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A brief survey of uncertainty quantification

Teresa Portone

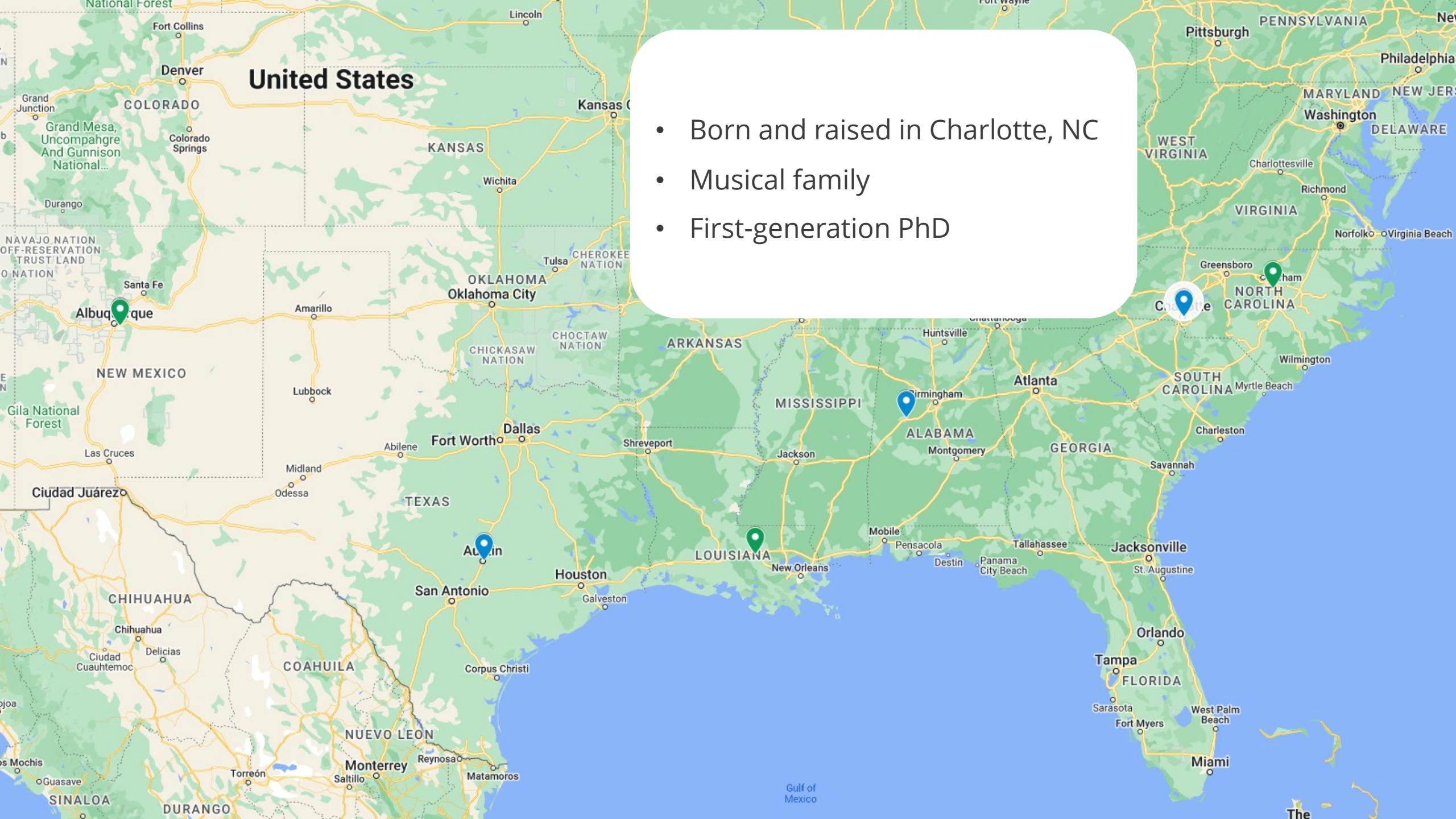
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University of Alabama Mathematics Colloquium



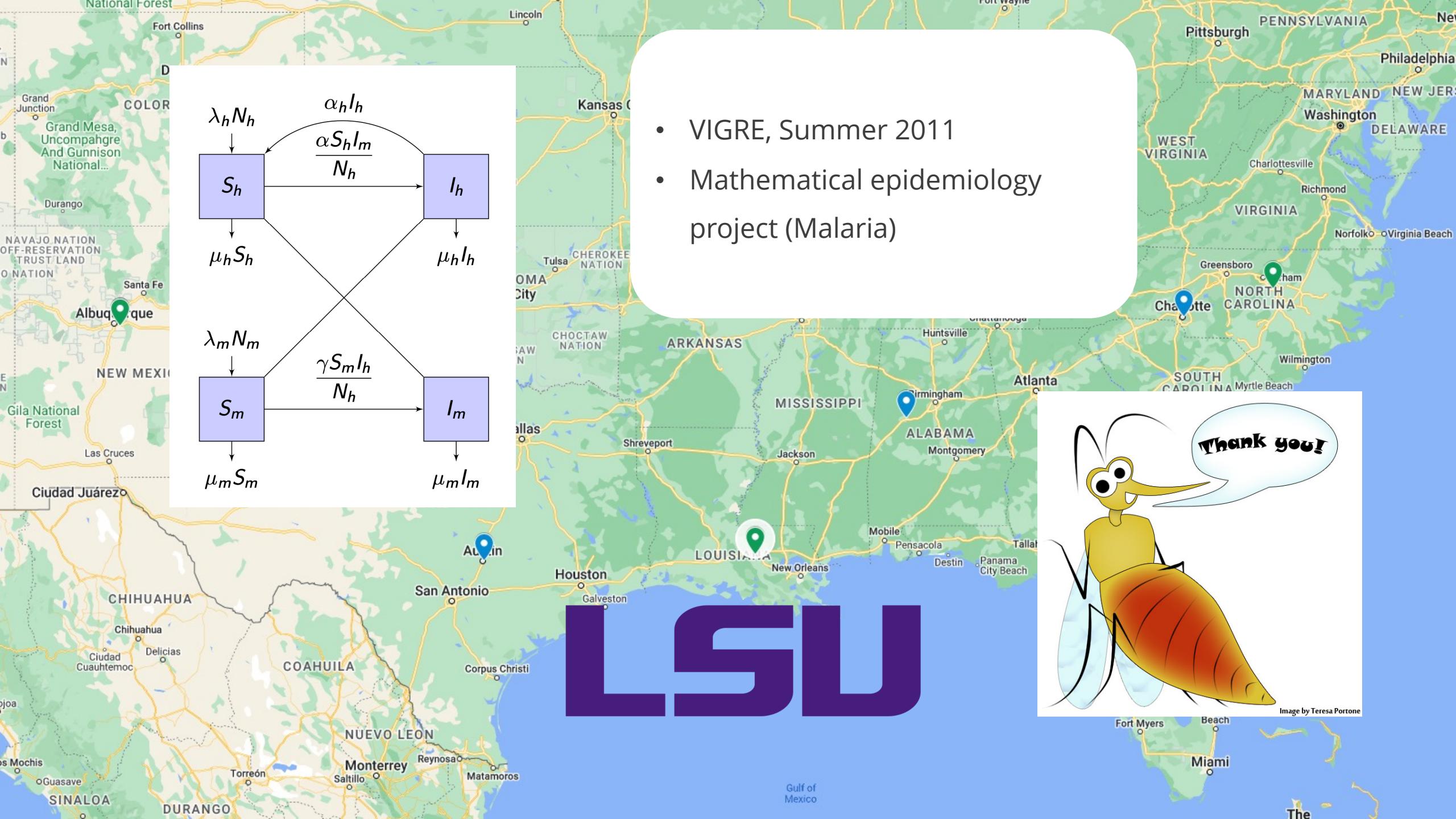
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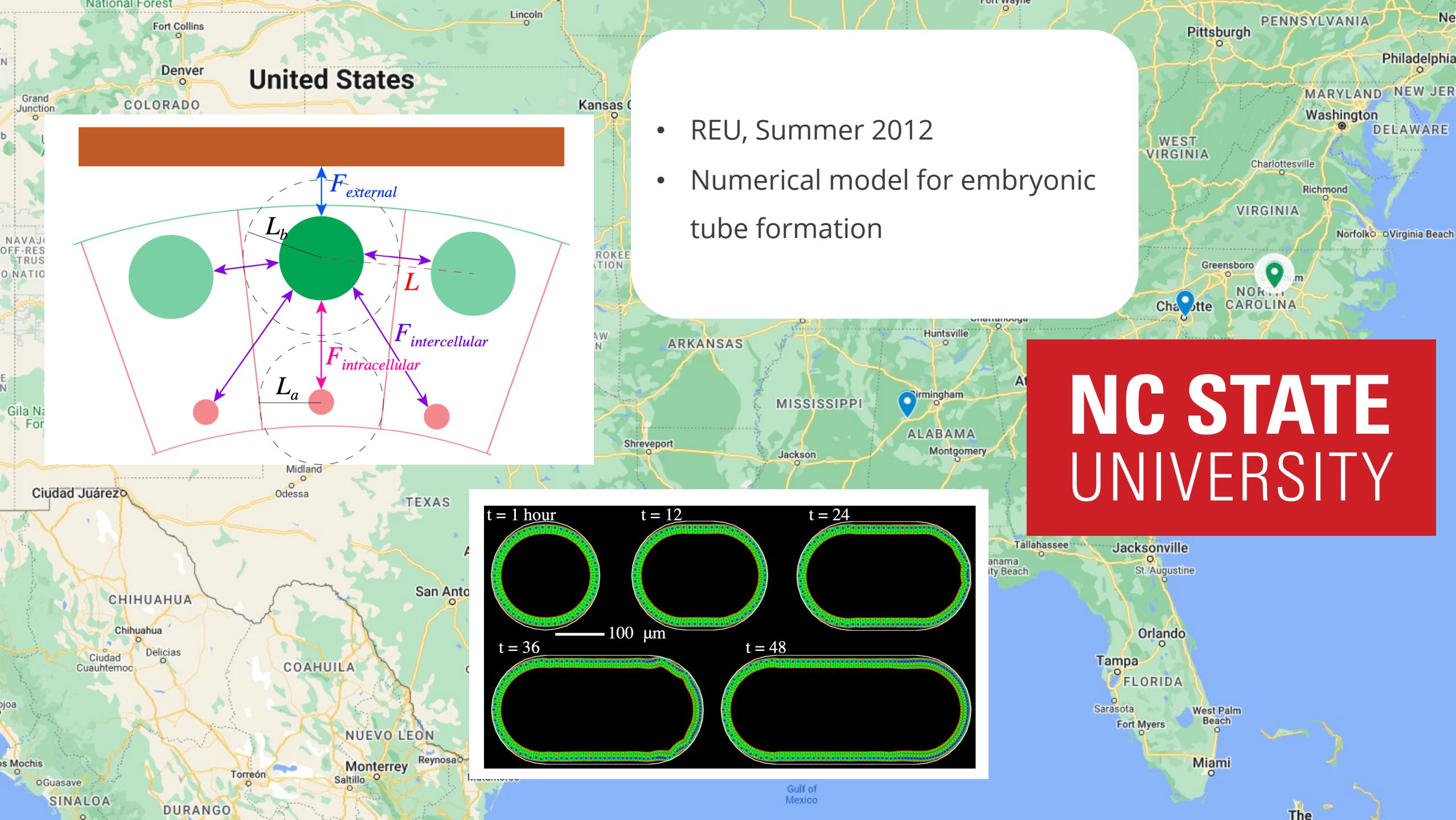
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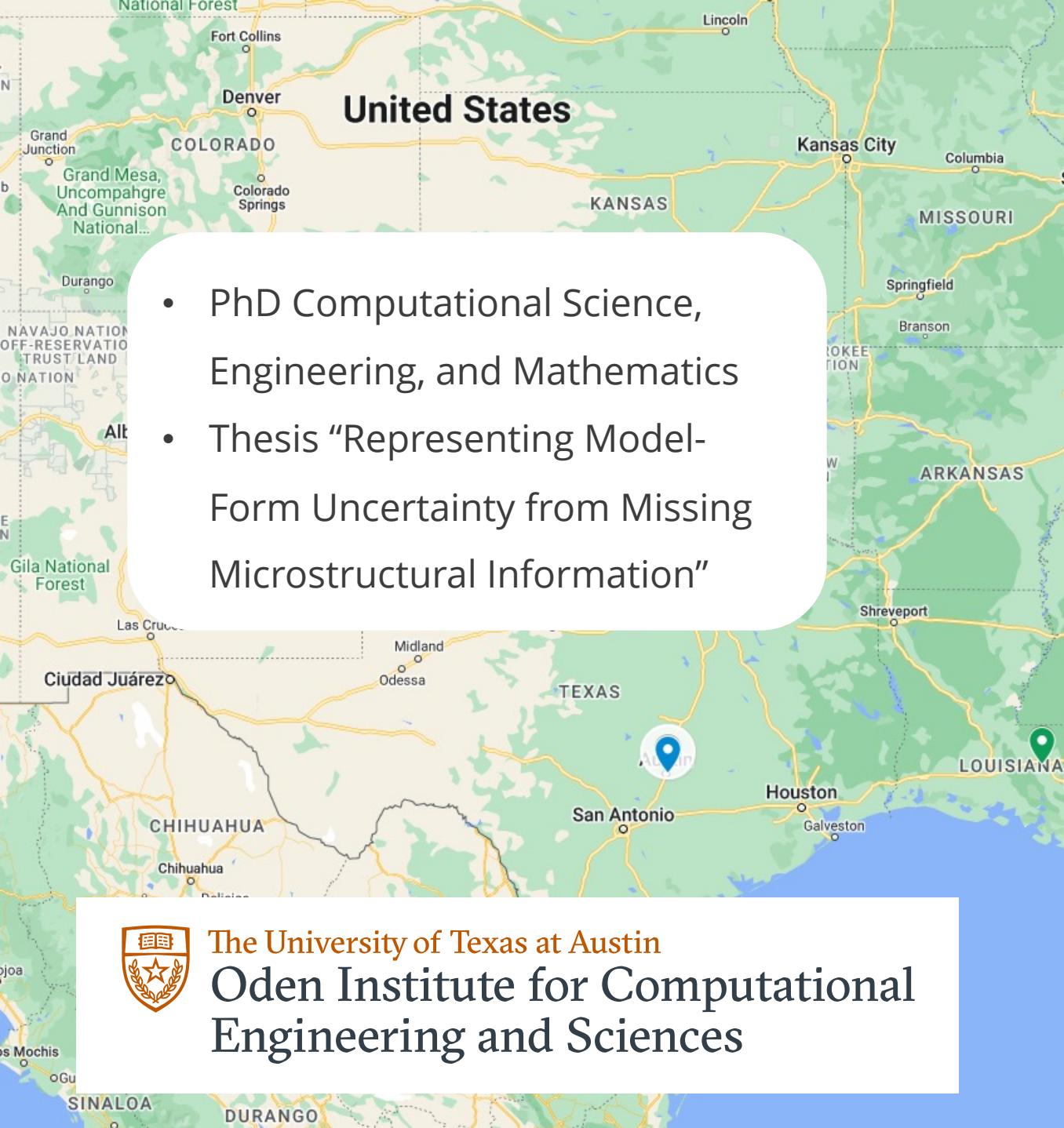


- Born and raised in Charlotte, NC
- Musical family
- First-generation PhD

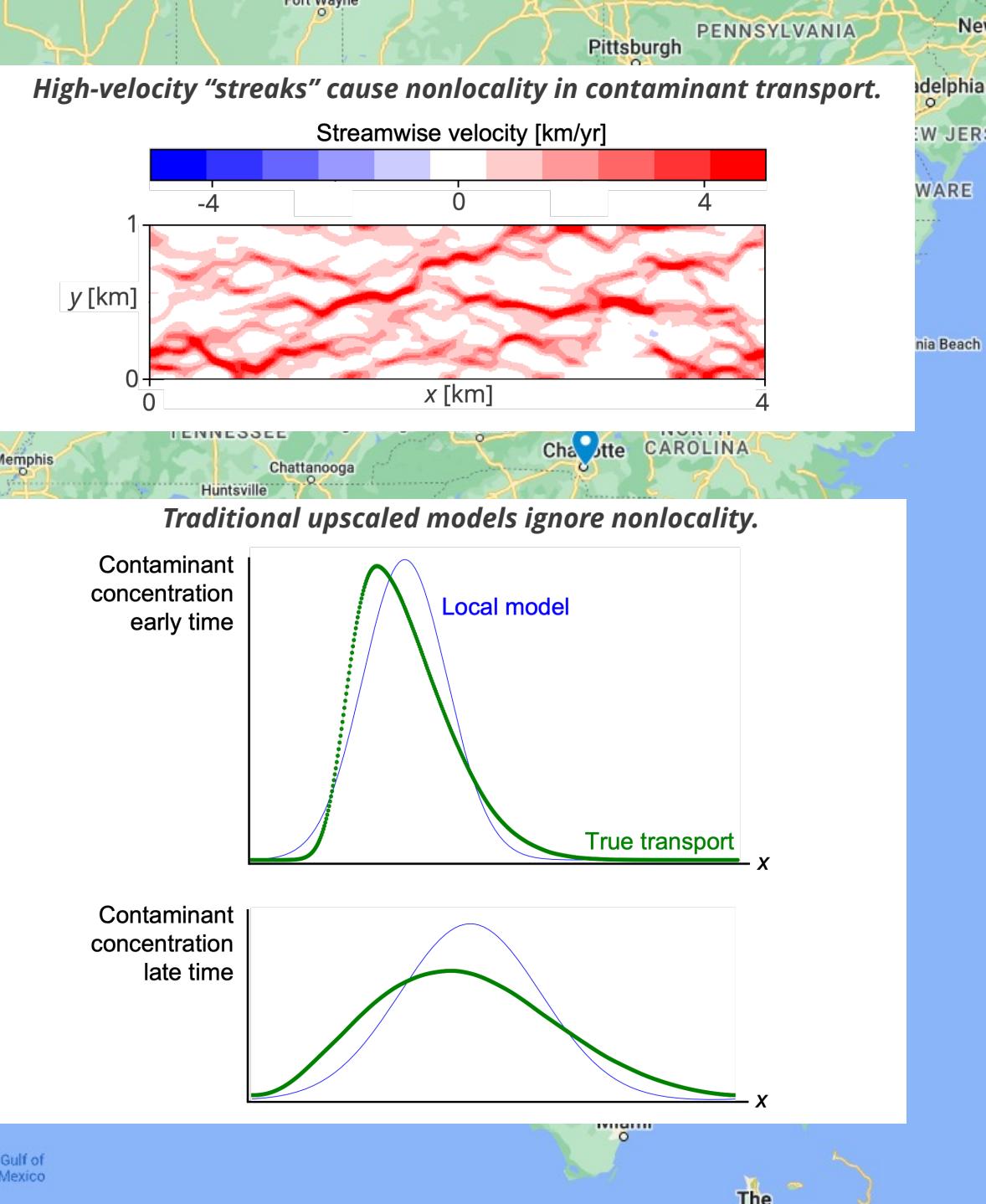




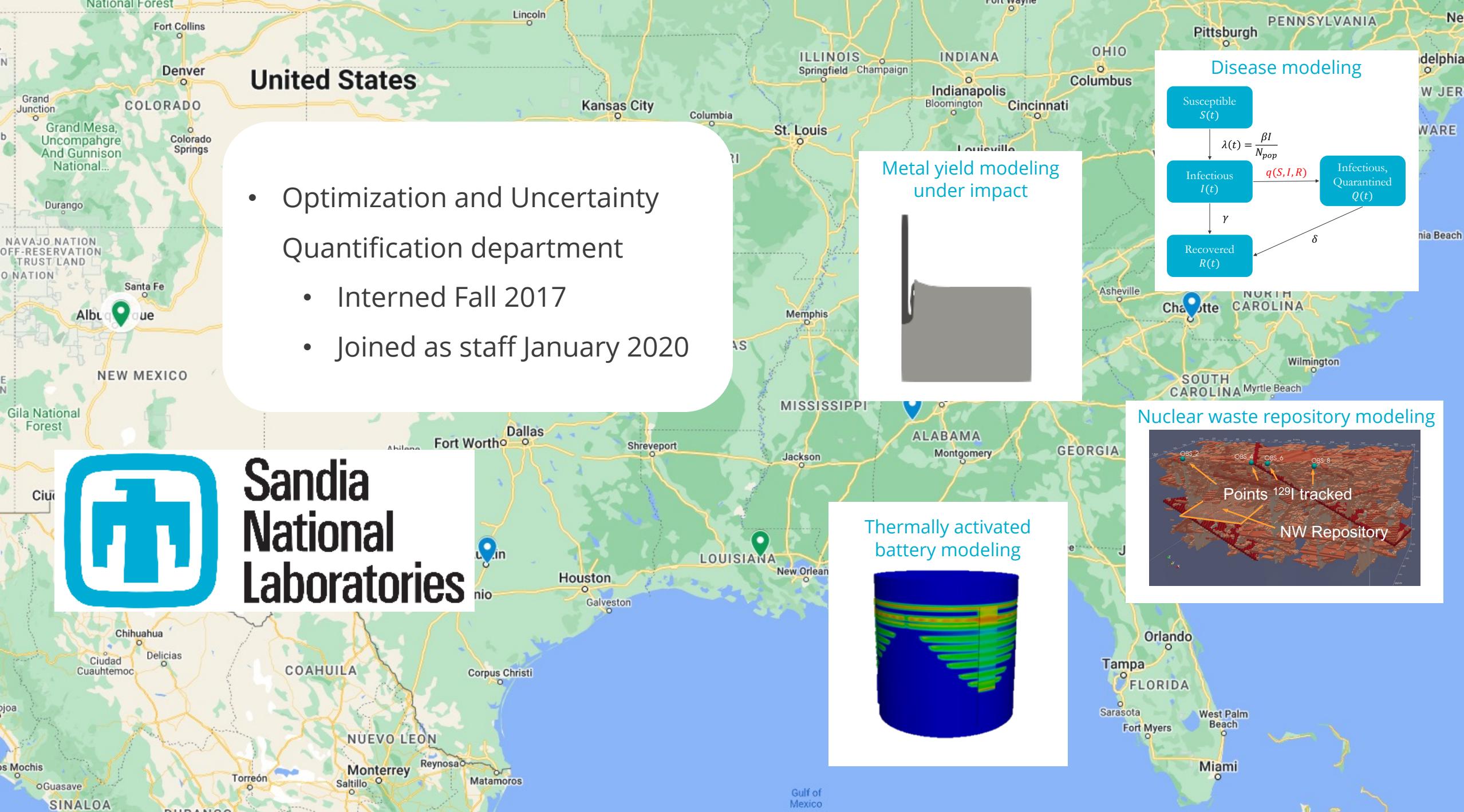




- PhD Computational Science, Engineering, and Mathematics
- Thesis “Representing Model-Form Uncertainty from Missing Microstructural Information”



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

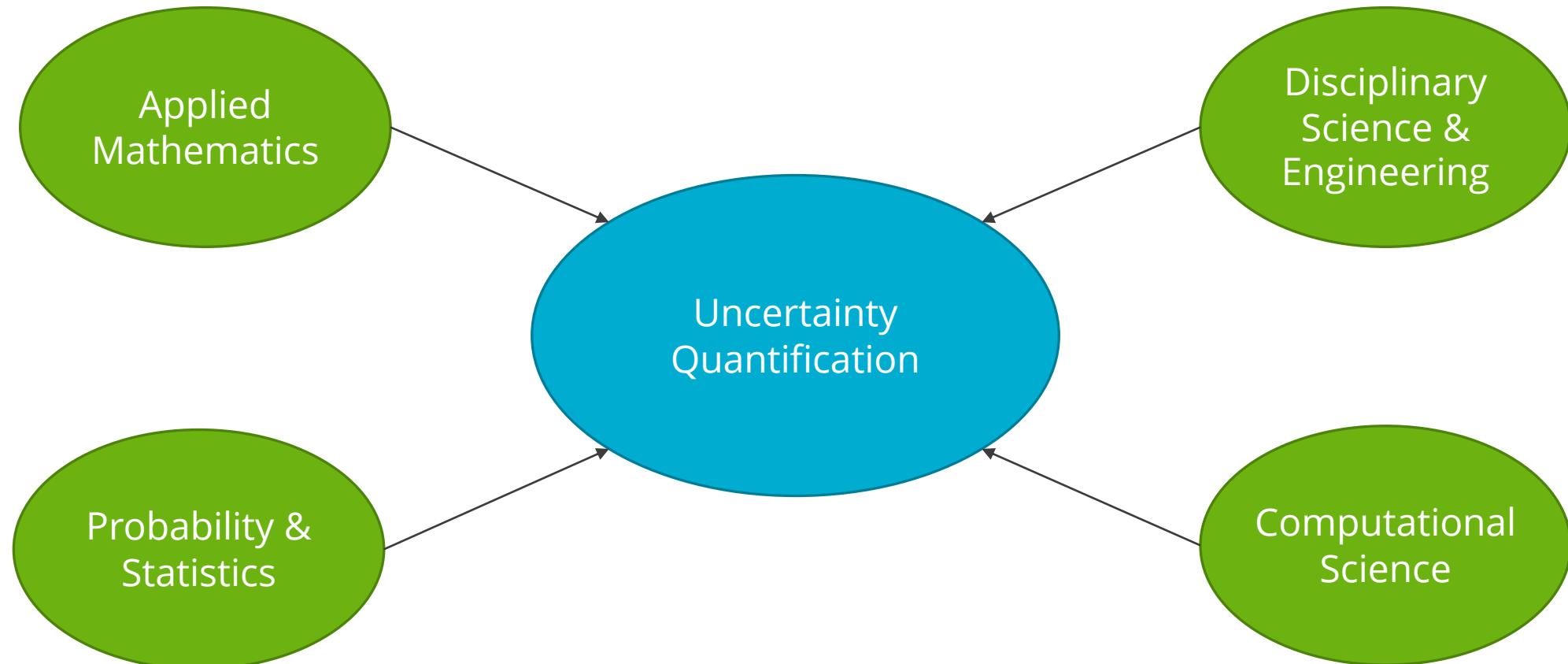


What is uncertainty quantification (UQ)?



My definition:

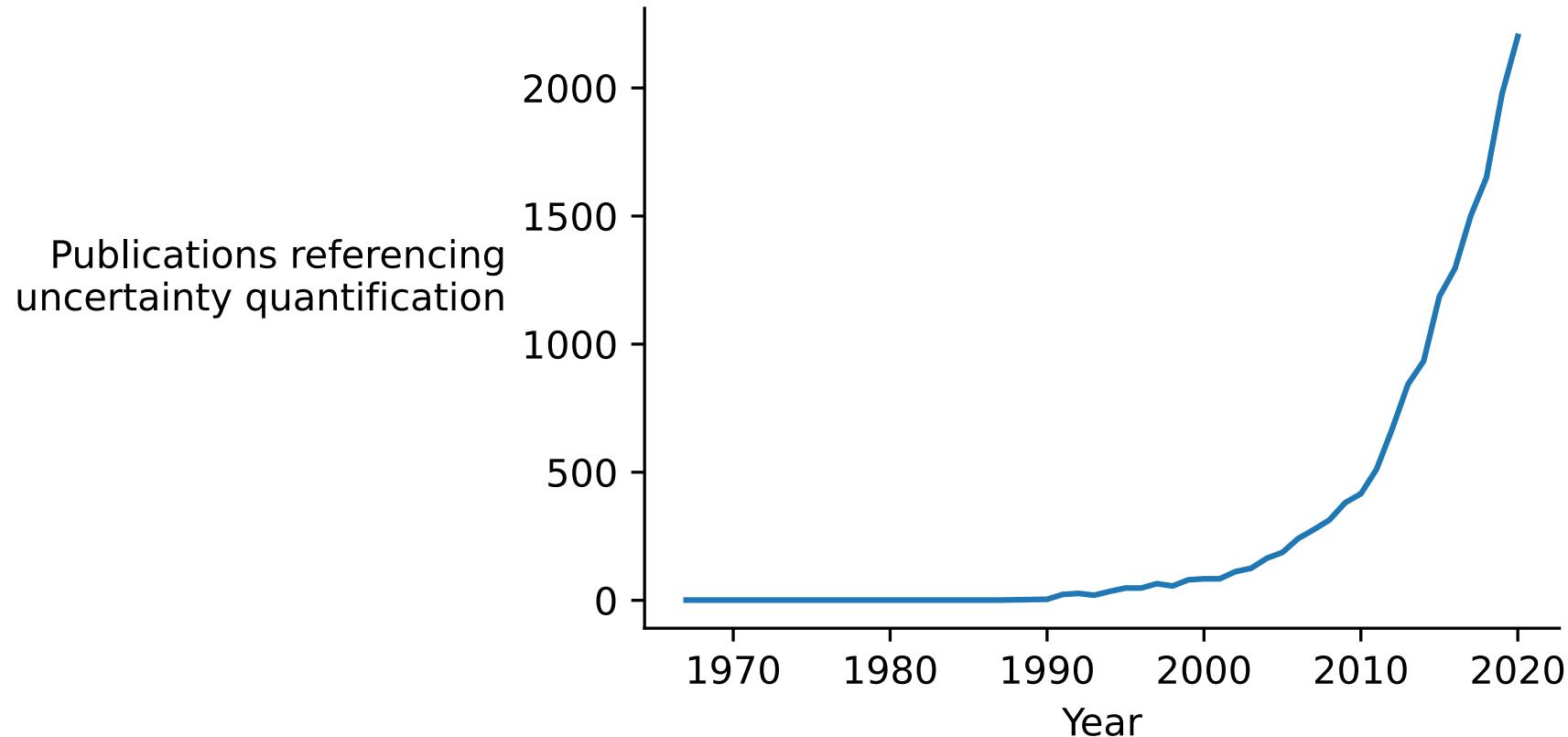
The science of characterizing, quantifying, and reducing uncertainties in mathematical models.



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]





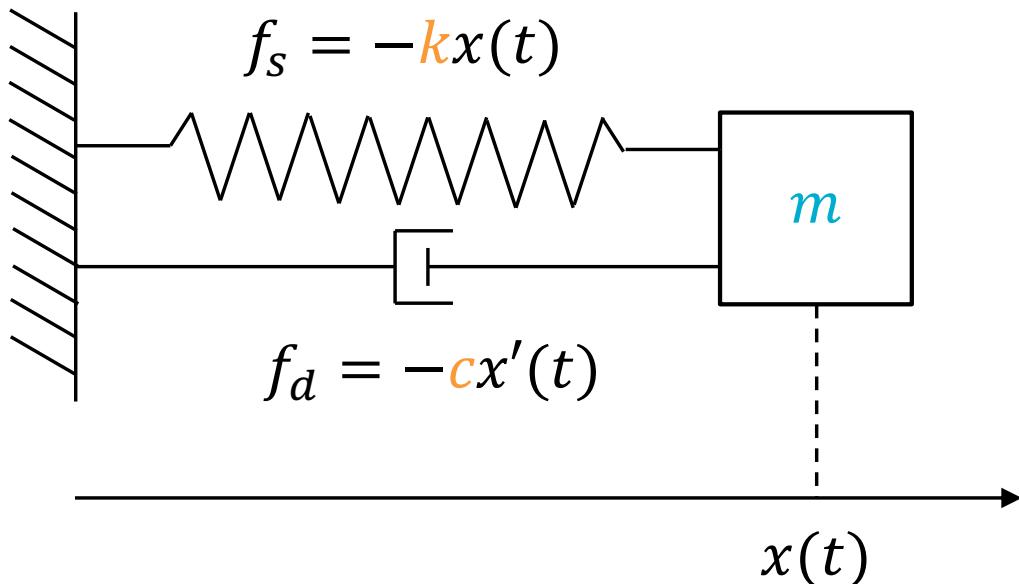
What is uncertainty?

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

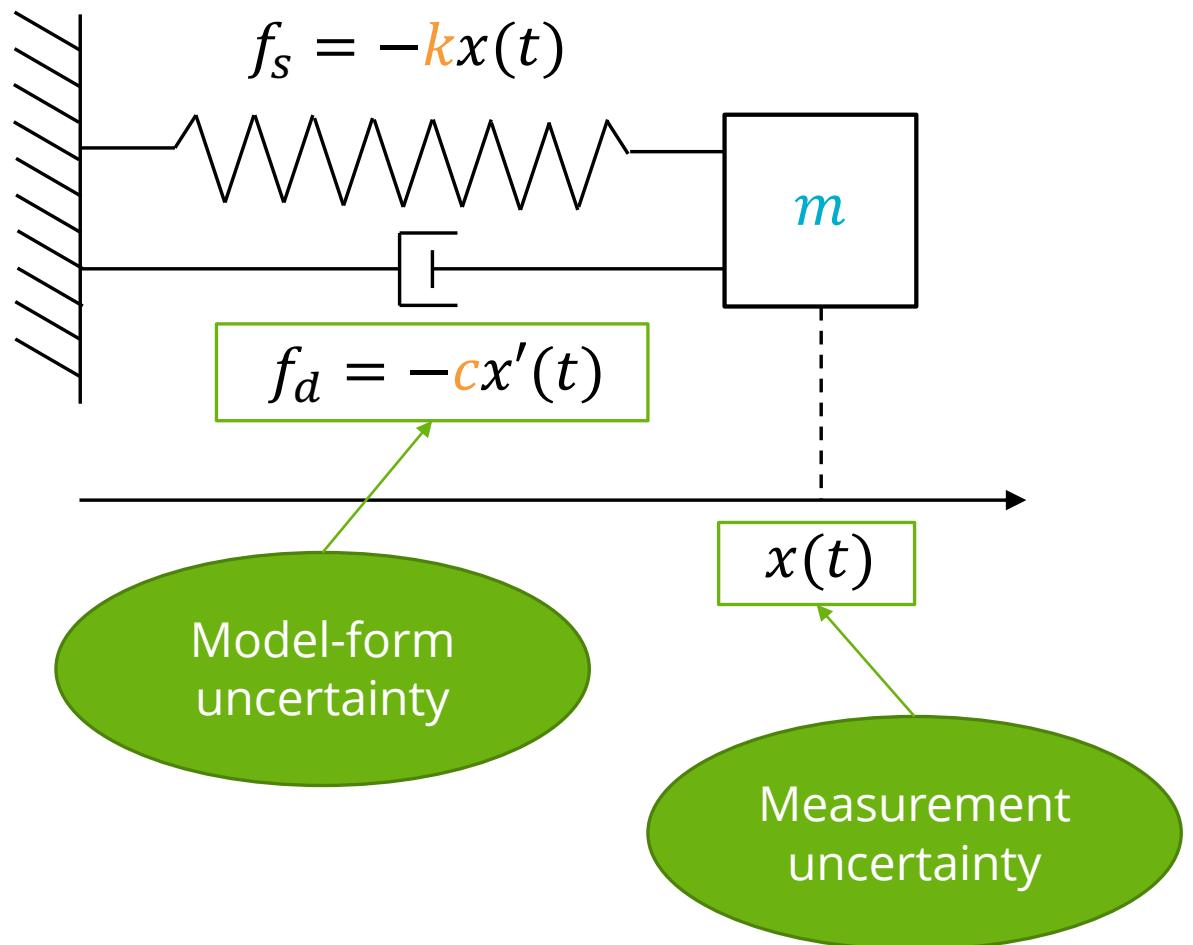
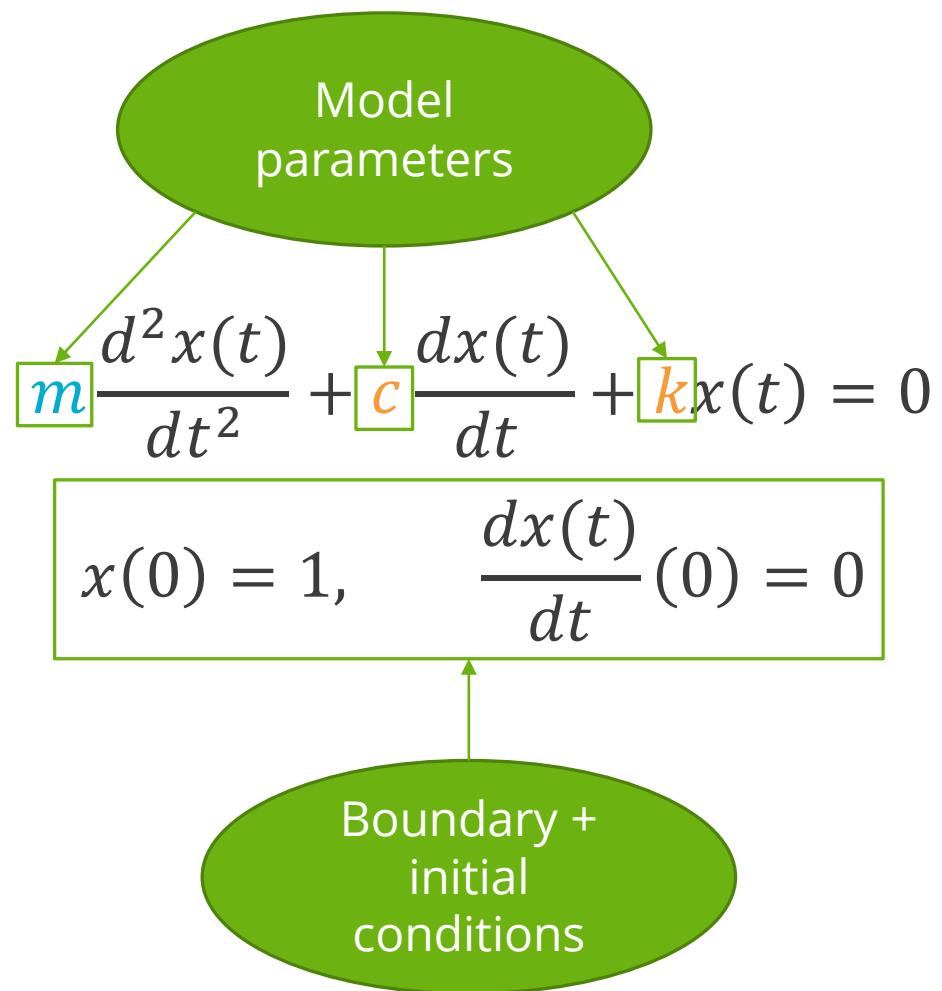


$$f_s + f_d \equiv F = ma \equiv m \frac{d^2x(t)}{dt^2}$$

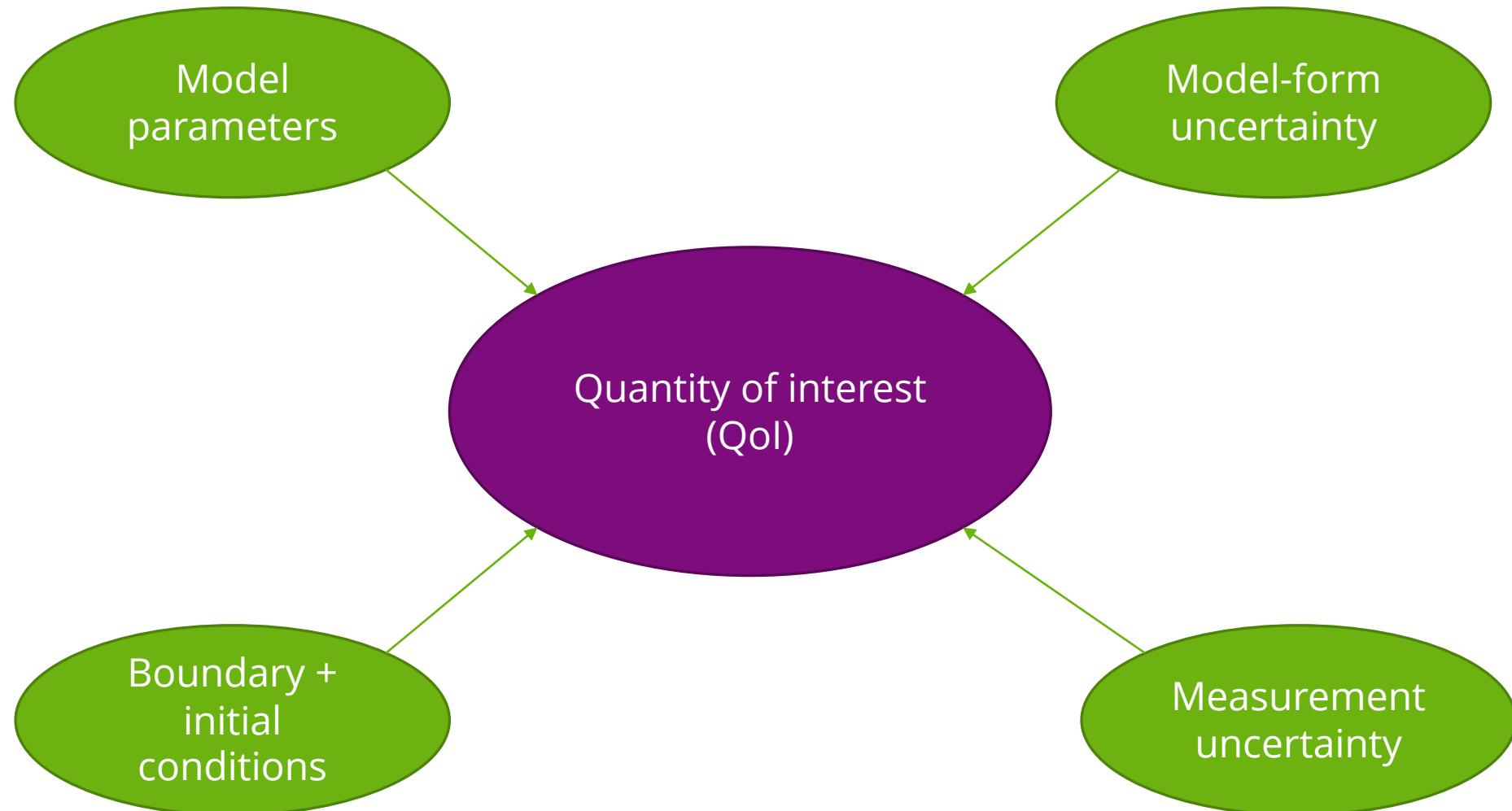
$$m \frac{d^2x(t)}{dt^2} + c \frac{dx(t)}{dt} + kx(t) = 0$$

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

Common sources of uncertainty



Result: uncertainty in model predictions



Real-world example

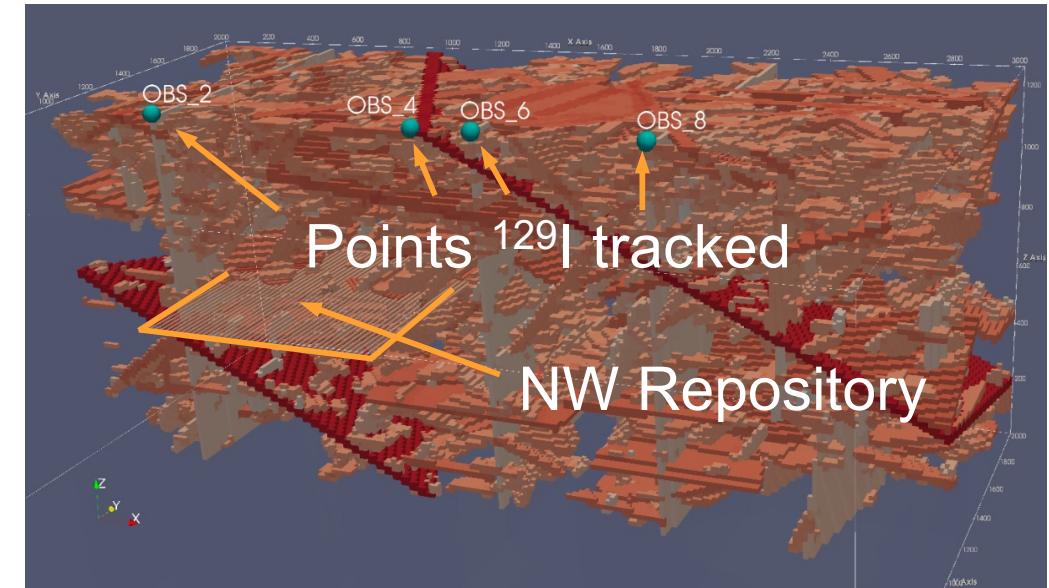
Quantity of Interest

- 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

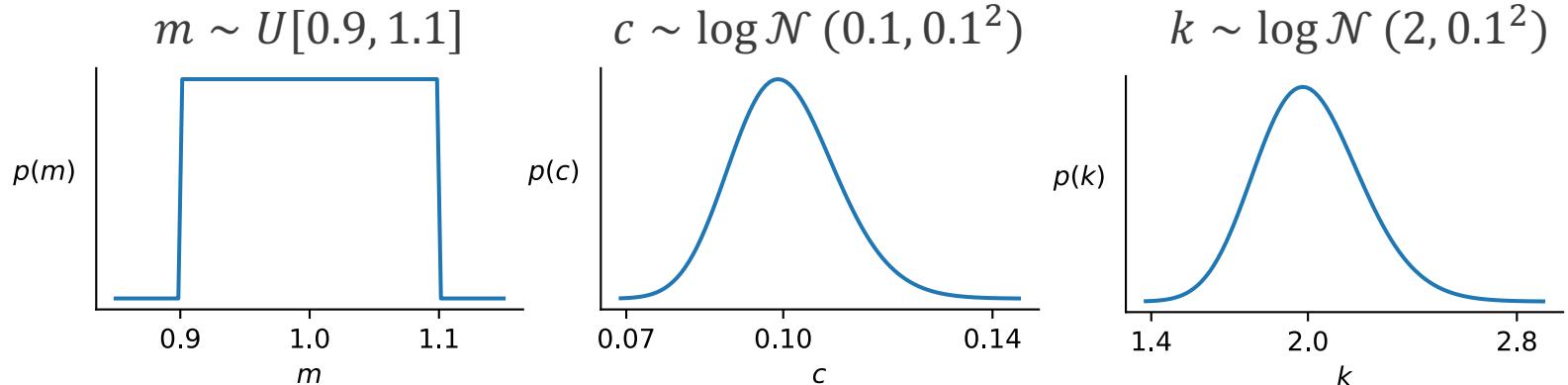




How do we *characterize* uncertainty?

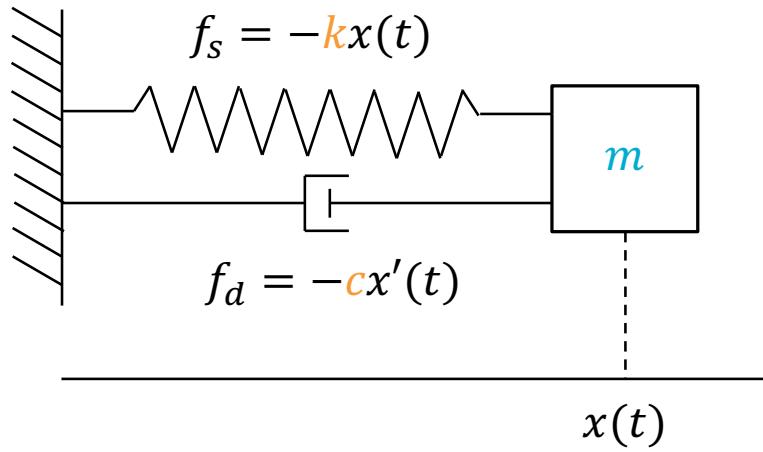
Represent sources of uncertainty as random variables (RVs)

Encode what is known through the parameterization of the RV

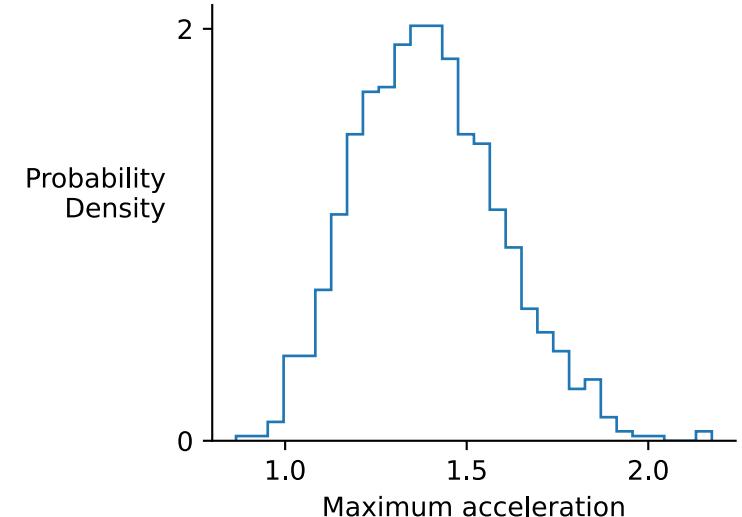
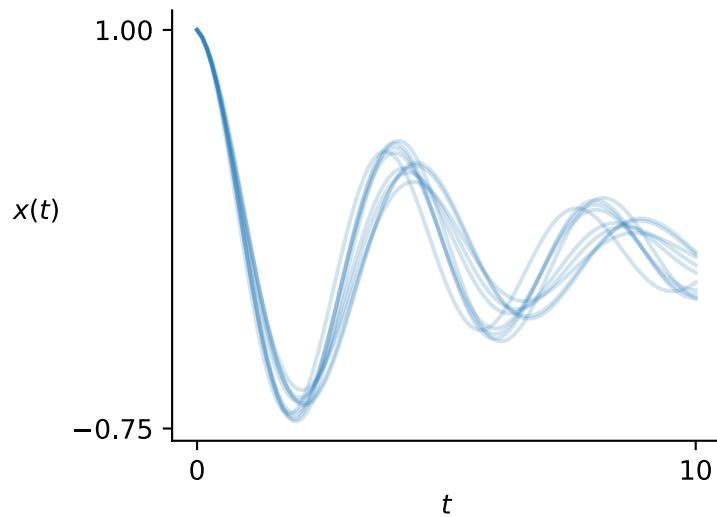


$$p_{\log \mathcal{N}(\mu, \sigma^2)}(x) \equiv \frac{1}{x \sigma \sqrt{2\pi}} \exp \left(-\frac{1}{2\sigma^2} (\log(x) - \mu)^2 \right)$$

How do we
quantify
uncertainty?



Propagate sources of uncertainty to Qols



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



How do we *reduce* uncertainty?

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

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

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

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

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

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

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

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



How do we
reduce
uncertainty?

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

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

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

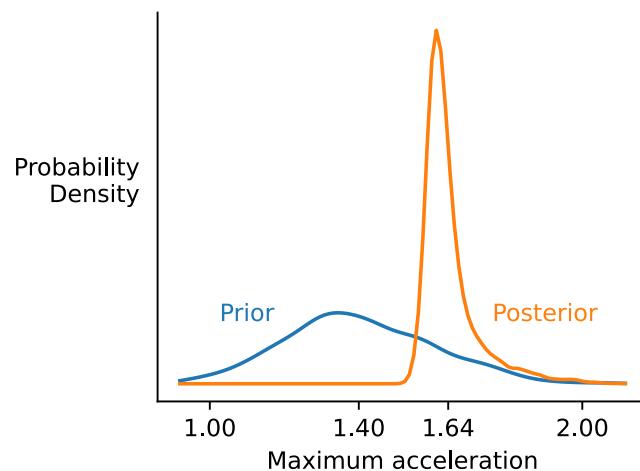
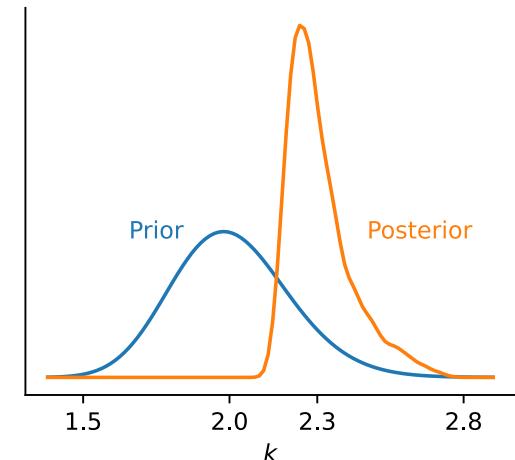
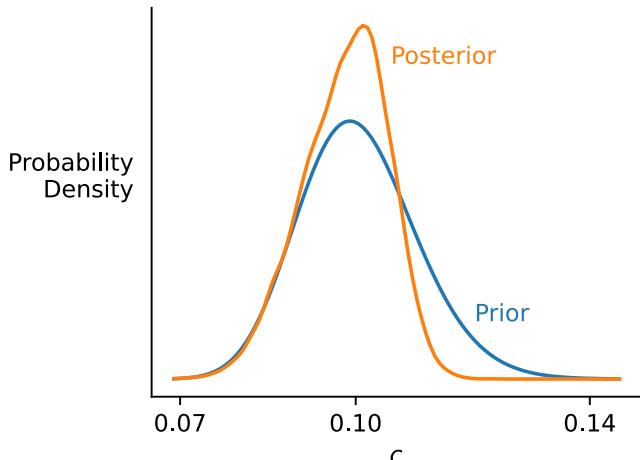
Bayes' Theorem

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



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



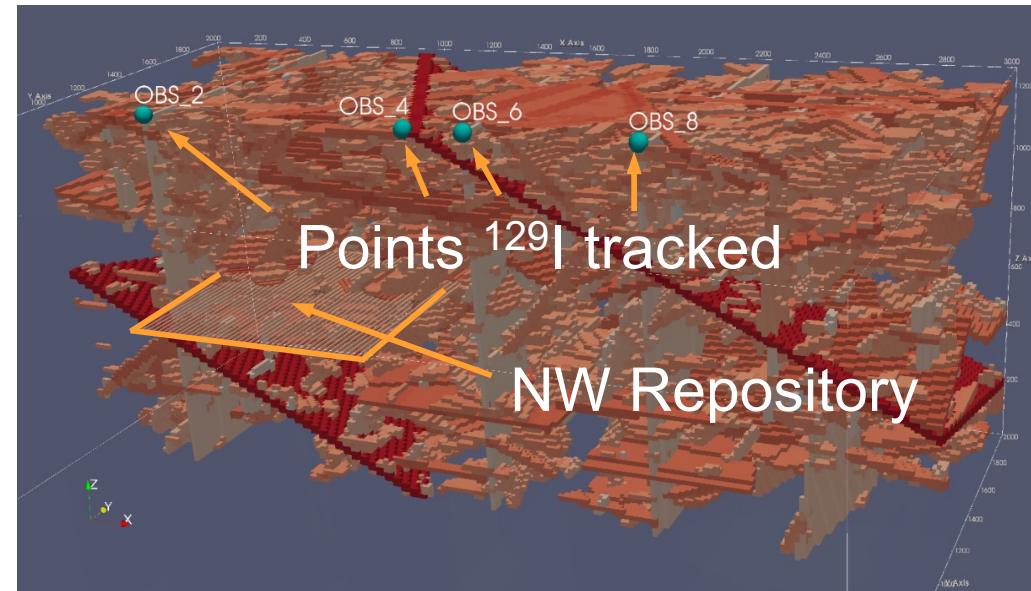
Data acquisition

- 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



Research areas in UQ



Reduc-order/surrogate
models

Bayesian inverse
problems

Multimodel methods

Optimal experimental
design

Sensitivity analysis

Algorithms for high
dimensionality

Model-form
uncertainty

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

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

Common statistical approaches

Gaussian processes [5,6]

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

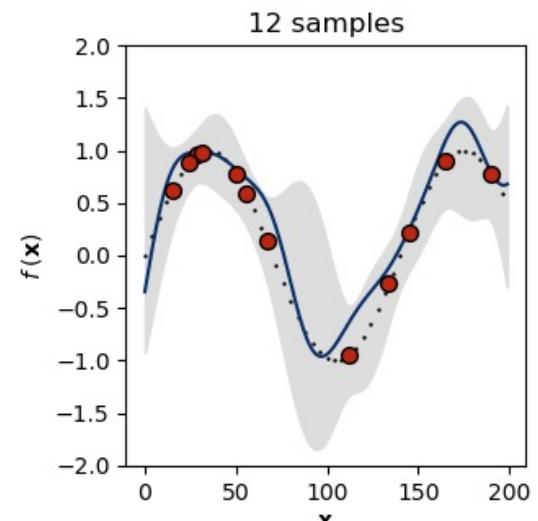
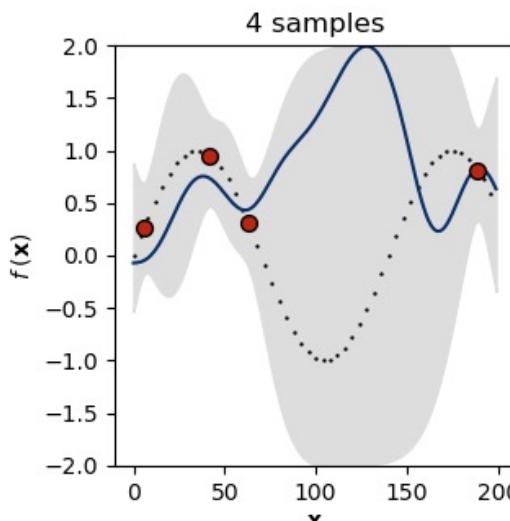
Common reduced-order model (ROM) approaches

Proper orthogonal decomposition [8,9]

Principal component analysis [10]

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

Reduc-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

Research areas in UQ



Reduc-order/surrogate
models

Bayesian inverse
problems

Multimodel methods

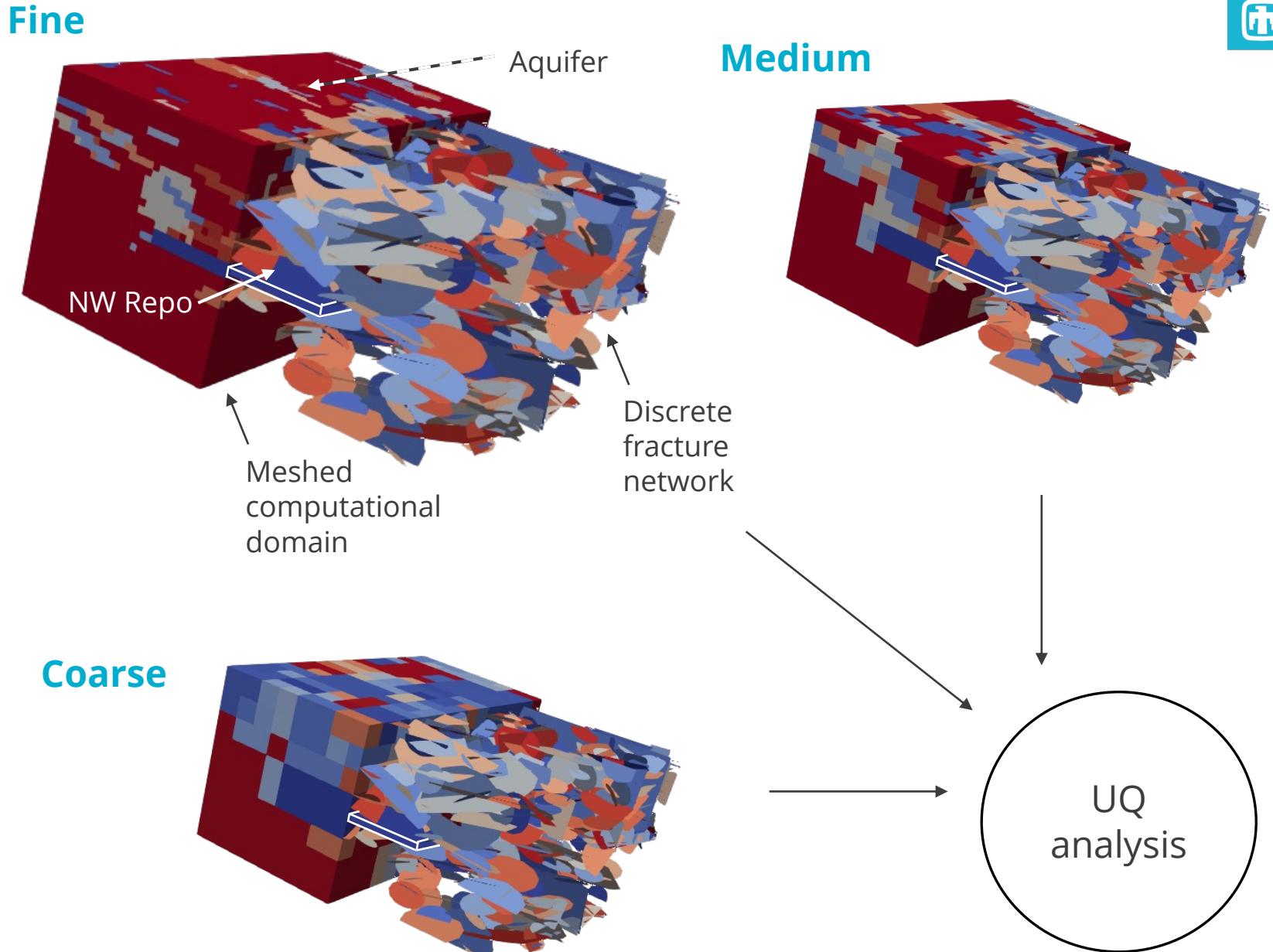
Optimal experimental
design

Sensitivity analysis

Algorithms for high
dimensionality

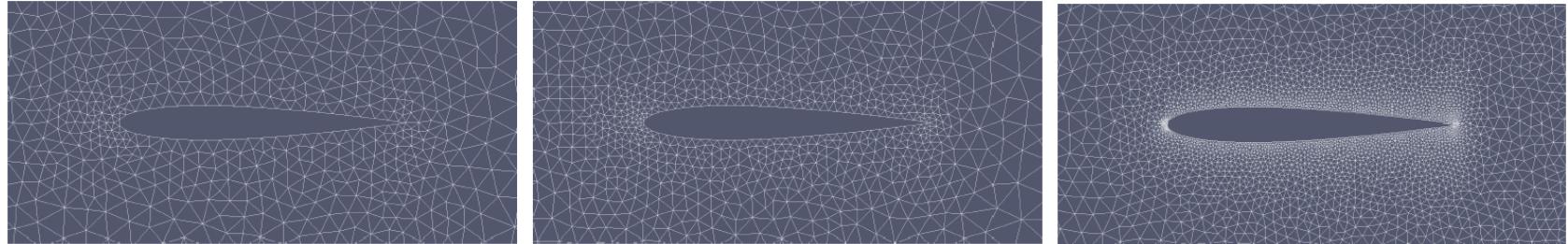
Model-form
uncertainty

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

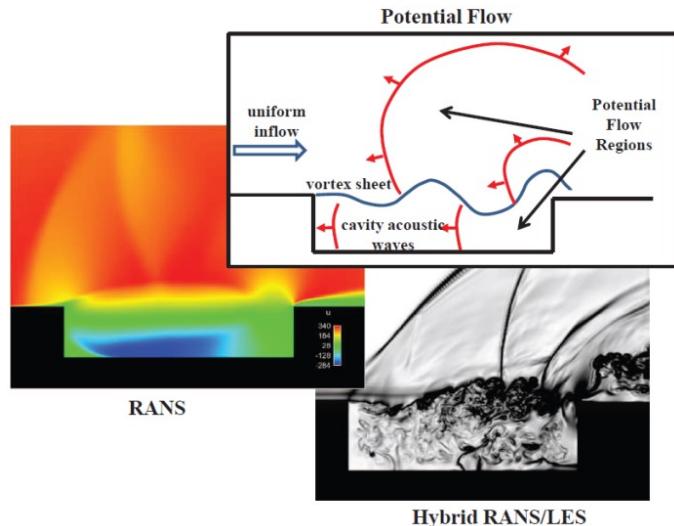


Idea: exploit lower-fidelity, cheaper models to lower cost for same accuracy

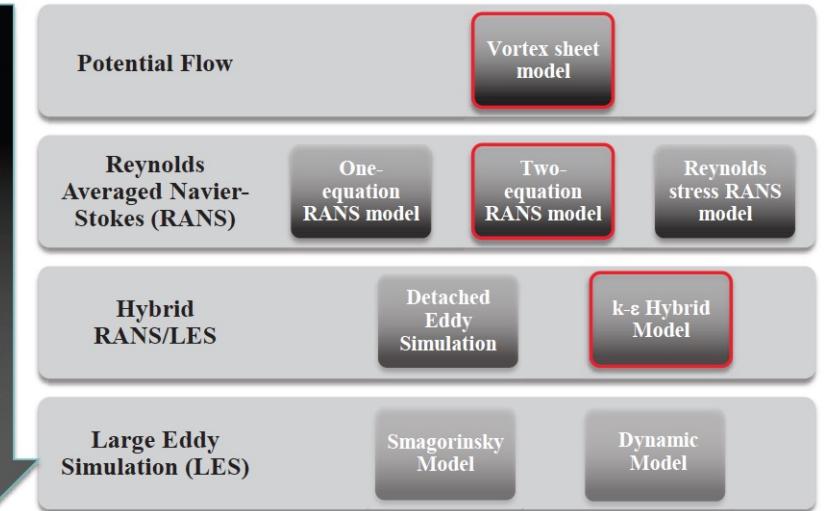
Discretization



Modeling assumptions



Increasing Model Fidelity



Sampling-based methods



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

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

Sampling-based methods – control variates

$$M_1(\theta)$$

$$c_1 = \frac{C_1}{C} \ll 1$$

$$\text{corr}(M, M_1) = \rho$$

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

$$\mathbb{E}[\widehat{M}_{CV}(\theta)] = \mathbb{E}[M] \quad \text{Unbiased}$$

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

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

$$\mathbb{V}[\widehat{M}_{CV}(\theta)] = \frac{\mathbb{V}[M]}{N}(1 - \rho^2)$$

$\rho^2 \approx 1 \rightarrow$ orders of magnitude reduction in variance

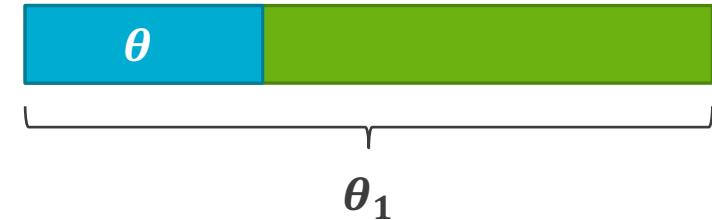
Sampling-based methods – beyond control variates



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

Multifidelity Monte Carlo [21]:

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



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

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

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

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)

Research areas in UQ



Reduc-order/surrogate
models

Bayesian inverse
problems

Multimodel methods

Optimal experimental
design

Sensitivity analysis

Algorithms for high
dimensionality

Model-form
uncertainty

Challenges and ongoing opportunities



$$p(d|\theta) = \frac{p(d|\theta)p(\theta)}{\int p(d|\theta)p(\theta)d\theta}$$

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

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

Markov Chain Monte Carlo [14,16-18,19] and Variational Inference [19] methods numerically approximate $p(\theta|d)$ --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

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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

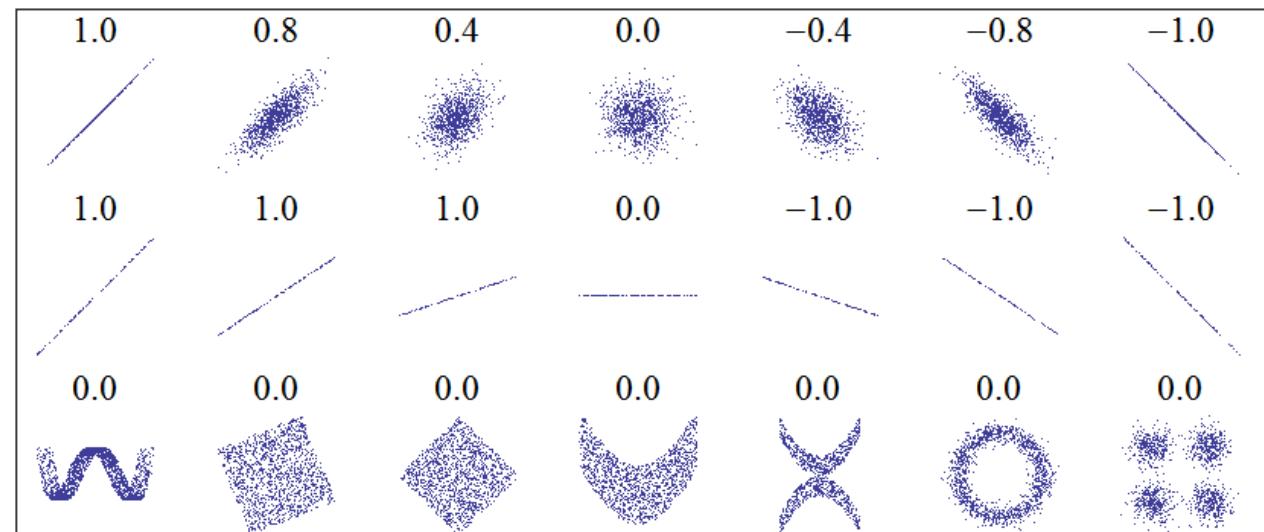
Correlation coefficients

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

Estimated from input/output samples

Slope doesn't matter, just strength of linear relationship

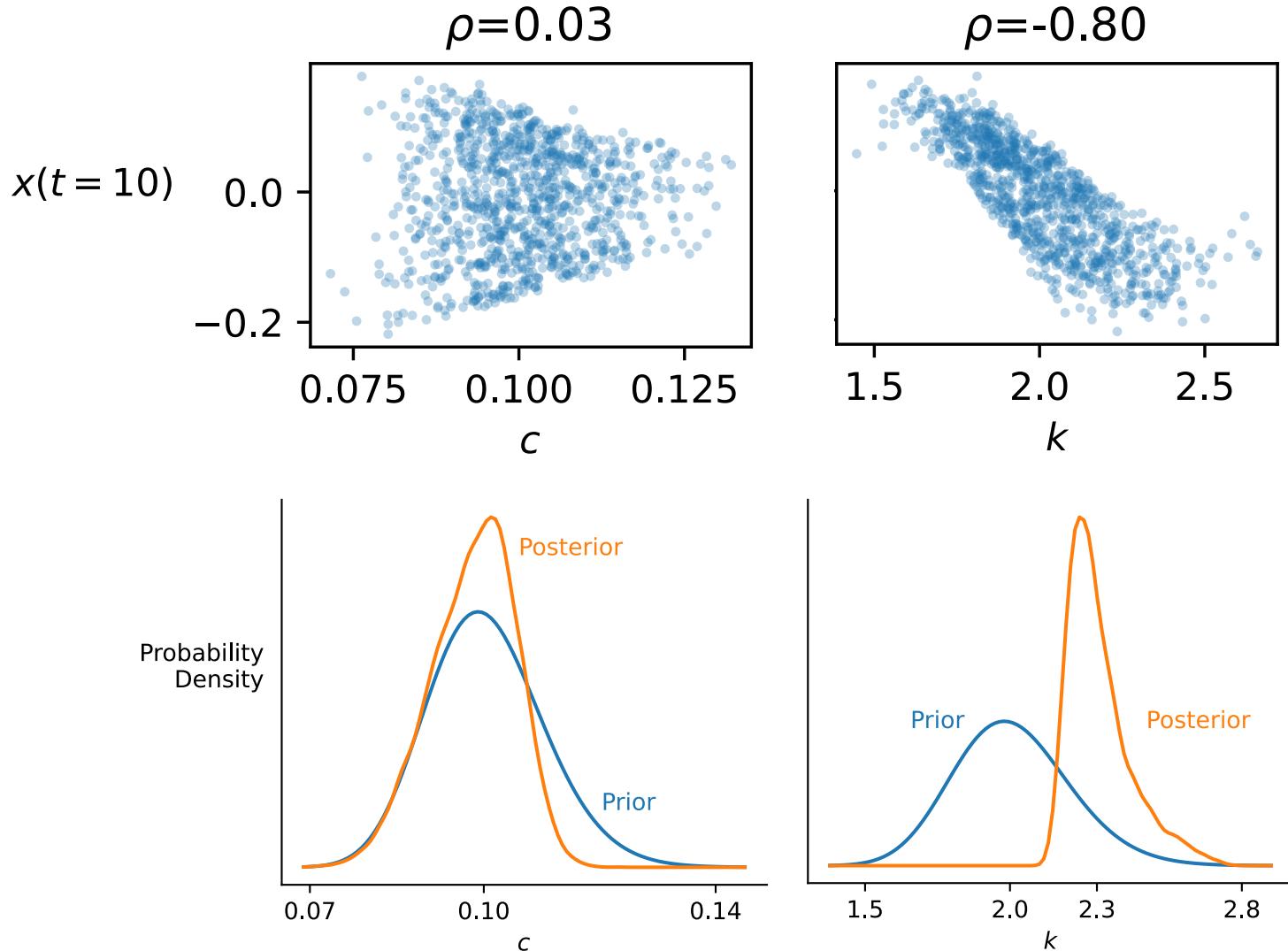
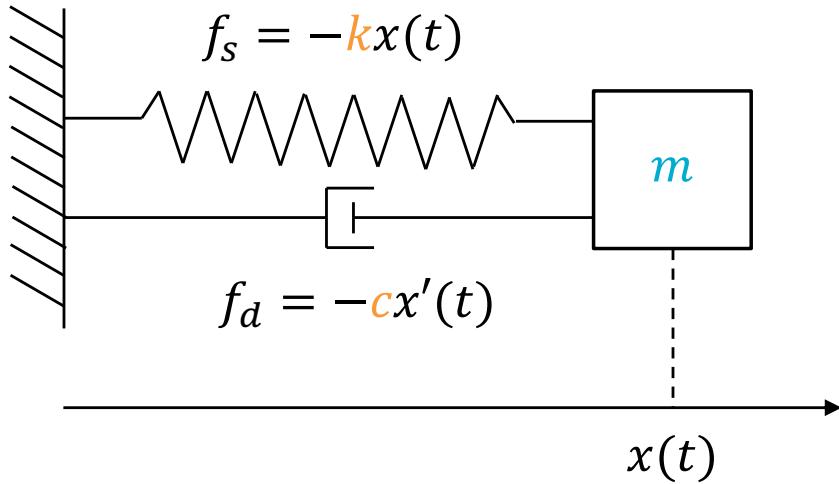
Nonlinear/nonmonotonic dependencies will not be detected.



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]

$$S_i = \frac{\mathbb{V}_{\theta_i} [\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[M|\theta_i]]}{\mathbb{V}[M]}$$

Effect of varying θ_i alone (averaging over other inputs)

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

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

Reduc-order/surrogate models

Optimal experimental design

Sensitivity analysis

Algorithms for high dimensionality

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

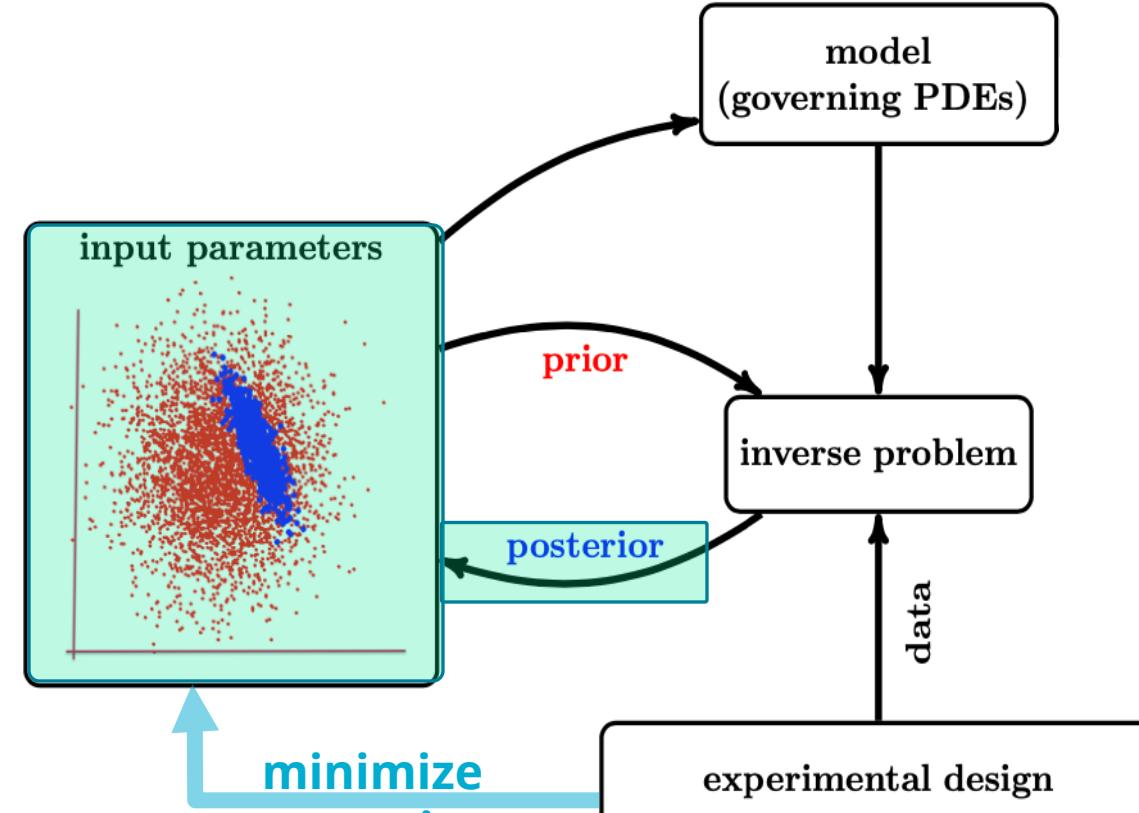


Figure courtesy of [34]

Slide courtesy of Rebekah White

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

$$d(w)$$

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

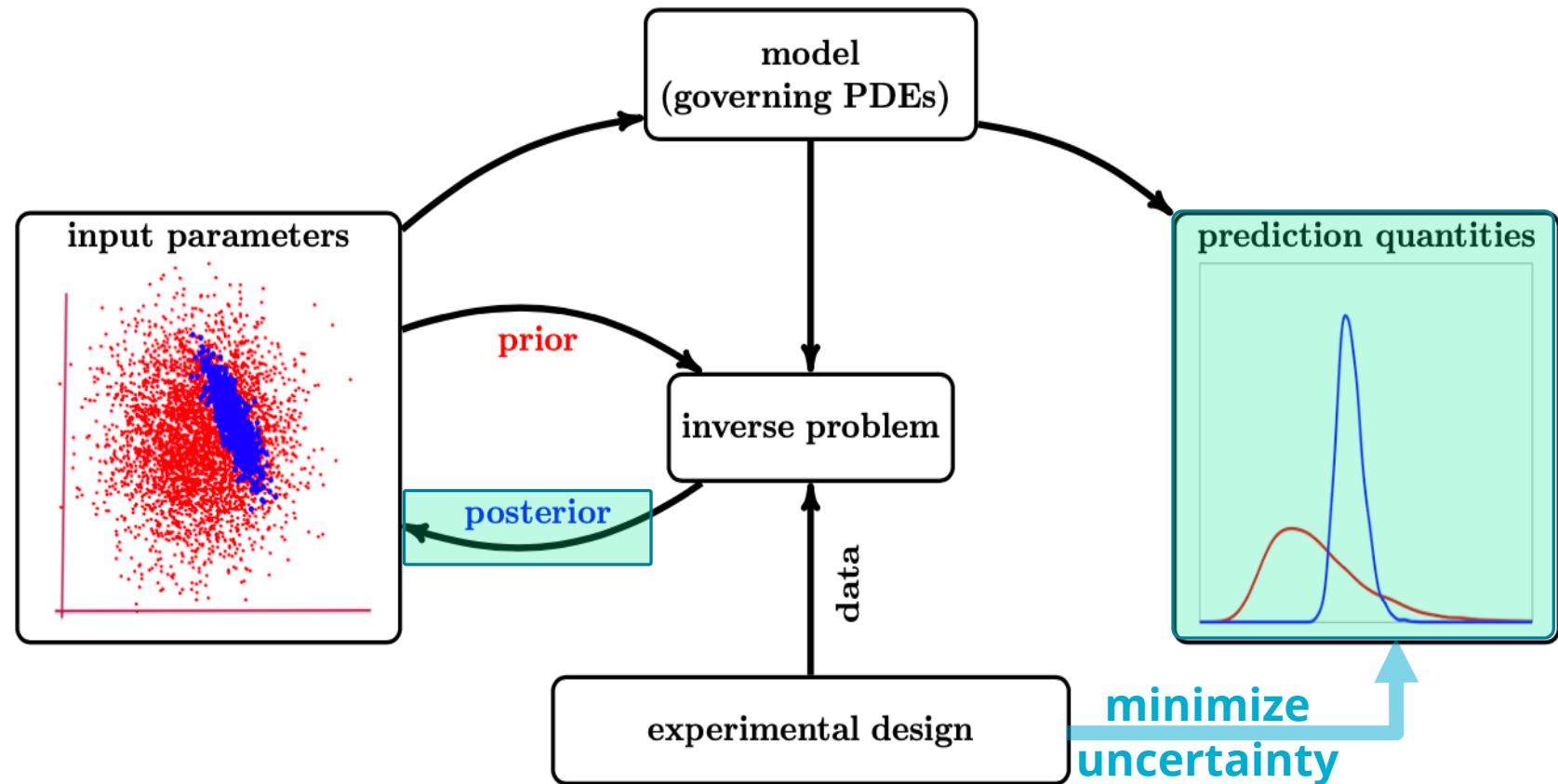


Figure courtesy of [34]

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Research areas in UQ



Efficient forward propagation

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Reduc-order/surrogate models

Optimal experimental design

Sensitivity analysis

Algorithms for high dimensionality

Model-form uncertainty

Come to my talk tomorrow!



Thanks!

teresaportone.com

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