

SAND2019-13961C

# UNCERTAINTY QUANTIFICATION: AN OVERVIEW

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ANU Uncertainty Quantification Workshop  
Canberra, Australia

November 25 2019

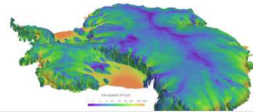
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# UQ IS ESSENTIAL TO ALL MODELING EFFORTS

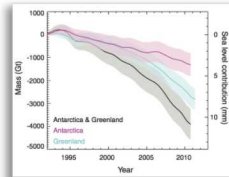
“All models are wrong; the practical question is how wrong do they have to be to not be useful” [BD86]

- Modeling is essential for understanding, predicting and designing complex systems
- Poor quality modeling can have catastrophic consequences
- Different models of the same system can produce vastly different predictions

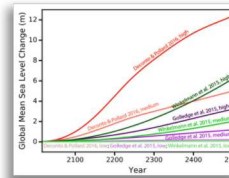
Credible modeling requires assessment of uncertainties



Prediction of ice-sheet velocities



Regional contributions to sea-level rise



Predictions of sea-level rise from high-profile studies

# APPLICATIONS



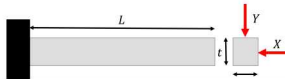
Tsunami/flood prediction



Aerospace design



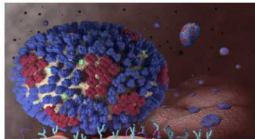
Acoustic testing



Material engineering



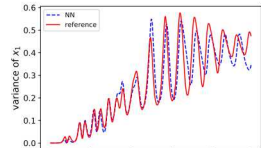
Groundwater flow



Biology and public health



Predicting burnt area from forest fires



Learning governing equations from data

# UQ WORKFLOW

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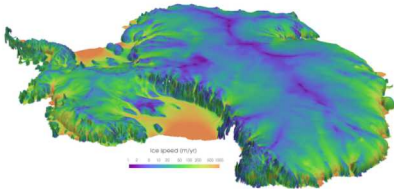
# CERTIFYING UQ ANALYSES

- |   |   |
|---|---|
| 1 Define objective  | 1 Design, prediction, discovery                               |
| 2 Define QoI  | 2 Sea level rise  |
| 3 Identify sources of uncertainty   | 3 Forcing, friction, geometry                                 |
| 4 Parameterize sources of uncertainty   | 4 Probabilistic, interval, fuzzy arithmetic                   |
| 5 Define metrics  | 5 VaR, CVaR   |
| 6 Condition prior uncertainty on data (inverse UQ)                                      | 6 Condition initial condition, friction on surface velocities |
| 7 Propagate posterior uncertainty through model to compute defined metrics (forward UQ) | 7 Monte Carlo sampling, Probabilistic arithmetic, Surrogates  |
| 8 Validate estimates of uncertainty   | 8 Does uncertainty estimates “bound” data                     |

# DEFINE OBJECTIVE AND QoI

## Prediction of sea-level rise

- Inform decision making
- Low accuracy requirements
- Single QoI - sea level rise



## Aerospace certification

- Certify system as safe
- High accuracy requirements
- Multiple QoI - Thrust, structural reliability, ...



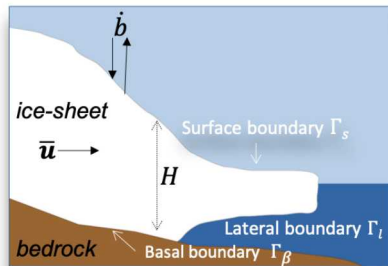
Focusing on a handful of well-defined QoI and significantly reduce the computational cost and data requirements of UQ

# IDENTIFYING SOURCES OF UNCERTAINTY

All potential sources of uncertainty must be documented

- Parametric uncertainty (uncertain conditions)
  - ▶ Forcing, boundary conditions, rate parameters, etc.
- Model for uncertainty (known unknowns and unknown unknowns)
  - ▶ Impact should be quantified during validation

Complexity of model should be continually evaluated. Less complex models can facilitate more accurate estimates of uncertainty

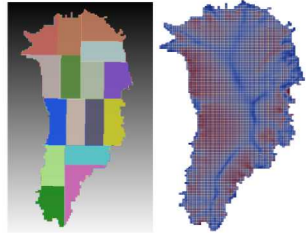


- Parametric - initial ice velocities  $u$ , forcing  $b$ , geometry  $H$ , basal friction  $\beta$
- Model form - Calving process, horizontal velocities, basal hydrology, unknown missing physics

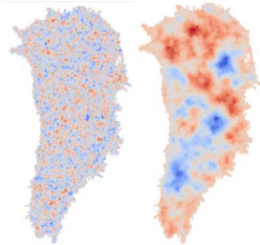
# CHARACTERIZATION OF UNCERTAINTY

- Model uncertainties must be parameterized
- The parameterization chosen (lumped, field, etc.) can significantly effect results
- The information provided (PDF, bounds, etc.) impacts interpretability of results
- Often little thought is given to this step

Chosen parameterization must be well justified and/or sensitivity of QoI uncertainty to the chosen parameterization must be investigated



Different parameterizations of Basal friction



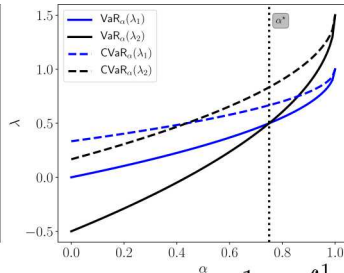
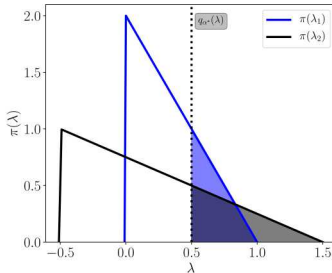
Different distributions (Gaussian random fields with different correlations)



# DEFINING MEASURES OF UNCERTAINTY

Measures used to communicate uncertainty must be tailored to stakeholder needs

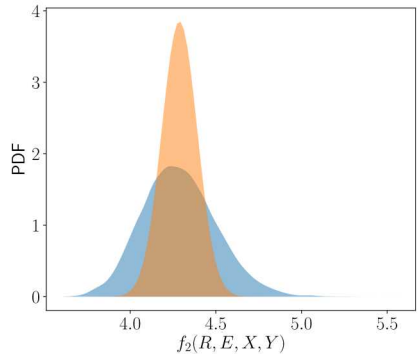
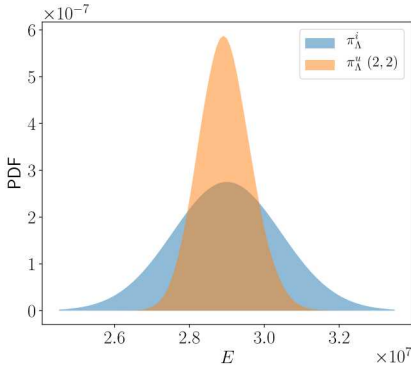
Need to determine if stakeholder cares about average performance or avoiding certain outcomes.



$$\text{VaR}_{\delta}(\lambda) = \inf\{\lambda \in \Lambda \mid F_{\lambda}(\lambda) \geq \delta\} \quad \text{CVaR}_{\alpha}(\lambda) = \frac{1}{1 - \alpha} \int_{\delta}^1 \text{VaR}_{\delta}(\lambda) d\delta$$

The choice of measure will impact the most efficient approach for quantifying uncertainty

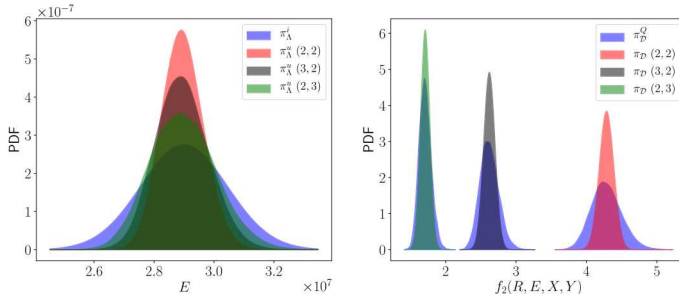
We can improve estimates of uncertainty and reduce impact of prior distributions by conditioning on observational data.



Probabilistic inference can be used to determine the input uncertainty that is in some sense consistent with observations. Bayesian inference is popular but there are a number of alternatives.

# OPTIMAL EXPERIMENTAL DESIGN (OED)

Data are not equally informative

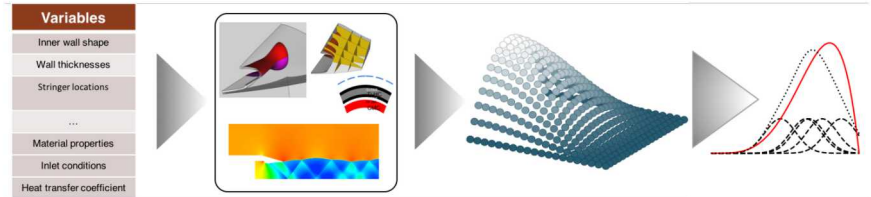


One should acquire data that maximize information gain whilst minimizing cost of experimentation.

Use measure of change in uncertainty

$$KL(\pi_{\Lambda}^i : \pi_{\Lambda}^u) := \int_{\Lambda} \pi_{\Lambda}^u \log \left( \frac{\pi_{\Lambda}^u}{\pi_{\Lambda}^i} \right) d\mu_{\Lambda}.$$

Given parameterization of input uncertainty estimate their impact on output QoI

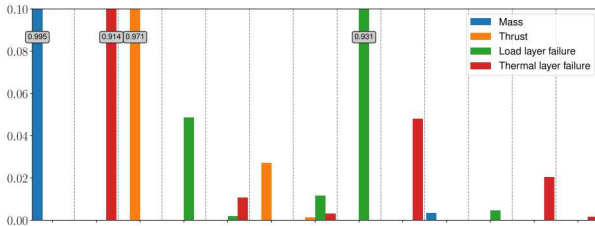


The appropriate approach depends on chosen uncertainty measures, accuracy requirements, number of uncertain parameters, “smoothness” of input-output map

# SENSITIVITY ANALYSIS

Sensitivity analysis (SA) is often an important phase of uncertainty quantification. SA can help

- Identify sources that significantly impact uncertainty in predictions
- Identify sources that are constrained by data
- Be used to guide dimension reduction and reduce the cost of UQ

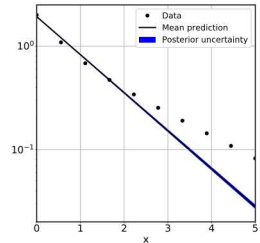


SA is often only applied to model parameters, however it can be generalized to investigate impact of assumptions, e.g. prior distributions, and the relative importance of components within a larger system.

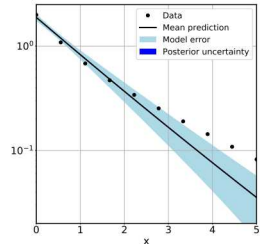
## Uncertainty estimates must be validated

- Interpolation - validate estimates on independent data set under same conditions.
  - ▶ Wrong assumptions such as incorrect error model (likelihood in inference) can lead to unjustified confidence.
- used to calibrate uncertainty
- Extrapolation - validate estimates under different conditions.
  - ▶ Models validated in interpolation regime can fail miserably under new scenarios

Embedded error models can limit over confidence and improve extrapolation



Gaussian error model



Embedded error model  
[SHN19]

# TABLE OF CONTENTS

1

UQ WORKFLOW

2

FUNCTION APPROXIMATION

3

MULTI-FIDELITY MODELING

4

INVERSE UNCERTAINTY QUANTIFICATION

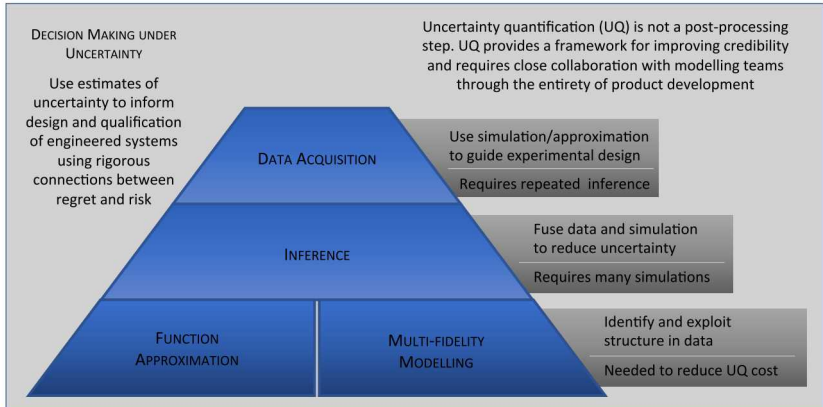
5

DATA ACQUISITION

6

DESIGN AND DECISION MAKING UNDER  
UNCERTAINTY

# UQ METHODS TAXONOMY





# ALGORITHMIC CHALLENGES

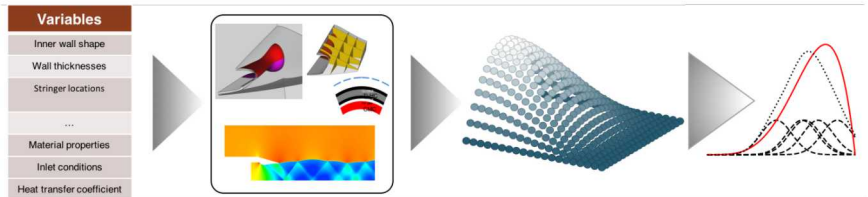
**Cost:** High-fidelity simulation is expensive. Must compute statistics from limited number of samples (simulations).

**High-Dimensionality:** Computational cost is often amplified as number of uncertainties increases.

**Inference:** Prior estimates of uncertainty can be overly conservative. Need to condition probabilistic estimates on observed data.

**Data Acquisition:** Determine experiments which are most informative.

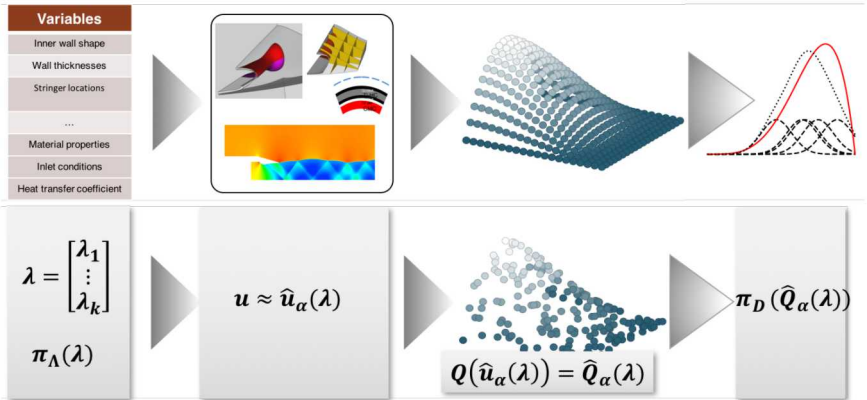
**Model Form Error:** Incorporate model inadequacy into uncertainty estimates



# FUNCTION APPROXIMATION

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# FORWARD UNCERTAINTY QUANTIFICATION FUNCTION APPROXIMATION



Must compute statistics from limited number of samples (simulations)  
Computational cost is amplified as number of uncertainties increases

# MULTIVARIATE POLYNOMIAL INTERPOLATION

## TENSOR-PRODUCT INTERPOLATION

Define a set of univariate points

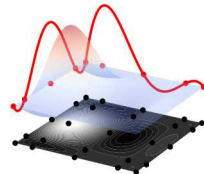
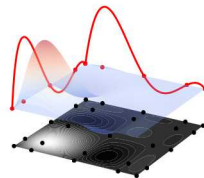
$$\mathcal{Z}_{m_{\beta_i}}^d = (\lambda_d^{(1)}, \dots, \lambda_d^{(m_{\beta_d})}), \quad d = 1, \dots, k$$

Univariate Lagrange polynomials

$$\phi_{d,j}(\lambda_d) = \prod_{i=1, i \neq j}^{m_{\beta_d}} \frac{\lambda_d - \lambda_d^{(i)}}{\lambda_d^{(j)} - \lambda_d^{(i)}},$$

Multivariate interpolant is given by

$$\hat{Q}_{\alpha, \beta}(\lambda) = \sum_{j \leq \beta} \hat{Q}_{\alpha}(\lambda^{(j)}) \prod_{d=1}^k \phi_{i, j_d}(\lambda_d).$$



Theorem

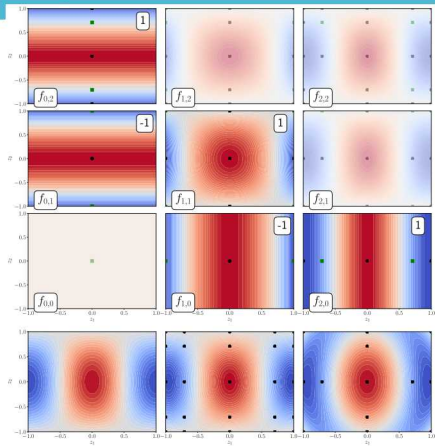
$$\left\| \hat{Q}_{\alpha} - \hat{Q}_{\alpha, \beta} \right\|_{L^{\infty}(\Lambda)} \leq C_{k, r} N_{\beta}^{-r/k}$$

# DELAYING THE CURSE OF DIMENSIONALITY SPARSE GRID INTERPOLATION

$$\hat{Q}_{\alpha, \mathcal{I}}(\lambda) = \sum_{\beta \in \mathcal{I}} c_{\beta} \hat{Q}_{\alpha, \beta}(\lambda)$$

$$c_{\beta} = (-1)^{n - \|\beta\|_1} \binom{k-1}{n - \|\beta\|_1}.$$

$$\mathcal{I}(n) = \{\beta \mid (\max(0, n-1) \leq \|\beta\|_1 \leq n-k-2)\}$$



Theorem [BNR00]

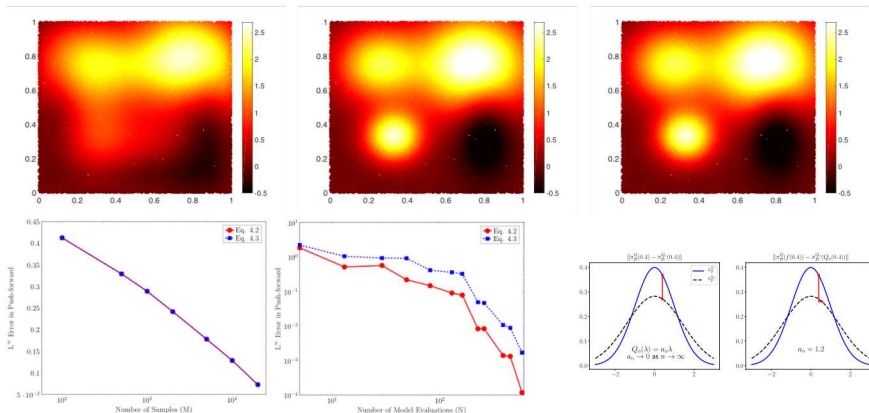
$$\left\| \hat{Q}_{\alpha} - \hat{Q}_{\alpha, \mathcal{I}(n)} \right\|_{L^{\infty}(\Lambda)} \leq C_{k,r} N_n^{-r} (\log N)^{(r+2)(k-1)+1}$$

# DENSITY ESTIMATION SAMPLING ON SPARSE GRIDS

Corollary [BJW18c]

Error in push-forward using isotropic level- $n$  CC sparse grid satisfies

$$\left\| \pi_{\mathcal{D}}^Q(Q(\lambda)) - \hat{\pi}_{\mathcal{D}}^{Q^n}(Q_n(\lambda)) \right\|_{L^\infty(\Lambda)} \leq C \left( \left( \frac{\log M}{M} \right)^{\frac{s}{2s+m}} + C_{k,r} N_n^{-r} (\log N)^{(r+2)(k-1)+1} \right).$$



# WEIGHTED APPROXIMATION HANDLING DEPENDENT PROBABILITY MEASURES

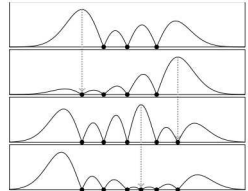
- Sparse grids can be used effectively for independent random variables
- Sparse grids can be improved upon when using dependent measures

## Theorem

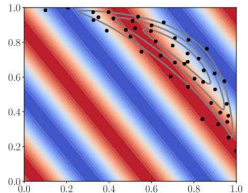
Let  $C_r := \max_{z \in \Gamma} \frac{\pi_\Lambda(\mathbf{y})}{g(\mathbf{y})}$ , and  $\epsilon := \|u - \hat{u}_g\|_{L_g^p}$ , then

$$\|u - \hat{u}_g\|_{L_{\pi_\Lambda}^p} \leq C_r^{1/p} \epsilon$$

- Sample complexity can be reduced by allocating samples in regions of high-probability while maintaining stability:
  - ▶ Leja sequences - polynomial approximation
  - ▶ power function sets - radial basis functions/Gaussian processes



Univariate weighted Leja sequence



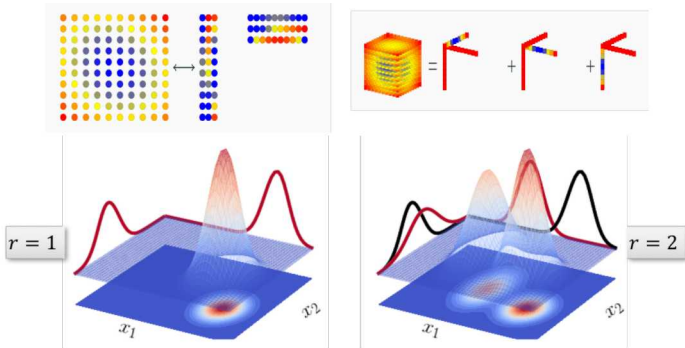
Multivariate weighted Leja sequence

# DELAYING THE CURSE OF DIMENSIONALITY

## LOW-RANK TENSOR DECOMPOSITIONS

The canonical tensor decomposition represents a tensor as the sum of outer product of  $d$  vectors

$$A = \sum_{i=1}^r v_1 \circ \cdots \circ v_d$$



Number of samples required grows quadratically with rank  $r$  and linearly with dimension  $d$  and number of univariate bases  $p$  [GJ18]



# DELAYING THE CURSE OF DIMENSIONALITY

## SPARSE APPROXIMATION

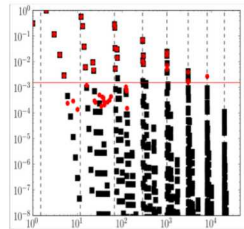
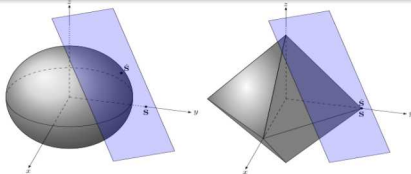
Approximate function with small number of nonzero terms  $f_\Lambda(\lambda) = \sum_{i \in I} \alpha_i \phi_i(\lambda)$   
 $s = \#\{i \mid |\alpha_i| > \delta\}$

$l_0$ -minimization (**NP HARD**)

$$\min_{\alpha} \|\alpha\|_0 \text{ s.t. } \|f - f_\Lambda\|_2 \leq \epsilon$$

$l_1$ -minimization (**Finds sparse solution under certain conditions**)

$$\min_{\alpha} \|\alpha\|_1 \text{ s.t. } \|f - f_\Lambda\|_2 \leq \epsilon$$



If a function is sparse the number of samples required to compute the coefficients only grows **linearly** with dimension

Sampling strategies for weighted probability spaces are needed [JNZ17]

# FUNCTION APPROXIMATION SUMMARY

## Goal

Build approximations from limited simulation data

## Challenge

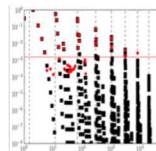
Growth of samples required can grow exponentially with dimension (curse of dimensionality)

## Solution

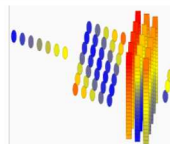
- Exploit structure in function
- Sample in regions of high-probability whilst maximizing conditioning

## Methods

- Sparse grids (smoothness) [JR13, NJ14]
- Compressive sensing (sparsity) [JES15, JNZ17]
- Low-rank decompositions (separability) [GJ18]



Find most sparse representation



Find low-rank representation

# MULTI-FIDELITY MODELING

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# MULTI-FIDELITY MODELING

## BALANCING SOURCES OF ERROR

Multi-fidelity modeling leverages simulations of lower-fidelity models of reduced cost to increase the tractability of sampling/approximating a high-fidelity model

$$\left\| Q - \hat{Q}_{\alpha, \mathcal{I}} \right\|_{L^p(\Lambda)} \leq \underbrace{\left\| Q - \hat{Q}_{\alpha} \right\|_{L^p(\Lambda)}}_I + \underbrace{\left\| \hat{Q}_{\alpha} - \hat{Q}_{\alpha, \mathcal{I}} \right\|_{L^p(\Lambda)}}_{II}$$

To minimize simulation cost we should balance physical error (I) with stochastic error (II). I.e. only sample highest fidelity model when stochastic error is smaller than deterministic error [JW15]

If models ensemble forms a hierarchy, i.e.

$$\left\| \hat{Q}_{\alpha} - Q \right\| \rightarrow 0 \quad \text{as} \quad \max \alpha \rightarrow \infty$$

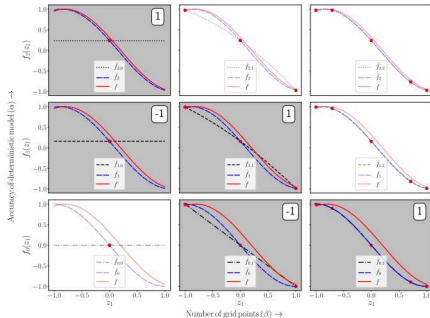
sparse grids can be naturally extended to multi-fidelity context

[HANTT16, dBR17, JEGG18]

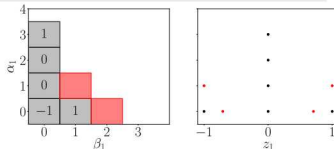


# MULTI-INDEX SPARSE GRIDS

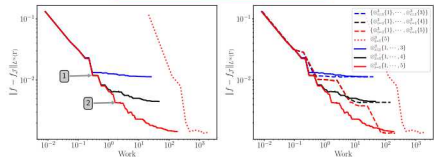
Balance stochastic and interpolation errors  
by refining in both spaces



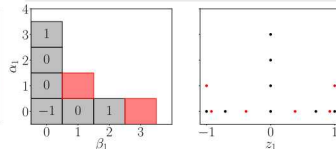
Adaptively refine to minimize error and  
cost



Despite lack of smoothness guarantees  
MISC can reduce cost by orders of  
magnitude



Adaptivity can be thought of using SA  
to increase efficiency of UQ



The MC estimate of the mean

$$\tilde{Q}_{\alpha} = N^{-1} \sum_{n=1}^N \hat{Q}_{\alpha}(\lambda^{(i)})$$

Central Limit Theorem implies error normally distributed with variance  $N^{-1}\mathbb{V}[\hat{Q}_{\alpha}]$ , as  $N \rightarrow \infty$ .

Leverage correlations of low-fidelity models to reduce variance of estimator.

$$\tilde{Q}_{\alpha}^{\text{CV}} = \tilde{Q}_{\alpha} + \gamma \left( \tilde{Q}_{\kappa} - \mu_{\kappa} \right)$$

Given  $r_{\alpha}$  samples of  $\hat{Q}_{\alpha}$  and  $r_{\kappa}$  of  $\hat{Q}_{\kappa}$ , variance in  $\tilde{Q}_{\alpha}^{\text{CV}}$  is

$$\mathbb{V}[\tilde{Q}_{\alpha}^{\text{CV}}] = \left(1 - \frac{r_{\kappa} - r_{\alpha}}{r_{\kappa} r_{\alpha}} \rho^2\right) \mathbb{V}[\tilde{Q}_{\alpha}]$$

where  $\rho$  correlation between  $Q_{\alpha}$  and  $Q_{\kappa}$

# CONTROL VARIATE MONTE CARLO

## A GENERALIZED FRAMEWORK

For multiple models the CV estimator is

$$\tilde{Q}_\alpha^{\text{CV}} = \tilde{Q} + \sum_{\alpha \in \mathcal{A}} \gamma_\alpha (\tilde{Q}_\alpha - \tilde{\mu}_\alpha) = \tilde{Q}_\alpha + \gamma \vec{\Delta}$$

Theorem [GGEJ18]

The Optimal CV weights are

$$\gamma^* = -\text{Cov} [\vec{\Delta}, \vec{\Delta}]^{-1} \text{Cov} [\vec{\Delta}, \tilde{Q}]$$

Multi-level MC (MLMC) is a control variate algorithm  $\mathcal{A} = \{0, \dots, L\}$ ,  $\gamma = (1, \dots, 1)^T$

$$\mathbb{E} [\hat{Q}_L] = \mathbb{E} [\hat{Q}_0] + \sum_{\ell=1}^L \mathbb{E} [\hat{Q}_\ell - \hat{Q}_{\ell-1}]$$

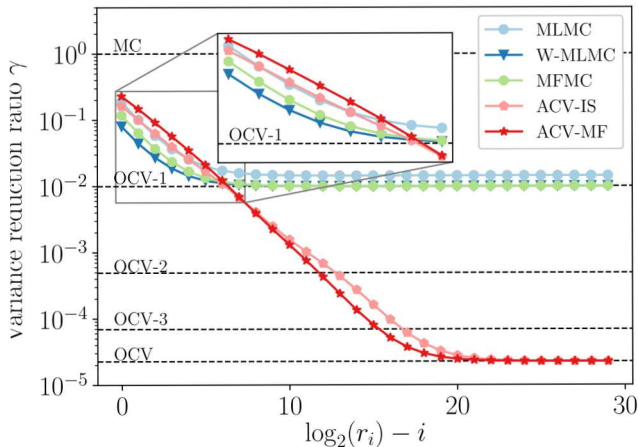
Theorem [GGEJ18]

Regardless of number of models  $M$ , variance of MLMC satisfies

$$\mathbb{V}[\tilde{Q}^{\text{MLMC}}] < (1 - \rho_{\max}^2) \mathbb{V}[\tilde{Q}]$$

$\rho_{\max}$  is max correlation of  $\hat{Q}_L$  with  $\hat{Q}_i$ ,  $i = 0, \dots, L-1$

Variance reduction for fixed high-fidelity samples of  $Q$  as a function of numbers of samples per level  $r_i(x) = 2^{i+x}$  for 4 low-fidelity models



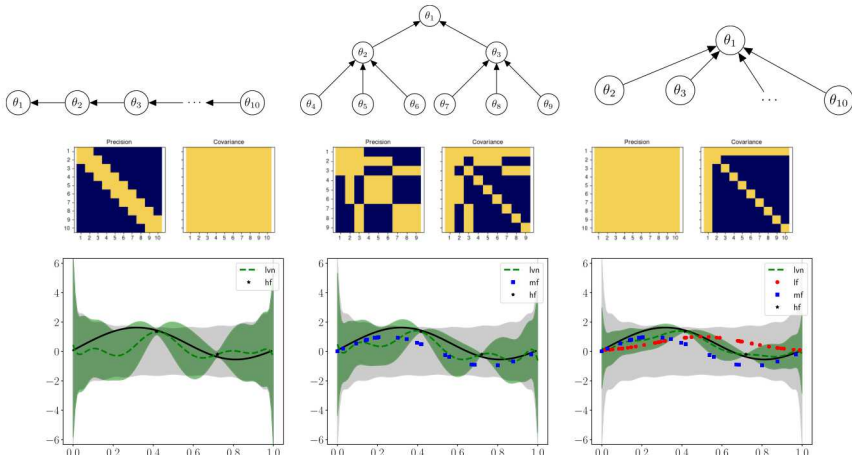


# MULTIFIDELITY MODELING

## EXPLOITING DIFFERENT MODEL RELATIONSHIPS

Use Bayesian networks to efficiently compute Bayesian regression basis coefficients. Bayesian generalization of MLMV and CVMC

Represent each model with polynomial basis with coefficients  $\theta_i$ .  
Estimate high-fidelity  $\theta$  using graph covariance on all models  $\theta$ .



# MULTIFIDELITY MODELING SUMMARY

## Goal

Use ensemble of models to reduce errors in statistics

## Challenge

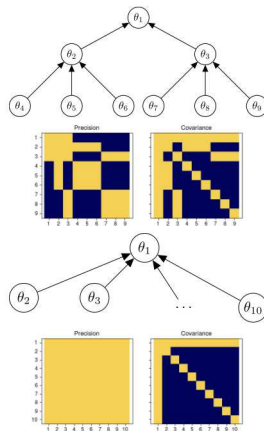
Relationship between models may not be known

## Solution

- Learn and exploit relationship between models
- Allocate samples between models to balance deterministic and stochastic errors

## Methods

- Variance reduction methods (MLMC, CVMC) [GEGJ18, GGEJ18]
- Multi-index approximation [JEGG18]
- Bayesian network learning [GJGE18]

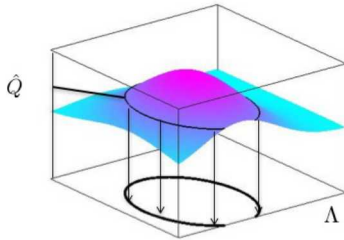


# INVERSE UNCERTAINTY QUANTIFICATION

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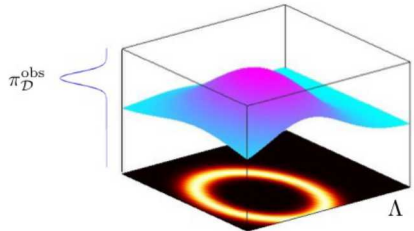
# PARAMETER INFERENCE

## Deterministic Inversion



Find parameter values that produce data. Ill posed must impose regularization.

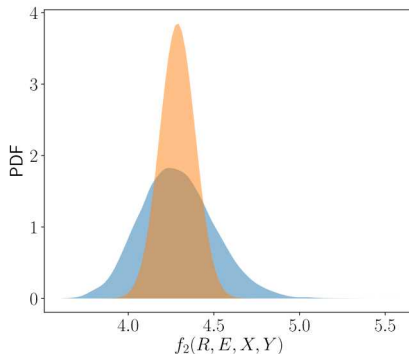
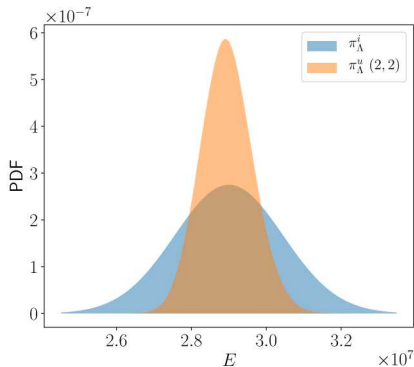
## Stochastic Inversion



Find probability of parameters producing data. Prior distribution is a form of regularization [Stu10].

## REDUCING UNCERTAINTY USING DATA

We can reduce estimates of uncertainty and improve the performance of design whilst still satisfying constraints.



Can we determine the probability density that when push forward through a model reproduces a given density on the observations?

# A NEW APPROACH FOR INVERSION

## PUSH-FORWARD BASED INFERENCE

### Theorem [BJW18b]

The consistent updated density is

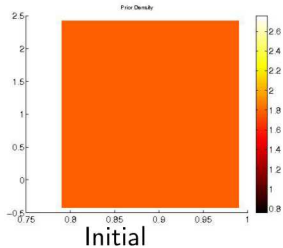
$$\pi_{\mathbf{\Lambda}}^u(\lambda) = \pi_{\mathbf{\Lambda}}^i(\lambda) \frac{\pi_{\mathcal{D}}^{\text{obs}}(Q(\lambda))}{\pi_{\mathcal{D}}^Q(Q(\lambda))}.$$

### Algorithm: Approximating the Push-forward of the Prior

- 1 Given a set of samples from the prior density:  $\{\lambda_i\}_{i=1}^M$ .
- 2 Evaluate the model and compute the Qols:  $q_i = Q(\lambda_i)$ .
- 3 Use the set of Qols and use a standard technique, such as a kernel density method, to estimate  $\pi_{\mathcal{D}}^Q(q)$ .

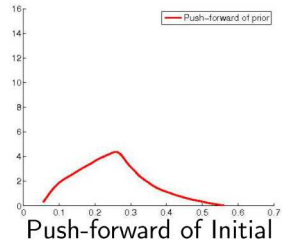
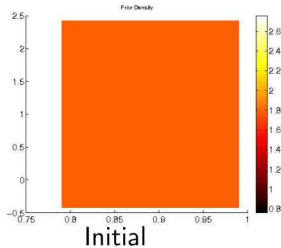
# EXAMPLE

## A SIMPLE NON-LINEAR SYSTEM



# EXAMPLE

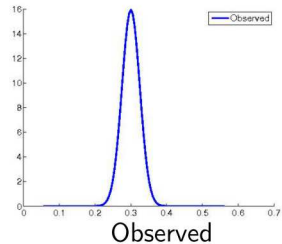
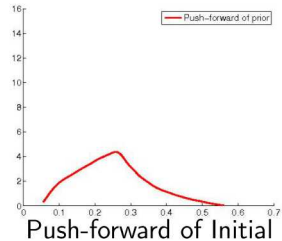
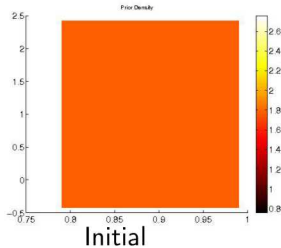
## A SIMPLE NON-LINEAR SYSTEM





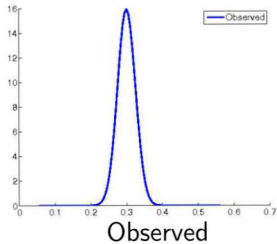
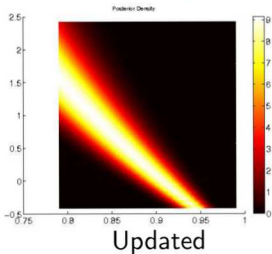
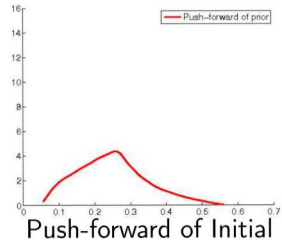
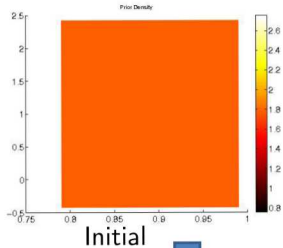
# EXAMPLE

## A SIMPLE NON-LINEAR SYSTEM



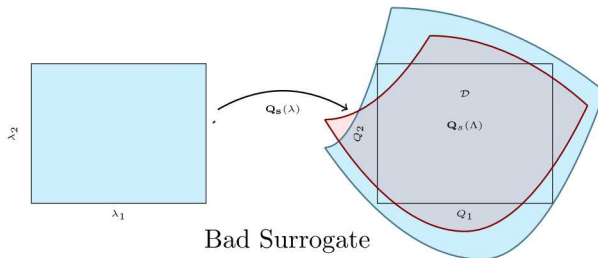
# EXAMPLE

## A SIMPLE NON-LINEAR SYSTEM



# UTILIZING SURROGATE MODELS

What happens when we use a surrogate model to compute the push-forward

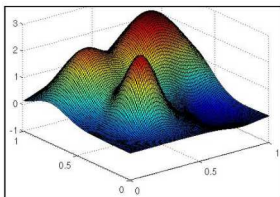


## Theorem [BJW18c]

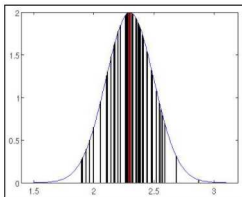
The error in the updated density using an isotropic level- $n$  CC sparse grid satisfies

$$\|\pi_{\mathbf{\Lambda}}^u(\lambda) - \hat{\pi}_{\mathbf{\Lambda}}^{u,n}(\lambda)\|_{L^1(\mathbf{\Lambda})} \leq C \left( \left( \frac{\log M}{M} \right)^{\frac{s}{2s+m}} + C_{k,r} N_n^{-r} (\log N)^{(r+2)(k-1)+1} \right).$$

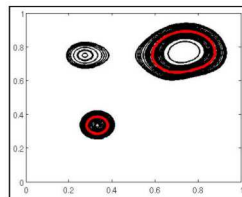
## EXAMPLE GAUSSIAN PEAKS



Gaussian peaks function



Density on observations



Contours in  $\Lambda$

- We let  $\Lambda = [0, 1]^2$  and consider a sum of Gaussian peaks.
- The initial density is uniform over  $\Lambda$ .
- The goal is to investigate how the accuracy of the surrogate model affects the updated density.

# EXAMPLE GAUSSIAN PEAKS

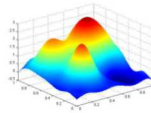
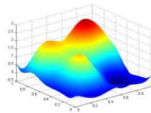
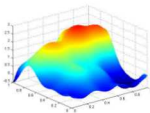
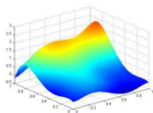
Level 2 (17 pts)

Level 3 (49 pts)

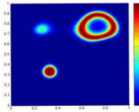
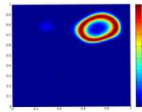
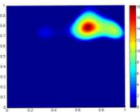
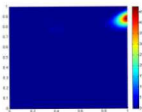
Level 4 (97 pts)

Level 5 (161 pts)

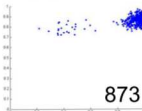
$Q_s(\lambda)$



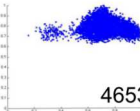
$\pi_{\Lambda}^{\text{post}}(\lambda)$



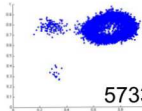
Samples from  
posterior



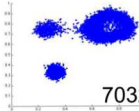
873



4653

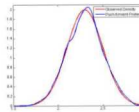
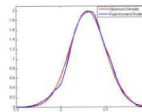
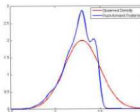
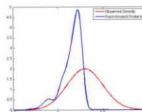


5733



7032

$\pi_{\mathcal{D}}^{\text{obs}}(q)$  and  
 $\pi_{\mathcal{D}}^{Q(\text{post})}(q)$



$$\int_{\Lambda} \pi_{\Lambda}^{\text{post}}(\lambda) d\mu_{\Lambda}$$

0.4789

0.8704

0.9787

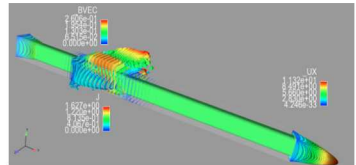
0.9825

# RESISTIVE MHD PROBLEM

- VMS stabilized finite element approximation
- Qol is the average induced magnetic energy.

$$Q = \frac{1}{2\mu_0} \int_{\Omega} (B_x^2 + B_y^2) d\Omega$$

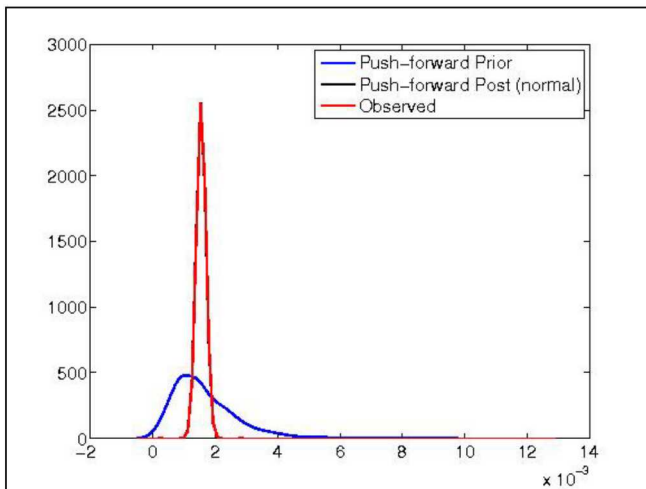
- Treat 4 input parameters as uncertain with uniform prior
- Use LHS study with 100 samples
- Build Gaussian process regression model as surrogate
- Use 50,000 samples of surrogate to compute push-forward of prior



Parameter	Min.	Max.
Viscosity	1.0E-3	1.0E-2
Vol. source	1.0E-1	5.0E-1
Resistivity	1.0E-1	1.0E1
Density	1.0E-1	1.0E1

## RESISTIVE MHD PROBLEM

We assume a Gaussian density for the Qol with mean  $1.55\text{E-}3$  and 10% standard deviation.



# INVERSE UNCERTAINTY QUANTIFICATION SUMMARY

## Goal

Condition estimates of uncertainty on experimental data

## Challenge

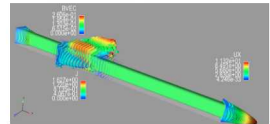
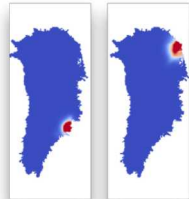
Develop new formulations and reduce sample complexity

## Solution

- Find input measure whose push-forward matches observed density
- Reduce inverse problem to one forward solve

## Methods

- Bayesian inference
- Push-forward based inference [BJW18a, BJW18c]

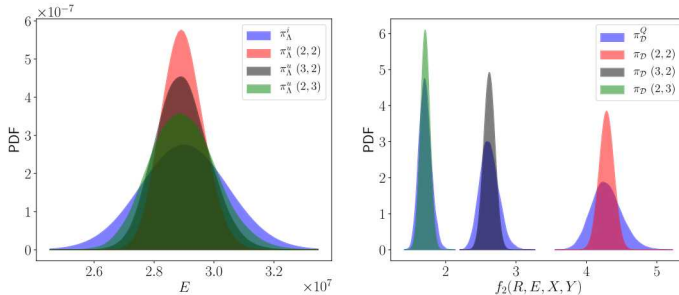




# DATA ACQUISITION

---

Data are not equally informative



How does one select the maximize information gain whilst minimizing cost of experimentation.

Use measure of change in uncertainty

$$KL(\pi_{\Lambda}^i : \pi_{\Lambda}^u) := \int_{\Lambda} \pi_{\Lambda}^u \log \left( \frac{\pi_{\Lambda}^u}{\pi_{\Lambda}^i} \right) d\mu_{\Lambda}.$$

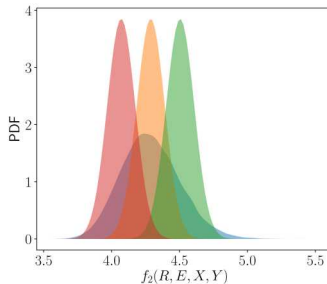
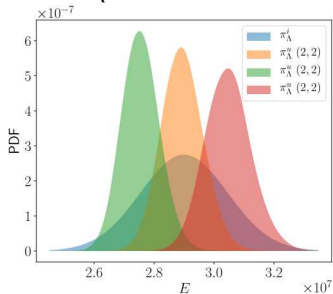
# INFORMATION THEORETIC DESIGN

OED must select a design before experimental data become available.

In the absence of data, we use the simulation model to quantify the information gain of a given experimental design for all possible realizations of data for that design.

Let  $\mathcal{O}$  denote the space of densities that may be observed in reality

$$\mathcal{O} = \left\{ \hat{N}(\mathbb{E}[\pi_D^Q] + \tau \mathbb{V}[\pi_D^Q]^{1/2}, \sigma^2) : \tau \in \{-1, 0, 1\} \right\},$$



## Expected Information Gain

$$EIG(Q) := \int_{\mathcal{D}} KL(d) \pi_{\mathcal{D}}^Q(d) d\mu_{\mathcal{D}}.$$

Given samples from push-forward:

$q^{(j)} = Q(\lambda^{(j)})$  compute

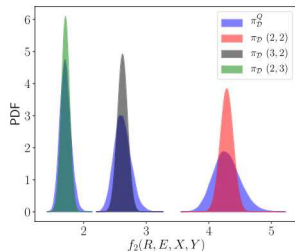
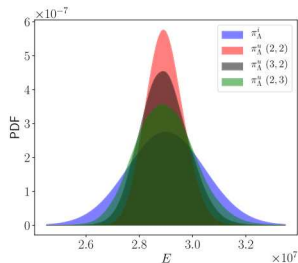
$$I_Q(\tau) \approx \frac{1}{N} \sum_{i=1}^N \frac{\pi_{\mathcal{D}}^{\text{obs}}(Q(\lambda^{(i)}))}{\pi_{\mathcal{D}}^Q(Q(\lambda^{(i)}))} \log \left( \frac{\pi_{\mathcal{D}}^{\text{obs}}(Q(\lambda^{(i)}))}{\pi_{\mathcal{D}}^Q(Q(\lambda^{(i)}))} \right)$$

## OED definition

Let  $Q^z \in \mathcal{Q}$  be a specific design in space of all possible designs, then OED solves

$$Q^{\text{opt}} := \arg \max_{Q^z \in \mathcal{Q}} E(I_{Q^z}).$$

We would choose (2,2)



# DATA ACQUISITION SUMMARY

## Goal

Determine data that maximizes reduction in uncertainty whilst minimizing cost

## Challenge

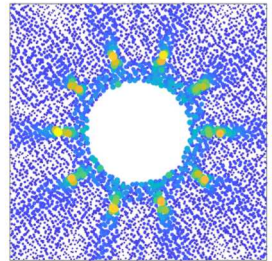
Requires solving many inverse problems

## Solution

- Use push-forward based inference - only one forward problem required
- Use gradient based optimization

## Methods

- OED using SVD of Jacobians [BJP<sup>+</sup>18]
- OED using Push-forward based inference [WWJ17]

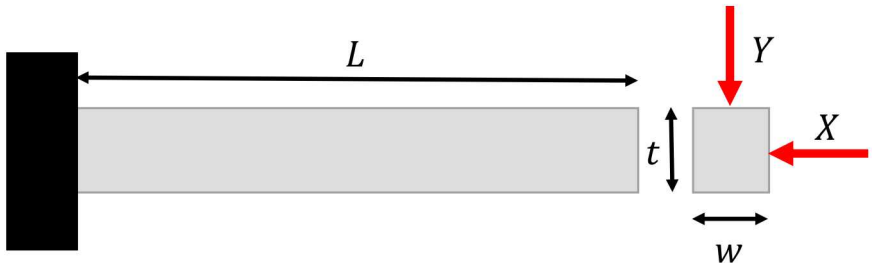


# DESIGN AND DECISION MAKING UNDER UNCERTAINTY

---

# A SIMPLE MOTIVATING EXAMPLE

## CANTILEVER BEAM



$$f_1(\boldsymbol{\lambda}) = 1 - \frac{6L}{Rwt} \left( \frac{X}{w} + \frac{Y}{t} \right) \geq 0 \quad f_2(\boldsymbol{\lambda}) = 1 - \frac{4L^3}{2.2535Ewt} \sqrt{\frac{X^2}{w^4} + \frac{Y^2}{t^4}} \geq 0$$

Uncertainty	Symbol	Prior
Yield stress	$R$	$N(40000, 2000)$
Young's modulus	$E$	$N(2.9e7, 1.45e6)$
Horizontal load	$X$	$N(500, 100)$
Vertical Load	$Y$	$N(1000, 100)$

# DESIGN UNDER UNCERTAINTY

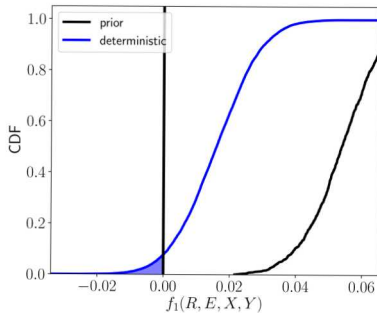
## Deterministic Design

$$\operatorname{argmin}_{w,t} wt$$

$$f_1(\lambda) \geq 0$$

$$f_2(\lambda) \geq 0$$

$$1 \leq w \leq 4 \quad 1 \leq t \leq 4$$



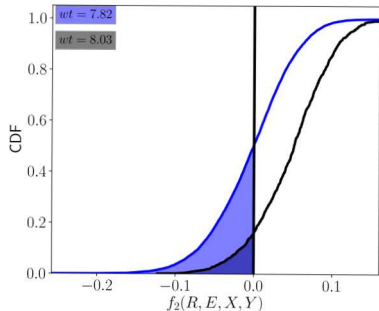
## Design under uncertainty

$$\operatorname{argmin}_{w,t} wt$$

$$P(f_1(\lambda) \leq 0) \leq \delta_1$$

$$P(f_2(\lambda) \leq 0) \leq \delta_2$$

$$1 \leq w \leq 4 \quad 1 \leq t \leq 4$$





# PUTTING IT ALL TOGETHER

## CANTILEVER BEAM

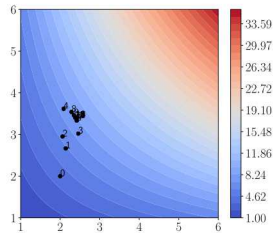
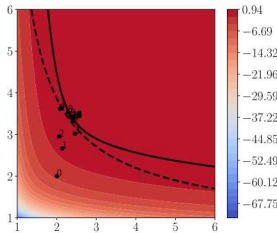
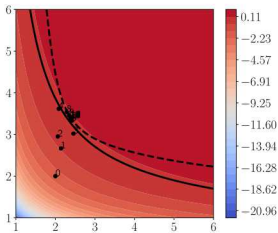
### Design under uncertainty

$$\operatorname{argmin}_{w,t} wt$$

$$P(f_1(\lambda) \leq 0) \leq \delta_1$$

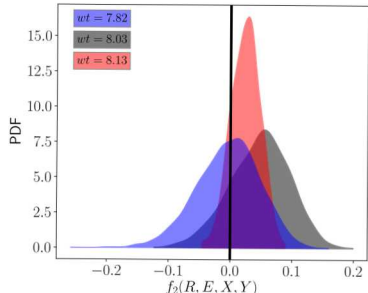
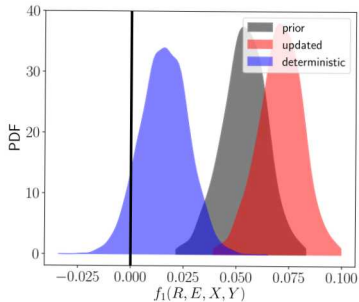
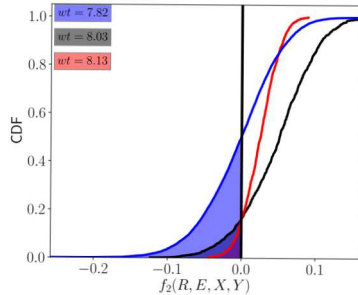
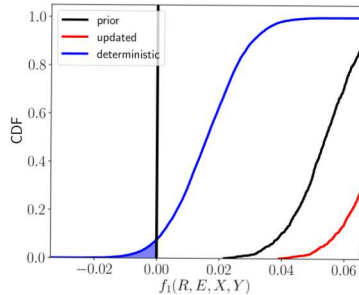
$$P(f_2(\lambda) \leq 0) \leq \delta_2$$

$$1 \leq w \leq 4 \quad 1 \leq t \leq 4$$



# PUTTING IT ALL TOGETHER

## CANTILEVER BEAM



# DESIGN UNDER UNCERTAINTY APPLICATION

Minimize weight subject to thrust and thermal and structural failure constraints



# ACKNOWLEDGMENTS









## Contributors

- Troy Butler (University of Colorado, Denver)
- Mike Eldred (SNL)
- Gianluca Geraci (SNL)
- Alex Gorodetsky (University of Michigan)
- Helmut Harbrecht (University of Basel)
- Drew Kouri (SNL)
- John Lewis (SNL)
- Akil Narayan (University of Utah)
- Mauro Perego (SNL)
- Dirk Pflüger (University of Stuttgart)
- Steve Price (LANL)
- Georg Stadler (Courant)
- Irina Tezaur (SNL)
- Scott Walsh (University of Colorado, Denver)
- Tim Walsh (SNL)
- Tim Wildey (SNL)

## Funding

- Sandia National Laboratories (SNL), Laboratory Directed Research & Development (LDRD)
  - ▶ Learning Hidden Structure in Multifidelity Information Sources for Efficient Uncertainty Quantification
  - ▶ Risk-Adaptive Experimental Design for High-Consequence Systems
- Defense Advanced Research Projects Agency (DARPA), Enabling Quantification of Uncertainty in Physical Systems (EQUIPS)
  - ▶ Scalable Environment for Quantification of Uncertainty and Optimization in Industrial Applications (SEQUOIA)
- U.S. Department of Energy, Scientific Discovery through Advanced Computing (SciDAC) program
  - ▶ Frameworks, Algorithms and Scalable Technologies for Mathematics (FastMath)
  - ▶ Probabilistic Sea Level Projections from Ice Sheet and Earth System Models (ProSPect)

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