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A brief survey of uncertainty quantification

Teresa Portone

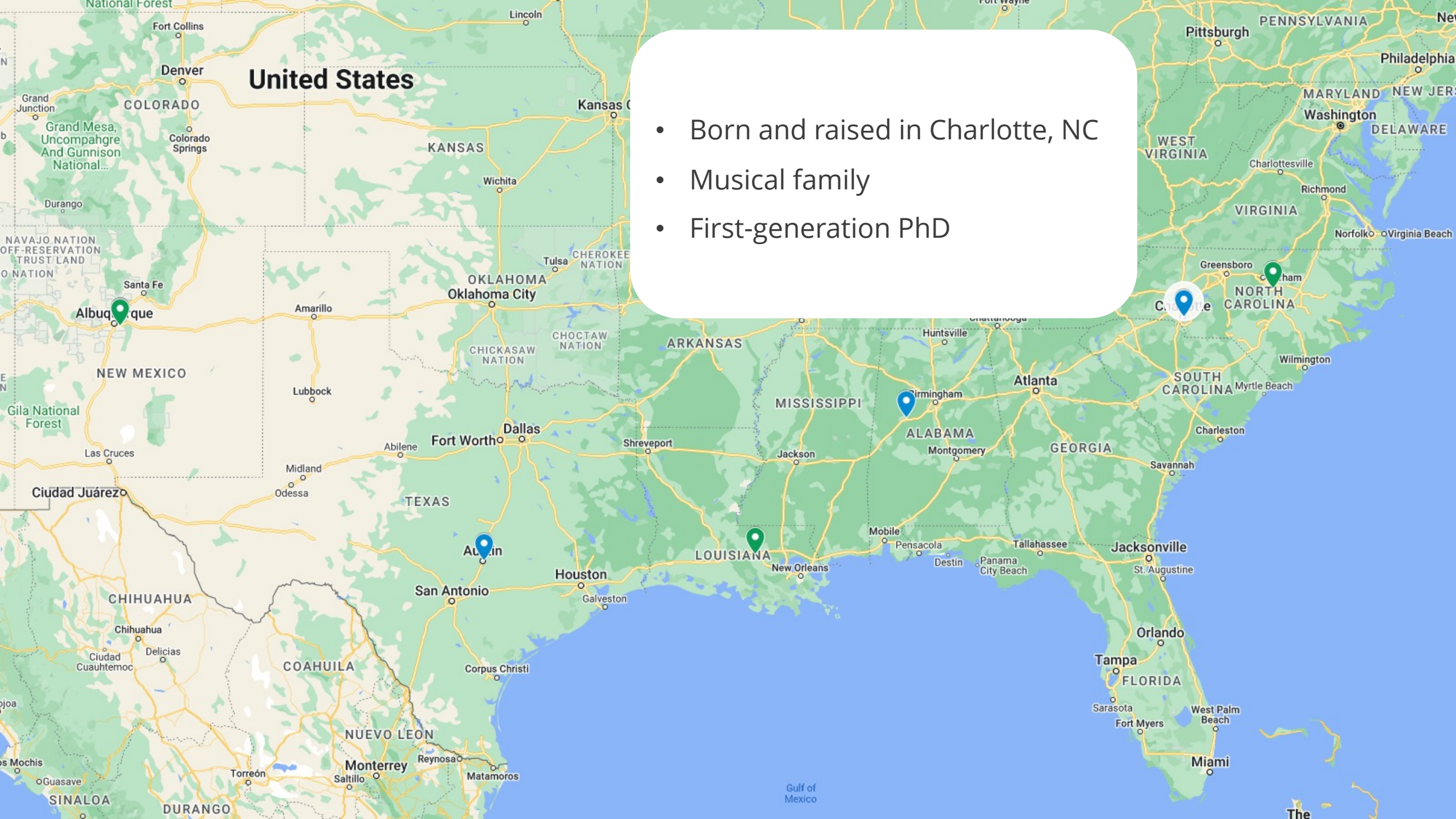
November 1, 2022

University of Alabama Mathematics Colloquium



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SAND2022-15190 PE



United States

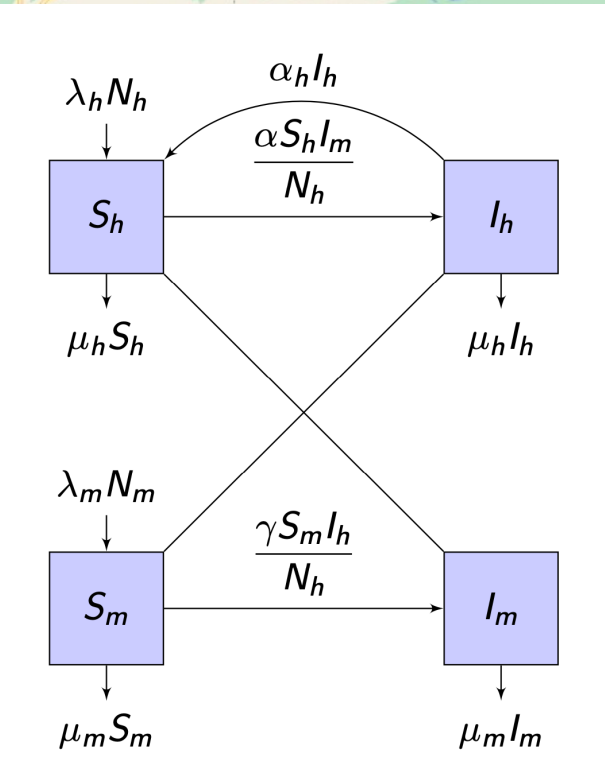
- Born and raised in Charlotte, NC
- Musical family
- First-generation PhD

United States

- Numerical Linear Algebra
- Theory of Probability
- Real Analysis I/II
- Mathematical Statistics
- Numerical Analysis
- Complex Calculus

- Major: Math, numerical track
- Minor: Italian, (almost) photography





- VIGRE, Summer 2011
- Mathematical epidemiology project (Malaria)

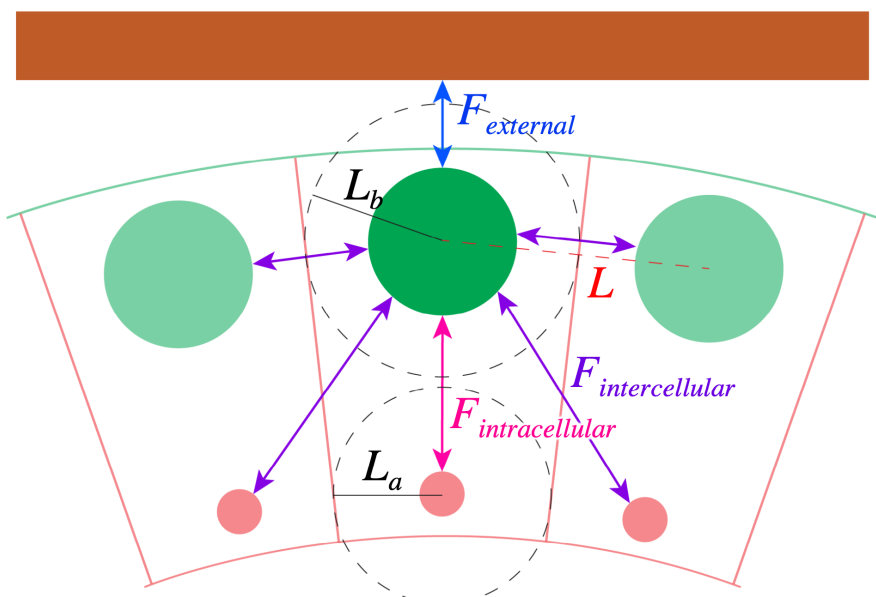
LSU



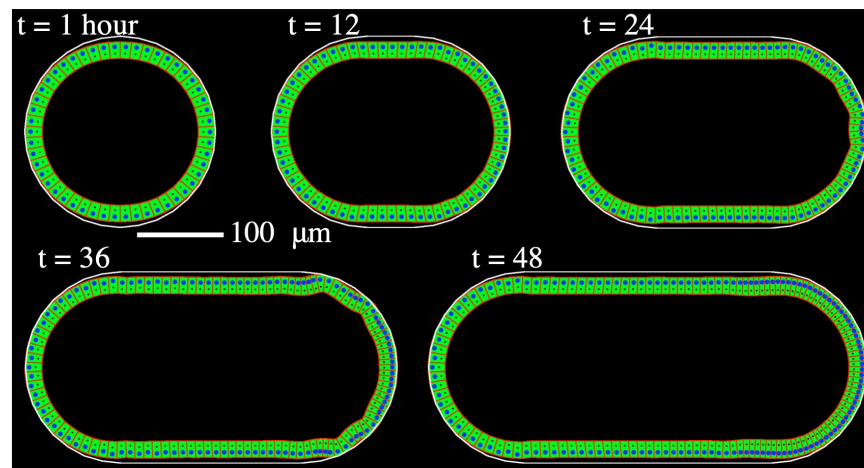
Image by Teresa Portone

United States

- REU, Summer 2012
- Numerical model for embryonic tube formation



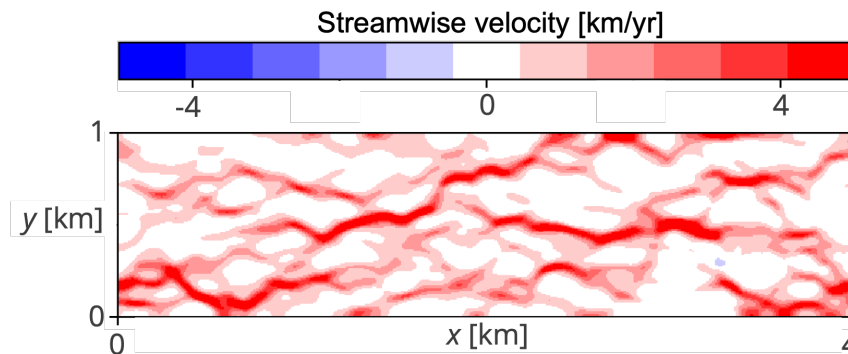
**NC STATE
UNIVERSITY**



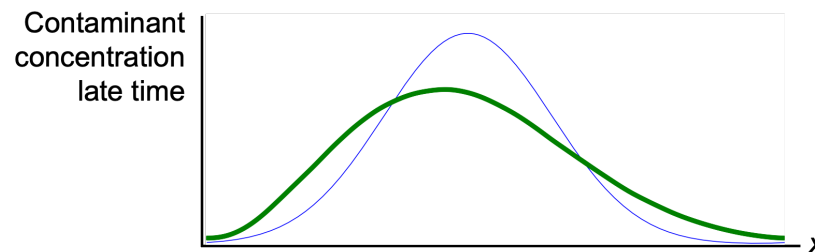
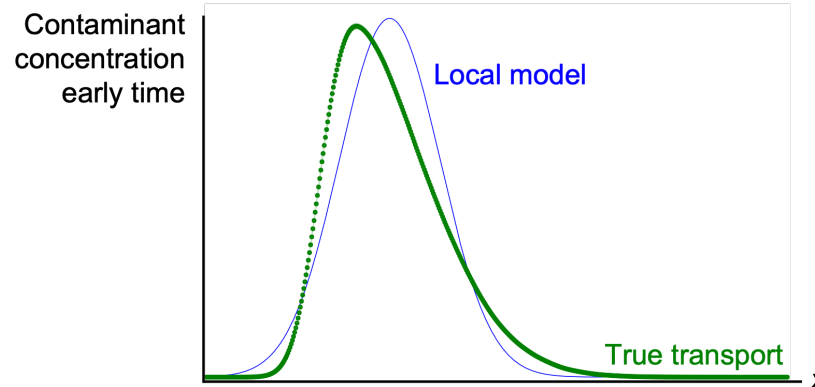
United States

- PhD Computational Science, Engineering, and Mathematics
- Thesis "Representing Model-Form Uncertainty from Missing Microstructural Information"

High-velocity "streaks" cause nonlocality in contaminant transport.



Traditional upscaled models ignore nonlocality.



The University of Texas at Austin
Oden Institute for Computational
Engineering and Sciences

United States

- Optimization and Uncertainty Quantification department
 - Interned Fall 2017
 - Joined as staff January 2020

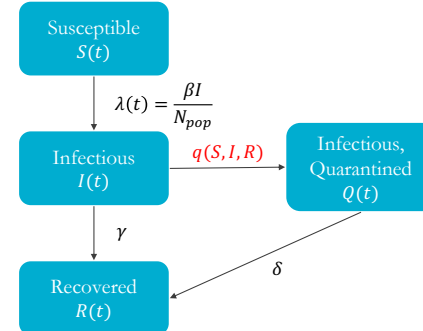


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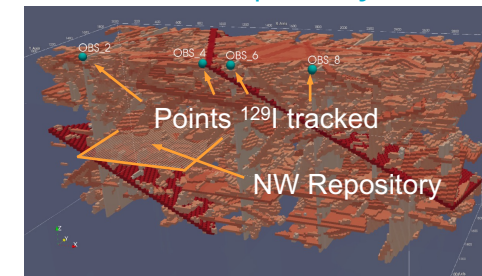
Metal yield modeling under impact



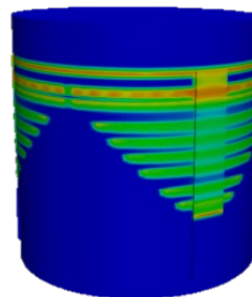
Disease modeling



Nuclear waste repository modeling



Thermally activated battery modeling

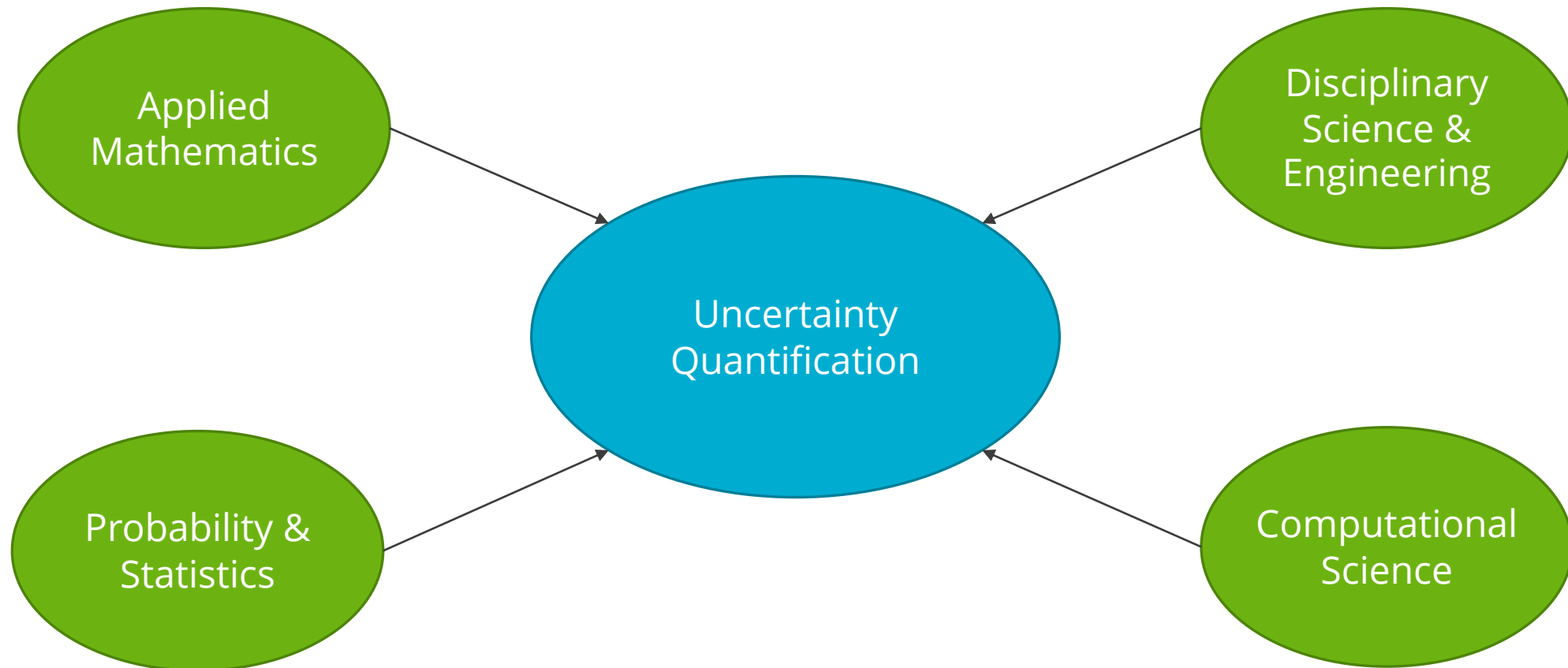


What is uncertainty quantification (UQ)?



My definition:

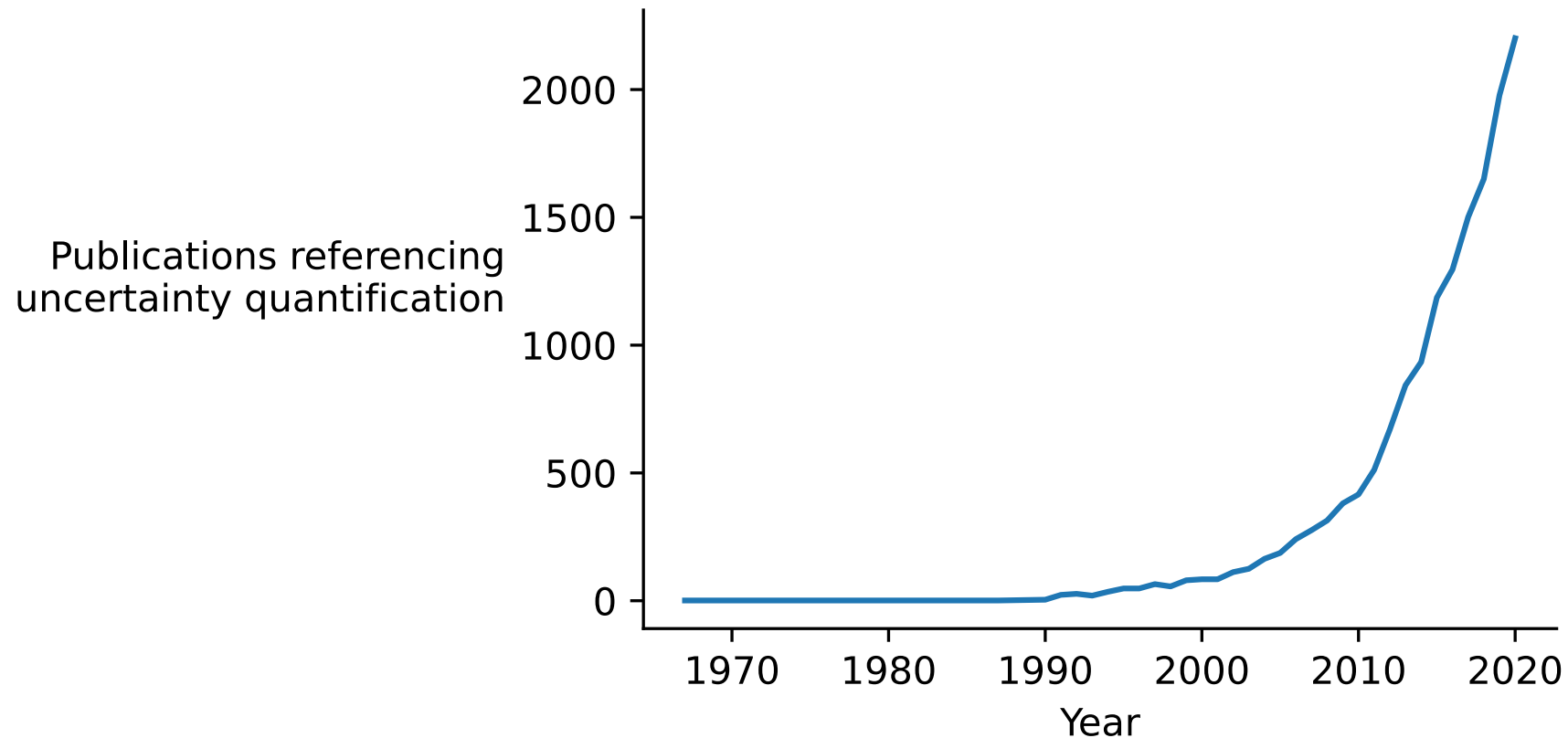
The science of characterizing, quantifying, and reducing uncertainties in mathematical models.



UQ has taken off in the last couple decades



“Uncertainty quantification is both a new field and one that is as old as the disciplines of probability and statistics.” (Smith 2013) [1]



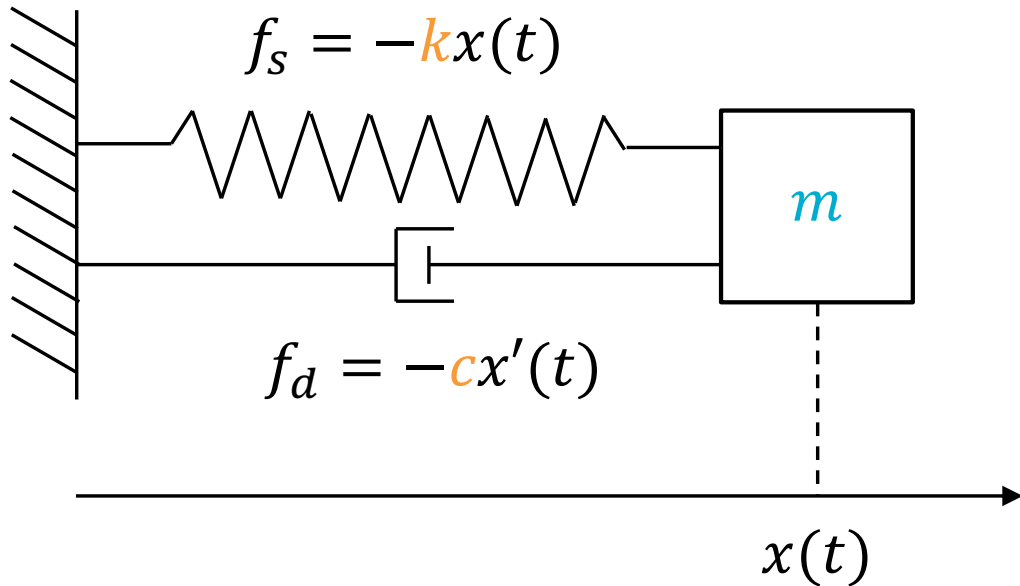
What is uncertainty?

Inability to assign an exact value to a modeled quantity.

How does uncertainty arise?

Intrinsic variability in a modeled quantity

Lack of precise knowledge of a modeled quantity

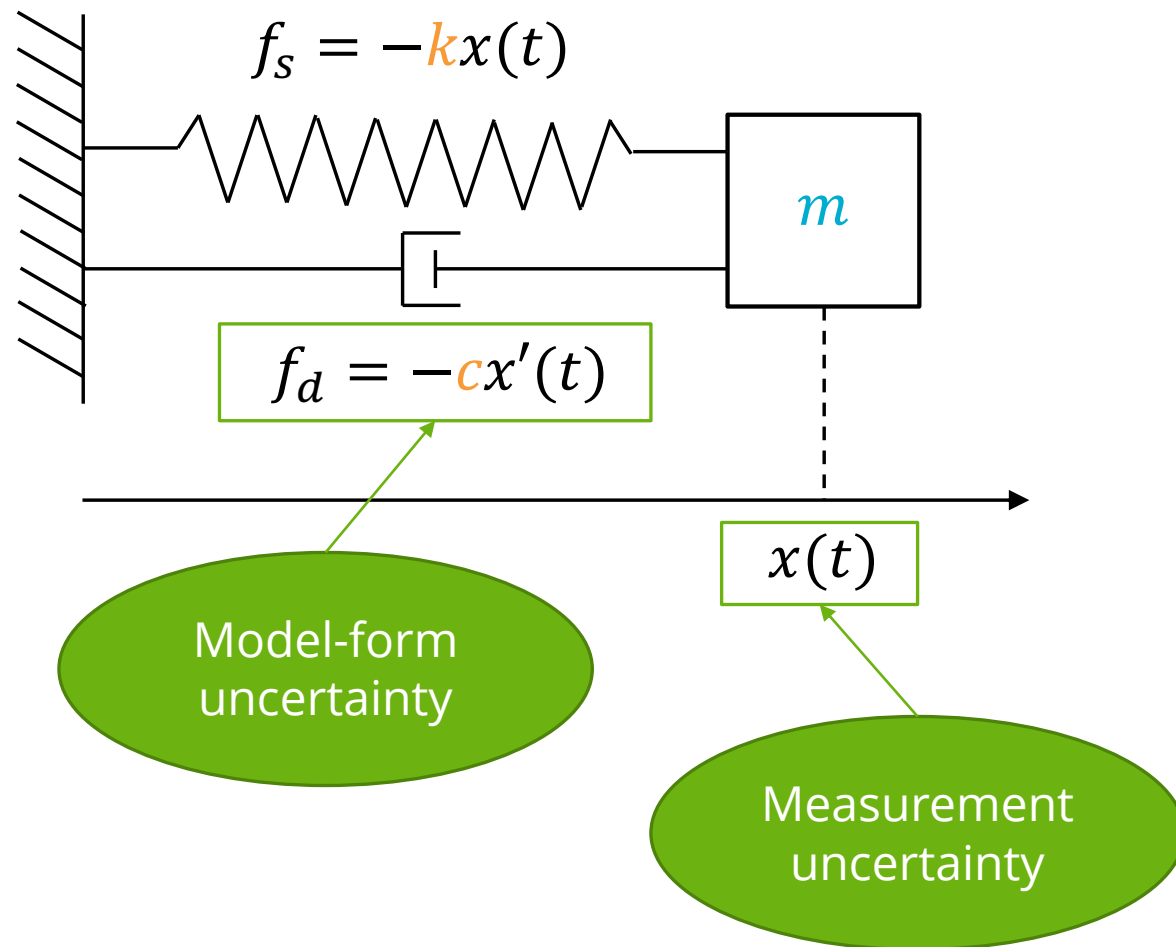
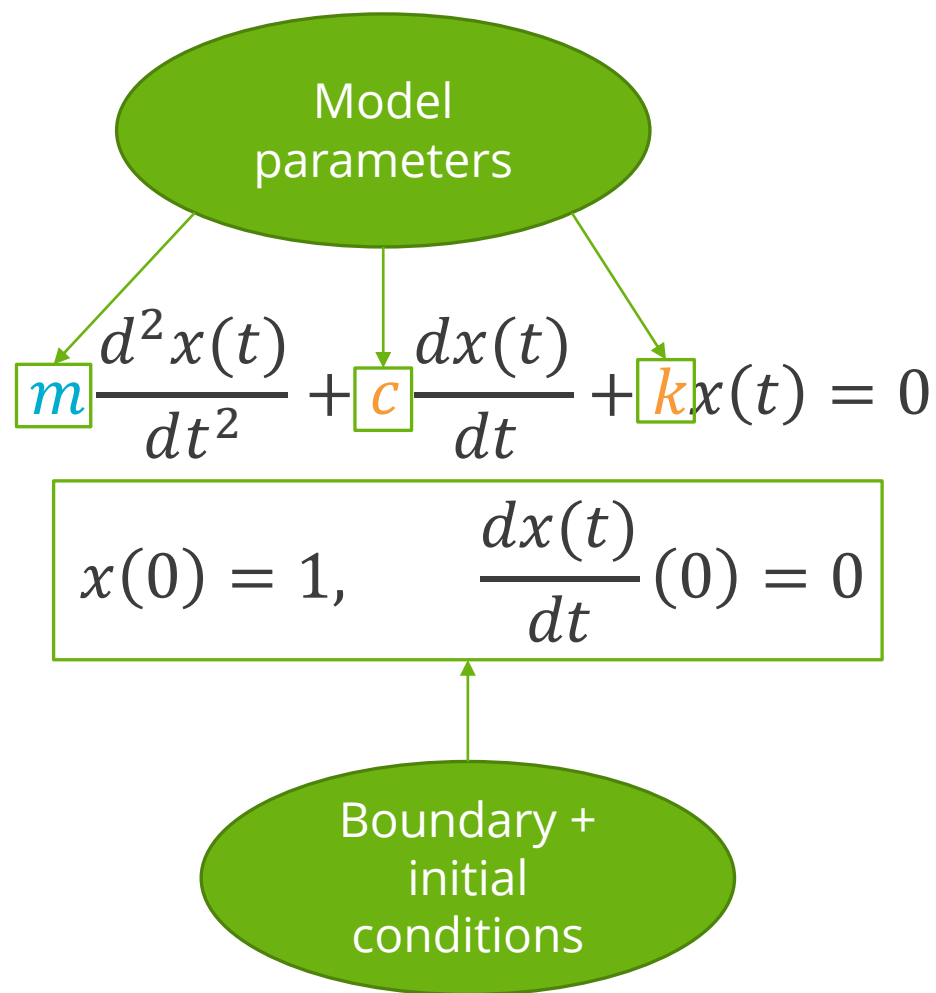


$$f_s + f_d \equiv F = ma \equiv m \frac{d^2x(t)}{dt^2}$$

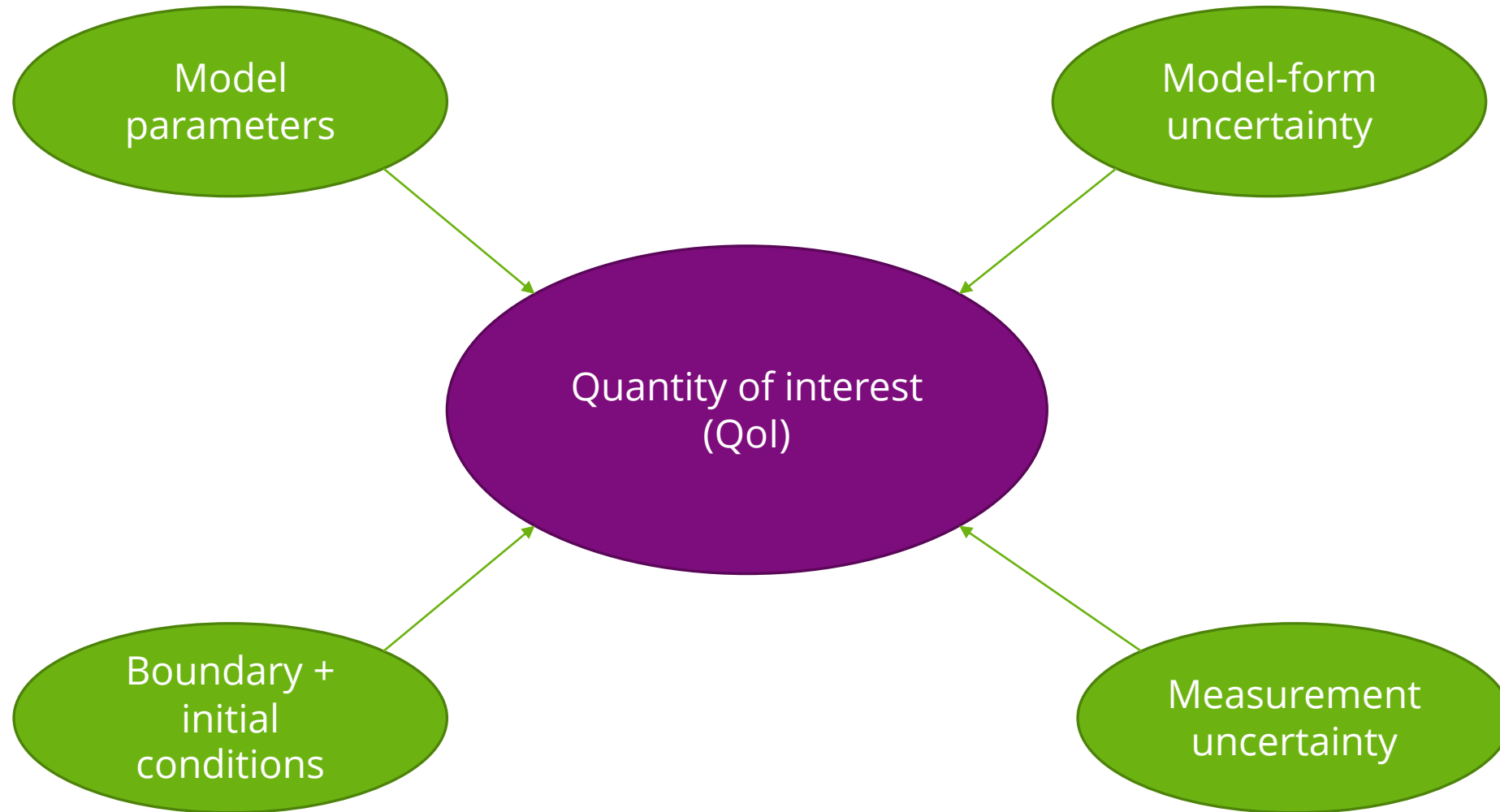
$$m \frac{d^2x(t)}{dt^2} + c \frac{dx(t)}{dt} + kx(t) = 0$$

$$x(0) = 1, \quad \frac{dx(t)}{dt}(0) = 0$$

Common sources of uncertainty



Result: uncertainty in model predictions



Real-world example

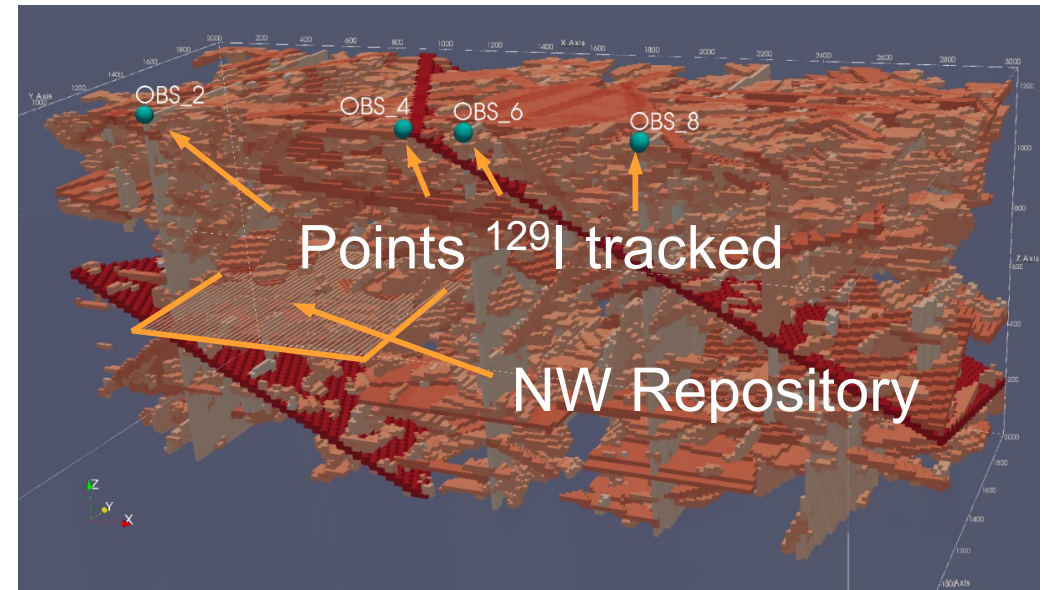
Quantity of Interest

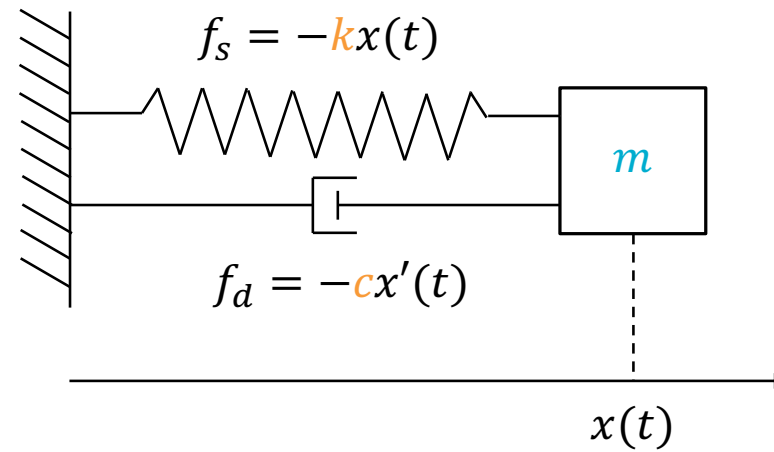
- Concentration of radionuclide ^{129}I in nearby aquifer after 10^6 years

Sources of uncertainty

- Properties of canisters holding nuclear waste (e.g. degradation rate)
- Subsurface properties (e.g. porosity, permeability)
- Environmental conditions (e.g. incidence of earthquake, glaciation)

Nuclear waste repository modeling

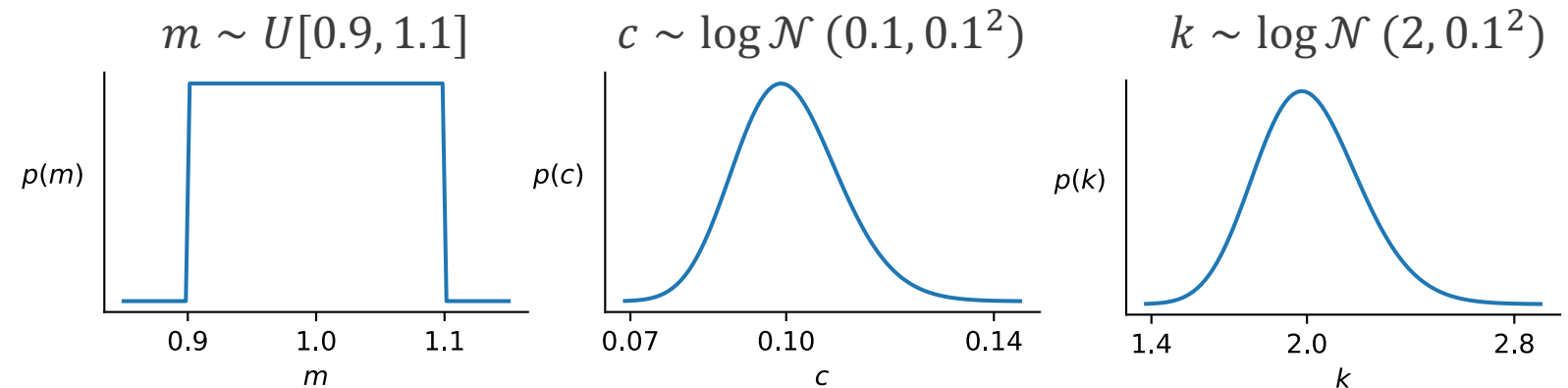




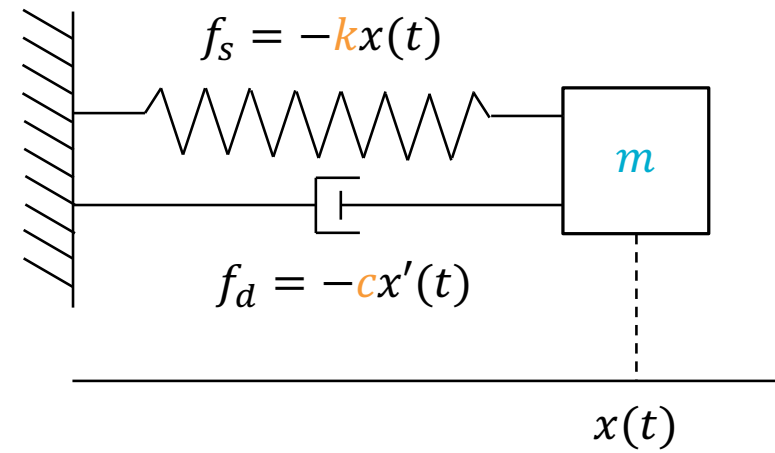
How do we
characterize
uncertainty?

Represent sources of uncertainty as random variables (RVs)

Encode what is known through the parameterization of the RV

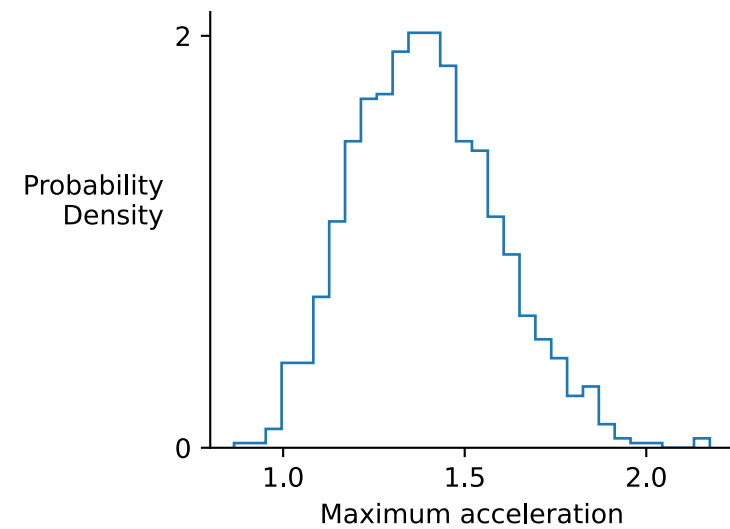
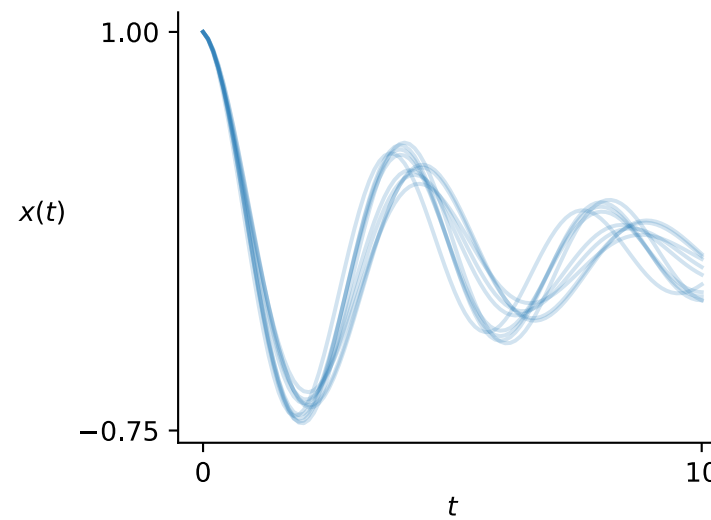


$$p_{\log \mathcal{N}(\mu, \sigma^2)}(x) \equiv \frac{1}{x\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2} (\log(x) - \mu)^2\right)$$



How do we
quantify
uncertainty?

Propagate sources of uncertainty to QoIs



Compute statistics of QoIs, e.g. mean, variance, tail probabilities

How do we
reduce
uncertainty?

Use data to gain **more precise knowledge** of sources of uncertainty

$$m \frac{d^2 x(t)}{dt^2} + c \frac{dx(t)}{dt} + kx(t) = 0$$

$$d = x_{true}(t = 10) + \epsilon_m, \quad \epsilon_m \sim \mathcal{N}(0, \sigma^2)$$

What is the **likelihood** the model produced the data for a given k, c ?

$$\mathcal{M}(k, c) \equiv x(t = 10; k, c)$$

$$d = \mathcal{M}(k, c) + \epsilon_m, \quad \epsilon_m \sim \mathcal{N}(0, \sigma^2)$$

$$d - \mathcal{M}(k, c) \sim \mathcal{N}(0, \sigma^2)$$

$$p(d|k, c) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(d - \mathcal{M}(k, c))^2}{2\sigma^2}\right)$$



How do we
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uncertainty?

Use data to gain **more precise knowledge** of sources of uncertainty

$$p(d|k, c) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(d - M(k, c))^2}{2\sigma^2}\right)$$

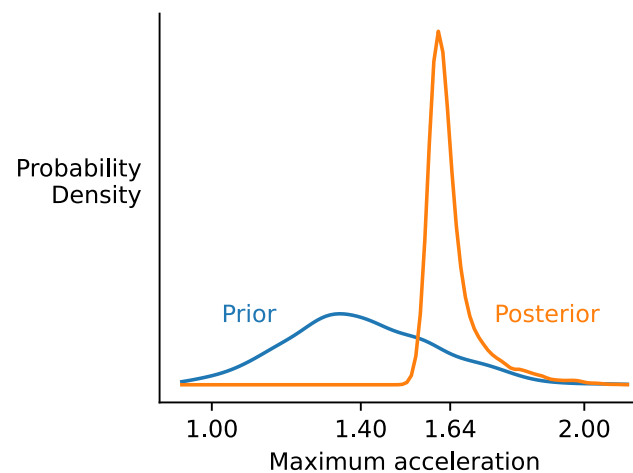
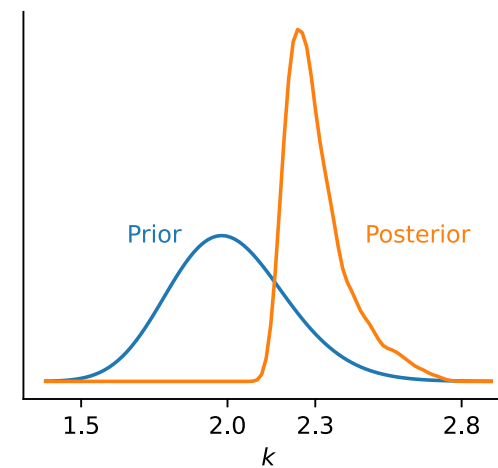
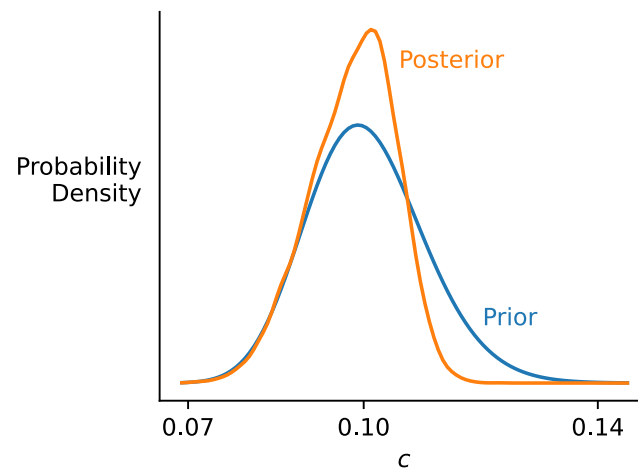
$$p(k, c) = p(k)p(c)$$

Bayes' Theorem

$$p(k, c|d) = \frac{p(d|k, c)p(k, c)}{\int p(d|k, c)p(k, c)dkdc}$$

How do we
reduce
uncertainty?

Use data to gain **more precise knowledge** of sources of uncertainty



This is also
called **Bayesian**
inference or
Bayesian
calibration

How do we

- characterize
 - quantify
 - reduce

uncertainty **in practice?**

Harsh reality



- Models for practical problems challenging
 - Nonlinear: propagating uncertainty + performing inference need many model evaluations
 - Computationally expensive; can afford few evaluations, causing poor statistical accuracy
 - High-dimensional problems
- Data expensive or impossible to attain
- Models imperfect representations of reality
 - Leads to unquantified error in predictions, biased Bayesian calibrations
 - But the correct model form is generally unknown (model-form uncertainty)
- Input/data uncertainties have to be modeled
 - If no quantitative information, have to encode prior belief through expert elicitation [4]

Real-world example



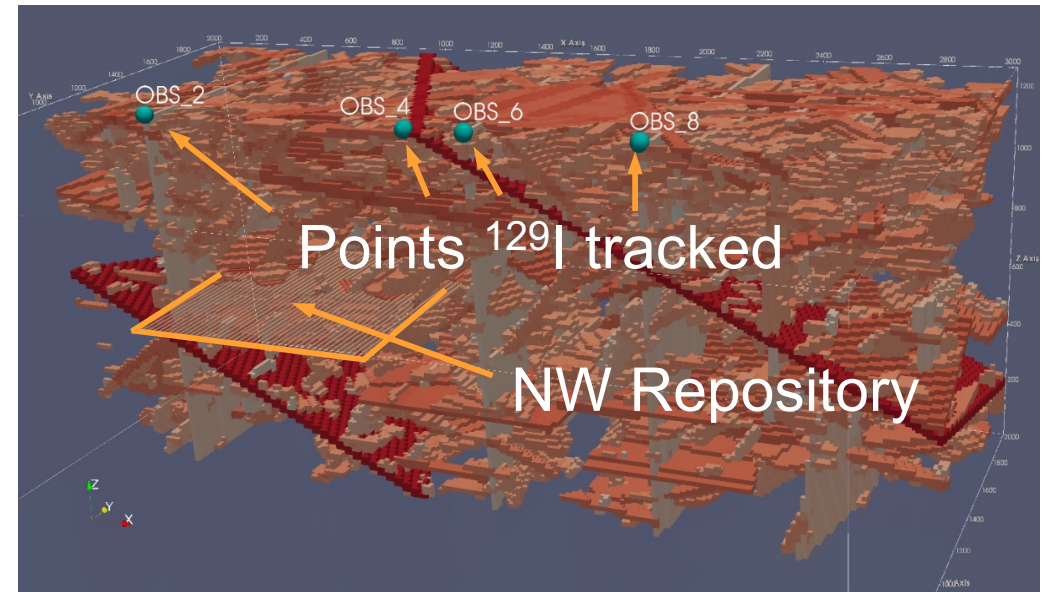
Data acquisition

- Subsurface properties: drill borehole(s)
- Canister properties: fabricate and test several canister specimens in the lab

Computational cost per model evaluation

- ~1.5 hours on 512 cores
- ~8 days on 4 cores
- ~22 years for 1000 samples on 4 cores

Nuclear waste repository modeling



Reduced-
order/surrogate
models

Bayesian inverse
problems

Multimodel methods

Optimal experimental
design

Sensitivity analysis

Algorithms for high
dimensionality

Model-form
uncertainty

$$M(\theta) \approx f(\theta)$$

Common statistical approaches

Gaussian processes [5,6]

Stochastic expansions
(polynomial chaos, stochastic
collocation) [7]

Common reduced-order model (ROM) approaches

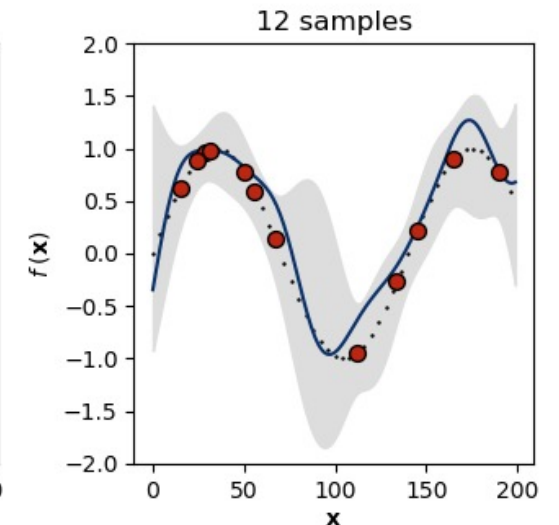
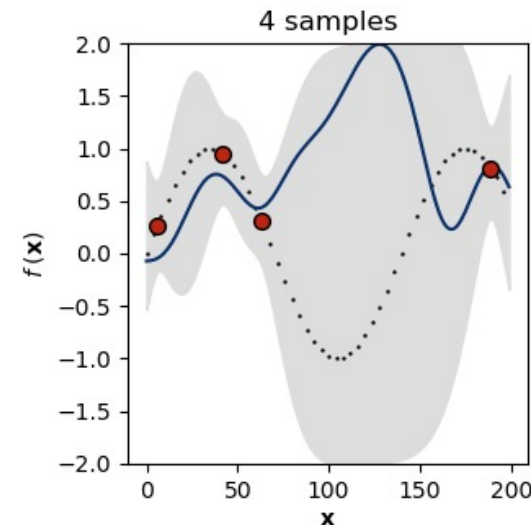
Proper orthogonal
decomposition [8,9]

Principal component analysis
[10]

Goal: reduce
computational burden
of UQ by using
approximate
representations of
model

And, more recently

Machine learning!



Ongoing opportunities



- Efficient surrogates/ROMs for high-dimensional models
- Adaptive/goal-oriented surrogate/ROM construction
- More theory for error incurred in UQ analyses by using approximation of $M(\theta)$
- Multimodel surrogates

Research areas in UQ



Efficient forward
propagation

Bayesian inverse
problems

Reduced-
order/surrogate
models

Optimal experimental
design

Sensitivity analysis

Algorithms for high
dimensionality

Model-form
uncertainty

Two types of high dimensionality



Infinite
dimensionality

High cardinality

Ongoing opportunities



- Dimension reduction (PCA [10], active subspaces [11], autoencoders [12], ISOMAP [13])
 - Methods encouraging/exploiting sparsity
- Expanded theory for infinite-dimensional problems with less restrictive assumptions (e.g. linearity, Gaussianity) [14,15]
- Improve on existing inference methods
 - Derivative-based (MALA/HMC, Stochastic Newton, VI) [16-19]
 - Data-informed (DILI) [20]
- Methods to address high cardinality, especially for
 - Surrogates
 - Bayesian inference
 - Sensitivity analysis



Reduced-order/surrogate models

Bayesian inverse problems

Multimodel methods

Optimal experimental design

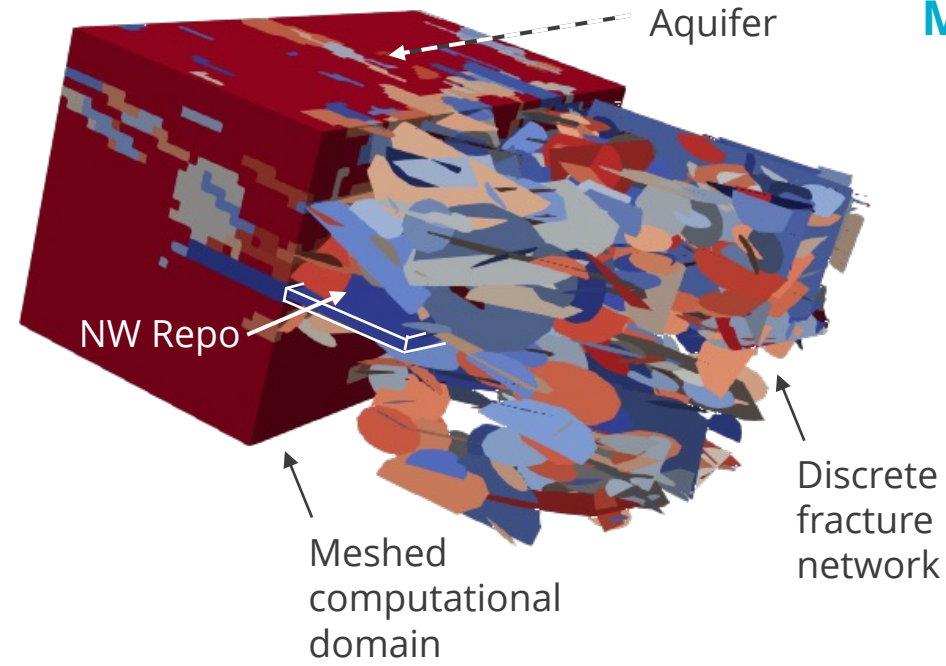
Sensitivity analysis

Algorithms for high dimensionality

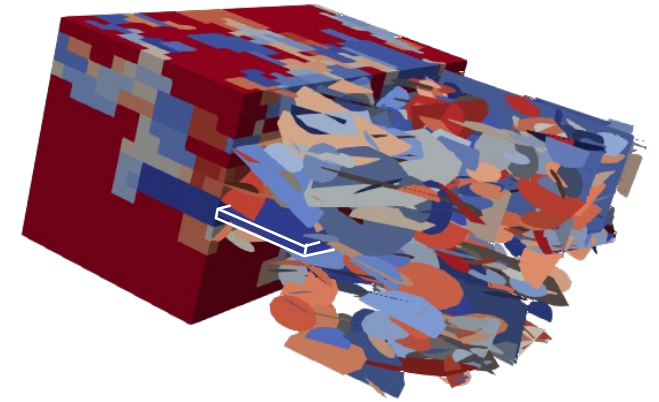
Model-form uncertainty

Idea: exploit lower-fidelity, cheaper models to lower cost for same accuracy

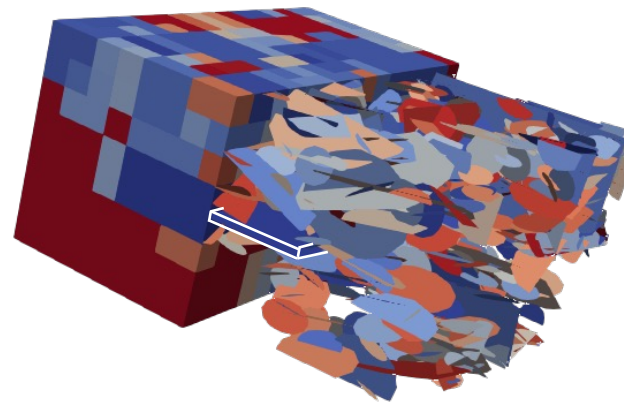
Fine



Medium



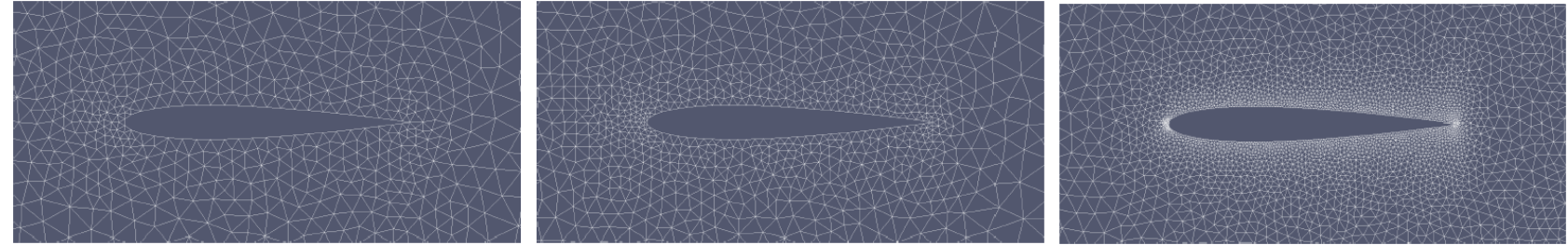
Coarse



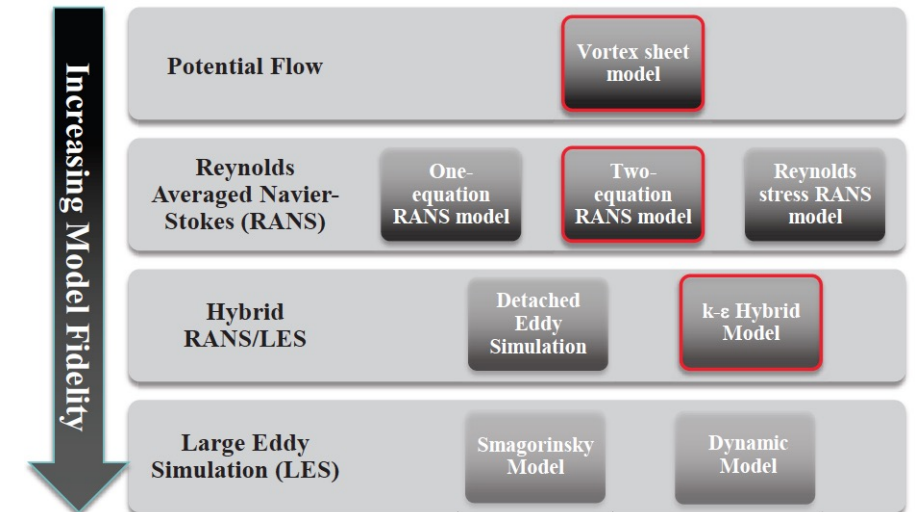
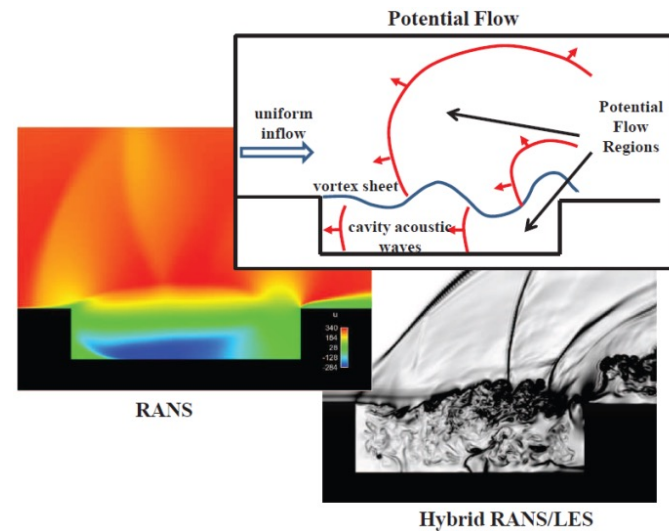
UQ
analysis

Idea: exploit lower-fidelity, cheaper models to lower cost for same accuracy

Discretization



Modeling assumptions





$$\hat{M}(\theta) = \frac{1}{N} \sum_{i=1}^N M(\theta^{(i)}), \quad \theta^{(i)} \sim p(\theta) \text{ i. i. d.}$$

$$\mathbb{V}[\hat{M}] = \frac{\mathbb{V}[M]}{N}$$

Sampling-based methods – control variates



$$M_1(\theta) \qquad c_1 = \frac{C_1}{C} \ll 1 \qquad \text{corr}(M, M_1) = \rho$$

$$\widehat{M}_{CV}(\theta) = \widehat{M}(\theta) + \alpha(\widehat{M}_1(\theta) - \mathbb{E}[M_1]) \qquad \mathbb{E}[\widehat{M}_{CV}(\theta)] = \mathbb{E}[M] \leftarrow \text{Unbiased}$$

$$\mathbb{V}[\widehat{M}_{CV}(\theta)] = \frac{1}{N} (\mathbb{V}[M] + \alpha^2 \mathbb{V}[M_1] + 2\alpha \text{Cov}[M, M_1])$$

$$\alpha^* = \min_{\alpha} \mathbb{V}[\widehat{M}_{CV}(\theta)] = -\frac{\text{Cov}[M, M_1]}{\mathbb{V}[M_1]}$$

$$\mathbb{V}[\widehat{M}_{CV}(\theta)] = \frac{\mathbb{V}[M]}{N} (1 - \rho^2) \leftarrow \rho^2 \approx 1 \rightarrow \text{orders of magnitude reduction in variance}$$

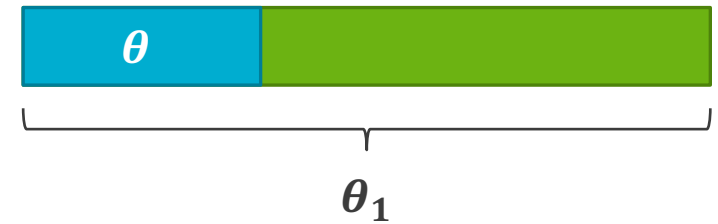
Sampling-based methods – beyond control variates



$$\widehat{M}_{CV}(\theta) = \widehat{M}(\theta) + \alpha(\widehat{M}_1(\theta) - \mathbb{E}[M_1]) \quad \text{Have to estimate this too}$$

Multifidelity Monte Carlo [21]:

$$\widehat{M}_{MFMC} = \widehat{M}(\theta) + \alpha(\widehat{M}_1(\theta) - \widehat{M}_1(\theta_1))$$



$$\alpha^* = -\frac{\rho\sqrt{\mathbb{V}[M]}}{\sqrt{\mathbb{V}[M_1]}}$$

$$r_1^* = \sqrt{\frac{\text{Cost}(M)\rho^2}{\text{Cost}(M_1)(1-\rho^2)}} \quad N_1 = \lceil r_1 N \rceil$$

$$\mathbb{V}[\widehat{M}_{MFMC}] = \frac{\mathbb{V}[M]}{N} \left(1 - \rho^2 \left(\frac{r_1 - 1}{r_1} \right) \right)$$

Multimodel methods



- Theory extends to multiple (nonhierarchical) models
- Many algorithms combining different models and sample sets in different ways [21-24]
- Recent focus on multifidelity surrogates, e.g. Gaussian processes [25], multifidelity polynomial chaos [26], and several others [27-29]

$$M(\theta) \approx f(\theta)$$

vs.

$$M_1(\theta) \approx f_1(\theta)$$

$$M(\theta) - M_1(\theta) \approx f_\Delta(\theta)$$

$$M(\theta) \approx f_1(\theta) + f_\Delta(\theta)$$

Multimodel methods: ongoing opportunities



- Moving beyond functions of moments, e.g. tail probabilities, CDFs
- Startup cost of sampling all models to compute sample correlations → exploration vs exploitation tradeoff to find optimal model ensemble
- Stochastic models: stochasticity weakens correlation, but averaging it out can models too costly
- Addressing dissimilar parametrization (high and low fidelity models don't have same uncertain parameters)



Reduced-order/surrogate models

Bayesian inverse problems

Multimodel methods

Optimal experimental design

Sensitivity analysis

Algorithms for high dimensionality

Model-form uncertainty

Challenges and ongoing opportunities



$$p(d|\boldsymbol{\theta}) = \frac{p(d|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(d|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}} \quad p(d|\boldsymbol{\theta}) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(d - M(\boldsymbol{\theta}))^2}{2\sigma^2}\right)$$

If $M(\boldsymbol{\theta})$ nonlinear, can't compute analytically.

Markov Chain Monte Carlo [14,16-18,19] and Variational Inference [19] methods numerically approximate $p(\boldsymbol{\theta}|d)$ --need many model evaluations

Much work in multimodel, derivative-based, & surrogate/reduced-order modeling methods to make this tractable. Methods in optimization can be leveraged

Opportunities for improvement: methods addressing multimodal and/or non-Gaussian posteriors; high dimensionality; model error



Reduced-
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Model-form
uncertainty

What model inputs (parameters) most affect model predictions?



Sensitivity analysis methods provide a quantitative measure of output sensitivity to each input [30]

Extremely powerful tool in mathematical modeling. Supports

- *Scientific discovery/model interpretation* – increase understanding of relationships between inputs + their interactions and outputs
- *Dimension reduction* – parameters identified to not affect model predictions can be screened out of further uncertainty analysis
- *Model improvement* – resources can be focused on reducing uncertainties where they will have the most impact

A range of methods



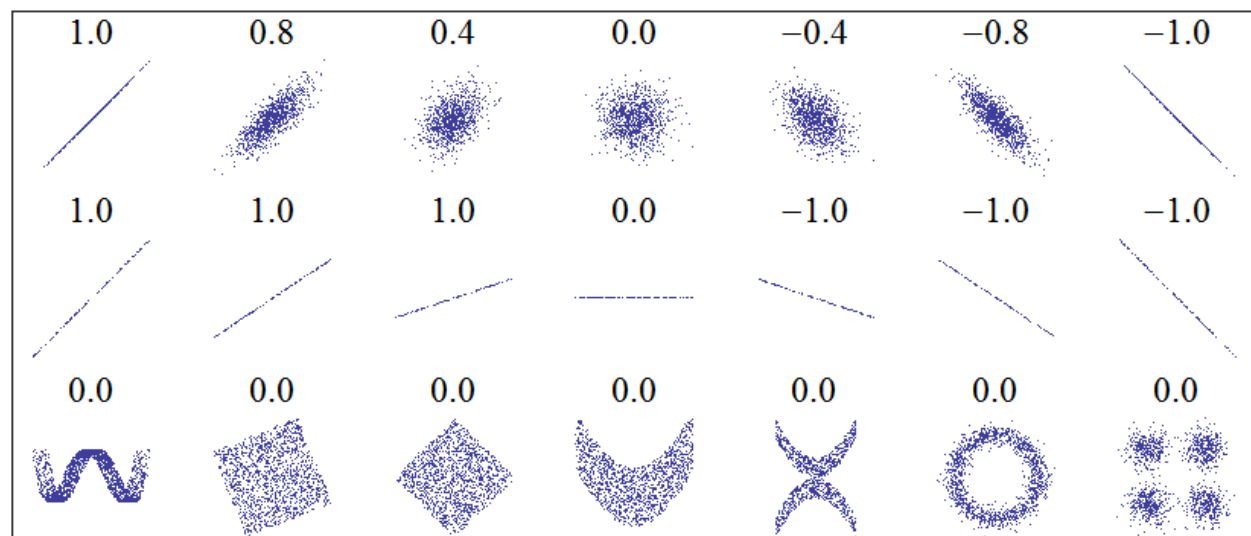
Correlation coefficients

$$\rho(\theta_i, M(\boldsymbol{\theta})) = \frac{\text{Cov}[\theta_i, M(\boldsymbol{\theta})]}{\sqrt{\text{Var}(\theta_i)\text{Var}(M(\boldsymbol{\theta}))}}$$

Estimated from input/output samples

Slope doesn't matter, just strength of linear relationship

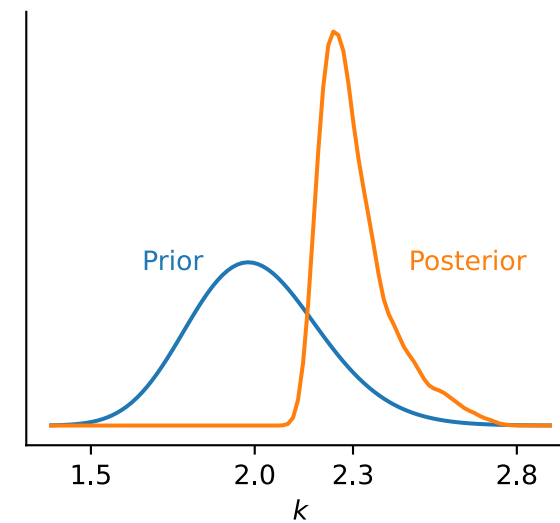
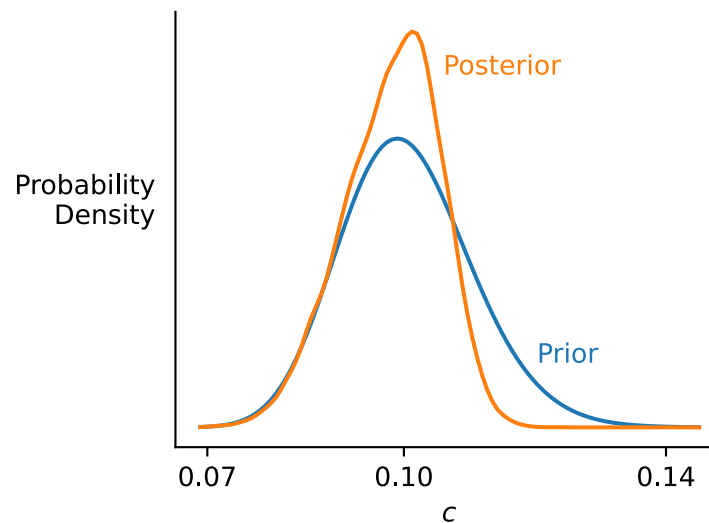
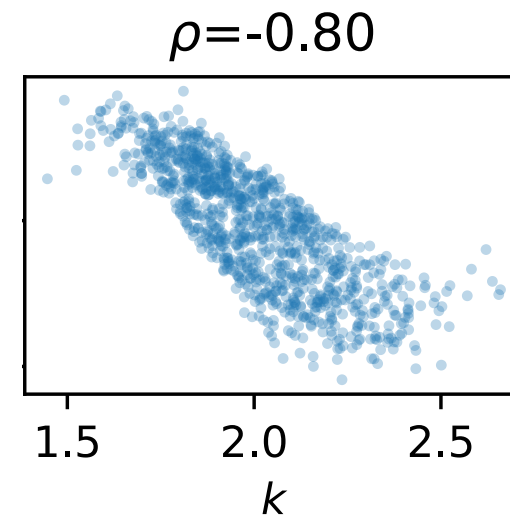
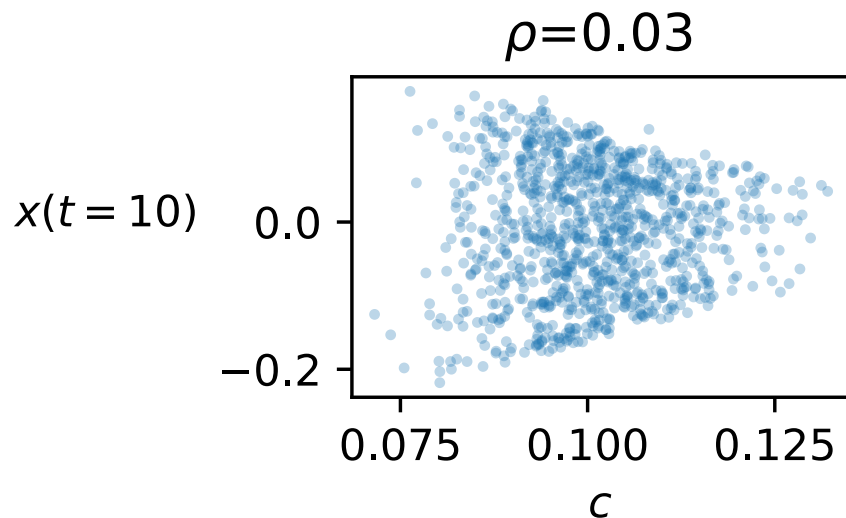
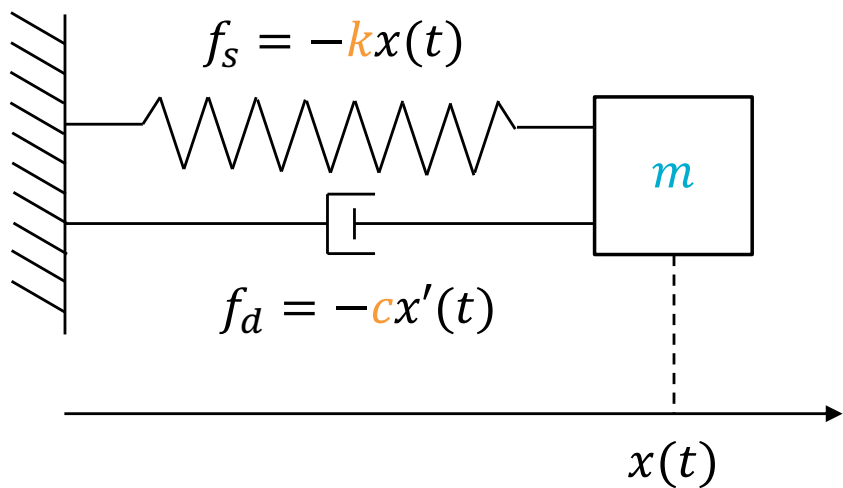
Nonlinear/nonmonotonic dependencies will not be detected.



Source: <http://en.wikipedia.org/wiki/Correlation>

Higher-order dependencies (i.e. dependence on two parameters varying together) won't be detected.

Can detect which parameter(s) would be informed in calibration before even collecting data!



A range of methods



Global Variance-Based Sensitivity Analysis [30]

$$S_i = \frac{\mathbb{V}_{\theta_i} \left[\mathbb{E}_{\theta_{\sim i}} [M | \theta_i] \right]}{\mathbb{V}[M]}$$

Effect of varying θ_i alone (averaging over other inputs)

$$T_i = 1 - \frac{\mathbb{V}_{\theta_{\sim i}} \left[\mathbb{E}_{\theta_i} [M | \theta_{\sim i}] \right]}{\mathbb{V}[M]}$$

Effect of varying θ_i alone and with all other inputs

Robust to nonlinearities and higher-order interactions between parameters

model evaluations: $N(d + 2)$, N independent samples, d -dimensional input space

Assumes inputs statistically independent

A range of methods



- Distribution-based method [31]
 - Instead measure sensitivity of model output *distribution*.
 - Requires distribution to be estimated—extremely challenging with high input dimension
- Shapley values [32]
 - Game-theory based method
 - Relaxes assumption of independent inputs
 - Computationally costly ($2^d - 1$ evaluations)

Ongoing opportunities [33]



- Computational cost high for more advanced methods, $\mathcal{O}(d^\alpha)$, $\alpha \geq 1$
- Computationally tractable methods for correlated inputs
- Unifying process to identify appropriate sensitivity method for a given task/goal

Research areas in UQ



Efficient forward
propagation

Bayesian inverse
problems

Reduced-
order/surrogate
models

Optimal experimental
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Sensitivity analysis

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Model-form
uncertainty

Bayesian OED overview

minimize uncertainty in parameter estimates

$$d(w)$$

$$\min_w \Psi(w) = f(p(\theta|d(w)))$$



Standard OED problem

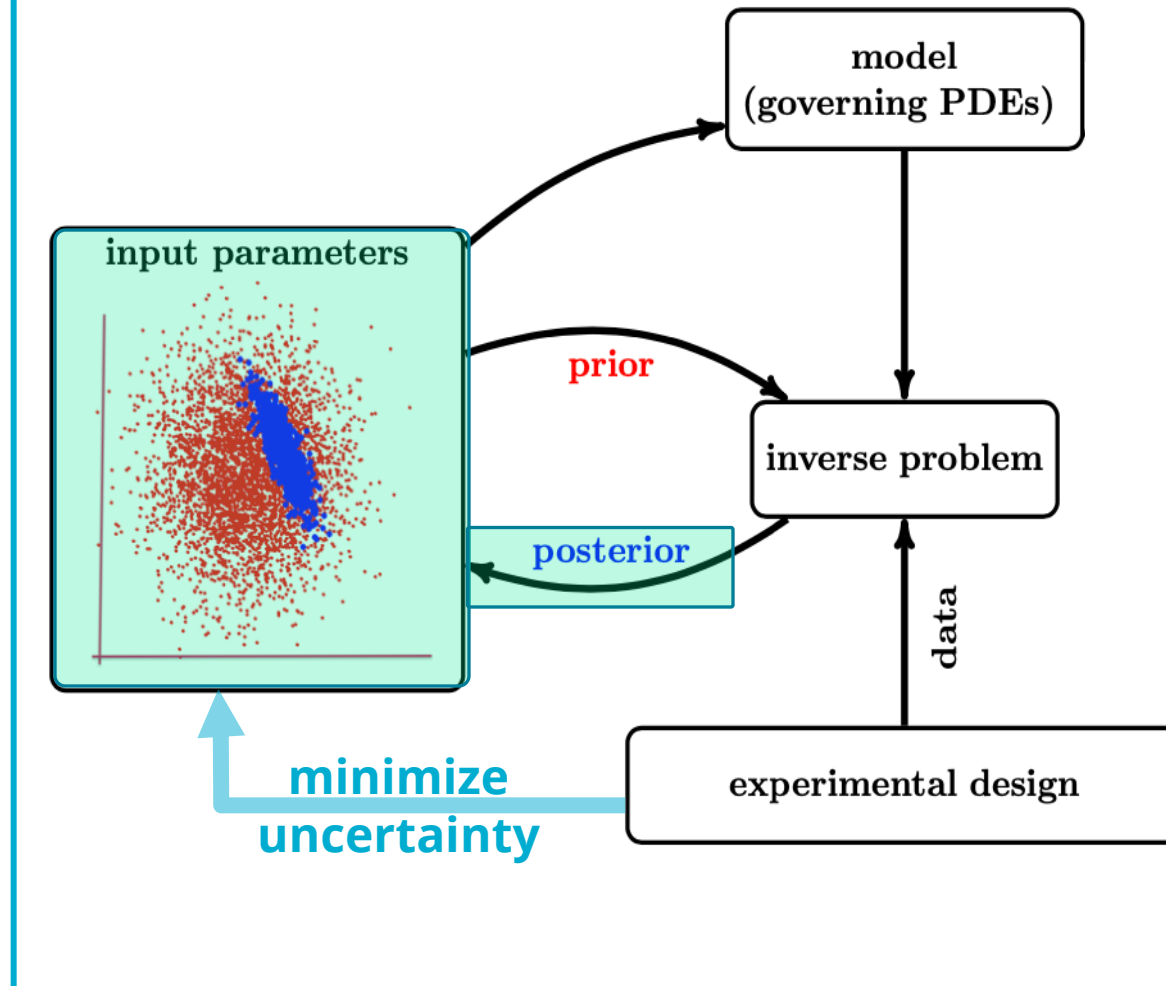


Figure courtesy of [34]

Ongoing opportunities



- Outer-loop analysis on expensive Bayesian inverse problem; leverage all efficiency gains possible
 - Surrogates/ROMs
 - Multimodel methods
 - Dimension reduction
 - Derivative-based methods
- Methods to efficiently search experimental design space (especially if it's high dimensional, e.g. many sensors)
- Methods to address heterogeneous data (i.e. sensor and satellite image data)
- Goal-oriented approaches [35]

Goal-oriented OED overview

minimize
uncertainty in
predictions

$d(w)$

$$\min_w \Psi^G(w) = f(p(M(\theta)|d(w)))$$

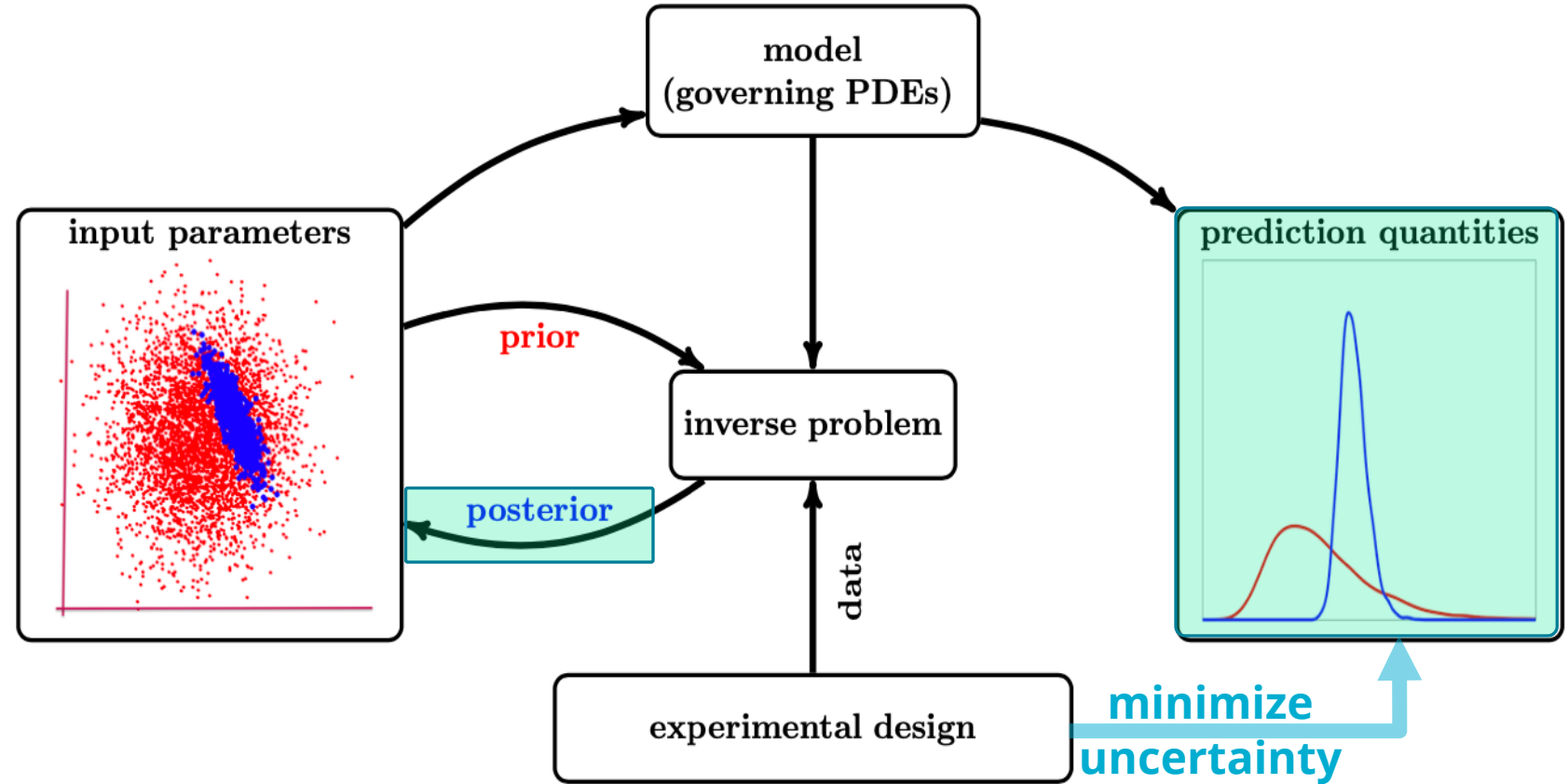


Figure courtesy of [34]

Research areas in UQ



Efficient forward
propagation

Bayesian inverse
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Reduced-
order/surrogate
models

Optimal experimental
design

Sensitivity analysis

Algorithms for high
dimensionality

Model-form
uncertainty

Come to my talk tomorrow!

Thanks!

teresaportone.com

References

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