorithms permits solution of some large-scale Bayesian inverse problems

## Ocean dynamics example: Observational data



# Ocean dynamics example: Model

## Navier-Stokes equations

- Conservation of mass
- Conservation of momentum
- Conservation of energy
- Conservation of salinity
- Equation of state
- Subgrid parameterizations



TACC Stampede supercomputer



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# Ocean dynamics example: Uncertain parameters

### 2D and 3D parameter fields

- 3D initial temperature and salinity fields
- 2D time-varying atmospheric state at ocean-atmosphere interface
  - surface air temperature
  - specific humidity
  - downwelling shortwave radiation
  - zonal and meridional wind speed
- 3D subgrid model parameter fields
  - vertical mixing coefficient
  - GM coefficient (geostrophic eddy mixing)
  - Redi coefficient (along-isypycnal mixing)

xx\_uwind\_timemean: mn:-6.9e+00,mx:1.2e+01,av:-8.2e-02,sd:9.8e-01





Courtesy Patrick Heimbach, ICES/GEO



Input parameters, computational model, and output observables

### The forward problem

• Given model parameters m, solve forward model  ${\mathcal F}$  to yield output observables d

 $\mathfrak{F}(m) \longrightarrow d$ 

- Well-posed: solution exists, is unique, and is stable to perturbations in inputs
- Causal: later-time solutions depend only on earlier time solutions
- Local: the forward operator includes derivatives that couple nearby solutions in space and time



Input parameters, computational model, and output observables

### The inverse problem

• Given output observations  $d_{\rm obs}$  and forward model  ${\mathcal F}$ , infer model parameters m

 $m \longleftarrow \mathcal{F}^{-1} d_{\mathsf{obs}}$ 

- Ill-posed: observations are usually sparse; many different parameter values may be consistent with the data
- Non-causal: the inverse operator couples earlier time solutions with later time ones
- Global: the inverse operator couples solution values across all of space and time

## Anatomy of an inverse problem



Input parameters, computational model, and output observables

### Occam's approach to ill-posedness

Employ regularization to penalize unwanted solution features, guarantee unique solution:

$$\min_{m} \ \frac{1}{2} \| \mathcal{F}(m) - d_{\mathsf{obs}} \|_{W}^{2} + \frac{\alpha}{2} \| m - m_{\mathsf{ref}} \|_{R}^{2}$$

### Bayesian approach to ill-posedness

Describe **probability** of all models that are consistent with the data and any prior knowledge of the parameters:

$$\begin{split} \pi(m|d_{\text{obs}}) \propto \\ \exp \! \left(\! - \frac{1}{2} \, \| \, \mathcal{F}(m) - d_{\text{obs}} \, \|_{C_{\text{d}}^{-1}}^2 \! - \! \frac{1}{2} \, \| \, m - m_{\text{pr}} \, \|_{C_{\text{m}}^{-1}}^2 \! \right) \end{split}$$



- forward model  $\mathcal{F}$ : blurring (convolution with a Gaussian)
- model parameters m: unknown left image
- observations  $d_{obs}$ : blurred and noisy right image





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$$\min \frac{1}{2} \|\mathcal{F}m - d_{\mathsf{obs}}\|^2 + \frac{\alpha}{2} \|m\|^2$$

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- forward model  $\mathcal{F}$ : blurring (convolution with a Gaussian)
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## Example: Inverse problem for Antarctic ice sheet

- Ice flows from interior of polar ice sheets to ocean is primary contributor to sea level rise (200 billion tons/yr currently)
- Flow rates of outlet glaciers in Antarctica have been increasing over past several decades
- Thinning of ice shelves due to increased mixing in ocean driven by intensification of polar winds, bringing warmer water to surface;
- Ice shelf thinning leads to loss of buttressing effect and retreat of ice sheet
- 0.5 m sea level rise by 2070 estimated to jeopardize 136 largest port cities, with 150M inhabitants and \$35 trillion in assets
- We need to develop predictive models, with quantified uncertainties, to better anticipate future sea level rise

- Recent evidence suggests that sea level rose abruptly at the end of the last interglacial ( $\sim$ 118 kyr ago) by  $\sim$ 5-6m; the likely cause is catastrophic collapse of polar ice sheets
  - Ice sheet collapse following a prolonged period of stable sea level during the last interglacial, MJ O'Leary, PJ Hearty, WG Thompson, ME Raymo, JX Mitrovica, JM Webster, Nature Geoscience, 6, 796800, 2013.
- Recent work indicates that retreat of the Amundsen Sea Embayment (a portion of the West Antarctic ice sheet) is accelerating with no major bed obstacles to prevent draw down of the entire basin.
  - Widespread, rapid grounding line retreat of Pine Island, Thwaites, Smith and Kohler glaciers, West Antarctica from 1992 to 2011, E. Rignot, J. Mouginot, M. Morlighem, H. Seroussi, and B. Scheuchl, Geophysical Research Letters, 41(10):3502–3509, 2014.

## Dynamics of the Antarctic ice sheet and sea level rise

Glaciers flow thousands of miles from the continent's deep interior to its coast

Credit: NASA Goddard Space Flight Center/JPL-Caltech

#### Balance of linear momentum, mass, and energy

$$\begin{aligned} -\boldsymbol{\nabla} \cdot [\eta(\theta, \boldsymbol{u}) \, \dot{\boldsymbol{\varepsilon}} - \boldsymbol{I} \boldsymbol{p}] &= \rho \boldsymbol{g} \qquad [\dot{\boldsymbol{\varepsilon}} = \frac{1}{2} (\boldsymbol{\nabla} \boldsymbol{u} + \boldsymbol{\nabla} \boldsymbol{u}^T)] \\ \boldsymbol{\nabla} \cdot \boldsymbol{u} &= 0 \\ \frac{\partial \theta}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \theta \right) - \boldsymbol{\nabla} \cdot (K \boldsymbol{\nabla} \theta) &= 2 \, \eta \, \mathrm{tr}(\dot{\boldsymbol{\varepsilon}}^2) \end{aligned}$$

## Constitutive relation

 $\rho c$ 

$$\eta(\theta, \boldsymbol{u}) = \left\{ A_0 \exp\left(-\frac{Q}{R\theta}\right) \right\}^{-\frac{1}{n}} \dot{\boldsymbol{\varepsilon}}_{\mathrm{II}}^{\frac{1-n}{2n}} \qquad [\dot{\boldsymbol{\varepsilon}}_{\mathrm{II}} = \frac{1}{2} \mathrm{tr}(\dot{\boldsymbol{\varepsilon}}^2)]$$

## Boundary conditions

$$\begin{split} \theta|_{\Gamma_{FS}} &= \theta_{FS} \quad \frac{Dz}{Dt}|_{\Gamma_{FS}} = a \qquad \qquad \boldsymbol{\sigma}\boldsymbol{n}|_{\Gamma_{FS}} = \boldsymbol{0} \\ K\boldsymbol{\nabla}\theta \cdot \boldsymbol{n}|_{\Gamma_{B}} &= q_{B} \qquad \boldsymbol{u} \cdot \boldsymbol{n}|_{\Gamma_{B}} = 0 \qquad (\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{n}) \left(\boldsymbol{\sigma}\boldsymbol{n} + \beta \boldsymbol{u}\right)|_{\Gamma_{B}} = \boldsymbol{0} \end{split}$$

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### Balance of linear momentum, mass, and energy

$$-\nabla \cdot [\eta(\theta, \boldsymbol{u}) \dot{\boldsymbol{\varepsilon}} - \boldsymbol{I}\boldsymbol{p}] = \rho \boldsymbol{g} \qquad [\dot{\boldsymbol{\varepsilon}} = \frac{1}{2} (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)]$$
$$\nabla \cdot \boldsymbol{u} = 0$$
$$\frac{\theta}{2} + \boldsymbol{u} \cdot \nabla \theta - \nabla \cdot (K\nabla \theta) = 2 \, \boldsymbol{n} \operatorname{tr}(\dot{\boldsymbol{\varepsilon}}^2)$$

$$\rho c \left( \frac{\partial \theta}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \theta \right) - \boldsymbol{\nabla} \cdot (K \boldsymbol{\nabla} \theta) = 2 \eta \operatorname{tr}(\dot{\boldsymbol{\varepsilon}}^2)$$

#### rrhenius-type thinning near melting point

$$\eta(\theta, \boldsymbol{u}) = \left\{ A_0 \exp\left(-\frac{Q}{R\theta}\right) \right\}^{-\frac{1}{n}} \dot{\boldsymbol{\varepsilon}}_{\mathrm{II}}^{\frac{1-n}{2n}} \qquad [\dot{\boldsymbol{\varepsilon}}_{\mathrm{II}} = \frac{1}{2} \mathrm{tr}(\dot{\boldsymbol{\varepsilon}}^2)]$$

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Constitutive relation

#### shear thinning with 2nd strain rate invariant

$$\eta(\theta, \boldsymbol{u}) = \left\{ A_0 \exp\left(-\frac{Q}{R\theta}\right) \right\}^{-\frac{1}{n}} \dot{\boldsymbol{\varepsilon}}_{\mathrm{II}}^{\frac{1-n}{2n}} \qquad [\dot{\boldsymbol{\varepsilon}}_{\mathrm{II}} = \frac{1}{2} \mathrm{tr}(\dot{\boldsymbol{\varepsilon}}^2)]$$

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### Balance of linear momentum, mass, and energy

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## Boundary conditions

#### dynamic free surface

$$\theta|_{\Gamma_{FS}} = \theta_{FS} \quad \frac{Dz}{Dt}|_{\Gamma_{FS}} = a \qquad \boldsymbol{\sigma}\boldsymbol{n}|_{\Gamma_{FS}} = \boldsymbol{0}$$
$$K\boldsymbol{\nabla}\theta \cdot \boldsymbol{n}|_{\Gamma_{B}} = q_{B} \qquad \boldsymbol{u} \cdot \boldsymbol{n}|_{\Gamma_{B}} = 0 \qquad (\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{n}) (\boldsymbol{\sigma}\boldsymbol{n} + \beta \boldsymbol{u})|_{\Gamma_{B}} = \boldsymbol{0}$$

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## Boundary conditions

#### basal sliding coefficient

$$\theta|_{\Gamma_{FS}} = \theta_{FS} \quad \frac{Dz}{Dt}|_{\Gamma_{FS}} = a \qquad \boldsymbol{\sigma}\boldsymbol{n}|_{\Gamma_{FS}} = \boldsymbol{0}$$
$$K\boldsymbol{\nabla}\theta \cdot \boldsymbol{n}|_{\Gamma_{B}} = q_{B} \qquad \boldsymbol{u} \cdot \boldsymbol{n}|_{\Gamma_{B}} = 0 \qquad (\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{n}) (\boldsymbol{\sigma}\boldsymbol{n} + \boldsymbol{\beta}\boldsymbol{u})|_{\Gamma_{B}} = \boldsymbol{0}$$

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# Regularization approach to ice sheet inverse problem

## Minimize regularized data misfit

$$\min_{oldsymbol{eta}} \mathcal{J}(oldsymbol{eta}) := \; rac{1}{2} \int_{\Gamma_t} (\mathfrak{B} oldsymbol{u}(oldsymbol{eta}) - oldsymbol{d}_{\mathsf{obs}})^2 \; doldsymbol{s} + rac{lpha}{2} \int_{\Gamma_b} 
abla_{\Gammaoldsymbol{eta}} \cdot 
abla_{\Gammaoldsymbol{eta}} \; doldsymbol{s}$$

where u and p satisfy the forward (nonlinear) Stokes equations

$\boldsymbol{ abla}\cdot \boldsymbol{u}=0$	in $\Omega$
$-\boldsymbol{\nabla}\cdot[\boldsymbol{\eta}(\boldsymbol{u})(\boldsymbol{\nabla}\boldsymbol{u}+\boldsymbol{\nabla}\boldsymbol{u}^T)-\boldsymbol{I}p]=\rho\boldsymbol{g}$	in $\Omega$
$\sigma_{u}n=0$	on $\Gamma_t$
$\boldsymbol{u} \cdot \boldsymbol{n} = 0, \ (\boldsymbol{\sigma}_{\boldsymbol{u}} \boldsymbol{n})_{\Gamma} + \exp(\boldsymbol{\beta}) \boldsymbol{u}_{\Gamma} = \boldsymbol{0}$	on $\Gamma_b$

- u: velocity,  $\beta$ : log basal sliding coefficient field
- $d_{\sf obs}$ : observed surface velocity, lpha: regularization parameter
- $\mathfrak{B}$ : observation operator,
- $\Gamma$ : indicates surface tangential component or surface operator



### Left: Synthetic surface velocity observations Right: "Truth" basal sliding field



### Left: Reconstructed surface velocity field Right: Inferred basal sliding field



Left: InSAR-based Antarctica ice surface velocity observations Right: Inferred basal sliding field



#### Left: Reconstructed ice surface velocity field Right: Inferred basal sliding field



InSAR-based Antarctica ice surface velocity observations



#### Reconstructed ice surface velocity field



#### Error in velocity observations

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Bayesian approach to inverse problem: Standard deviation of basal friction



Posterior standard deviation

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