Uncertainty Quantification via Optimal Experimental Design and Bayesian Neural Networks for Aerospace Applications

Xun Huan

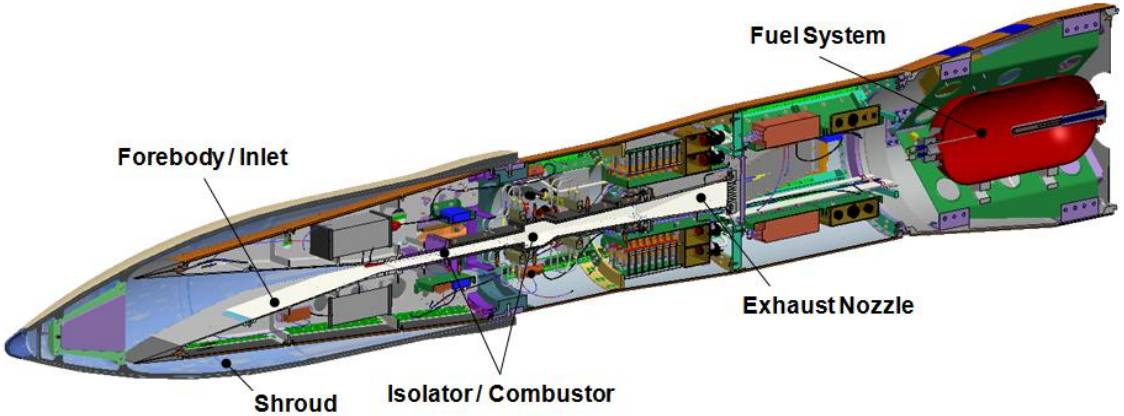
xhuan@umich.edu

University of Michigan
Mechanical Engineering

August 27, 2019

COLLEGE OF ENGINEERING
MECHANICAL ENGINEERING
UNIVERSITY OF MICHIGAN

Uncertainty in engineering and science



(Sources: 1. Argonne National Lab; 2. www.weather.com; 3. NASA Ames)

Uncertainty is everywhere

"Uncertainty is everywhere and you cannot escape from it."

— Dennis Lindley

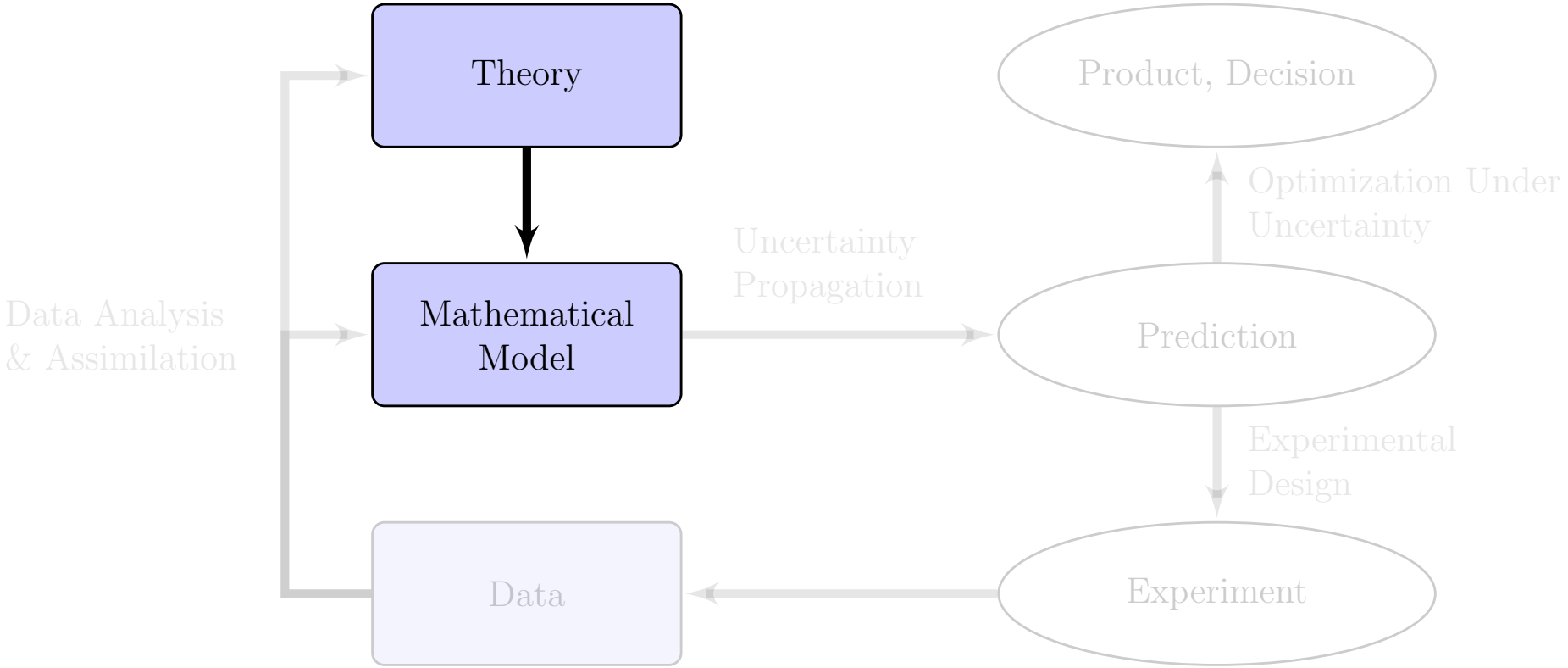
Uncertainty quantification (UQ) focuses on systematic approaches to bridge together **data** and **models**, and allows us to:

- characterize
- incorporate
- propagate
- reduce

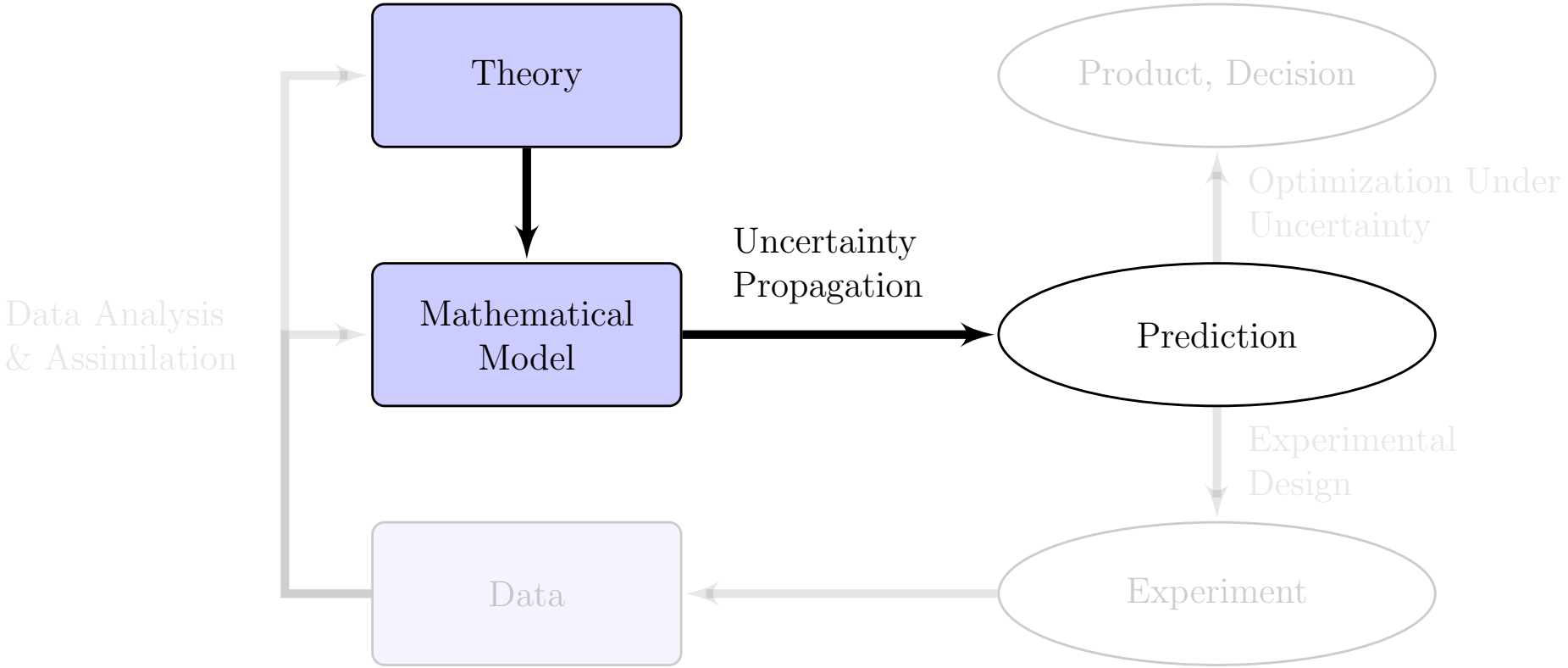
. . . uncertainty in complex engineering systems

To what extent can we trust a simulation and its prediction?
How can we continue to improve that trust?

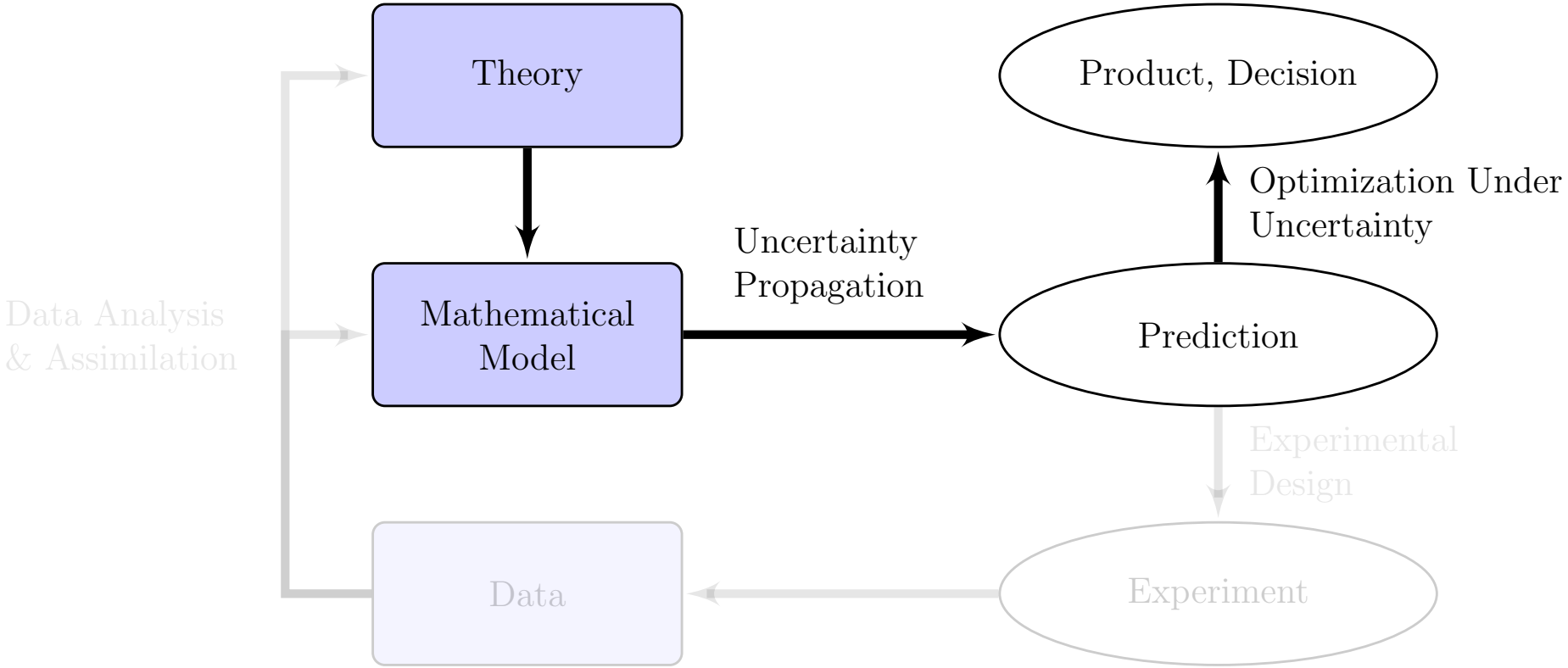
UQ in engineering and science: big picture



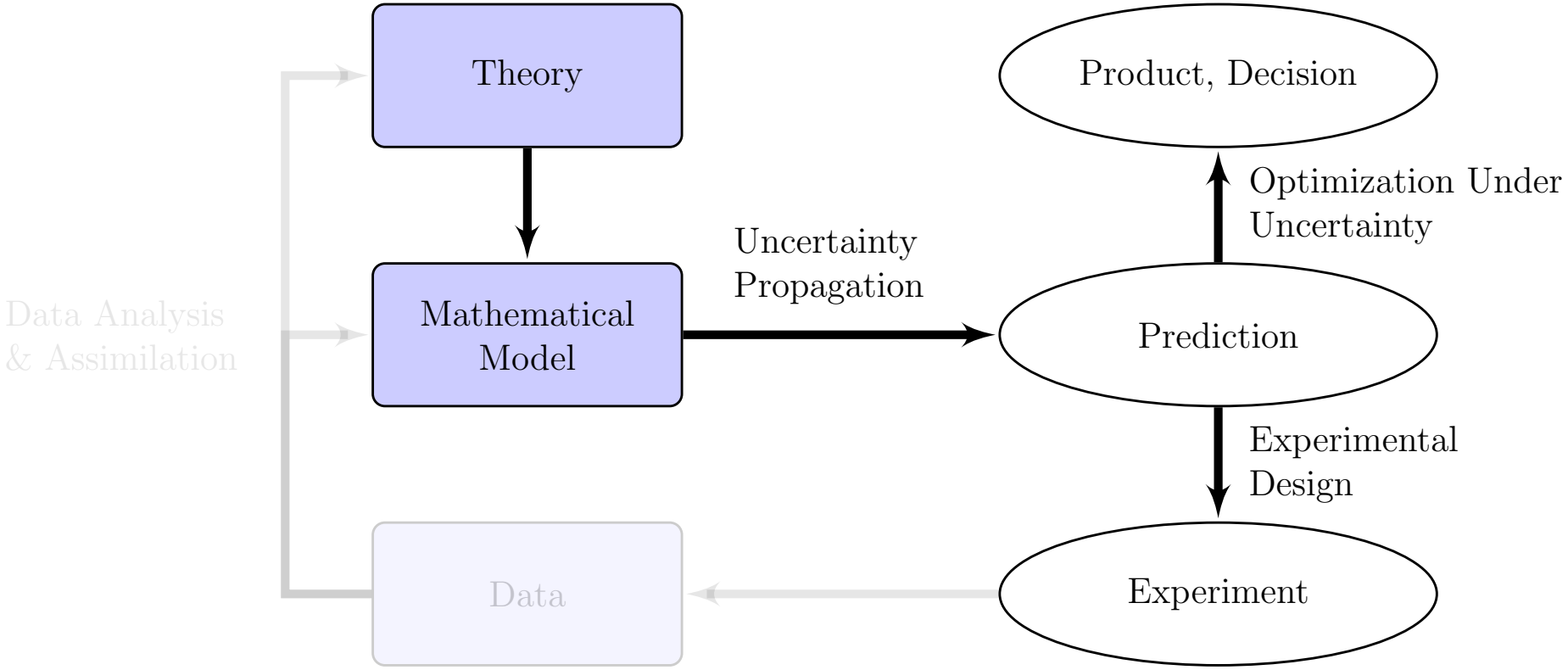
UQ in engineering and science: big picture



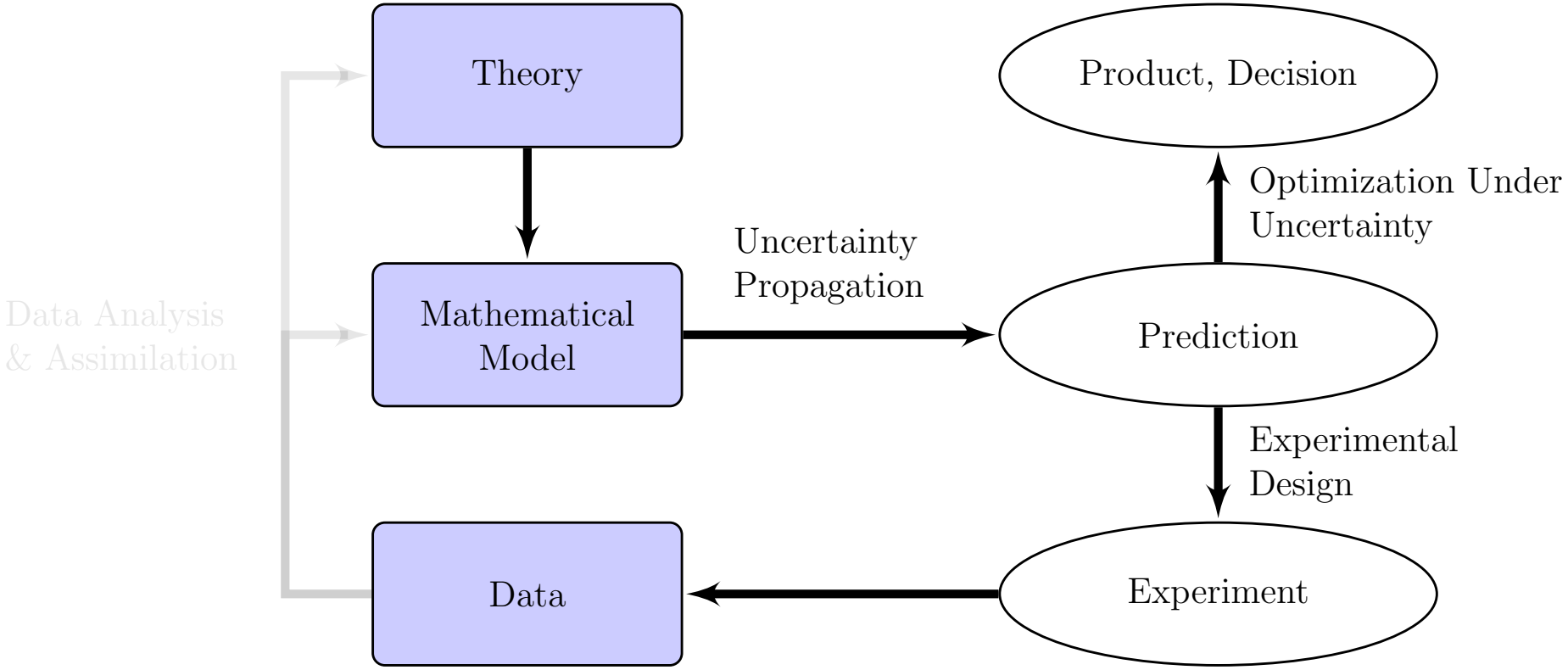
UQ in engineering and science: big picture



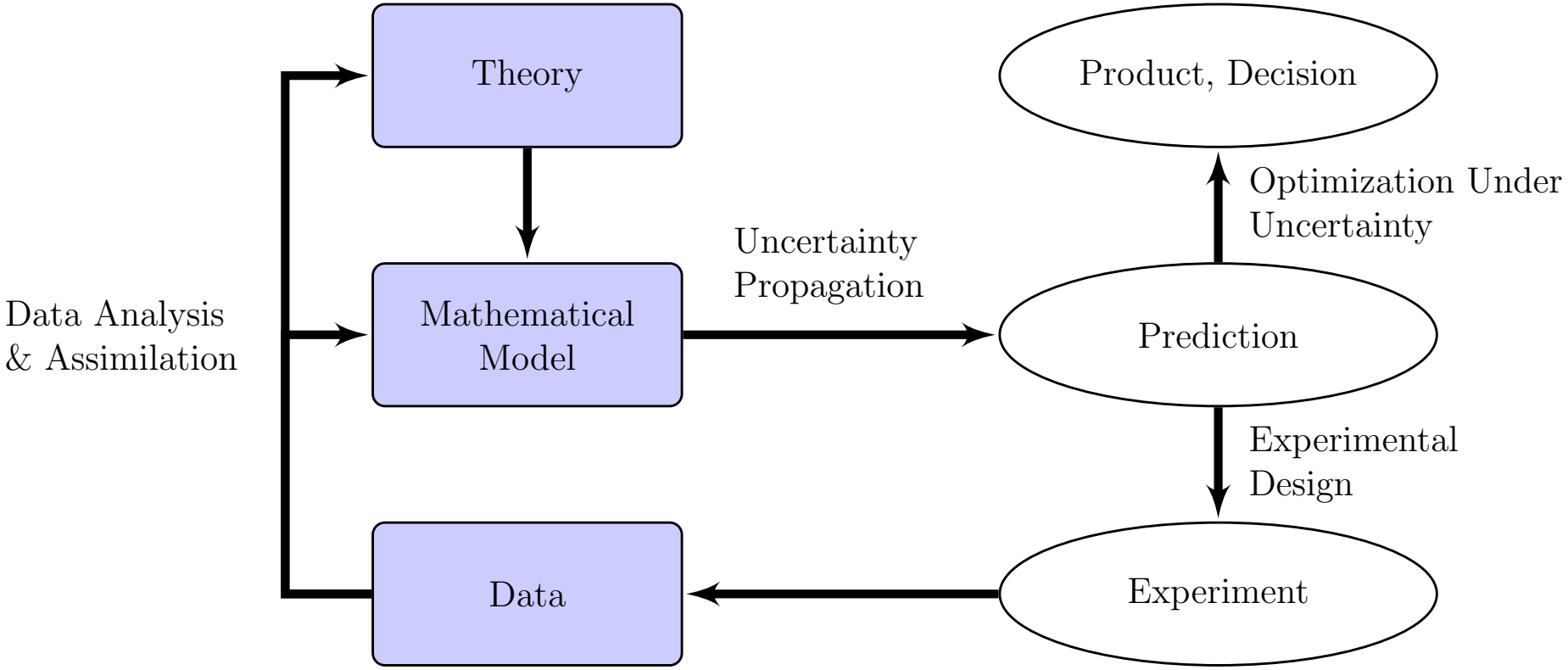
UQ in engineering and science: big picture



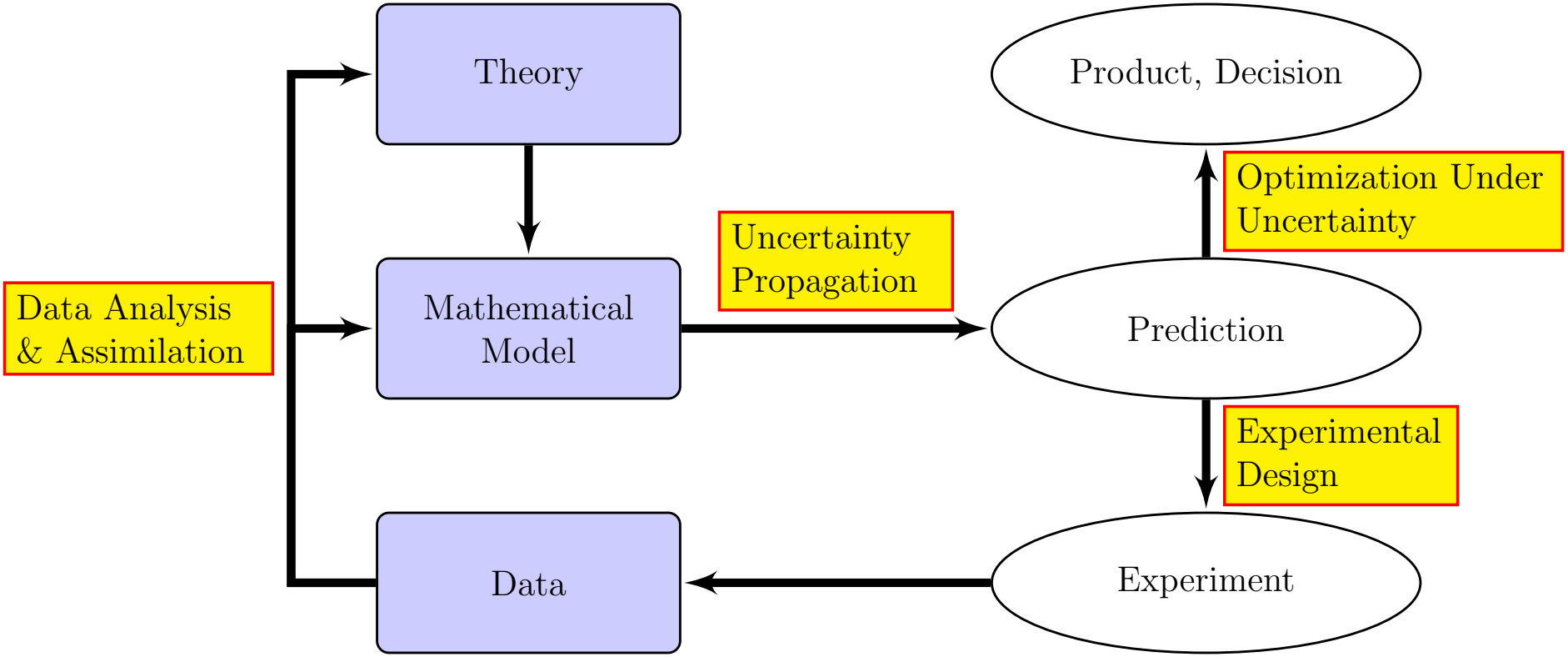
UQ in engineering and science: big picture



UQ in engineering and science: big picture



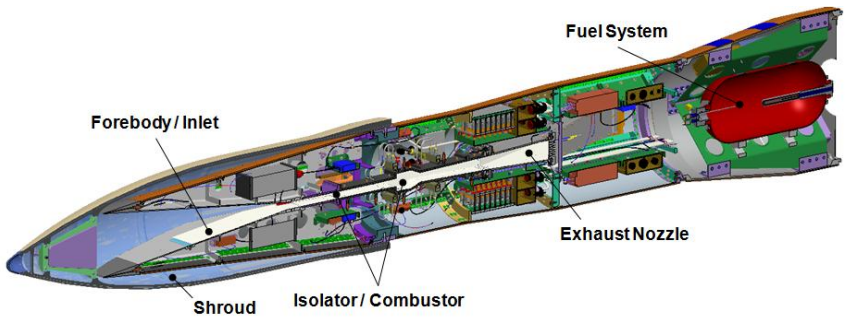
UQ in engineering and science: big picture

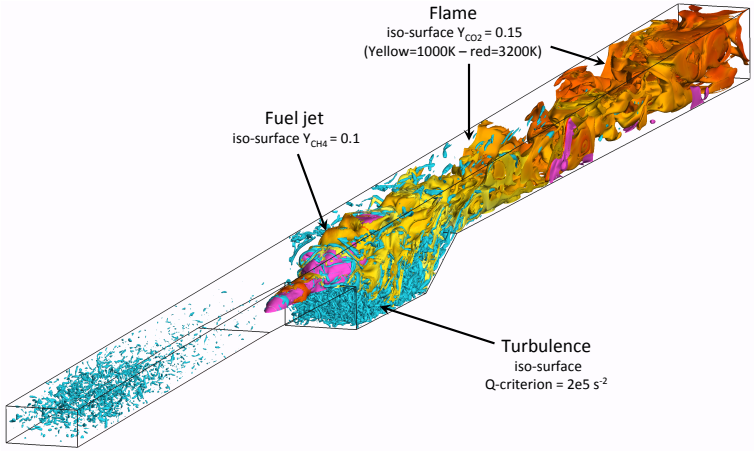


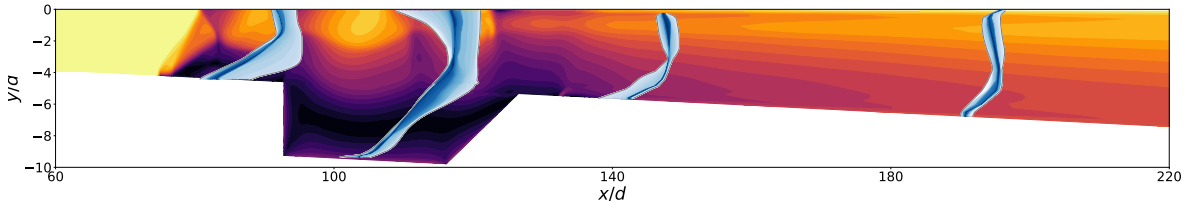
UQ work in hypersonics research

UQ for scramjet design—supersonic turbulent reactive flow

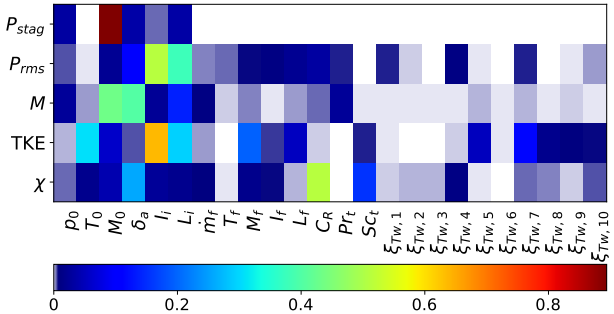
HIFiRE: [Dolvin 08, Dolvin 09, Gruber 08, Jackson 11, Ferlemann 08, Gruber 09]; Scramjet UQ: [Witteveen 11, Constantine 15]
RAPTOR flow solver: [Oefelein 06, Oefelein 07, Lacaze 17]







Uncertainty propagation through flow-field



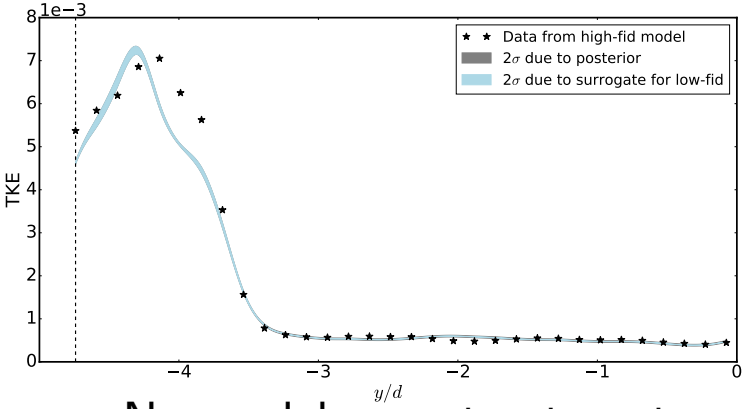
Global sensitivity analysis

Huan *et al.*, "Global Sensitivity Analysis and Estimation of Model Error, Toward UQ in Scramjet Computations," *AIAA Journal*, 56(3):1170–1180, 2018. [Huan 18a]

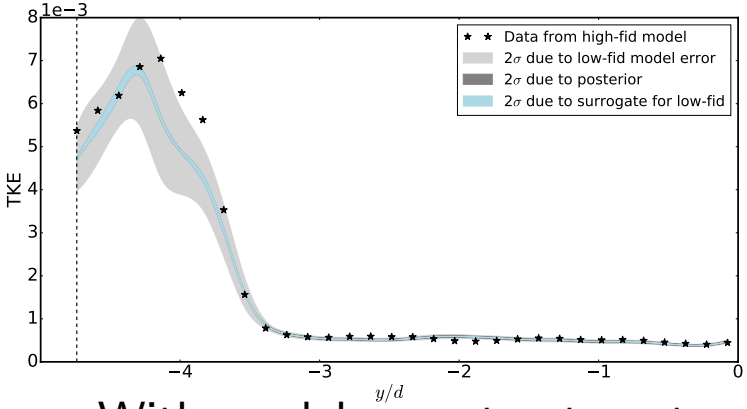
Huan *et al.*, "Compressive Sensing with Cross-Validation and Stop-Sampling for Sparse Polynomial Chaos Expansions," *SIAM/ASA Journal on Uncertainty Quantification*, 6(2):907–936, 2018. [Huan 18b]

UQ work in hypersonics research

Bayesian inference of model-form uncertainty:



No model error treatment

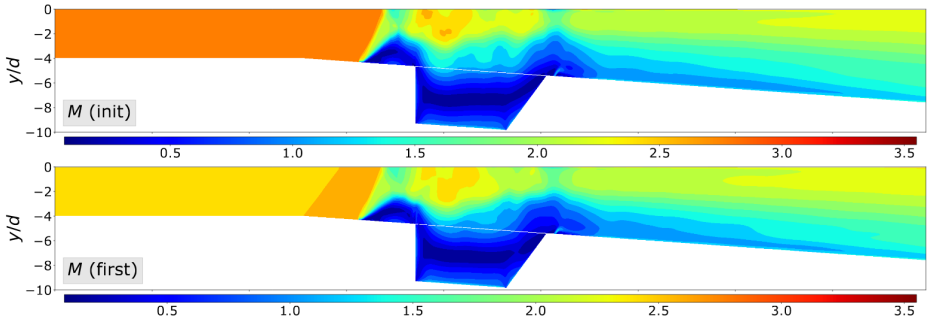


With model error treatment

max η_c design optimization:

Design parameter
ϕ_G
ϕ_R
x_1
x_2
a_1

QoI	Allowable
ϕ_{burn}	≥ 0.1843 (nominal d/8)
max P_{rms}	≤ 0.1677 (nominal d/8)
x_{shock}	$\geq 32d$
P_{stagloss}	≤ 0.3768 (nominal d/8)

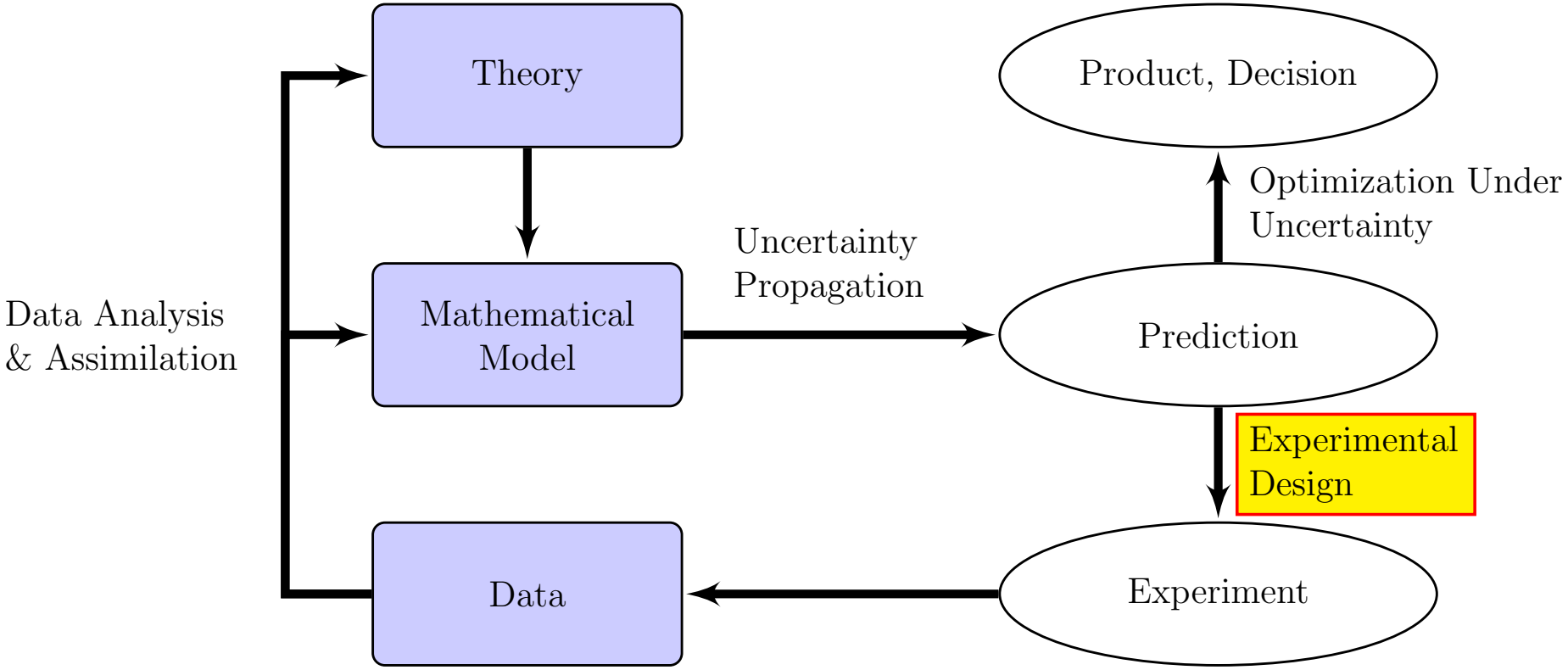


Sargsyan, **Huan**, & Najm, "Embedded model error representation for model calibration," *International Journal on Uncertainty Quantification*, published online, 2019. [Sargsyan 19]

Geraci, Menhorn, **Huan** *et al.*, "Progress in Scramjet Design Optimization Under Uncertainty Using Simulations of the HDCR," *AIAA Scitech 2019 Forum*, AIAA paper 2019—0725, 2019. [Geraci 19]

Ghanem, Soize, Safta, **Huan** *et al.*, "Design optimization of a scramjet under uncertainty using probabilistic learning manifolds," under revision in *Journal of Computational Physics*, 2019.

UQ in engineering and science: big picture



Outline

Outline

Some experiments are more useful than others

Experiments can be:

- Expensive
- Time-consuming
- Delicate to perform
- Dangerous or controversial

(Statistical) experimental design focuses on questions such as:

- Under what **conditions** (how) to perform the experiments?
- **What**, **where**, and **when** to measure?
- **How many** experiments?

Experimental design may have an entirely different meaning to experimentalists

Batch (non-sequential) design landscape

Classical statistical **design of experiments** often non simulation-based (e.g. space-filling) [Fisher 35, Box 87, Cox 00, Box 05, Santner 18]

Optimal experimental design: criterion based on a model/simulator

- Linear: information matrix (e.g., A-, D-optimal) [Fedorov 72, Atkinson 07]
- Nonlinear: intractable [Box 59, Ford 89, Chaloner 95, Müller 05, Ryan 16]
- Bayesian and decision-theoretic: maximize expected utility [Lindley 56, Berger 85, Clyde 96, Müller 04, Amzal 06, Parmigiani 09, Santner 18]
- Recent numerical advances (and many more. . .) [Ryan 03, Huan 13, Long 15, Weaver 16, Alexanderian 16, Tsilifis 17, Beck 18]

Scope of this talk:

- Nonlinear and expensive (e.g., physics-based) models
- Continuous parameter, design, and data spaces of multiple dimensions
- Bayesian information objective with non-Gaussian distributions

Step 1: Define experimental goals

What is a good experiment?

Depends on the experimental goals

Examples:

Goal	Quantifiable objective
learn model parameter	minimize parameter uncertainty
make accurate prediction	minimize QoI variance
discriminate between models	maximize Bayes factor
customized performance assessment	minimize a loss function
⋮	⋮

Huan & Marzouk, "Simulation-based optimal Bayesian experimental design for nonlinear systems," *Journal of Computational Physics*, 232(1):288–317, 2013. [Huan 13]

Step 1: Define experimental goals

What is a good experiment?

Depends on the experimental goals

Examples:

Goal	Quantifiable objective
learn model parameter	minimize parameter uncertainty
make accurate prediction	minimize QoI variance
discriminate between models	maximize Bayes factor
customized performance assessment	minimize a loss function
⋮	⋮

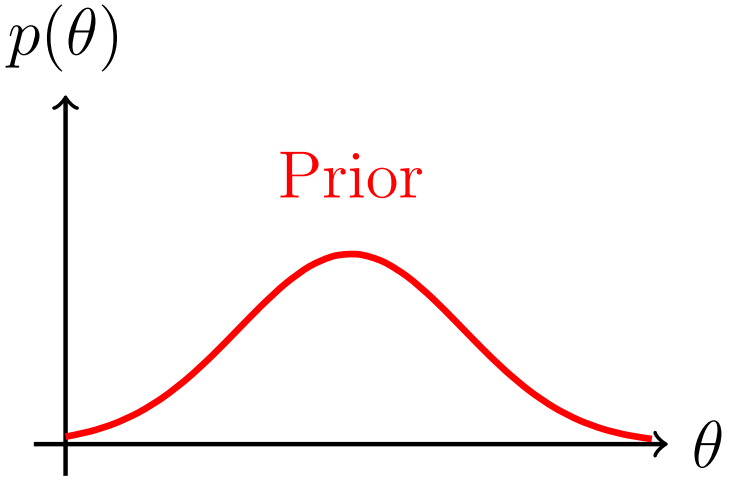
Huan & Marzouk, "Simulation-based optimal Bayesian experimental design for nonlinear systems," *Journal of Computational Physics*, 232(1):288–317, 2013. [Huan 13]

Step 2: Formulate objective function

Characterize uncertainty using **Bayes' Theorem**:

$$\overbrace{p(\theta \quad)}^{prior}$$

θ — parameters $\quad$ y — noisy data

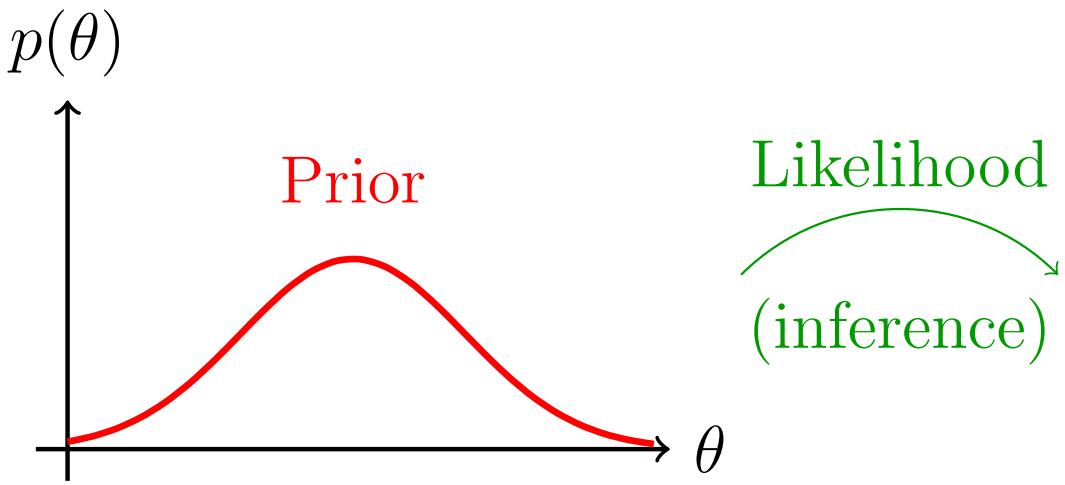


Step 2: Formulate objective function

Characterize uncertainty using **Bayes' Theorem**:

$$\frac{\overbrace{p(y|\theta)}^{likelihood}\,\overbrace{p(\theta)}^{prior}}{}$$

θ — parameters $\quad$ y — noisy data

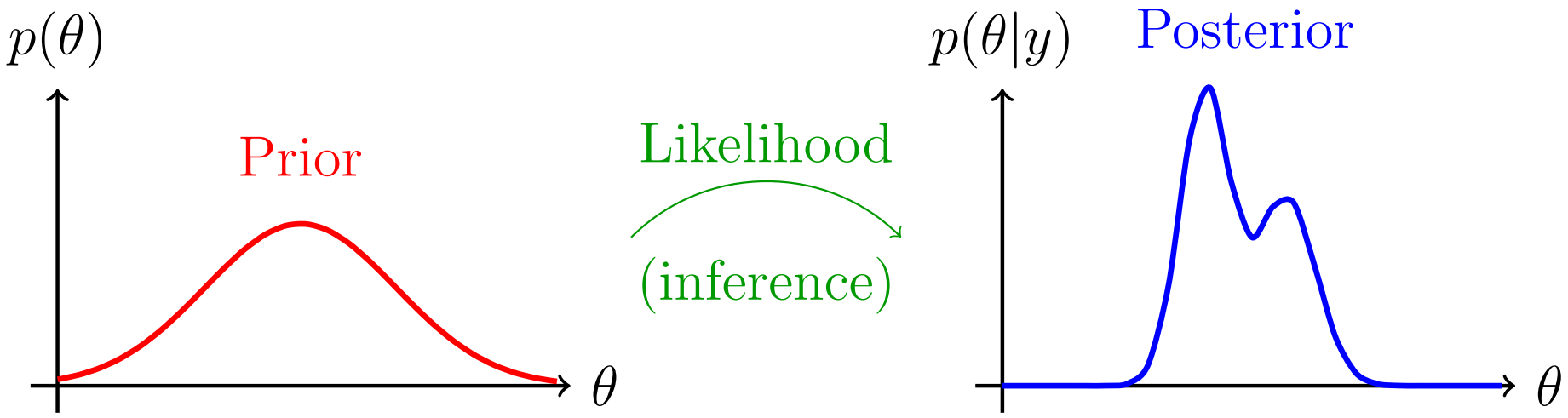


Step 2: Formulate objective function

Characterize uncertainty using **Bayes' Theorem**:

$$\overbrace{p(\theta|y)}^{posterior} = \frac{\overbrace{p(y|\theta)}^{likelihood}\overbrace{p(\theta)}^{prior}}{\underbrace{p(y)}_{evidence}}$$

θ — parameters $\quad$ y — noisy data

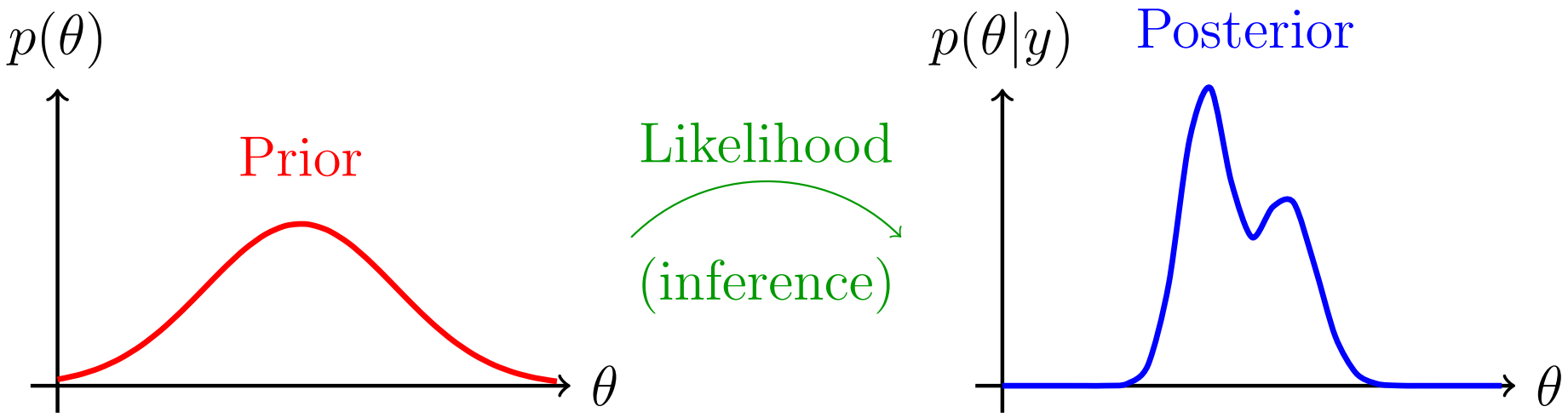


Step 2: Formulate objective function

Characterize uncertainty using **Bayes' Theorem**:

$$\overbrace{p(\theta|y,d)}^{posterior} = \frac{\overbrace{p(y|\theta,d)}^{likelihood}\overbrace{p(\theta|d)}^{prior}}{\underbrace{p(y|d)}_{evidence}}$$

θ — parameters $\quad$ y — noisy data $\quad$ d — design (experimental conditions)



Step 2: Formulate objective function

Expected **Kullback-Leibler (KL)** divergence between posterior and prior ($\Longleftrightarrow$ **mutual information** between data and parameters)

$$
\begin{aligned}
U(d) &= \mathbb{E}_{y|d}\left[D_{\mathrm{KL}}(p(\theta|y,d)||p(\theta|d))\right] \\
&= \int_{\mathcal{Y}} \left[\int_{\Theta} \ln\left[\frac{p(\theta|y,d)}{p(\theta)}\right] p(\theta|y,d)\, d\theta\right] p(y|d)\, dy \\
&\approx \frac{1}{N}\sum_{i=1}^{N}\left\{\ln\left[p(y^{(i)}|\theta^{(i)},d)\right] - \ln\left[p(y^{(i)}|d)\right]\right\}
\end{aligned}
$$

$$
p(y^{(i)}|d) \approx \frac{1}{M}\sum_{j=1}^{M} p(y^{(i)}|\theta^{(i,j)},d) \qquad \text{(nested Monte Carlo!)}
$$

U — expected utility

θ — parameters of interest
y — noisy data
d — design variables

Step 3: Approximate objective function numerically

Expected **Kullback-Leibler (KL)** divergence between posterior and prior ($\Longleftrightarrow$ **mutual information** between data and parameters)

$$
\begin{aligned}
U(d) &= \mathbb{E}_{y|d}\left[D_{\mathrm{KL}}(p(\theta|y,d)||p(\theta|d))\right] \\
&= \int_{\mathcal{Y}} \left[\int_{\Theta} \ln\left[\frac{p(\theta|y,d)}{p(\theta)}\right] p(\theta|y,d)\, d\theta\right] p(y|d)\, dy \\
&\approx \frac{1}{N}\sum_{i=1}^{N}\left\{\ln\left[p(y^{(i)}|\theta^{(i)},d)\right] - \ln\left[p(y^{(i)}|d)\right]\right\}
\end{aligned}
$$

$$
p(y^{(i)}|d) \approx \frac{1}{M}\sum_{j=1}^{M} p(y^{(i)}|\theta^{(i,j)},d) \qquad \text{(nested Monte Carlo!)}
$$

U — expected utility

θ — parameters of interest
y — noisy data
d — design variables

Step 3: Approximate objective function numerically

Likelihood evaluation is the most expensive part:

$$p(y|\theta, d)$$

Need to specify a likelihood model:

- statistical description of mismatch between
  model prediction vs. observed data
- e.g., additive Gaussian noise $\epsilon \sim \mathcal{N}(0, \sigma_\epsilon^2)$

$$y = G(\theta, d) + \epsilon$$

- Each evaluation $p(y|\theta, d) = p_\epsilon(y - G(\theta, d))$ requires a model solve

U — expected utility

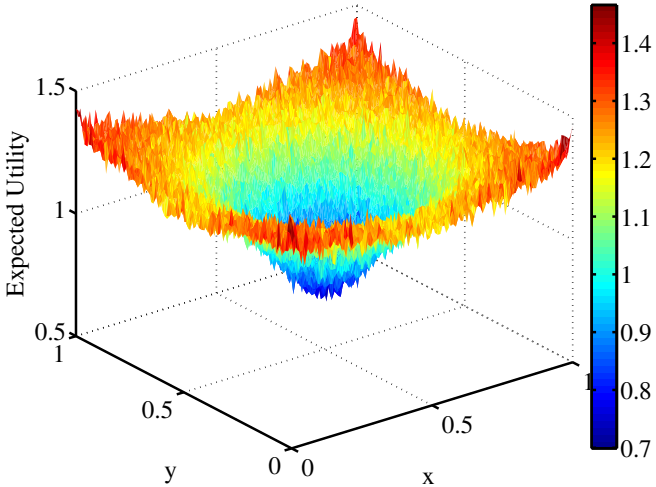
θ — parameters of interest
y — noisy data
d — design variables

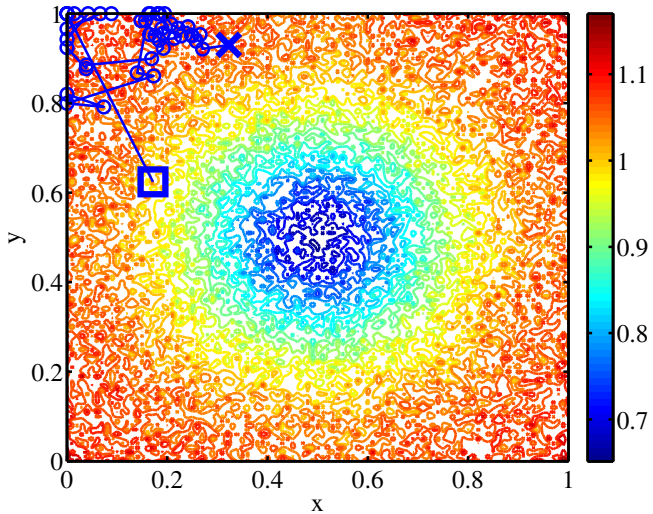
Step 4: Perform stochastic optimization

Find optimal design: $$d^* = \underset{d \in \mathcal{D}}{\operatorname{argmax}}\ U(d)$$

$\Rightarrow$ **noisy** objective function due to Monte Carlo

Robbins-Monro stochastic approximation [Robbins 51]





- Needs to derive gradient
- Can approximate by building certain types of surrogate models

(Optional): Accelerate using surrogate models

Example: polynomial chaos expansions [Ghanem 91, Xiu 02, Najm 09, Marzouk 09]

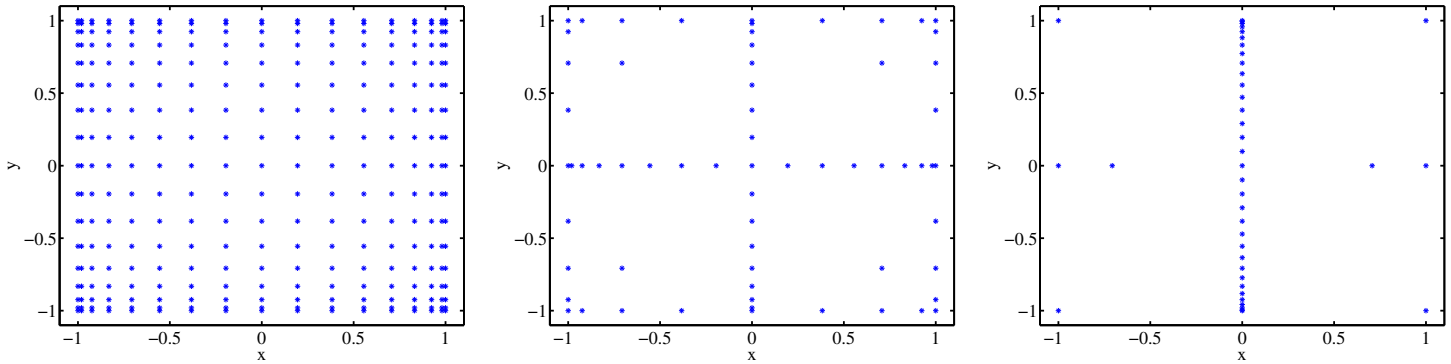
$$g(\theta(\xi)) = \sum_{\beta \in \mathcal{J}} c_\beta \Psi_\beta(\xi)$$

- c_β: coefficients (β polynomial order multi-index)
- ξ: reference random vector (e.g., uniform, Gaussian)
- Ψ_β: multivariate orthonormal polynomial (e.g., Legendre, Hermite)

Non-intrusive approach to compute coefficients

$$c_\beta = \langle G \Psi_\beta \rangle = \int G(\theta(\xi), d(\xi)) \Psi_\beta(\xi) p(\xi)\, d\xi$$

Integrate using adaptive sparse quadrature [Gerstner 98, Barthelmann 00, Gerstner 03]



Design of shock tube experiment for combustion kinetics

H_2-O_2 homogeneous ignition, no transport, constant pressure, adiabatic

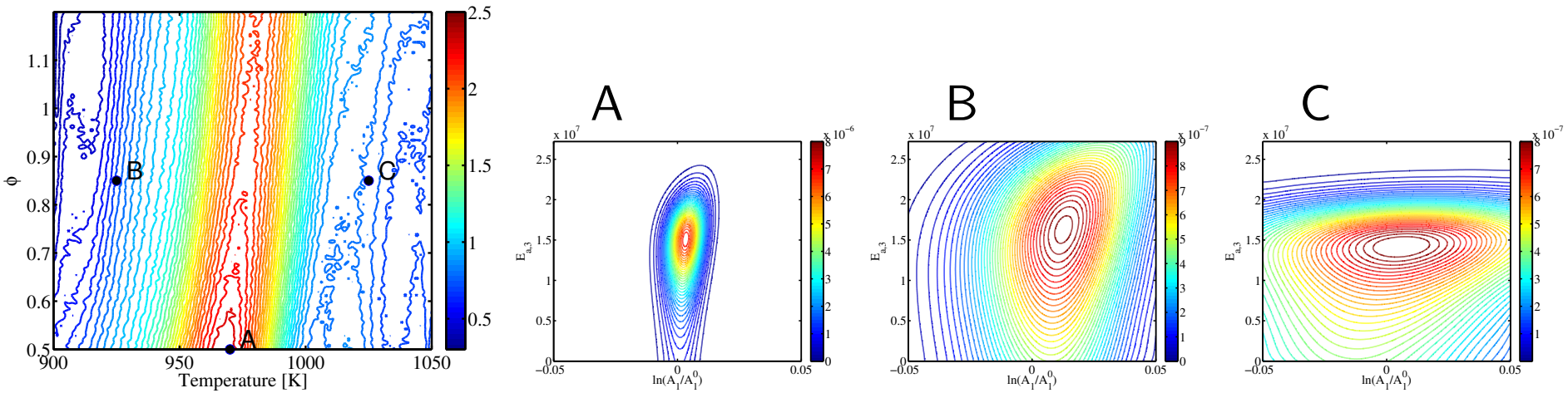
Goal: learn 2 kinetic parameters in a 19-reaction mechanism [Yetter 91]

- $\ln A$ of $R1$: $H + O_2 \Longleftrightarrow O + OH$
- E_a of $R3$: $H_2 + OH \Longleftrightarrow H_2O + H$

System of stiff ODEs, numerically solved using Cantera with CVODE

Measurement: ignition delay time

Design variables: initial T and ϕ (fuel amount used)



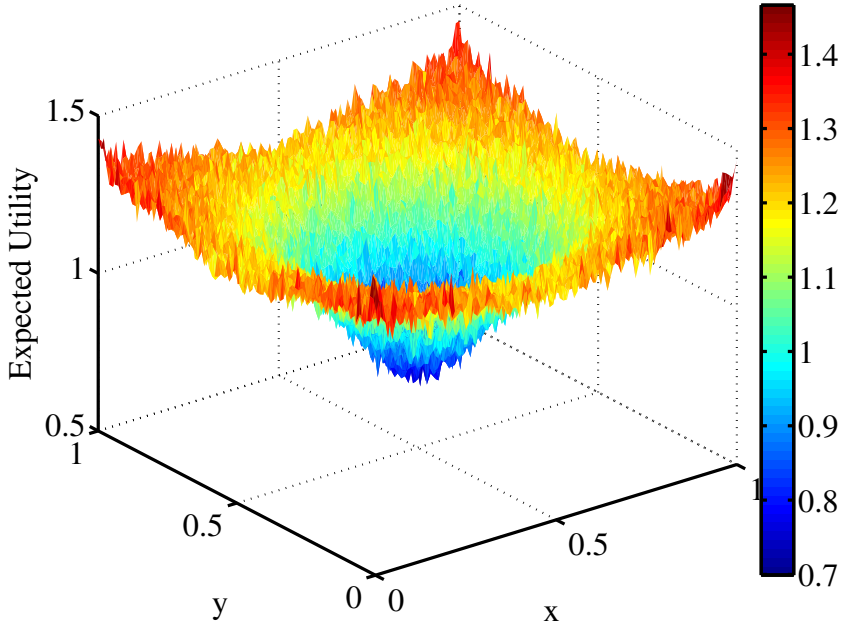
Huan & Marzouk, "Simulation-based optimal Bayesian experimental design for nonlinear systems," *Journal of Computational Physics*, 232(1):288–317, 2013. [Huan 13]

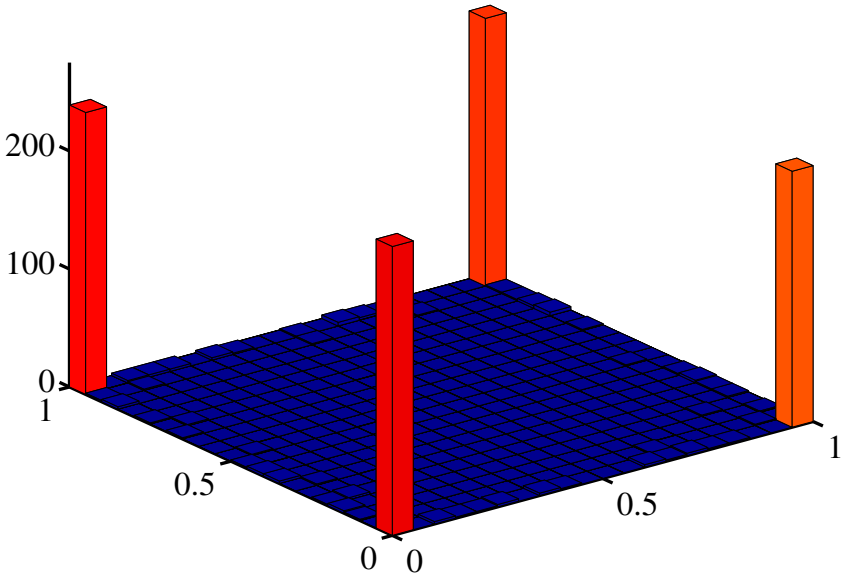
Sensor placement for source inversion

2D scalar diffusion PDE in a square domain with a time-limited source

Goal: infer uncertain source location

Measurements: concentrations at 5 equally spaced sample times
Design variables: sensor coordinates

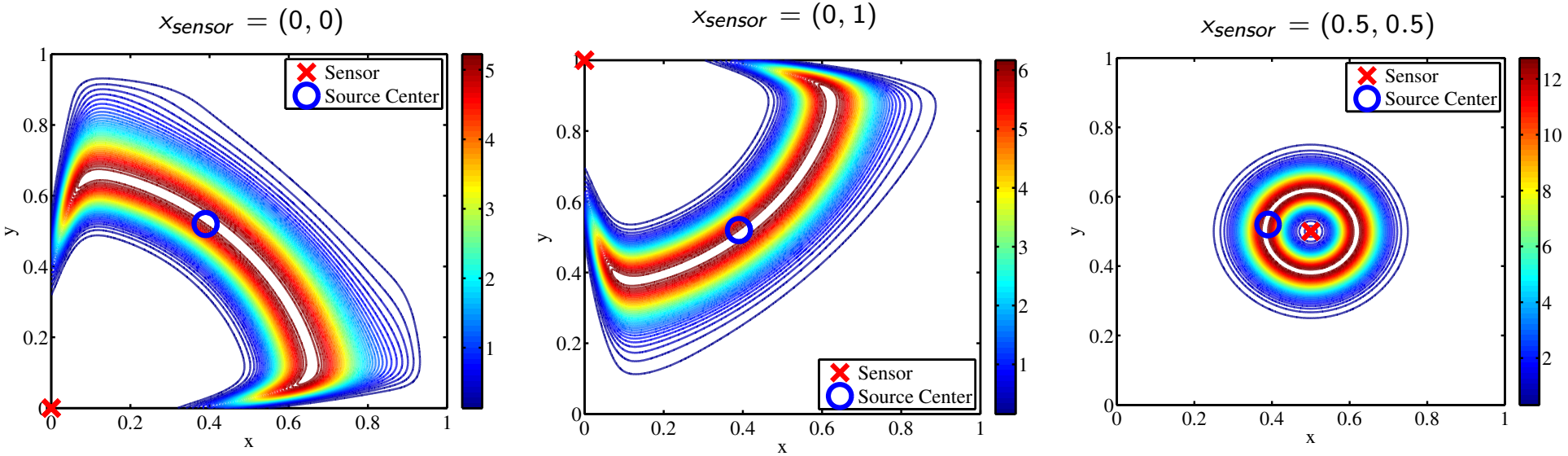




Huan & Marzouk, "Gradient-Based Stochastic Optimization Methods in Bayesian Experimental Design," *International Journal of Uncertainty Quantification*, 4(6):479–510, 2014. [Huan 14]

Sensor placement for source inversion: 1 sensor

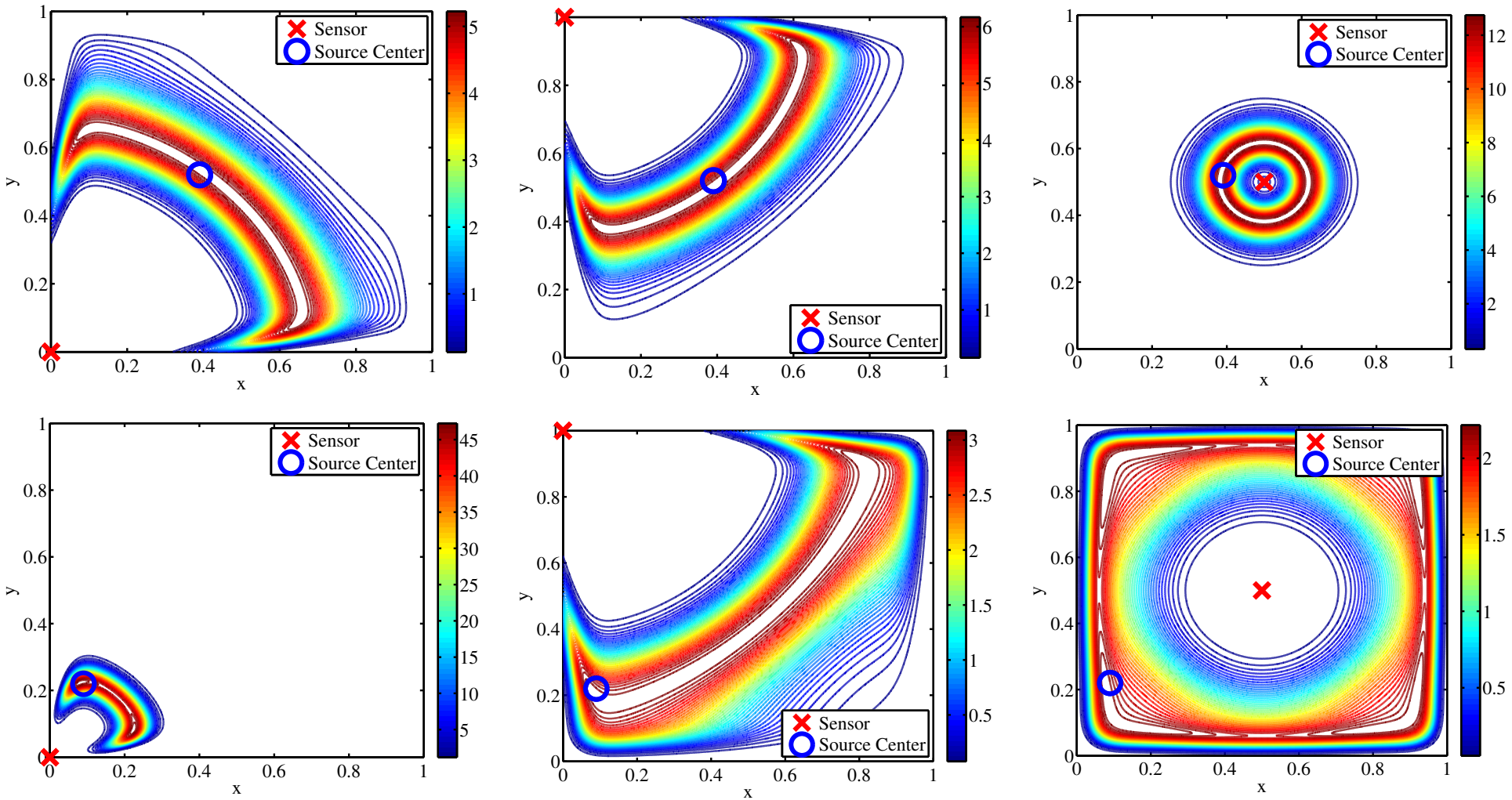
Posterior PDFs: $x_{src} = (0.39, 0.52)$



Sensor placement for source inversion: 1 sensor

Posterior PDFs: $x_{src} = (0.39, 0.52)$ (row 1) and $x_{src} = (0.09, 0.22)$ (row 2):

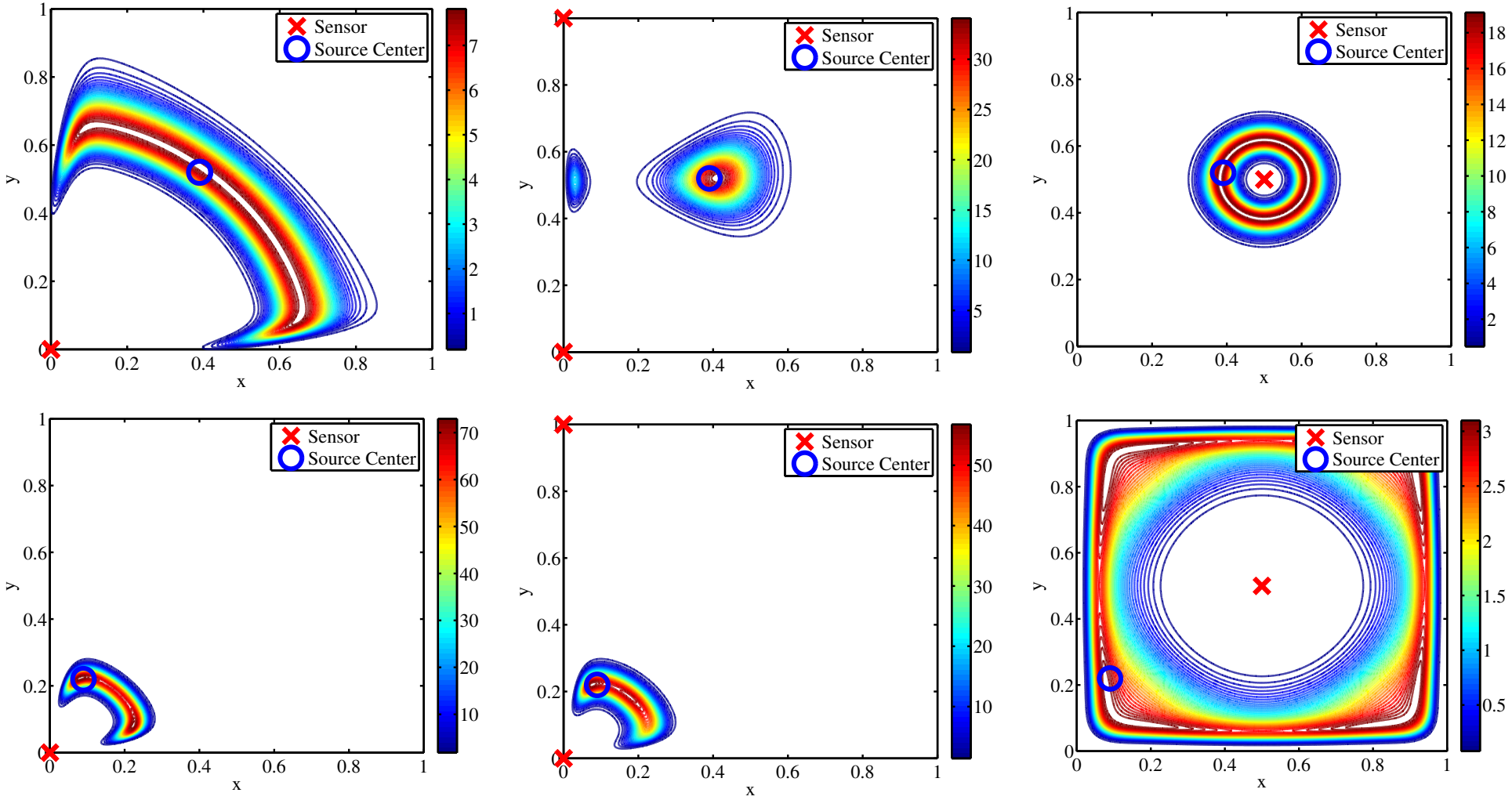
$x_{sensor} = (0, 0)$ $x_{sensor} = (0, 1)$ $x_{sensor} = (0.5, 0.5)$



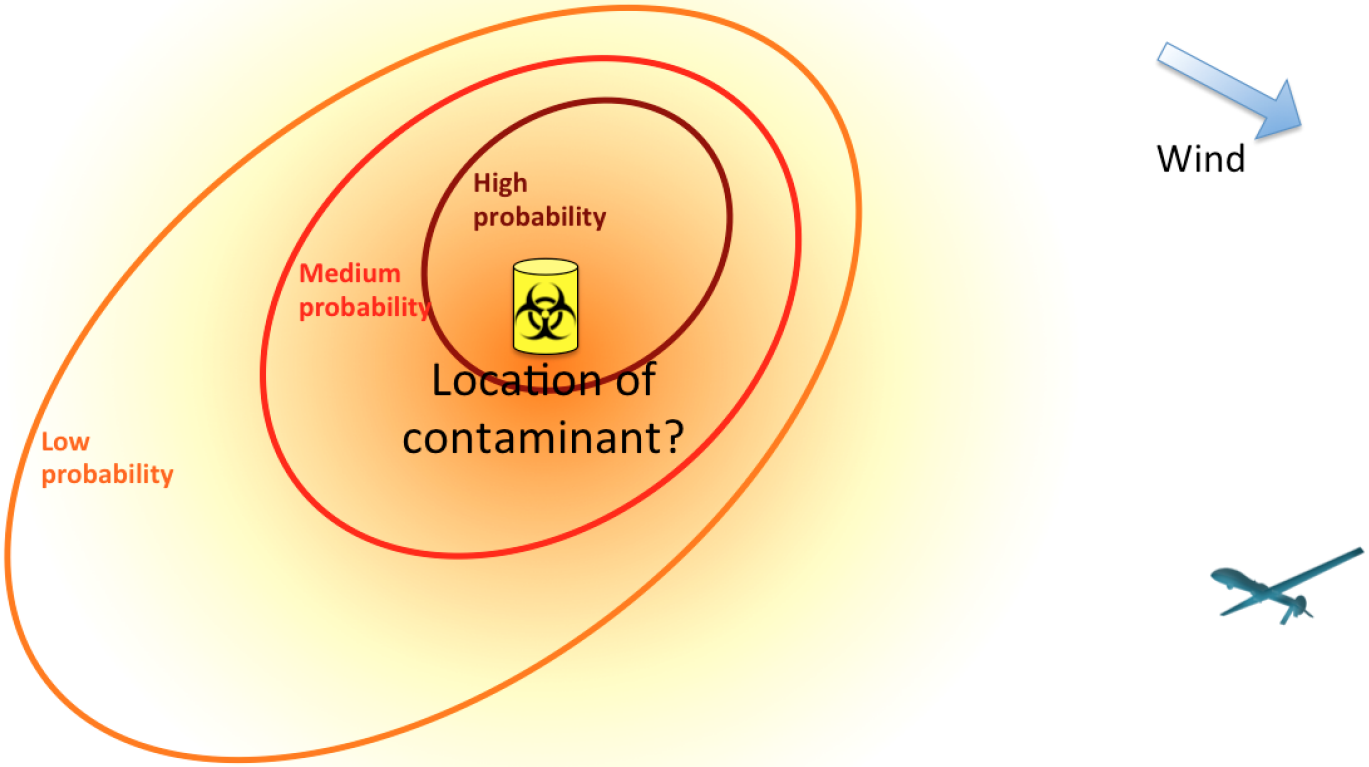
Sensor placement for source inversion: 2 sensors

Posterior PDFs: $x_{src} = (0.39, 0.52)$ (row 1) and $x_{src} = (0.09, 0.22)$ (row 2):

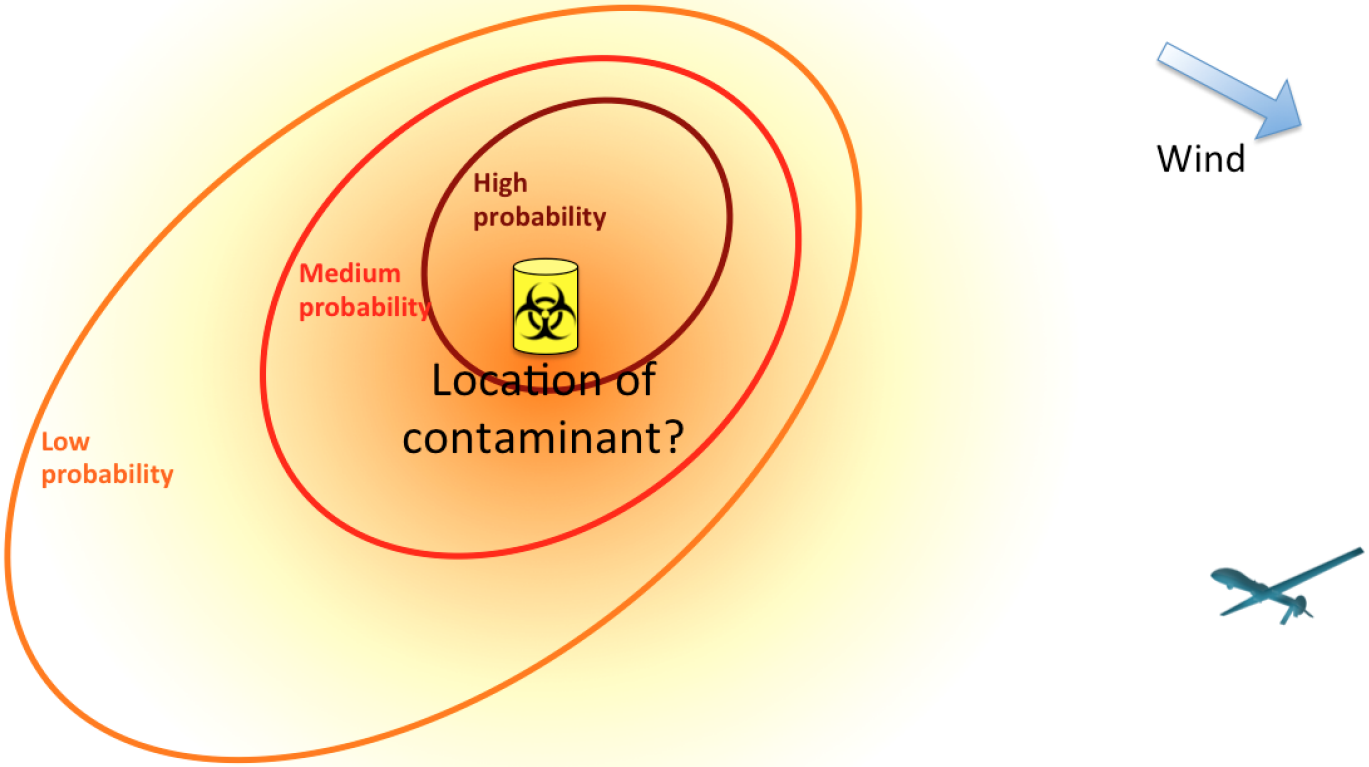
$x_{sensors} = (0,0), (0,0)$ $\quad$ $x_{sensors} = (0,0), (0,1)$ $\quad$ $x_{sensor} = (0.5,0.5), (0.5,0.5)$



Planning measurements: batch (non-sequential) design



Planning measurements: sequential design



Planning measurements: sequential design

Sequential experimental design much more challenging

- Greedy (myopic) design generally sub-optimal
- Incorporate 1. feedback and 2. lookahead
- Utilize dynamic programming and reinforcement learning

Huan & Marzouk, "Sequential Bayesian Optimal Experimental Design via Approximate Dynamic Programming," *arXiv: 1604.08320*, 2016. [Huan 16]

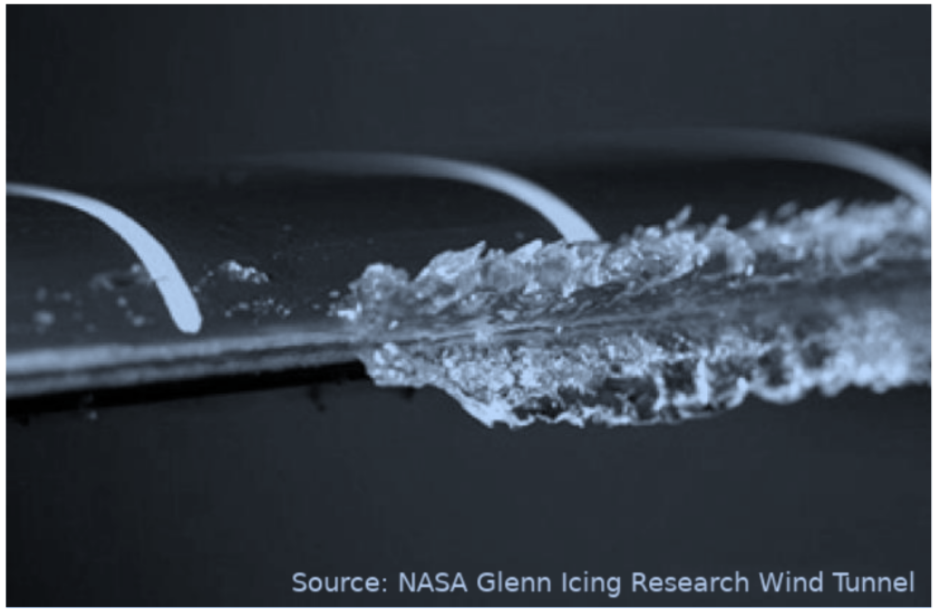
Outline

Motivation: in-flight rotorcraft icing

Collaboration with: **B. Y. Zhou, N. R. Gauger (TU-Kaiserslautern), M. Morelli, A. Guardone (Polytecnico di Milano), J. Hauth, X. Huan (U-Michigan). AIAA paper 2019–3103, 2019.** [Zhou 19a]

- In-flight rotorcraft icing is extremely dangerous:
  - alters leading-edge shape of rotor blades
  - severely degrades aerodynamic performance
  - is difficult to escape from/recover
- Many icing-induced fatal accidents in recent years
- Real-time in-flight ice detection system is of paramount importance

Source: BBC NEWS, Mar 2nd 2006


Source: NASA Glenn Icing Research Wind Tunnel

Motivation: in-flight rotorcraft icing

In-flight visual inspection nearly impossible due to high rotor RPM

Promising route: detection using **acoustic signals** enabled by simulations

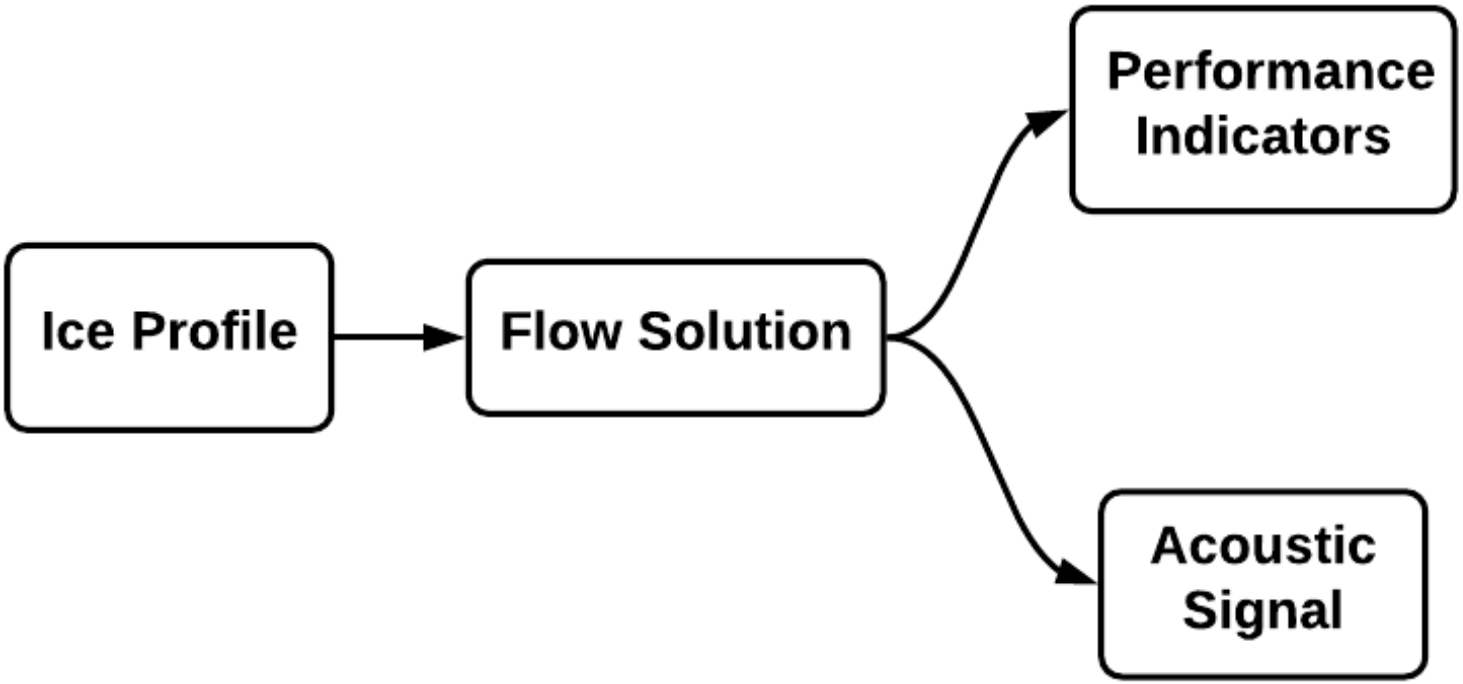
- computational fluid dynamics (CFD)
- computational aeroacoustics (CAA)

Motivation: in-flight rotorcraft icing

In-flight visual inspection nearly impossible due to high rotor RPM

Promising route: detection using **acoustic signals** enabled by simulations

- computational fluid dynamics (CFD)
- computational aeroacoustics (CAA)

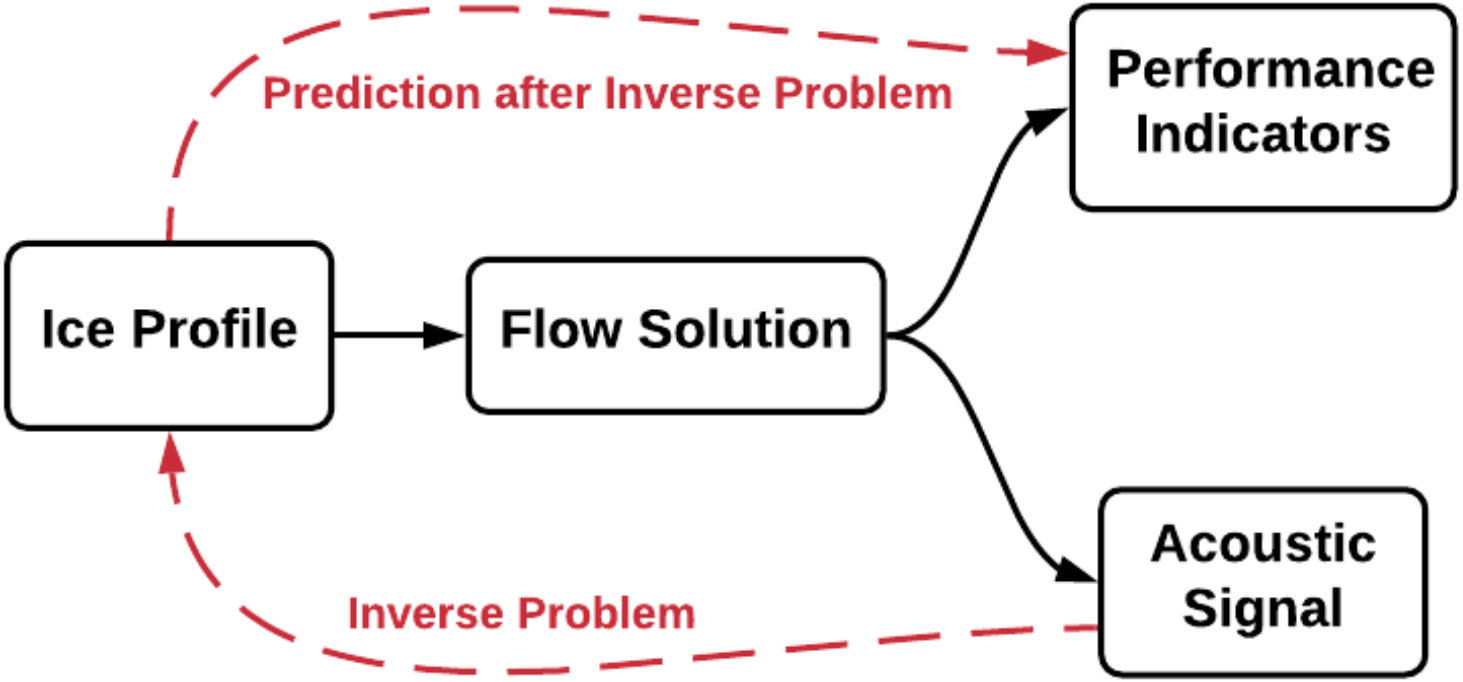


Motivation: in-flight rotorcraft icing

In-flight visual inspection nearly impossible due to high rotor RPM

Promising route: detection using **acoustic signals** enabled by simulations

- computational fluid dynamics (CFD)
- computational aeroacoustics (CAA)



Motivation: in-flight rotorcraft icing

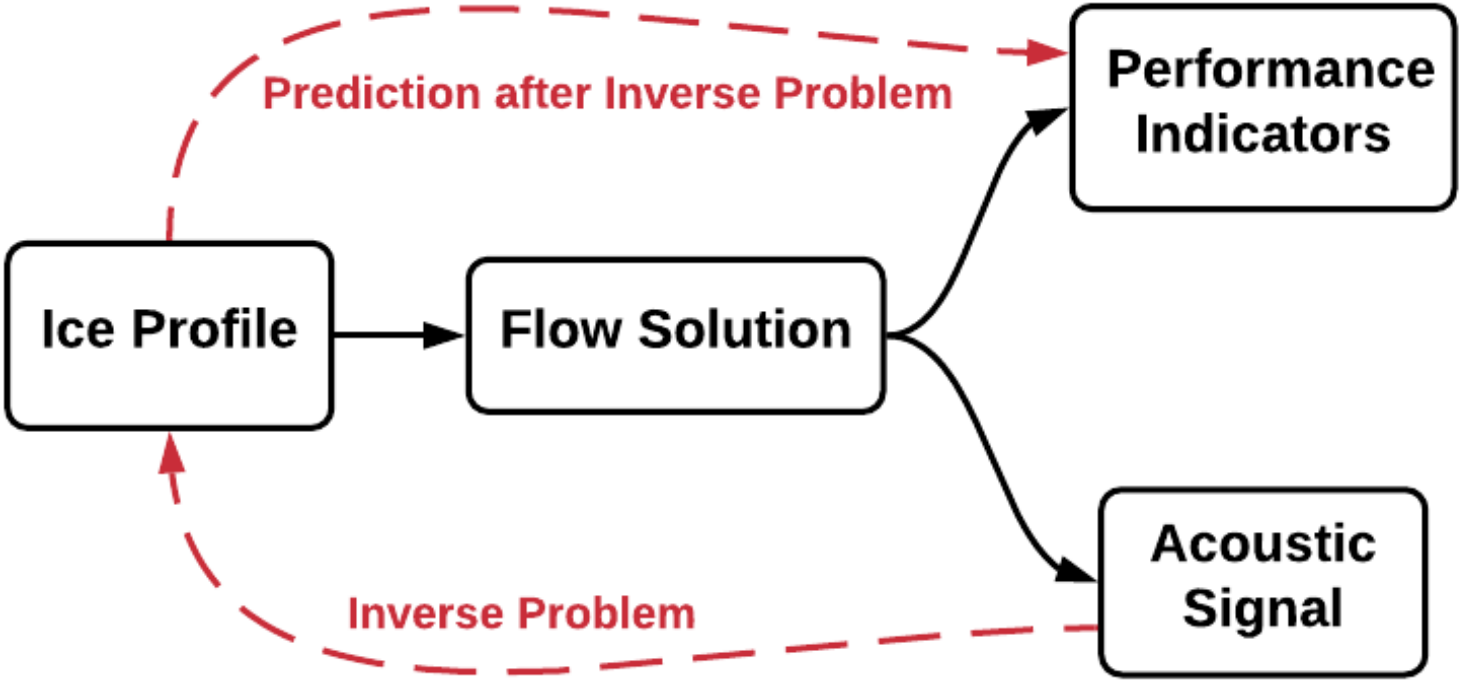
In-flight visual inspection nearly impossible due to high rotor RPM

Promising route: detection using **acoustic signals** enabled by simulations

- computational fluid dynamics (CFD)
- computational aeroacoustics (CAA)

But: physics-based solutions very expensive (min/hours)

$\Longrightarrow$ accelerate via **machine-learning (ML)** models



Motivation: in-flight rotorcraft icing

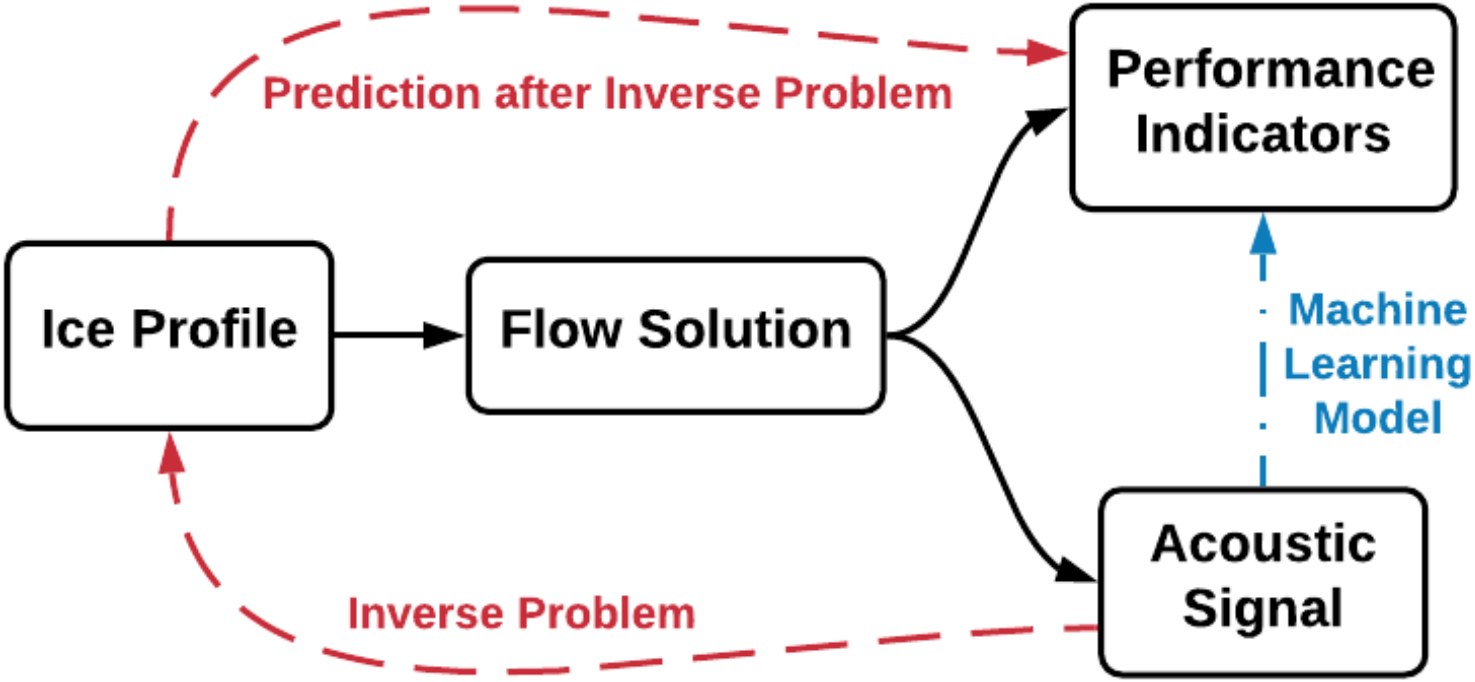
In-flight visual inspection nearly impossible due to high rotor RPM

Promising route: detection using **acoustic signals** enabled by simulations

- computational fluid dynamics (CFD)
- computational aeroacoustics (CAA)

But: physics-based solutions very expensive (min/hours)

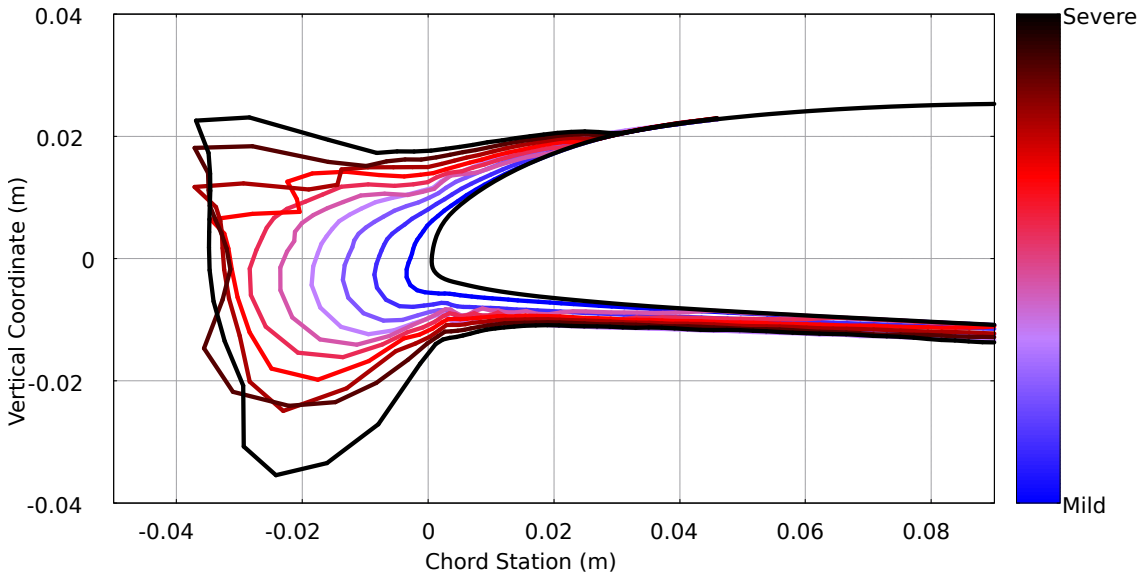
$\Longrightarrow$ accelerate via **machine-learning (ML)** models



Numerical modeling and simulations

Key components (omitting much details, please see [Zhou 19a]):

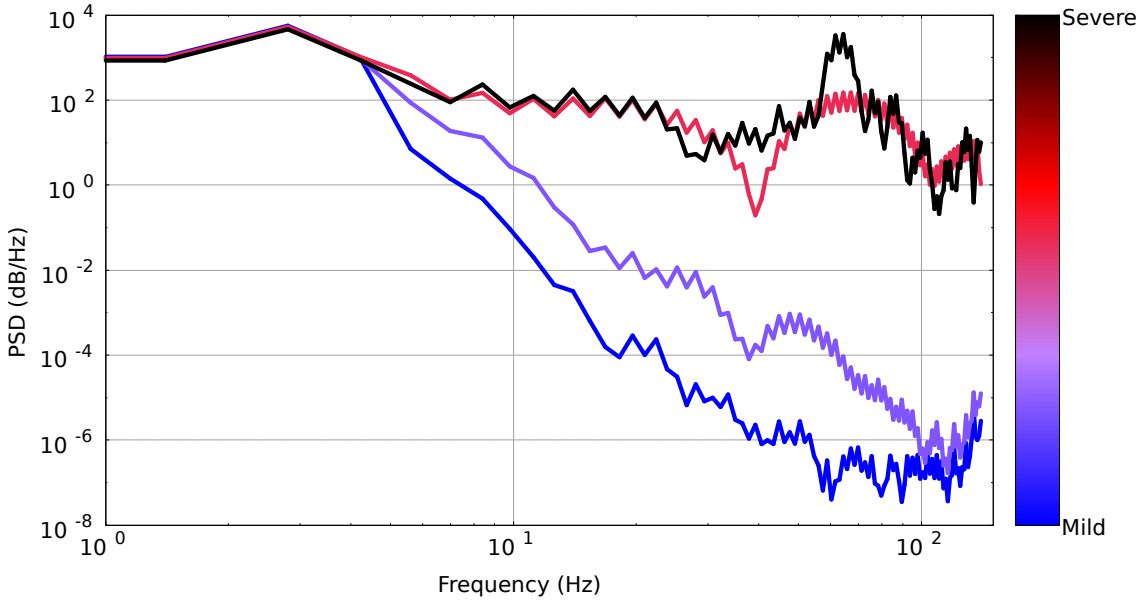
- PoliDrop, PoliMIce—ice seeding and accretion
- URANS/DES—turbulent flow solve for near field
- FW-H (Ffowcs Williams-Hawking)—acoustics solver propagate signals to far field
- Coupled through open-source software SU2 [Zhou 15]



Numerical modeling and simulations

Key components (omitting much details, please see [Zhou 19a]):

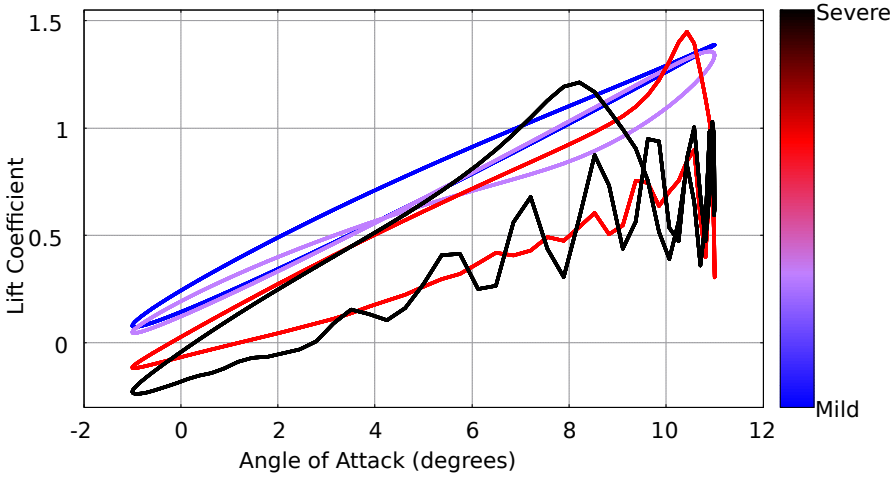
- PoliDrop, PoliMIce—ice seeding and accretion
- URANS/DES—turbulent flow solve for near field
- FW-H (Ffowcs Williams-Hawking)—acoustics solver propagate signals to far field
- Coupled through open-source software SU2 [Zhou 15]

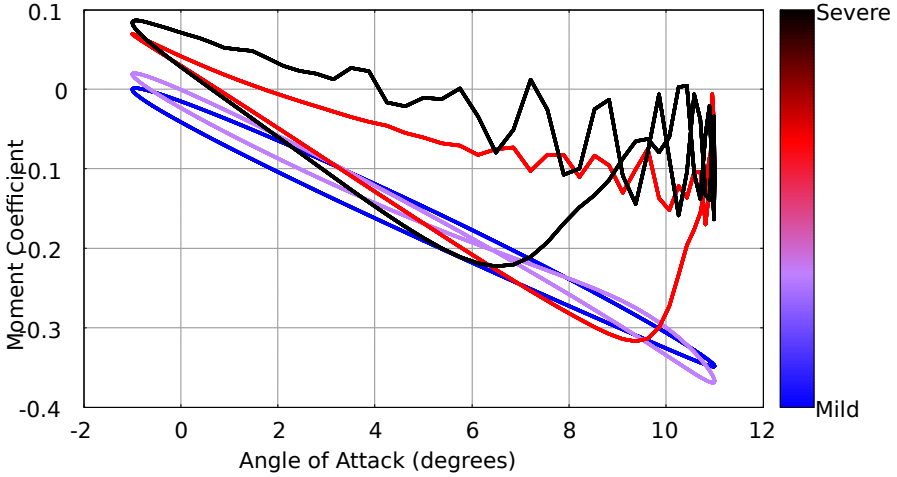


Numerical modeling and simulations

Key components (omitting much details, please see [Zhou 19a]):

- PoliDrop, PoliMIce—ice seeding and accretion
- URANS/DES—turbulent flow solve for near field
- FW-H (Ffowcs Williams-Hawking)—acoustics solver propagate signals to far field
- Coupled through open-source software SU2 [Zhou 15]

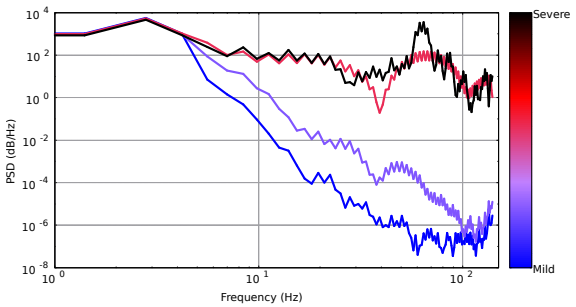




Numerical modeling and simulations

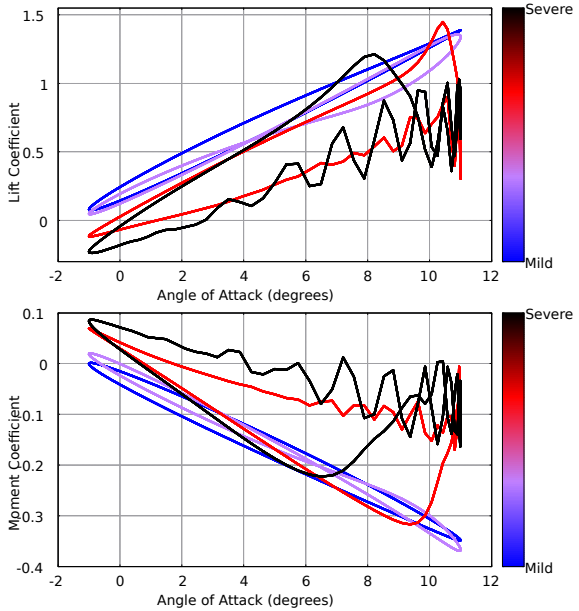
Key components (omitting much details, please see [Zhou 19a]):

- PoliDrop, PoliMIce—ice seeding and accretion
- URANS/DES—turbulent flow solve for near field
- FW-H (Ffowcs Williams-Hawking)—acoustics solver propagate signals to far field
- Coupled through open-source software SU2 [Zhou 15]



$\Longrightarrow$

Deep Learning

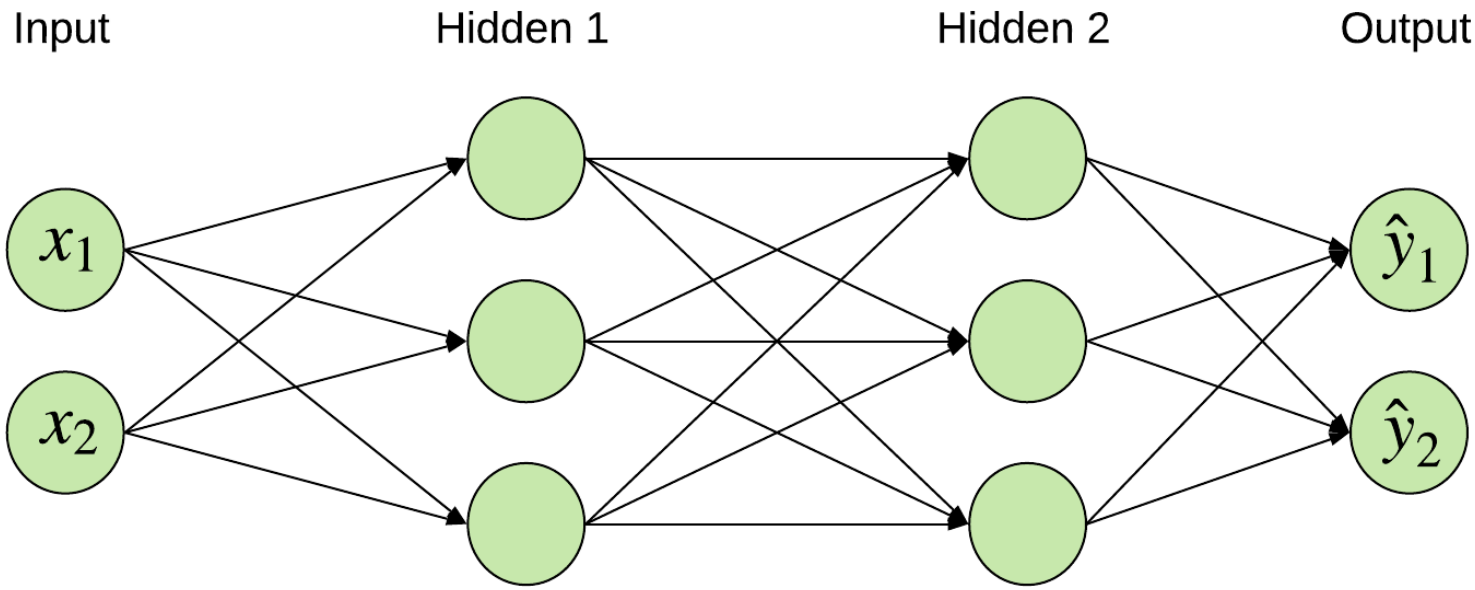


Deep neural networks (DNNs)

A neural network (NN) is a function $f : x \in \mathbb{R}^m \to \hat{y} \in \mathbb{R}^n$:

$$\hat{y} = f(x)$$

- $\hat{y}$ here denotes DNN *prediction*
- Example below: fully connect feed-forward NN
- NN generally considered "deep" with 2+ hidden layers



Deep neural networks (DNNs)

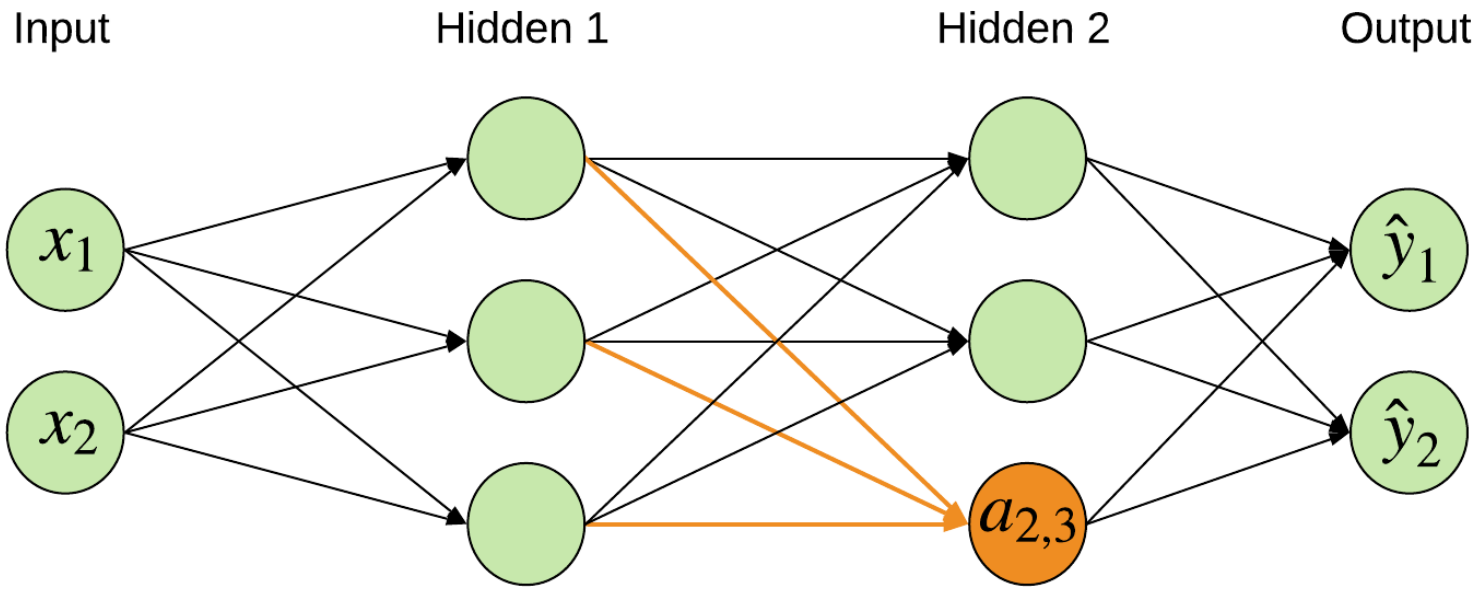
Computation at node j in layer ℓ:

$$a_{\ell,j} = \phi_\ell \left(\sum_i W_{\ell,ij} a_{\ell-1,i} + b_{\ell,j} \right)$$

- $a_{\ell,j}$: nodal output
- $W_{\ell,ij}$: weight on $a_{\ell-1,i}$
- ϕ_ℓ: activation function (e.g., rectified linear unit, tanh)

$a_{\ell-1,i}$: nodal input from previous layer

$b_{\ell,j}$: bias (offset) term

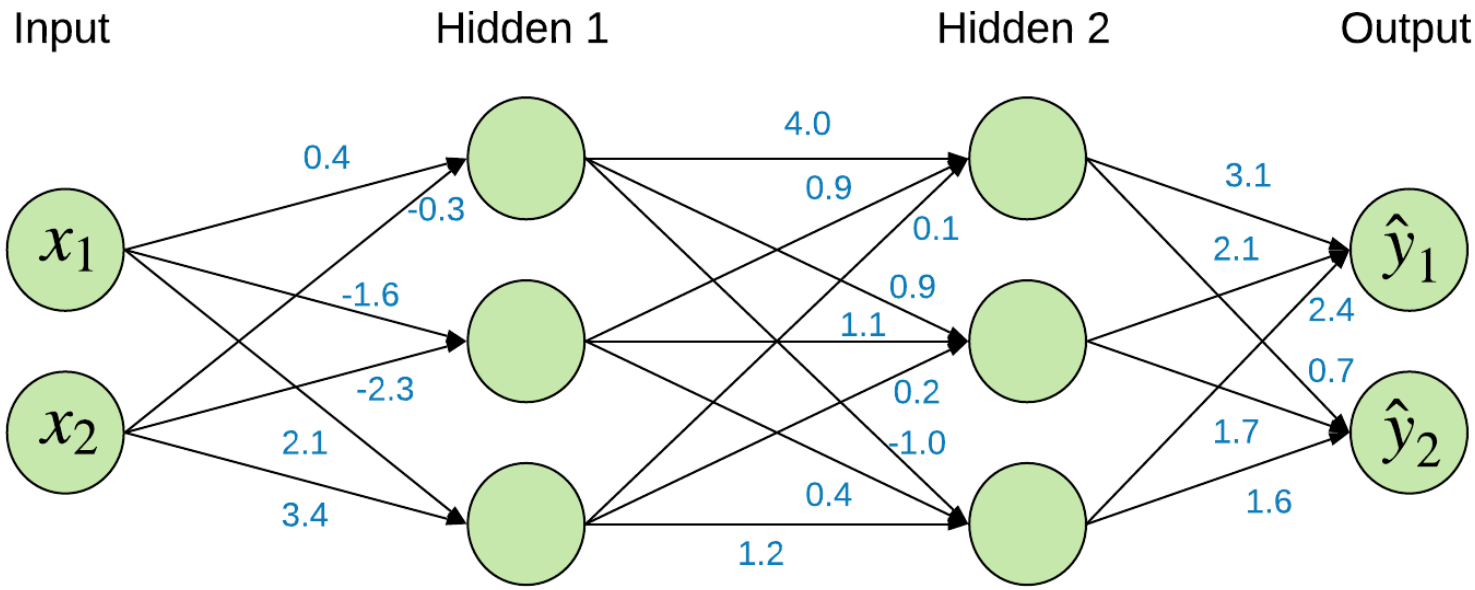


Deep neural networks (DNNs)

In this example:

$$a_0 = x$$
$$a_1 = \phi_1(W_1^T a_0 + b_1)$$
$$a_2 = \phi_2(W_2^T a_1 + b_2)$$
$$a_3 = \phi_3(W_3^T a_2 + b_3) = \hat{y}$$

Training a DNN: find the best $w \equiv \{W_\ell, b_\ell\}$

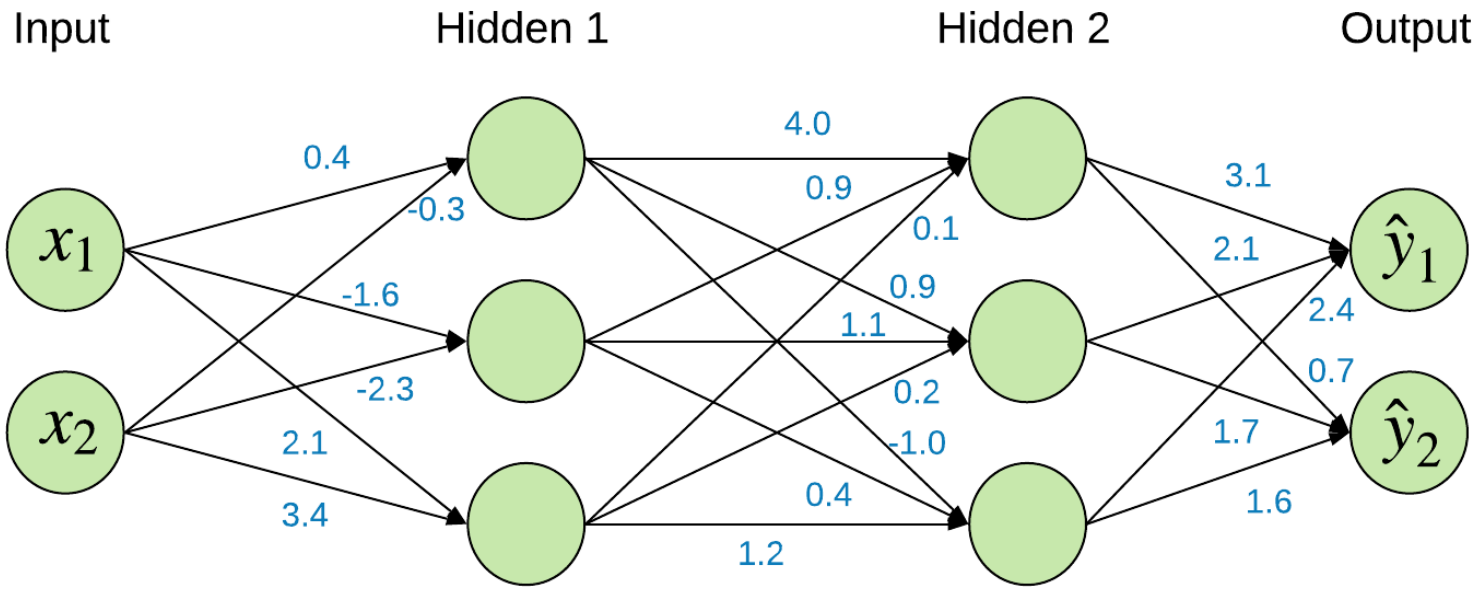


Deep neural networks (DNNs)

Given training data $(x_T, y_T) = \{x_n, y_n\}_{n=1}^N$, solve regression problem:

$$w^* = \underset{w}{\operatorname{argmin}} \left\{ \frac{1}{N} \sum_{n=1}^{N} \| f(x_n; w) - y_n \|_2^2 \right\}$$

- Popular algorithm: stochastic gradient descent [LeCun 12, Robbins 51]
- Gradient $\nabla_w f$ computed from chain rule (back-propagation)



Deep neural networks (DNNs)

However, after training, only single-valued predictions available:

$$\hat{y} = f(x; w^*)$$

- DNN does not offer uncertainty information to indicate the quality and credibility of output value
- We expect the prediction uncertainty to vary depending on:
  - architecture of the DNN
  - quantity, quality, and informativeness of the training data
  - input/operating regime, etc.

How much can we trust this DNN prediction?

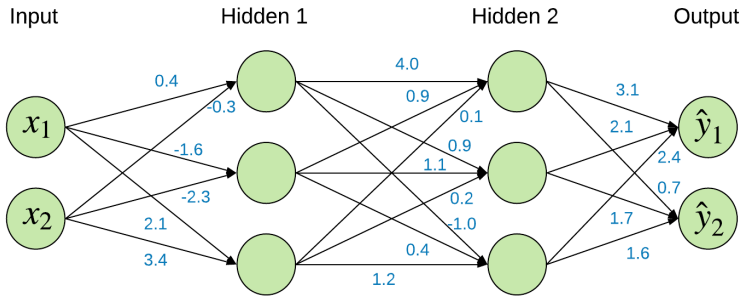
This question is crucial for mission- and safety-critical scenarios, and must be addressed before certifying and deploying ML-based technology

$\Rightarrow$ **need UQ for ML**

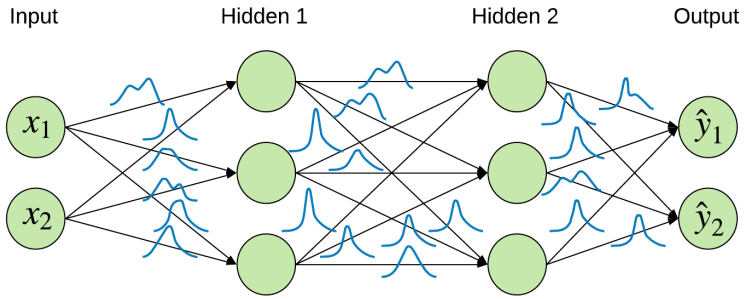
Bayesian neural networks (BNNs)

Bayesian neural networks (BNNs): treat w as random variables

[MacKay 92, Neal 96, Graves 11, Blundell 15, Gal 16]



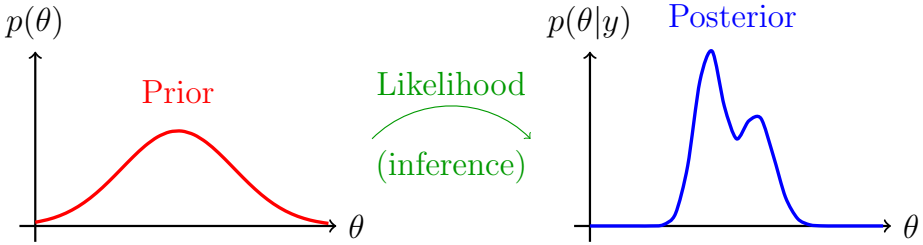
DNN



BNN

- w now has distribution of values
- $\hat{y} = f(x; w)$ then is also a distribution of predictions
  - $\Rightarrow$ uncertainty information for each prediction
- Update distribution of w from training data, via Bayes' theorem:

$$p(w|x_T, y_T) = \frac{p(y_T|x_T, w)p(w)}{p(y_T|x_T)}$$



Variational Bayesian inference

Major challenge: # of DNN weight parameters $\sim \mathcal{O}(\mathbf{10^3} - \mathbf{10^6}+)$:

- extremely high dimensional inference problem
- mainstream Markov chain Monte Carlo (MCMC) methods intractable

Variational inference (VI) more scalable:

- approximate posterior $p(w|x_T, y_T)$ with parametric family $q(w;\lambda)$
- e.g., mean-field (independent) 1D Gaussians

$$q(w;\lambda) = \prod_{k=1}^{K} q(w_k;\lambda_k) = \prod_{k=1}^{K} \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left[-\frac{(w_k-\mu_k)^2}{2{\sigma_k}^2}\right]$$

- find best approximation: inference problem $\rightarrow$ optimization

Variational Bayesian inference

Find best approximation by minimizing KL divergence:

$$\lambda^* = \underset{\lambda}{\operatorname{argmin}}\ D_{\mathrm{KL}}\left[q(w;\lambda) \parallel p(w|x_T, y_T)\right]$$

$$\approx \underset{\lambda}{\operatorname{argmin}} \left\{ \frac{1}{M} \sum_{m=1}^{M} \left[\log q\left(w^{(m)};\lambda\right) - \log p\left(y_T|x_T, w^{(m)}\right)\right] - \log p\left(w^{(m)}\right) \right\}$$

where $w^{(m)} \sim q(w;\lambda)$

- above known as the **evidence lower bound (ELBO)**
- for DNN, gradient available through chain rule
  $\rightarrow$ can use stochastic gradient descent

Results

Input: power spectral density of noise signal, discretized into 151 bins covering the frequency range 0–140 Hz

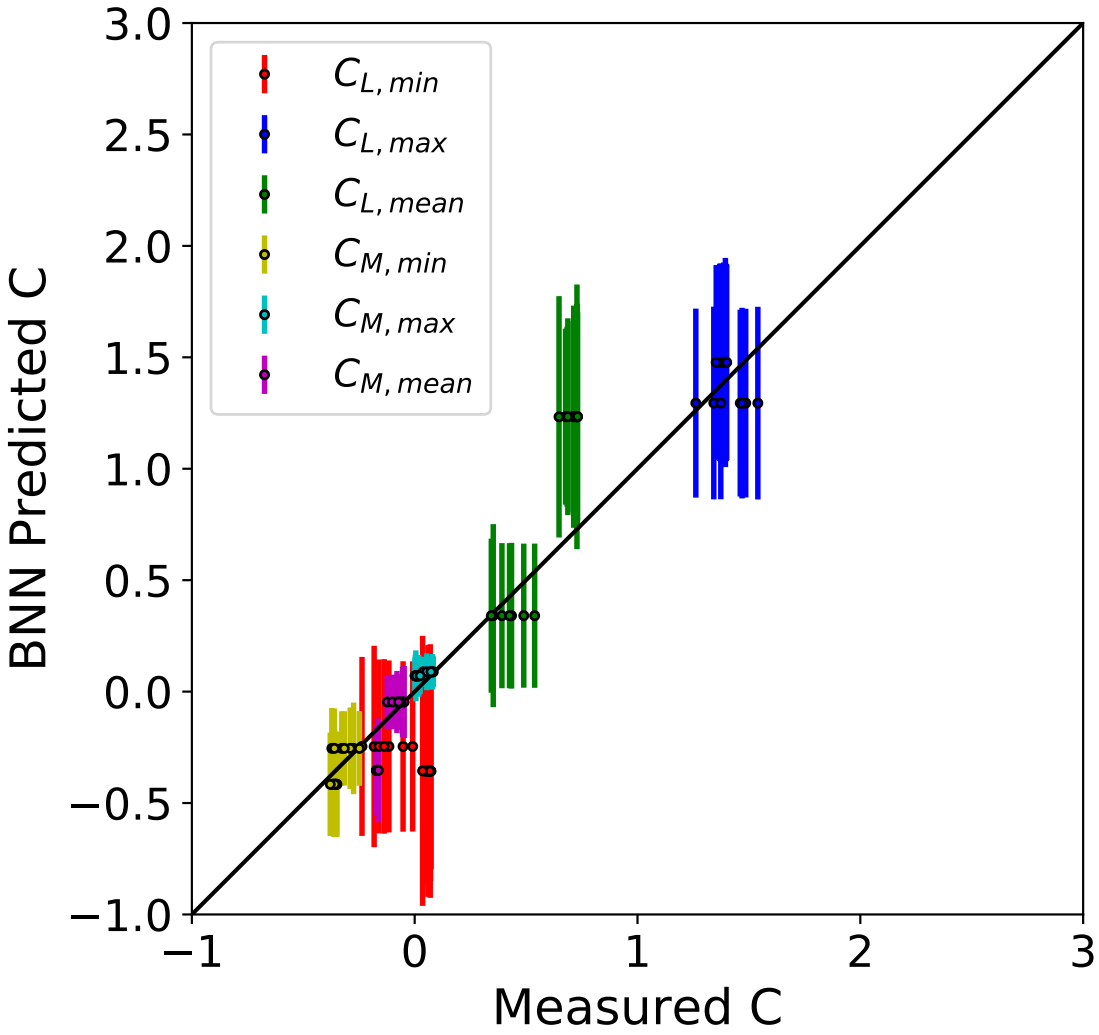
Output: minimum, maximum, and mean values of C_L and C_M

Layer	Name	No. of Neurons	Activation Fcn.
1	input	151	-
2	hidden 1	50	tanh
3	hidden 2	50	tanh
4	output	6	linear

- Total 10,456 weight parameters
- $M = 1000$ samples in computing ELBO
- ADAM optimizer [Kingma 15] (variant of stochastic gradient descent)
- Database: 101 CFD-CAA simulations available, trained on subsets

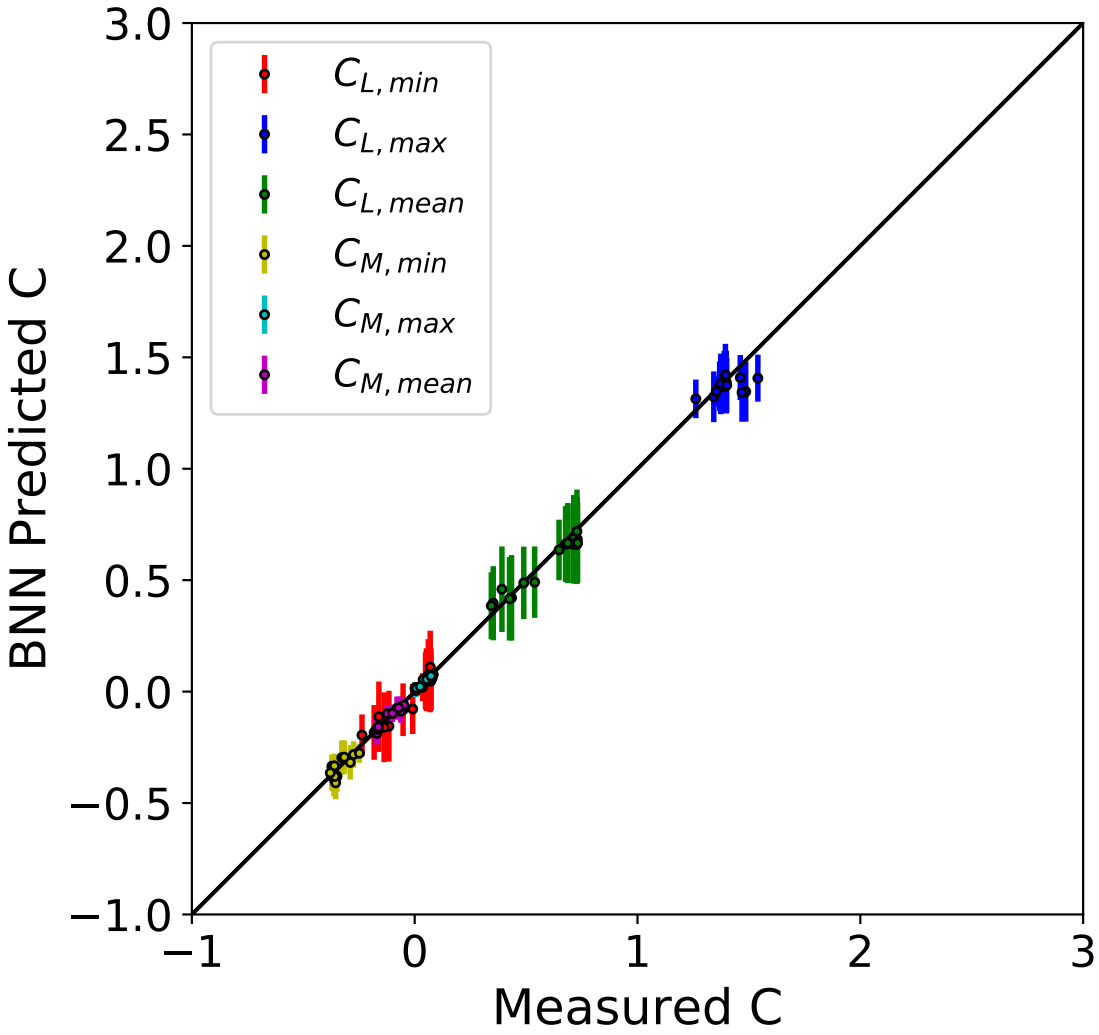
Predictive uncertainty intervals (all validation runs)

1 training datum



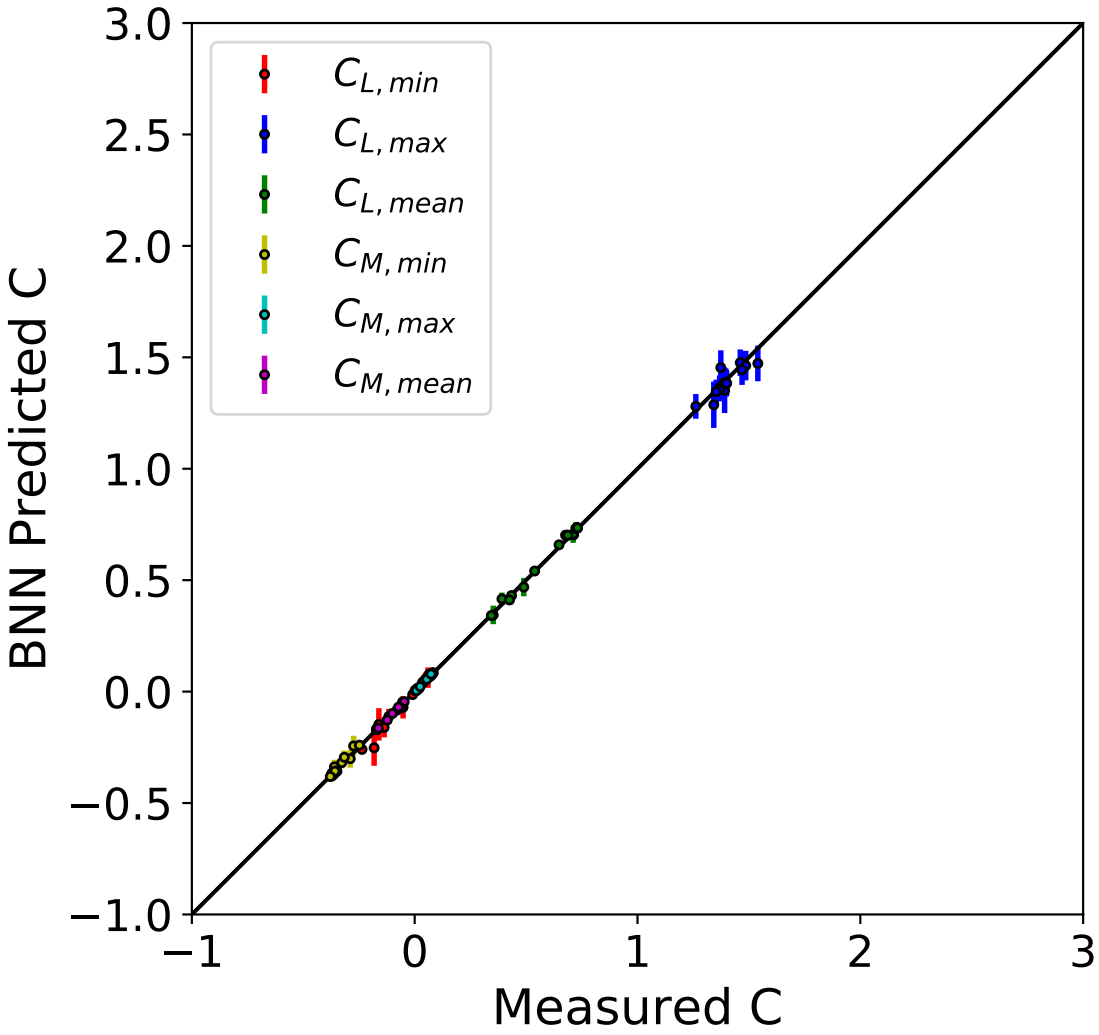
Predictive uncertainty intervals (all validation runs)

20 training data



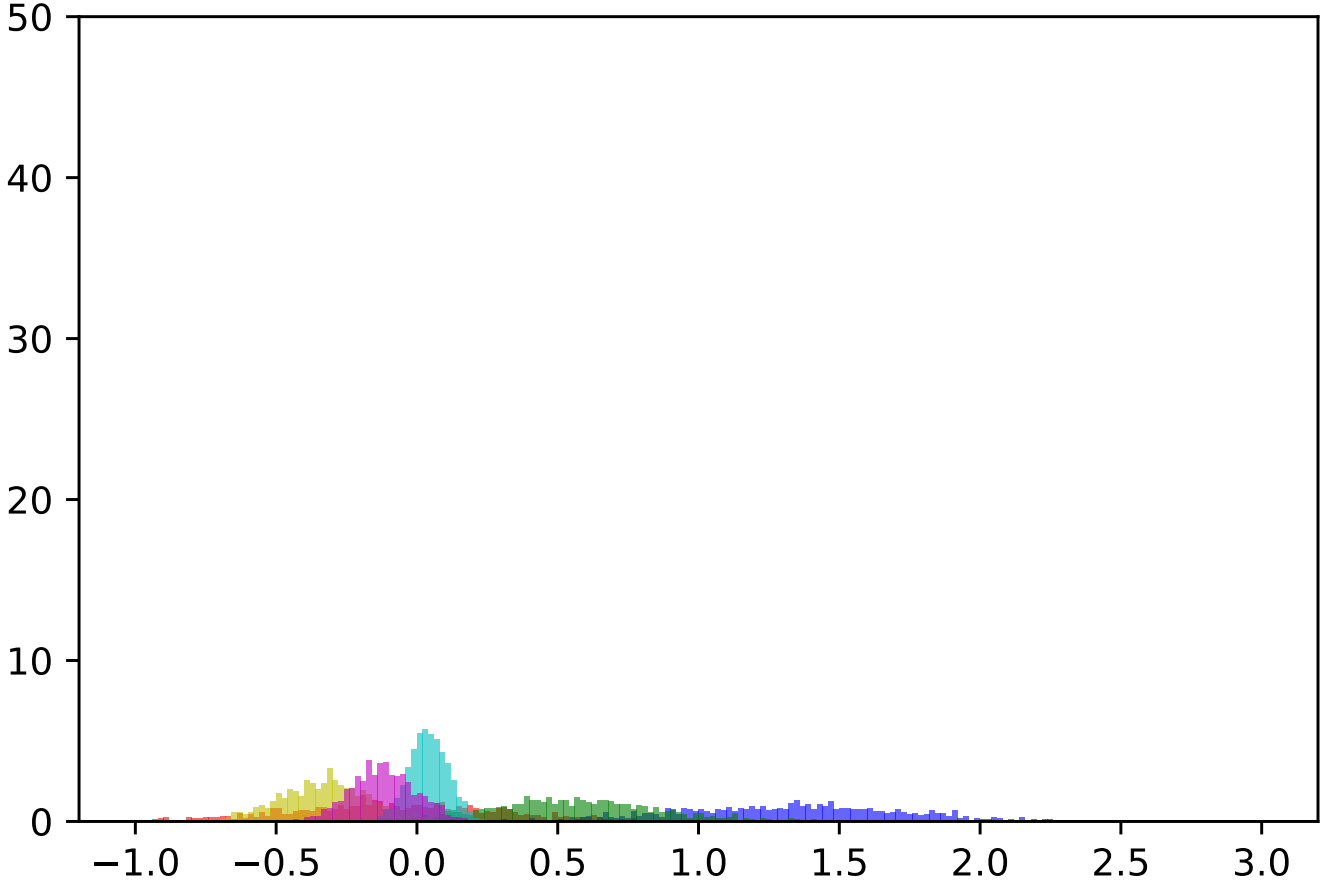
Predictive uncertainty intervals (all validation runs)

80 training data



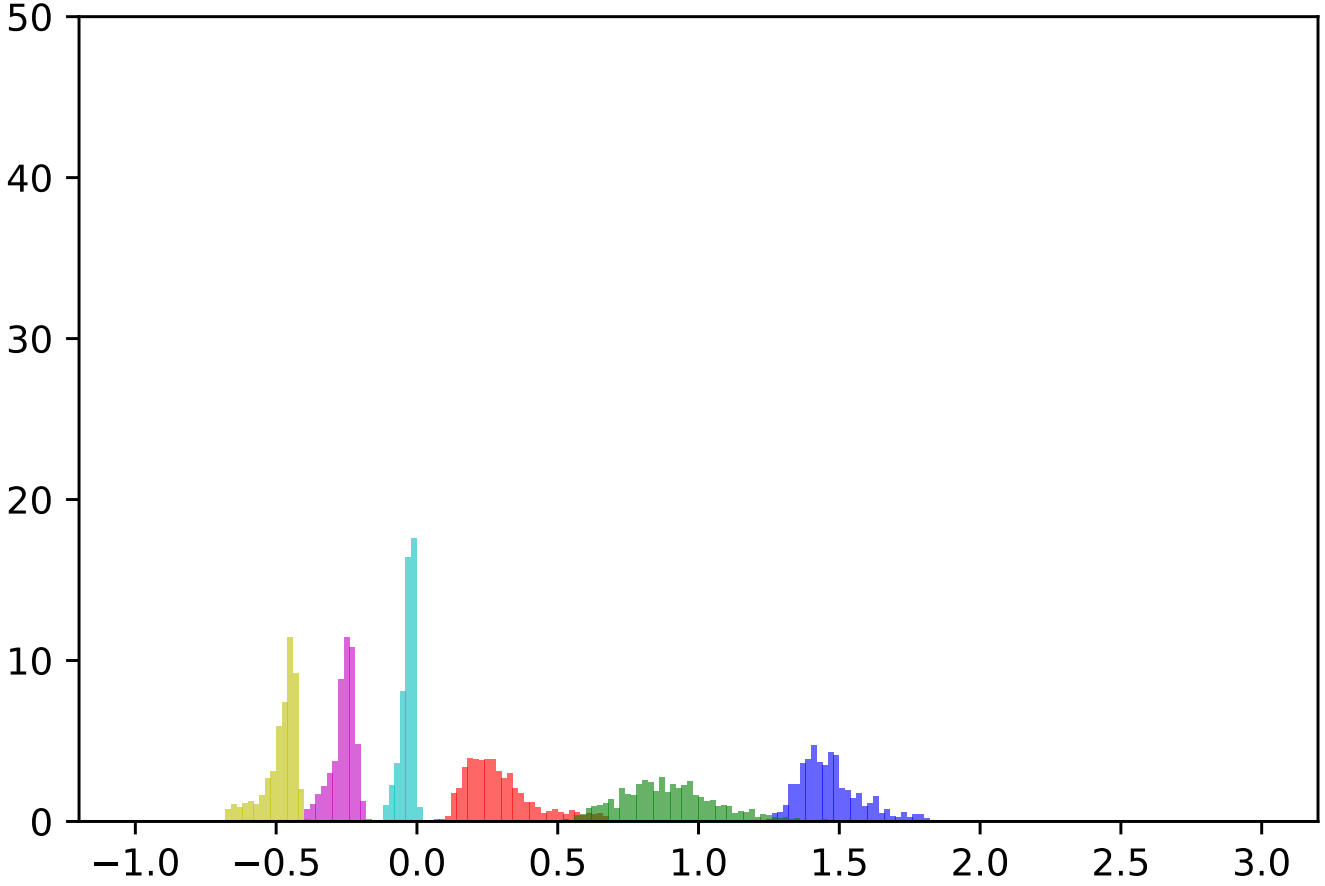
Predictive uncertainty distributions (specific runs)

1 training datum



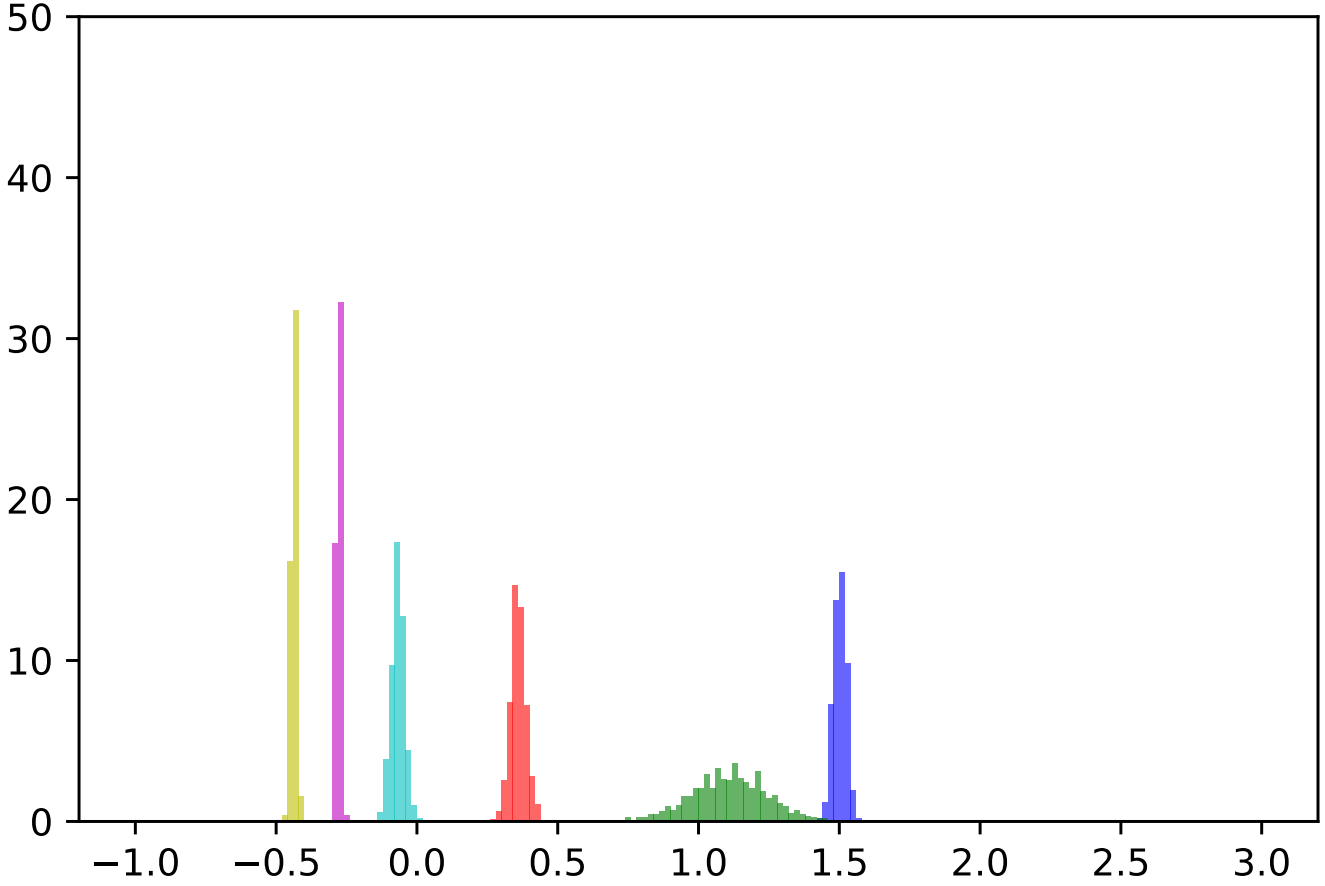
Predictive uncertainty distributions (specific runs)

20 training data



Predictive uncertainty distributions (specific runs)

80 training data



Timing and outlook

- Given noise signal input, perform 1000 DNN evaluations to generate these 6 prediction distributions: $\sim$ 3.8 ms (MacBook Pro)
- Positive outlook for meeting real-time detection requirements
- Plan to seek higher-fidelity simulations, and bigger databases
- Will investigate other ML architectures for feature detection, e.g.
  - recurrent neural network (RNN): suitable for time-dependent data
  - convolutional neural network (CNN): suitable for image-like signals

Outline

Motivation: stochastic noise generation

Collaboration with: **B. Y. Zhou, N. R. Gauger (TU-Kaiserslautern), J. Hauth, X. Huan (U-Michigan)**

Preliminary work (mainly formulation currently)

- Aircraft noise is important for design optimization
- High number of design variables motivates adjoint-based approaches
- Dilemma:
  - Scale-resolving simulations required for noise prediction, but adjoint diverges due to chaotic turbulent content [Blonigan 12]
  - Adjoint divergence benign in RANS, but noise generation suppressed

Approach: reconstruct turbulent fluctuations through **stochastic noise generation (SNG)** [Bechara 94, Bailly 99, Rossignol 13]

$$\vec{u}'(\vec{x},t) = 2\sum_{n=1}^{N_F} \hat{u}_n \cos\left[\vec{k}_n \cdot (\vec{x} - \vec{U}t) + \psi_n\right] \vec{\sigma}_n$$

where $\vec{k}_n$, ψ_n, $\vec{\sigma}_n$ randomly generated, and Fourier mode magnitudes are

$$\hat{u}_n = \sqrt{E(k_n, K, \epsilon)\Delta k_n}$$

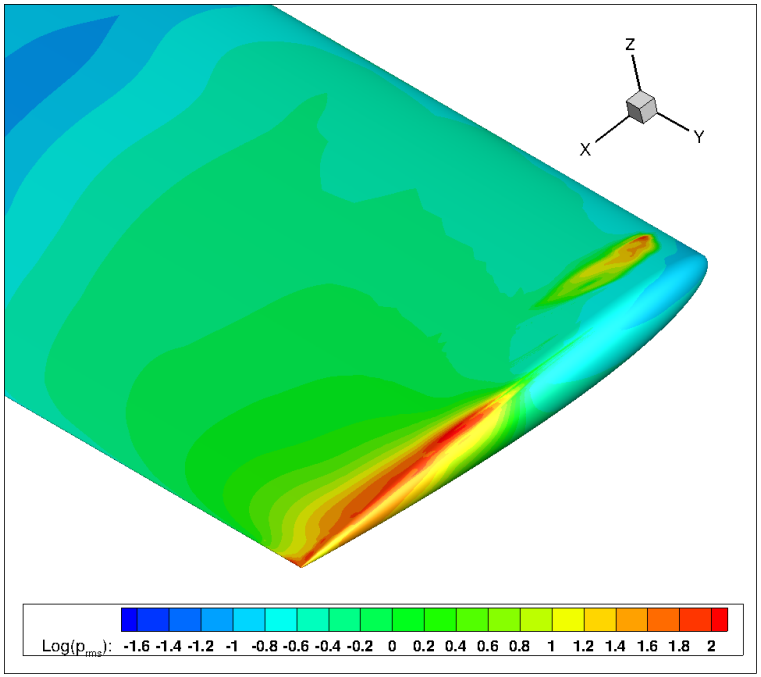
and K and ϵ are computed from RANS

Turbulence energy spectrum

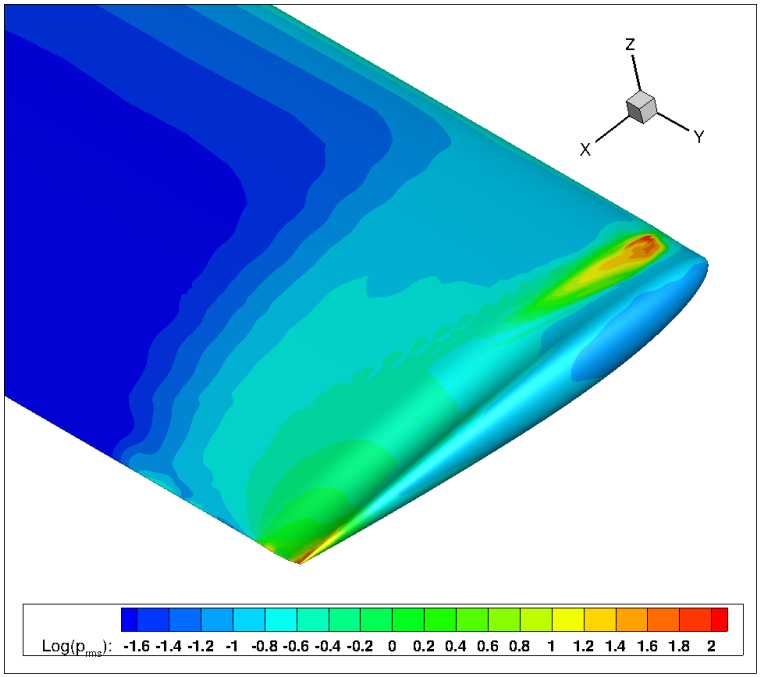
Turbulence energy spectrum generally adopts (isotropic) Von Kármán-Pao

$$E(k, K, \epsilon) = \frac{2A}{3}\frac{K}{k_e}\left(\frac{k}{k_e}\right)^4 \exp\left[-2\left(\frac{k}{k_\eta}\right)^2\right]\left[1+\left(\frac{k}{k_e}\right)^2\right]^{-\frac{17}{6}}$$

RANS-SNG: demonstrated design for noise reduction with weakly anisotropic cases [Zhou 19b] "Adjoint-based Broadband Noise Minimization using SNG", AIAA Paper 2019–2697



Baseline



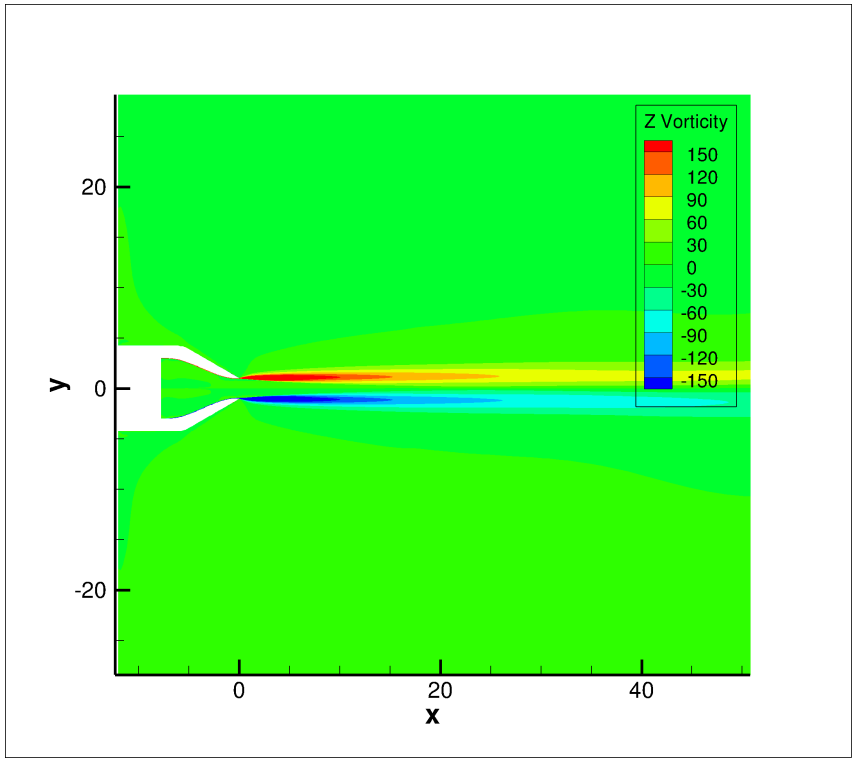
Optimized

Turbulence energy spectrum

Turbulence energy spectrum generally adopts (isotropic) Von Kármán-Pao

$$E(k, K, \epsilon) = \frac{2A}{3}\frac{K}{k_e}\left(\frac{k}{k_e}\right)^4 \exp\left[-2\left(\frac{k}{k_\eta}\right)^2\right]\left[1+\left(\frac{k}{k_e}\right)^2\right]^{-\frac{17}{6}}$$

. . . however, isotropic assumption may not hold in scenarios with strong shear layers (e.g., jet flow in NASA Acoustic Research Nozzle 2)



Turbulence energy spectrum

Machine learning (data-driven) idea:

- learn scenario-specififc energy spectrum $E_{\mathrm{DNN}}(k, K, \epsilon)$ from relevant (and low number of) LES run(s), then use it in RANS-SNG
- e.g., construct $E_{\mathrm{DNN}}(k, K, \epsilon)$ by minimizing loss function

$$\min_{\theta} \| E_{\mathrm{LES}}(k, K, \epsilon) - E_{\mathrm{DNN}}(k, K, \epsilon; \theta) \|_2^2$$

- lots of data points from a single LES run (each $\vec{x}$ can provide a $E_{\mathrm{LES}}(k, K, \epsilon)$ datum)
- ongoing work: plan to start with feed-forward DNN
- hypothesis: hybrid isotropic-DNN form may provide more accurate representations (combining physics with ML)

Outline

Summary

- Enabled tractable computation of optimal experimental designs targeting nonlinear and computationally intensive models
- Demonstrated design of combustion experiments for learning kinetic parameters, sensor placement for source inversion
- Advanced towards real-time in-flight rotorcraft icing detection using aeroacoustic computations
- Constructed Bayesian neural network machine learning models that achieve rapid online predictions with uncertainty information
- Presented plans for data-driven ML modeling of turbulence energy spectrum to improve RANS-SNG under anisotropic turbulence

Acknowledgment

- NIA, NASA Langley, Boris Diskin, Hiroaki Nishikawa
- Collaborators: Jeremiah Hauth, Beckett Zhou, Nicolas Gauger, Myles Morelli, Alberto Guardone, Youssef Marzouk, Wanggang Shen, Cosmin Safta, Khachik Sargsyan, Gianluca Geraci, Mike Eldred, Roger Ghanem, Habib Najm
- Defense Advanced Research Projects Agency (DARPA) Artificial Intelligence Research Associate (AIRA) Program (X. Huan)
- Computing resources provided by the "Alliance of High Performance Computing Rheinland-Pfalz" (AHRP), via the "Elwetritsch" Cluster at the TU Kaiserslautern (collaborators B. Zhou and N. Gauger)
- EU H2020 Funding and Marie Skodowska-Curie Grant (collaborators M. Morelli and A. Guardone)

Thank You!

References I

Alen Alexanderian, Noemi Petra, Georg Stadler & Omar Ghattas.
A Fast and Scalable Method for A-Optimal Design of Experiments for Infinite-dimensional Bayesian Nonlinear Inverse Problems.
SIAM Journal on Scientific Computing, vol. 38, no. 1, pages A243–A272, 2016.

Billy Amzal, Frédéric Y. Bois, Eric Parent & Christian P. Robert.
Bayesian-Optimal Design via Interacting Particle Systems.
Journal of the American Statistical Association, vol. 101, no. 474, pages 773–785, 2006.

Anthony C. Atkinson, Alexander N. Donev & R. D. Tobias.
Optimum Experimental Designs, With SAS.
Oxford University Press, New York, NY, 2007.

Christophe Bailly & Daniel Juve.
A Stochastic Approach To Compute Subsonic Noise Using Linearized Euler's Equations.
In 5th AIAA/CEAS Aeroacoustics Conference and Exhibit, numéro 1999-1872, Bellevue, WA, 1999.

Volker Barthelmann, Erich Novak & Klaus Ritter.
High dimensional polynomial interpolation on sparse grids.
Advances in Computational Mathematics, vol. 12, pages 273–288, 2000.

Walid Bechara, Christophe Bailly, Philippe Lafon & Sebastien M. Candel.
Stochastic Approach to Noise Modeling for Free Turbulent Flows.
AIAA Journal, vol. 32, no. 3, pages 455–463, mar 1994.

Joakim Beck, Ben Mansour Dia, Luis F. R. Espath, Quan Long & Raúl Tempone.
Fast Bayesian experimental design: Laplace-based importance sampling for the expected information gain.
Computer Methods in Applied Mechanics and Engineering, vol. 334, pages 523–553, 2018.

References II

James O. Berger.
Statistical Decision Theory and Bayesian Analysis.
Springer New York, New York, NY, 1985.

P. J. Blonigan, R. Chen, Q. Wang & J. Larsson.
Towards adjoint sensitivity analysis of statistics in turbulent flow simulation.
Rapport technique, 2012.

Charles Blundell, Julien Cornebise, Koray Kavukcuoglu & Daan Wierstra.
Weight Uncertainty in Neural Networks.
In Proceedings of the 32nd International Conference on Machine Learning, volume 37, pages 1613–1622, 2015.

George Edward Pelham Box & H. L. Lucas.
Design of Experiments in Non-Linear Situations.
Biometrika, vol. 46, no. 1-2, pages 77–90, 1959.

George Edward Pelham Box & Norman Richard Draper.
Empirical Model-Building and Response Surfaces.
John Wiley & Sons, Inc., Hoboken, NJ, 1987.

George Edward Pelham Box, J. Stuart Hunter & William G. Hunter.
Statistics for Experimenters: Design, Innovation and Discovery.
John Wiley & Sons, Inc., Hoboken, NJ, 2nd edition, 2005.

Kathryn Chaloner & Isabella Verdinelli.
Bayesian Experimental Design: A Review.
Statistical Science, vol. 10, no. 3, pages 273–304, 1995.

References III

Merlise A. Clyde, Peter Müller & Giovanni Parmigiani.
Exploring Expected Utility Surfaces by Markov Chains.
Rapport technique, Duke University, 1996.

Paul G. Constantine, M. Emory, J. Larsson & G. Iaccarino.
Exploiting active subspaces to quantify uncertainty in the numerical simulation of the HyShot II scramjet.
Journal of Computational Physics, vol. 302, pages 1–20, 2015.

D. R. Cox & N. Reid.
The Theory of the Design of Experiments.
Chapman & Hall/CRC, Boca Raton, FL, 2000.

Douglas J. Dolvin.
Hypersonic International Flight Research and Experimentation (HIFiRE).
In 15th AIAA International Space Planes and Hypersonic Systems and Technologies Conference, numéro 2008-2581, Dayton, OH, 2008.

Douglas J. Dolvin.
Hypersonic International Flight Research and Experimentation.
In 16th AIAA/DLR/DGLR International Space Planes and Hypersonic Systems and Technologies Conference, numéro 2009-7228, Bremen, Germany, 2009.

V. V. Fedorov.
Theory of Optimal Experiments.
Academic Press, New York, NY, 1972.

Paul G. Ferlemann.
Forebody and Inlet Design for the HIFiRE 2 Flight Test.
In JANNAF Airbreathing Propulsion Subcommittee Meeting, Boston, MA, 2008.

References IV

Ronald Aylmer Fisher.
The Design of Experiments.
Oliver & Boyd, Edinburgh, United Kingdom, 1935.

Ian Ford, D. M. Titterington & Christos P. Kitsos.
Recent Advances in Nonlinear Experimental Design.
Technometrics, vol. 31, no. 1, pages 49–60, 1989.

Yarin Gal.
Uncertainty in Deep Learning.
PhD thesis, University of Cambridge, 2016.

Gianluca Geraci, Friedrich Menhorn, Xun Huan, Cosmin Safta, Youssef Marzouk, Habib N. Najm & Michael S. Eldred.
Progress in Scramjet Design Optimization Under Uncertainty Using Simulations of the HIFiRE Direct Connect Rig.
In AIAA Scitech 2019 Forum, numéro 2019-0725, 2019.

Thomas Gerstner & Michael Griebel.
Numerical integration using sparse grids.
Numerical Algorithms, vol. 18, pages 209–232, 1998.

T. Gerstner & M. Griebel.
Dimension-Adaptive Tensor-Product Quadrature.
Computing, vol. 71, no. 1, pages 65–87, 2003.

Roger G. Ghanem & Pol D. Spanos.
Stochastic Finite Elements: A Spectral Approach.
Springer New York, New York, NY, 1st edition, 1991.

References V

Alex Graves.
Practical Variational Inference for Neural Networks.
In Advances in Neural Information Processing Systems 24 (NIPS 2011), pages 2348–2356, Granada, Spain, 2011.

Mark R. Gruber, Kevin Jackson & Jiwen Liu.
Hydrocarbon-Fueled Scramjet Combustor Flowpath Development for Mach 6-8 HIFiRE Flight Experiments.
Rapport technique, AFRL, 2008.

Mark R. Gruber, Paul G. Ferlemann & Keith McDaniel.
HIFiRE Flight 2 Flowpath Design Update.
Rapport technique, AFRL, 2009.

Xun Huan & Youssef M. Marzouk.
Simulation-based optimal Bayesian experimental design for nonlinear systems.
Journal of Computational Physics, vol. 232, no. 1, pages 288–317, 2013.

Xun Huan & Youssef M. Marzouk.
Gradient-Based Stochastic Optimization Methods in Bayesian Experimental Design.
International Journal for Uncertainty Quantification, vol. 4, no. 6, pages 479–510, 2014.

Xun Huan & Youssef M. Marzouk.
Sequential Bayesian optimal experimental design via approximate dynamic programming.
arXiv preprint arXiv:1604.08320, 2016.

Xun Huan, Cosmin Safta, Khachik Sargsyan, Gianluca Geraci, Michael S. Eldred, Zachary P. Vane, Guilhem Lacaze, Joseph C. Oefelein & Habib N. Najm.
Global Sensitivity Analysis and Estimation of Model Error, Toward Uncertainty Quantification in Scramjet Computations.
AIAA Journal, vol. 56, no. 3, pages 1170–1184, 2018.

References VI

Xun Huan, Cosmin Safta, Khachik Sargsyan, Zachary P. Vane, Guilhem Lacaze, Joseph C. Oefelein & Habib N. Najm.
Compressive Sensing with Cross-Validation and Stop-Sampling for Sparse Polynomial Chaos Expansions.
SIAM/ASA Journal on Uncertainty Quantification, vol. 6, no. 2, pages 907–936, 2018.

Kevin R Jackson, Mark R Gruber & Salvatore Buccellato.
HIFiRE Flight 2 Overview and Status Update 2011.
In 17th AIAA International Space Planes and Hypersonic Systems and Technologies Conference, numéro 2011-2202, San Francisco, CA, 2011.

Diederik P. Kingma & Jimmy Ba.
Adam: A Method for Stochastic Optimization.
In 3rd International Conference on Learning Representations, {ICLR} 2015, San Diego, CA, 2015.

Guilhem Lacaze, Zachary P. Vane & Joseph C. Oefelein.
Large Eddy Simulation of the HIFiRE Direct Connect Rig Scramjet Combustor.
In 55th AIAA Aerospace Sciences Meeting, numéro 2017-0142, Grapevine, TX, 2017.

Yann A. LeCun, Léon Bottou, Genevieve B. Orr & Klaus-Robert Müller.
Efficient BackProp.
In Grégoire Montavon, Geneviève B. Orr & Klaus-Robert Müller, editeurs, Neural Networks: Tricks of the Trade, pages 9–48. Springer-Verlag Berlin Heidelberg, 2012.

Dennis V. Lindley.
On a Measure of the Information Provided by an Experiment.
The Annals of Mathematical Statistics, vol. 27, no. 4, pages 986–1005, 1956.

Quan Long, Marco Scavino, Raúl Tempone & Suojin Wang.
A Laplace method for under-determined Bayesian optimal experimental designs.
Computer Methods in Applied Mechanics and Engineering, vol. 285, pages 849–876, 2015.

References VII

David J. C. MacKay.
A Practical Bayesian Framework for Backpropagation Networks.
Neural Computation, vol. 4, no. 3, pages 448–472, 1992.

Youssef M. Marzouk & Habib N. Najm.
Dimensionality reduction and polynomial chaos acceleration of Bayesian inference in inverse problems.
Journal of Computational Physics, vol. 228, no. 6, pages 1862–1902, 2009.

Peter Müller, Bruno Sansó & Maria De Iorio.
Optimal Bayesian Design by Inhomogeneous Markov Chain Simulation.
Journal of the American Statistical Association, vol. 99, no. 467, pages 788–798, 2004.

Peter Müller.
Simulation Based Optimal Design.
Handbook of Statistics, vol. 25, pages 509–518, 2005.

Habib N. Najm.
Uncertainty Quantification and Polynomial Chaos Techniques in Computational Fluid Dynamics.
Annual Review of Fluid Mechanics, vol. 41, pages 35–52, 2009.

Radford M. Neal.
Bayesian Learning for Neural Networks.
Springer-Verlag New York, New York, NY, 1996.

Joseph C. Oefelein.
Large eddy simulation of turbulent combustion processes in propulsion and power systems.
Progress in Aerospace Sciences, vol. 42, no. 1, pages 2–37, 2006.

References VIII

Joseph C. Oefelein, Vaidyanathan Sankaran & Tomasz G. Drozda.
Large eddy simulation of swirling particle-laden flow in a model axisymmetric combustor.
Proceedings of the Combustion Institute, vol. 31, pages 2291–2299, 2007.

Giovanni Parmigiani & Lurdes Y. T. Inoue.
Decision Theory: Principles and Approaches.
John Wiley & Sons, Inc., West Sussex, United Kingdom, 2009.

Herbert Robbins & Sutton Monro.
A Stochastic Approximation Method.
The Annals of Mathematical Statistics, vol. 22, no. 3, pages 400–407, 1951.

Karl-Stephane Stéphane Rossignol.
Flow Field Measurements to Characterize Flap Side-Edge Noise Generation.
In 19th AIAA/CEAS Aeroacoustics Conference, numéro 2013-2061, Berlin, Germany, 2013.

Kenneth J. Ryan.
Estimating Expected Information Gains for Experimental Designs With Application to the Random Fatigue-Limit Model.
Journal of Computational and Graphical Statistics, vol. 12, no. 3, pages 585–603, 2003.

Elizabeth G. Ryan, Christopher C. Drovandi, James M. Mcgree & Anthony N. Pettitt.
A Review of Modern Computational Algorithms for Bayesian Optimal Design.
International Statistical Review, vol. 84, no. 1, pages 128–154, 2016.

Thomas J. Santner, Brian J. Williams & William I. Notz.
The Design and Analysis of Computer Experiments.
Springer New York, New York, NY, 2nd edition, 2018.

References IX

Khachik Sargsyan, Xun Huan & Habib N. Najm.
Embedded Model Error Representation for Bayesian Model Calibration.
International Journal for Uncertainty Quantification, 2019.

Panagiotis Tsilifis, Roger G. Ghanem & Paris Hajali.
Efficient Bayesian Experimentation Using an Expected Information Gain Lower Bound.
SIAM/ASA Journal on Uncertainty Quantification, vol. 5, no. 1, pages 30–62, 2017.

Brian P. Weaver, Brian J. Williams, Christine M. Anderson-Cook & David M. Higdon.
Computational Enhancements to Bayesian Design of Experiments Using Gaussian Processes.
Bayesian Analysis, vol. 11, no. 1, pages 191–213, 2016.

Jeroen Witteveen, Karthik Duraisamy & Gianluca Iaccarino.
Uncertainty Quantification and Error Estimation in Scramjet Simulation.
In 17th AIAA International Space Planes and Hypersonic Systems and Technologies Conference, numéro 2011-2283, San Francisco, CA, 2011.

Dongbin Xiu & George Em Karniadakis.
The Wiener-Askey Polynomial Chaos for Stochastic Differential Equations.
SIAM Journal on Scientific Computing, vol. 24, no. 2, pages 619–644, 2002.

R. A. Yetter, F. L. Dryer & H. Rabitz.
A Comprehensive Reaction Mechanism For Carbon Monoxide/Hydrogen/Oxygen Kinetics.
Combustion Science and Technology, vol. 79, no. 1-3, pages 97–128, 1991.

Beckett Yx Zhou, Tim A. Albring, Nicolas R. Gauger, Thomas D. Economon, Francisco Palacios & Juan J. Alonso.
A Discrete Adjoint Framework for Unsteady Aerodynamic and Aeroacoustic Optimization.
In 16th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, numéro 2015-3355, 2015.

References X

Beckett Y. Zhou, Nicolas R. Gauger, M. Morelli, A. Guardone, J. Hauth & X. Huan.
Towards a Real-Time In-Flight Ice Detection System via Computational Aeroacoustics and Bayesian Neural Networks.
In AIAA/ISSMO Multidisciplinary Analysis and Optimization at the AVIATION Forum, numéro 2019-3103, Dallas, TX, 2019.

Beckett Yx Zhou, Nicolas R. Gauger, Huadong Yao, Shia-Hui Peng & Lars Davidson.
Adjoint-based Broadband Noise Minimization using Stochastic Noise Generation.
In 25th AIAA/CEAS Aeroacoustics Conference, numéro 2697, Delft, The Netherlands, 2019.