05/15/2022

Active learning for computational simulations: Application to TRISO fuel failure analysis

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Workshop on scientific machine learning for nuclear engineering applications

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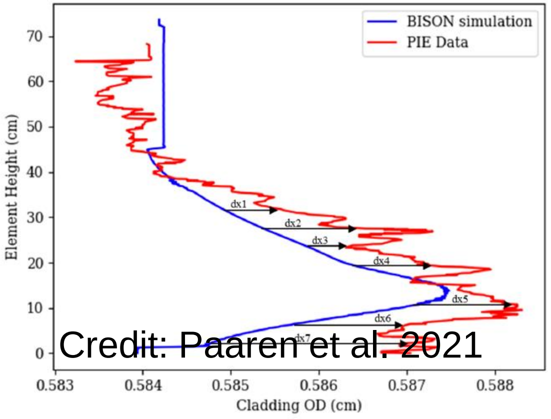
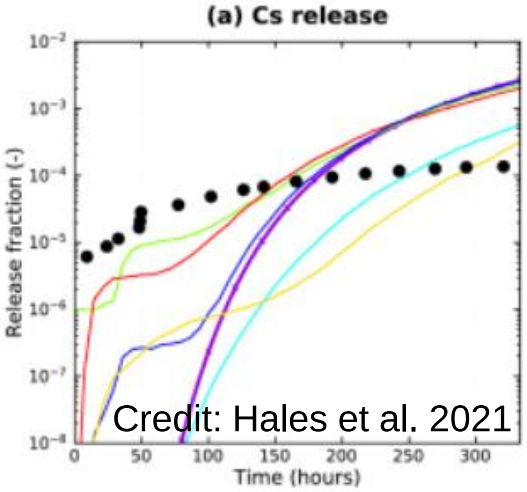
Motivation: Computational Modeling and Simulations

Forward modeling

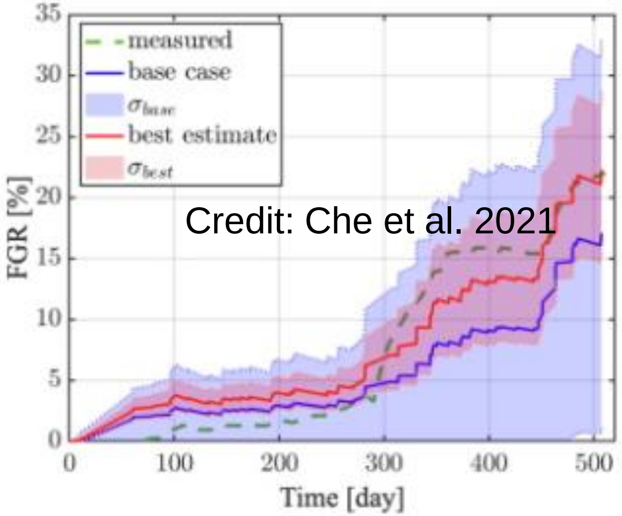


Credit: Paaren et al. 2021



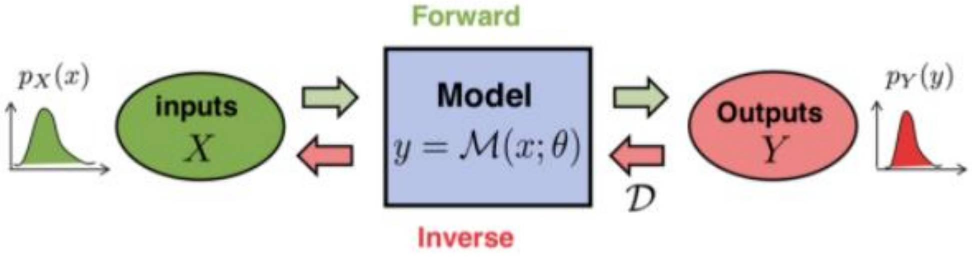
Credit: Hales et al. 2021

Inverse modeling



Credit: Che et al. 2021

Coupled modeling



Credit: Zhang 2020

Probabilistic ML: UQ + ML

- Data
  - High quality, small amount
  - Low quality, large (or small) amount

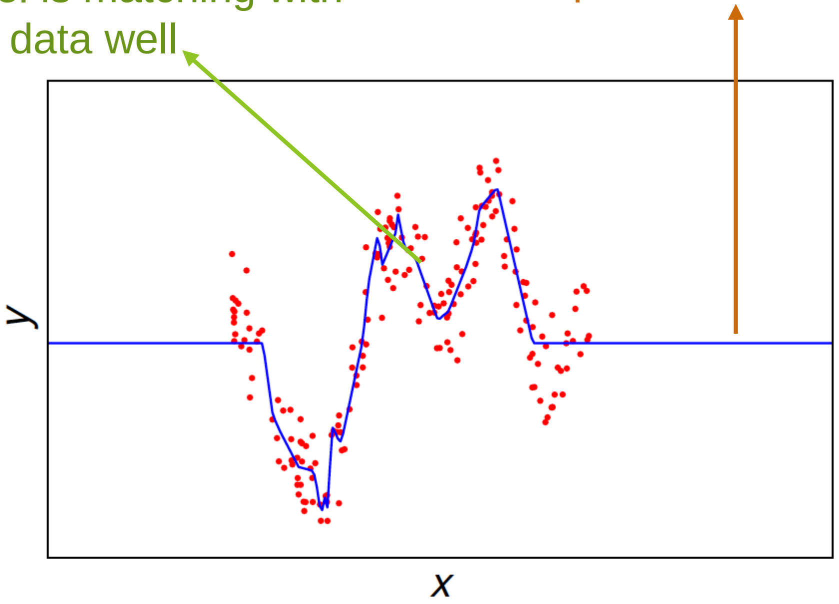
- Computational simulations are inherently inaccurate (Hendrickson 2020 DOE ASCR@40)
  - Modeling uncertainties (known knowns)
  - Epistemic uncertainties (known unknowns)
  - Aleatoric uncertainties (unknown unknowns)

- Increased complexity with the use of ML to accelerate modeling and simulations

- **UQ critical to assess the reliability of model predictions**

UQ ML

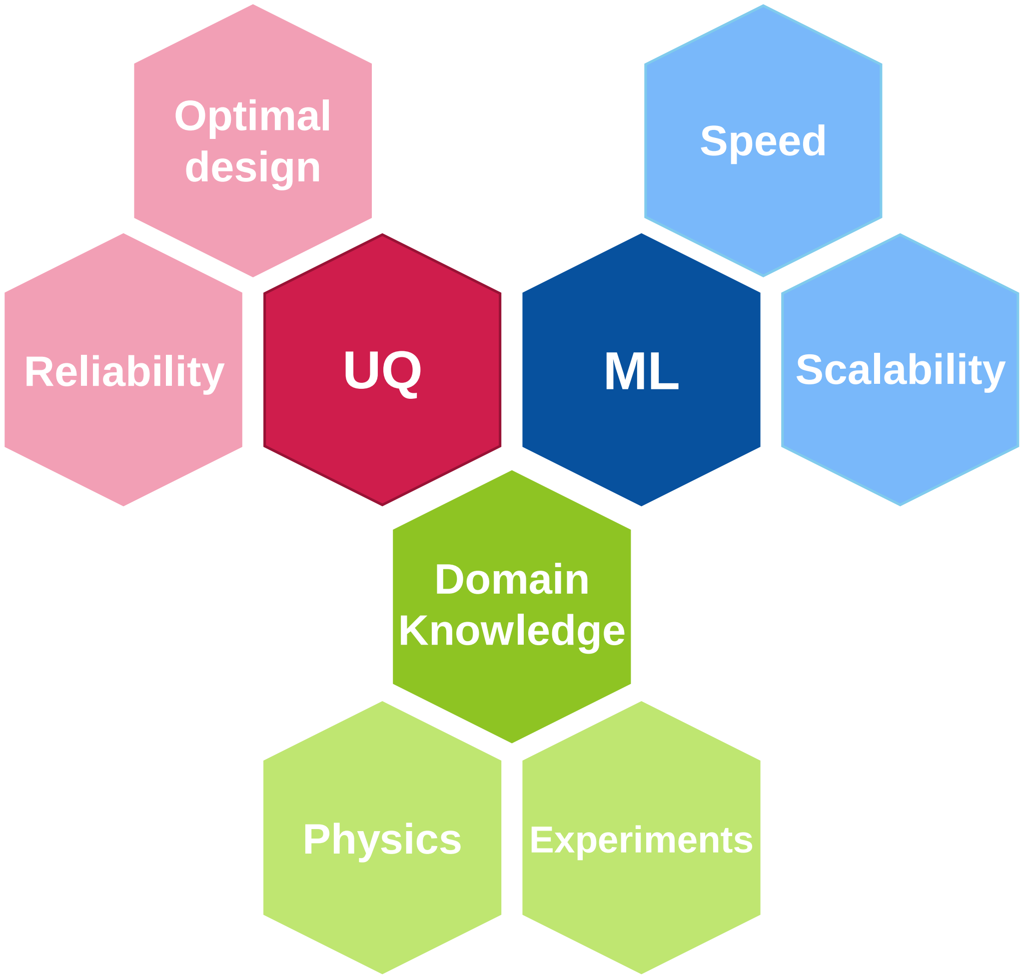
- All models are wrong, but models that know when they're wrong are useful (Lakshminarayanan et al. 2021)



(Credit: Ober et al. 2021)

Outline

- **Prediction**
  - Deterministic and Bayesian predictions
  - A simple Bayesian surrogate: Gaussian Process
  - Beyond Gaussian Processes
- **Inference**
  - Sampling
  - Markov Chain Monte Carlo
  - Beyond MCMC: Hybrid MCMC and sampling as optimization
- **Active learning and Multifidelity modeling**
- **TRISO nuclear fuel failure analysis**
- **Ongoing work:**
  - **MOOSE stochastic tools module**
  - **Monte Carlo with Hamiltonian Neural Nets**



Combo of the above three benefits computational tasks

Prediction

- Prediction problem:

$$\boldsymbol{y} = f(\boldsymbol{x};\, \boldsymbol{\theta})$$

$$\boldsymbol{\theta}^* = Argmin_{\boldsymbol{\theta}}\, \boldsymbol{L} \qquad [= Argmax_{\boldsymbol{\theta}}\, p(\boldsymbol{y}|\boldsymbol{x};\, \boldsymbol{\theta})]$$

- **Blackbox prediction**

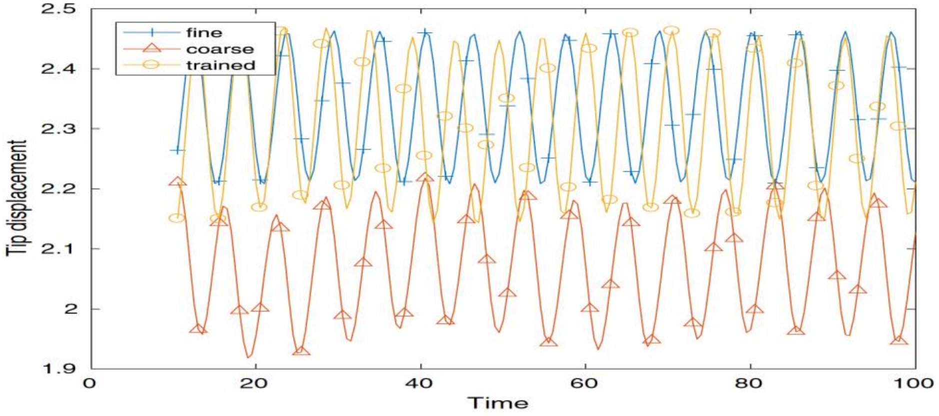
- **Auxiliary mesh refinement:** Baiges et al. 2019 Neural network correction term in linear algebraic equations

- **Constitutive relations:** Wang et al. 2019 Reinforcement Learning to combine phenomenological and data-driven relations

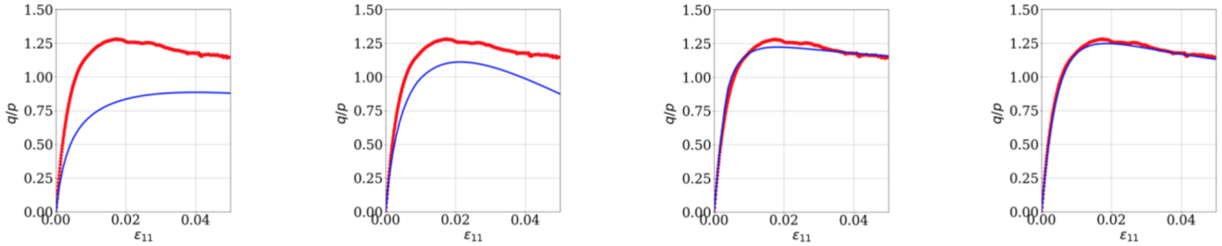
- **Physics in loss function:** Raissi et al. 2019 With training set loss, incorporate differential eq loss and IC/BC loss (Perdikaris 2020, LLNL seminar)

- **Eighty Years of FEM by Liu, Li, and Park 2021**

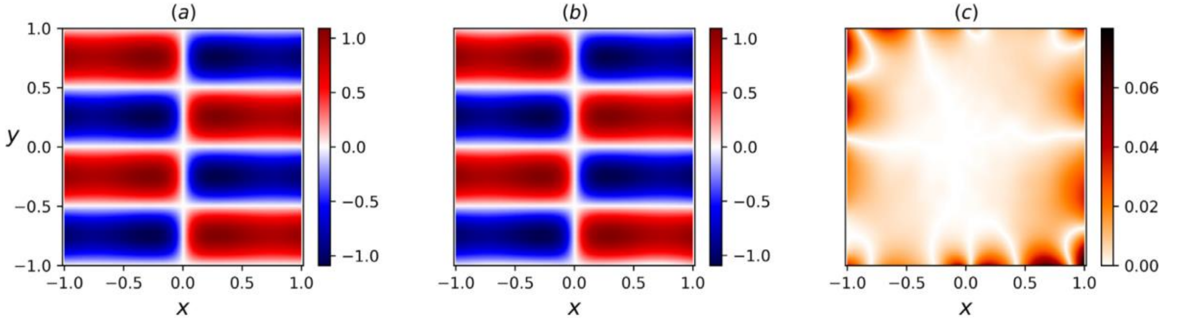
Fluid-structure interaction Credit: Baiges et al. 2019



Soil constitutive behavior prediction Credit: Wang et al. 2019

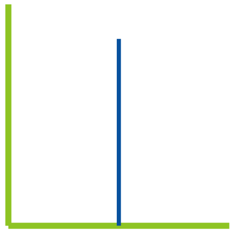


Heat eqn. Credit: Haghighat and Juanes 2019



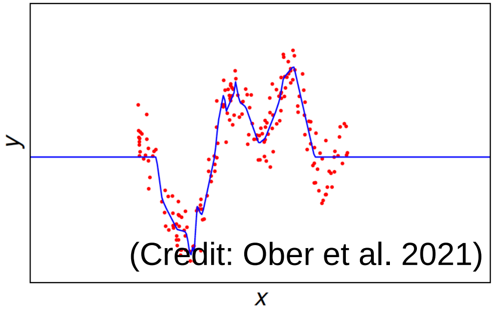
Deterministic and Bayesian predictions

- Define $\boldsymbol{y} = f(\boldsymbol{x};\ \boldsymbol{\theta})$
- Solve $\boldsymbol{\theta}^* = Argmax_{\boldsymbol{\theta}}\, p(\boldsymbol{y}|\boldsymbol{x};\ \boldsymbol{\theta})$



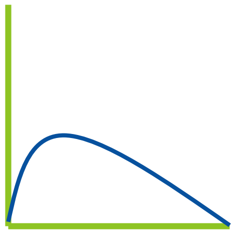
θ^*

- Predict $\boldsymbol{y} = f(\boldsymbol{x}; \boldsymbol{\theta}^*)$



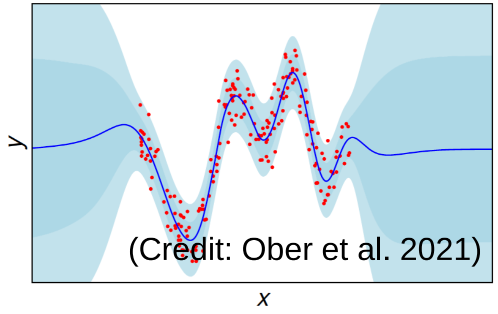
(Credit: Ober et al. 2021)

- Define $\boldsymbol{y} = f(\boldsymbol{x};\ \boldsymbol{\theta})$
- Solve $p(\boldsymbol{\theta}|\boldsymbol{x}, \boldsymbol{y}) \propto p(\boldsymbol{y}|\boldsymbol{x};\ \boldsymbol{\theta})\, p(\boldsymbol{\theta})$ [Hoff 2009]



θ

- Predict $p(\boldsymbol{y}|\boldsymbol{x}) = \int p(\boldsymbol{y}|\boldsymbol{x};\ \boldsymbol{\theta})\, p(\boldsymbol{\theta}|\boldsymbol{x}, \boldsymbol{y})\ d\theta$ [Do 2008]

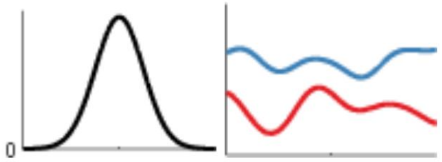


(Credit: Ober et al. 2021)

A simple Bayesian surrogate: Gaussian Process

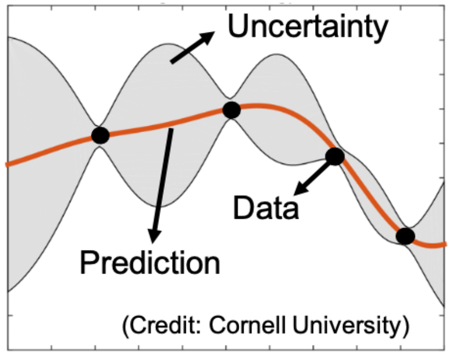
- Probabilities over functions: $f(\boldsymbol{X}) \sim \mathcal{N}(m(\boldsymbol{X}), k(\boldsymbol{X}, \boldsymbol{X}'))$
- Predictive distribution:

$$p(\boldsymbol{y}_* \mid \boldsymbol{X}, \boldsymbol{X}_*, \boldsymbol{y}) \sim \mathcal{N}\Big(k(\boldsymbol{X}_*, \boldsymbol{X})\, k(\boldsymbol{X}, \boldsymbol{X})^{-1}\, \boldsymbol{y},\; k(\boldsymbol{X}_*, \boldsymbol{X}_*) - k(\boldsymbol{X}_*, \boldsymbol{X})\, k(\boldsymbol{X}, \boldsymbol{X})^{-1}\, k(\boldsymbol{X}, \boldsymbol{X}_*) \Big)$$



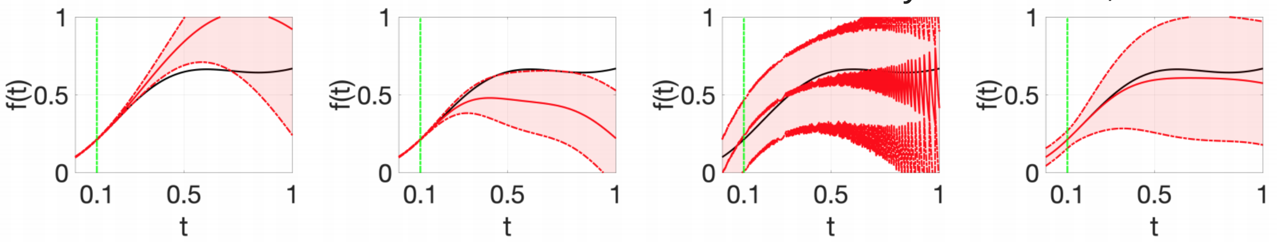
$$k_{\mathrm{SE}}(x, x') = \sigma^2 \exp\left(-\frac{(x-x')^2}{2\ell^2}\right)$$

(Kernel Cookbook by Duvenaud)



- Closed form solution; kernel params optimized using SGD
- SE kernel: Universal approximator [Micchelli et al. 2006]
- Robust UQ

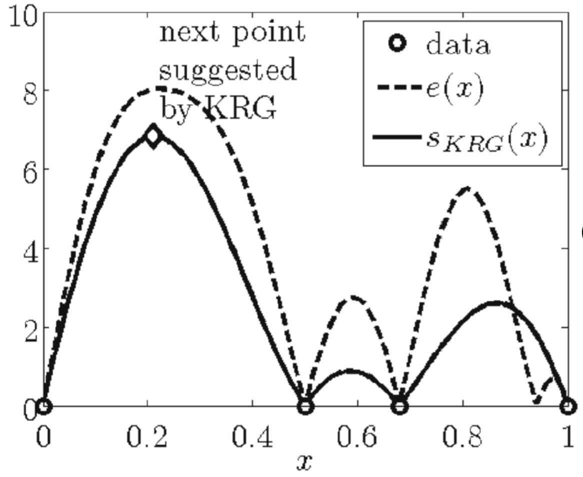
1st order ODE Credit: Anonymous 2021, ICLR



(a) SKL (b) DKL (c) LFM (d) PI-DKL

- **Physics in Gaussian Process:** Anonymous 2021, ICLR Physics informed neural network embedded in GP kernel (technically called deep kernel learning)

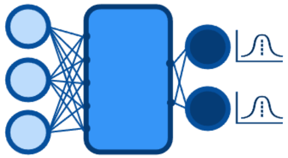
- **Optimal design:** Viana et al. 2021 Gaussian process UQ estimate tells the next best training point



Credit: Viana et al. 2021

Beyond Gaussian Processes

- GP limitations: Excessive smoothing, high-dimensional data, Complexity O(n^3)
- BNN: Bayesian Neural Network

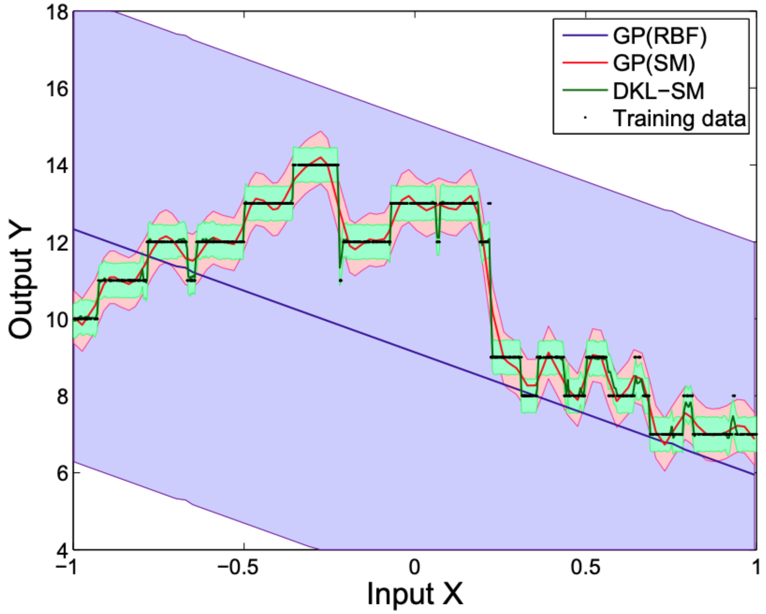


- Bayesian surrogates:

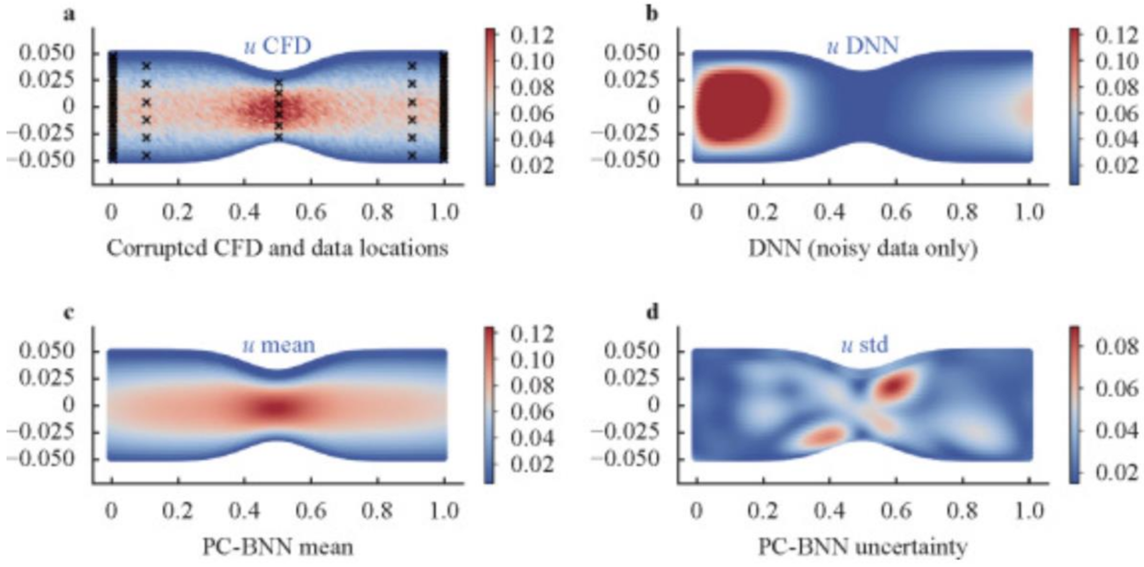
A spectrum of Bayesian predictive models* [Dhulipala et al. 2021]

- **Navier-Stokes embedded BNN:** Sun and Wang 2020 Flow reconstruction from sparse and noisy data

Step function Credit: Wilson et al. 2016



BNN with Navier-Stokes Credit: Sun and Wang 2020



*This is incomplete and for illustration only

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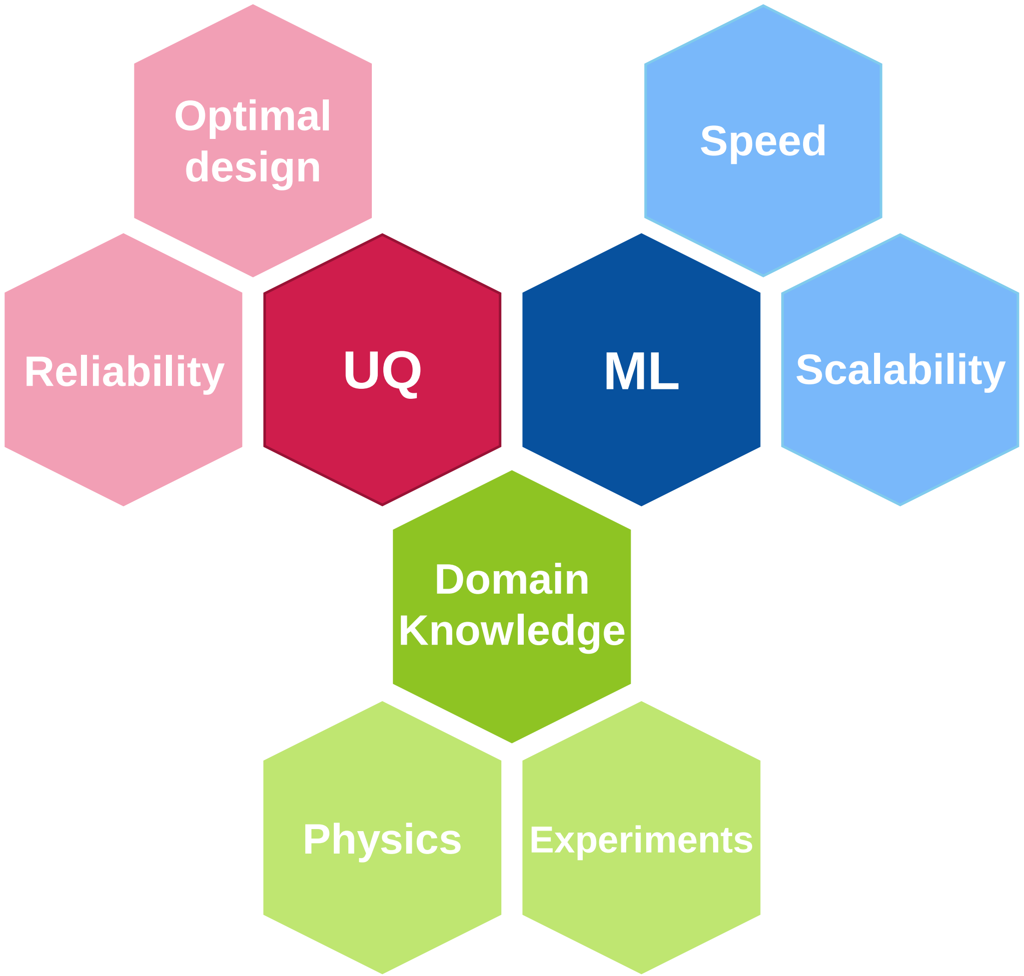

Combo of the above three benefits computational tasks

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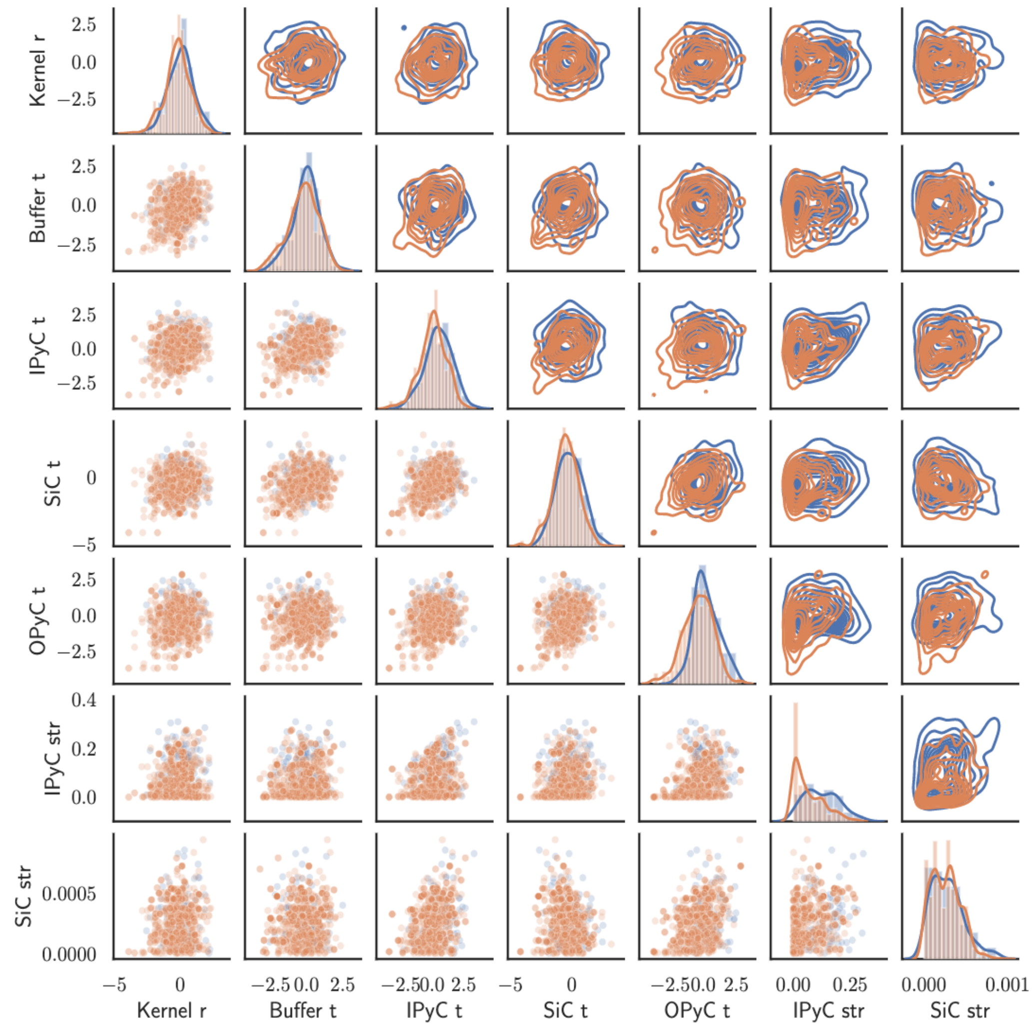
Inference: Sampling

- Probability distributions of input parameters that cause TRISO particle failure (Jiang et al. 2021)
- Update BISON fission gas release models given experimental data (Che et al. 2021)
- Parameter distributions of a Bayesian Neural Network

$$f(\boldsymbol{\theta}|\boldsymbol{Data})$$

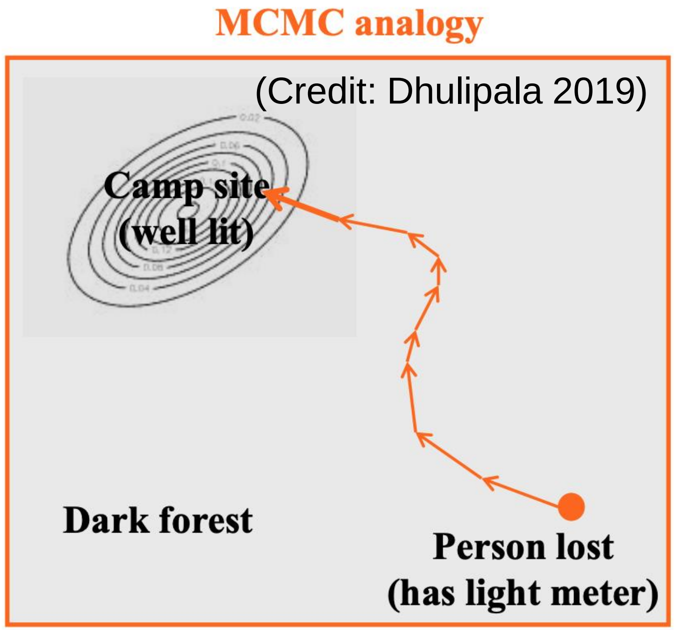
- Standard methods like Monte Carlo or Latin Hypercube very expensive or not applicable
- So, how do we sample efficiently from conditional distributions?

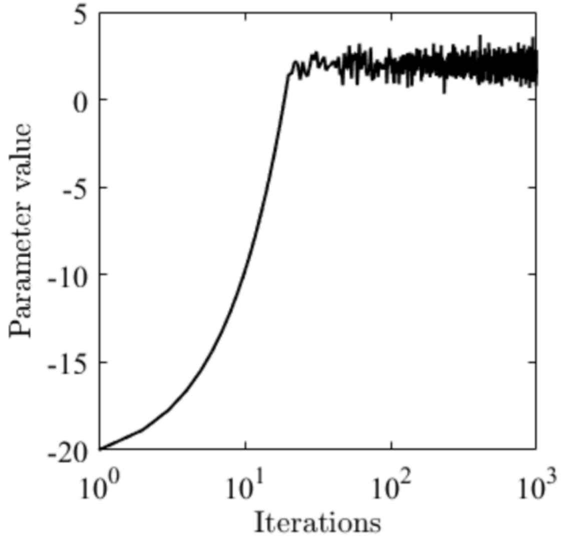


Distributions of input parameters causing TRISO particle failures

Markov Chain Monte Carlo

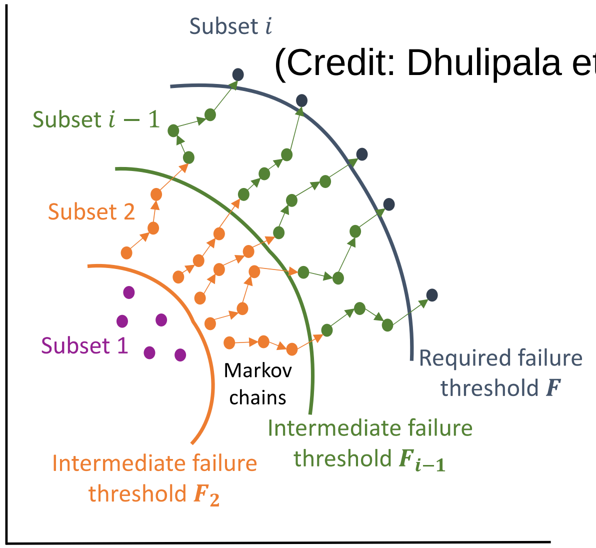
- Sample efficiently from conditional distributions $f(\boldsymbol{\theta}|\boldsymbol{Data})$
- **Dark forest:** Parameter space
- **Well lit camp site:** Required distribution to be sampled from
- **Light meter:** Acceptance ratio (or transition operator)
- Metropolis-Hastings: Popular MCMC algorithm (being implemented in MOOSE)
- **Does an MCMC algorithm always converge to the required distribution?**
  - Neal 1993 Detailed balance sufficient condition
  - Acceptance ratio satisfies detailed balance
- Variants of MCMC exist on how acceptance ratio designed



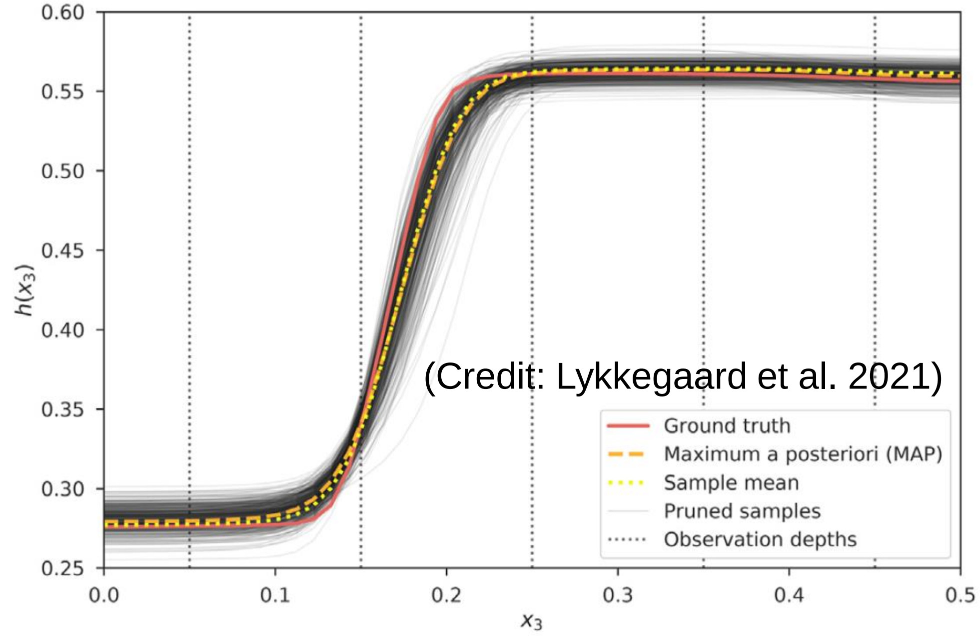


MCMC: Applications in the Computational Sciences

- **Rare events:** Dhulipala et al. 2021 Sample from parameter spaces that causes FE model to fail (Subset Simulation)
- **Inverse analysis:** Lykkegaard et al. 2021 Update porous flow model given ground water data
- **High-dimensional integration:** Mancang et al. 2011 Neutron transport equation using MCNP with MCMC techniques



(Credit: Dhulipala et al. 2021)



(Credit: Lykkegaard et al. 2021)

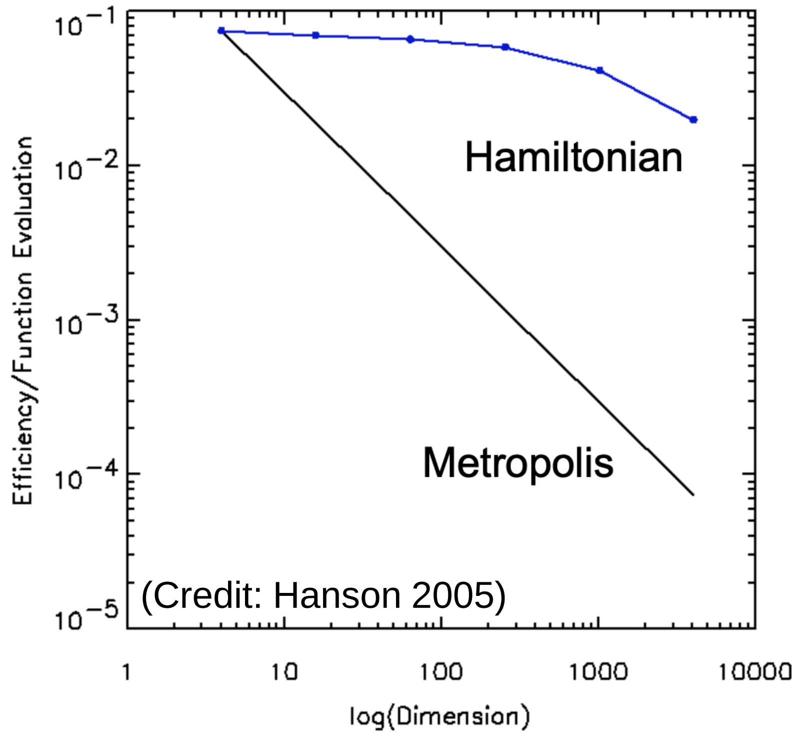
Beyond MCMC: Hybrid MCMC and sampling as optimization

- **MCMC limitations:** Poor high-dimensional scalability (convergence issues), many model evaluations required

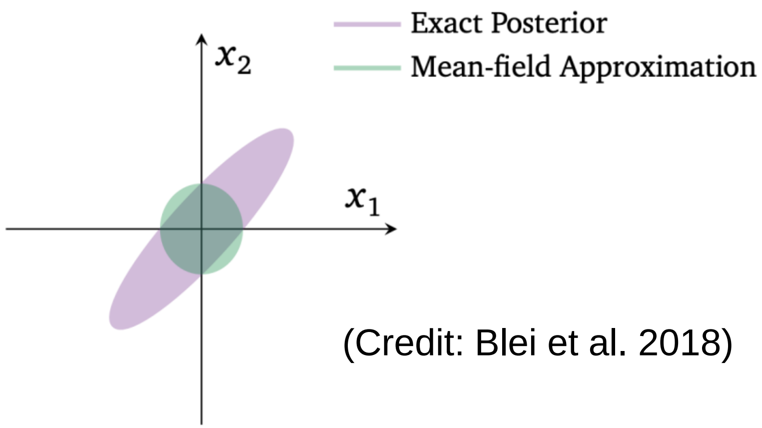
- **Hybrid MCMC (Hamiltonian Monte Carlo):** Neal 2011 Hamiltonian dynamics solved to propose the next sample. Very good scalability (Current “gold standard” for Bayesian Neural Networks)

$$z_1 = z_0 + \int_{t_0}^{t_1} \boldsymbol{I}\ \nabla H(\boldsymbol{z})\ dt$$

- **Optimization (approximate):** Blei et al. 2018 Variational inference transforms sampling to optimization. A variational family of distributions is assumed (e.g., exponential family). Distribution parameters are optimized



(Credit: Hanson 2005)



(Credit: Blei et al. 2018)

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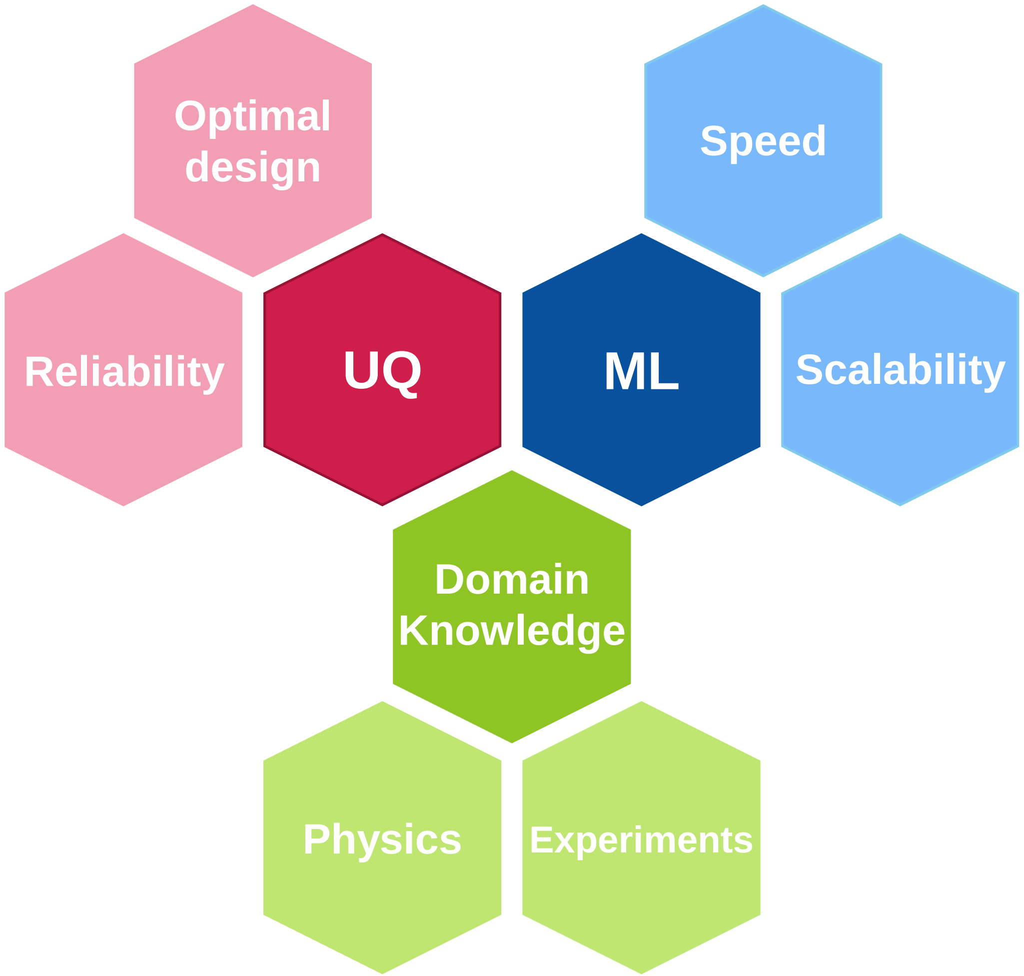
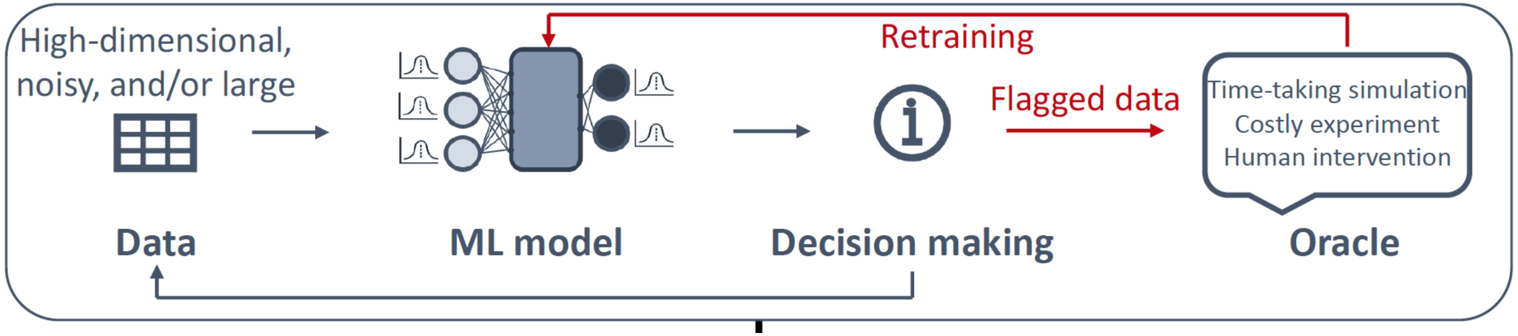


Combo of the above three benefits computational tasks

Active learning

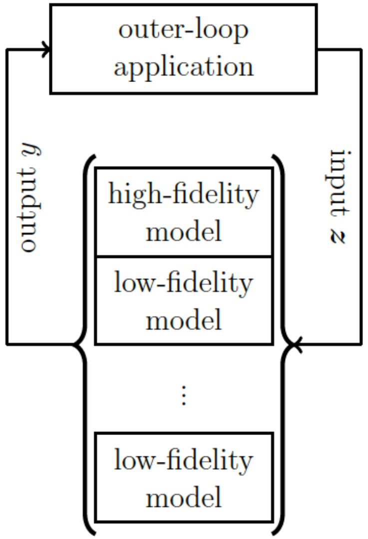
Principle of active learning (Bayesian ML model preferred)



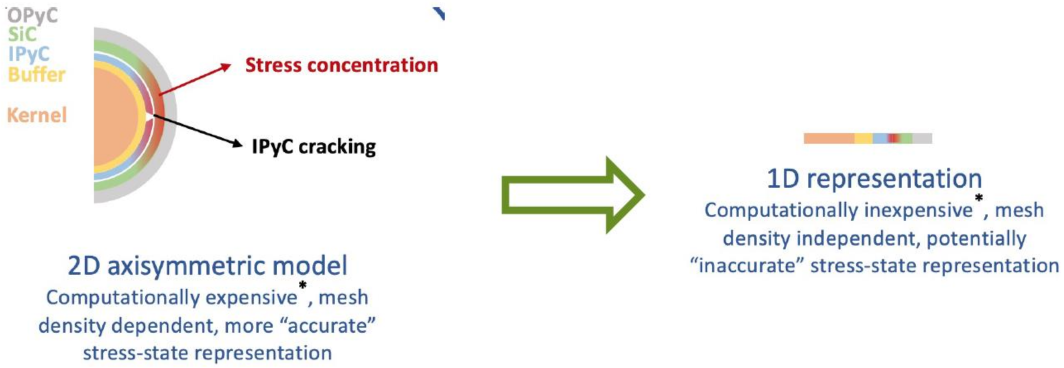
- ML model actively decides the next optimal training point
- Useful when dealing with expensive computational models or costly experiments as the ML model identifies the training point such that the information gain is optimized
- Probabilistic (Bayesian) ML preferred as it provides prediction uncertainty estimates---useful for designing learning functions

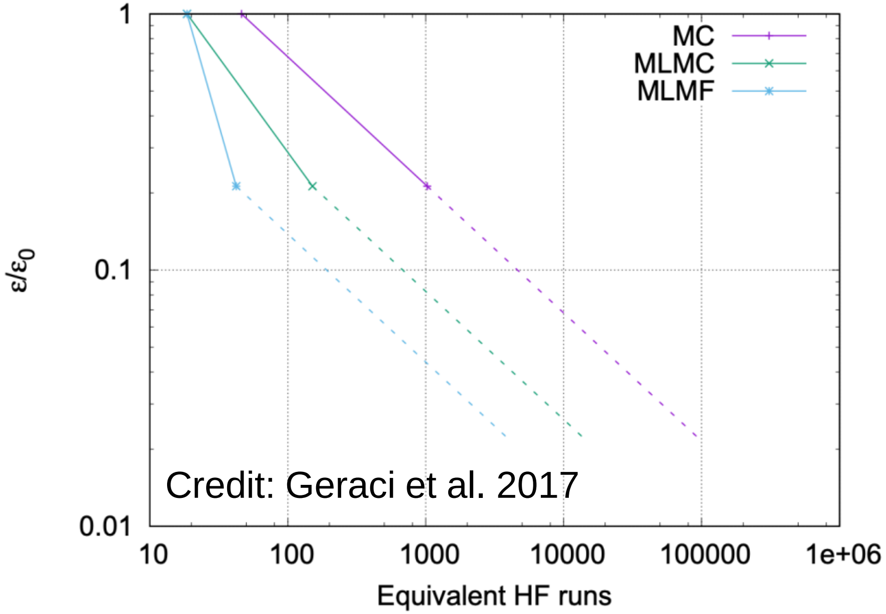
Multifidelity modeling

- TRISO model is a good example
- Pehertorfer et al. 2018 Multiple low-fidelity models can be considered
- Computational budget across multiple fidelity models constrained. Gorodetsky et al. 2020 approximate control variates framework
- Actively decide which modeling fidelity to call



Credit: Pehertorfer et al. 2018





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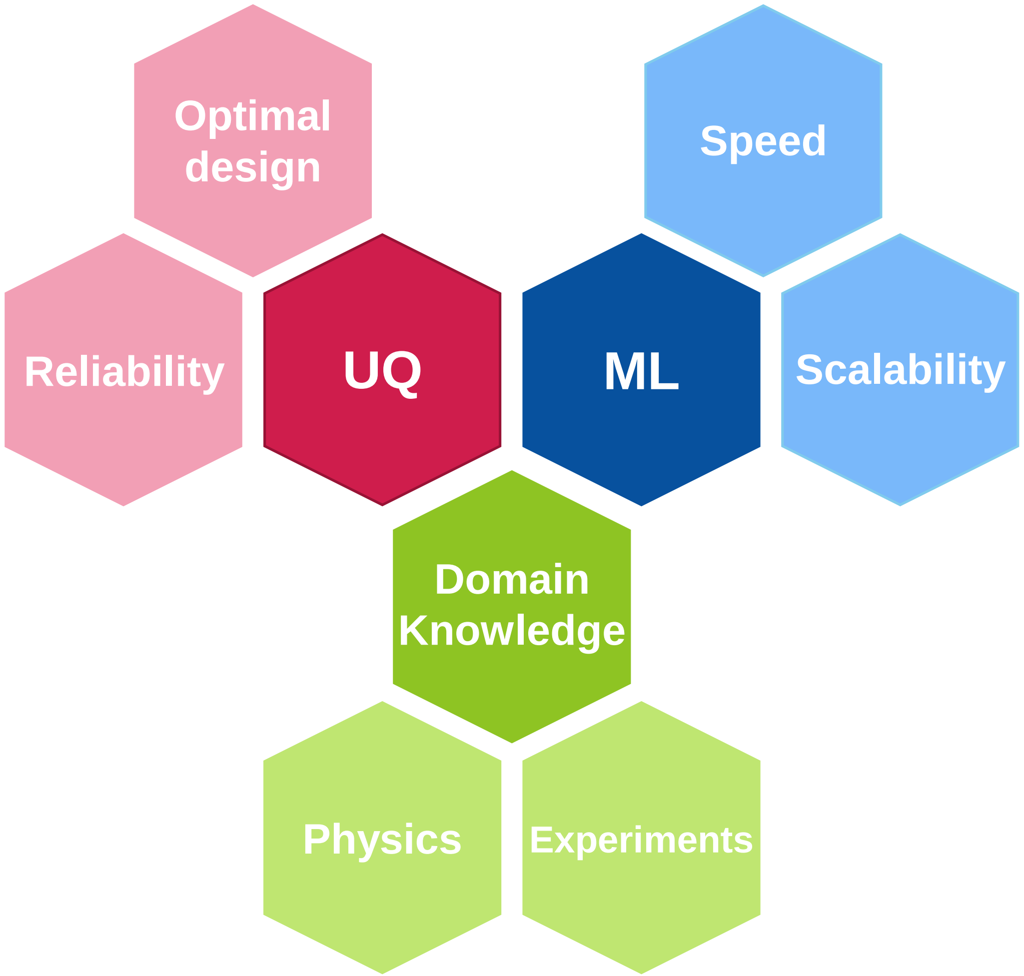
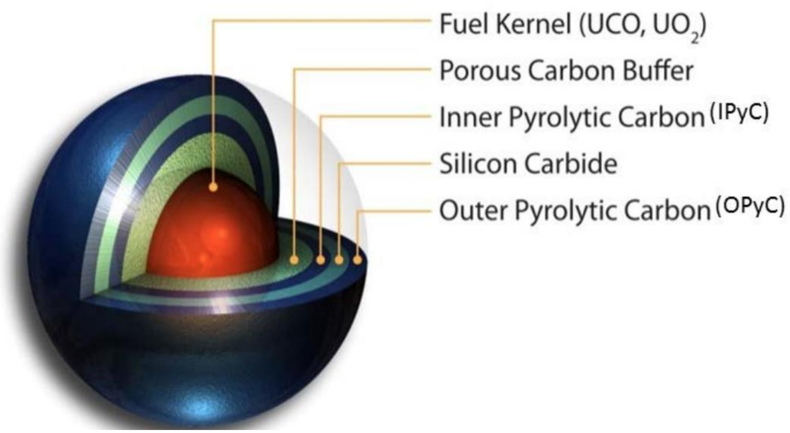
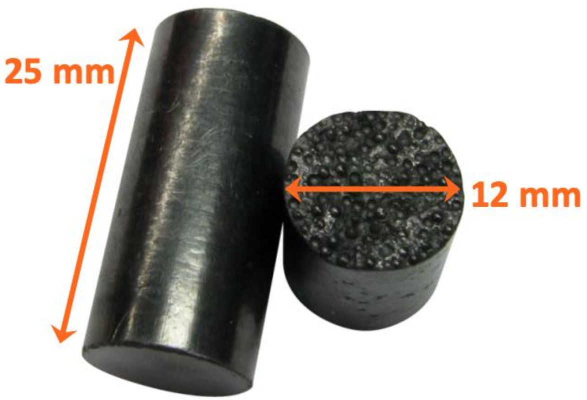


Combo of the above three benefits computational tasks

Motivation: TRISO, a robust nuclear fuel



Single TRISO particle of radius ~400 μm (Davenport 2016)



Fuel compact with numerous TRISO particles (Demkowicz 2016)

- TRISO stands for TRI-structural iSOtropic particle fuel
- Proposed for use in many advanced reactor concepts like micro-reactors owing to its robustness
- Interest from the DOE, DOD, and industries like Kairos Power, Xenergy
- Fuel kernel surrounded by several protective layers
- A fuel compact can have 1000s of tiny TRISO particles
- **Critical to analyze the failure rates of TRISO particle**: Impacts to reactor operation

Motivation: Expensive models, low failure rates

Heat

$$\rho\, C_p\, \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) - E_f\, \dot{F} = 0$$

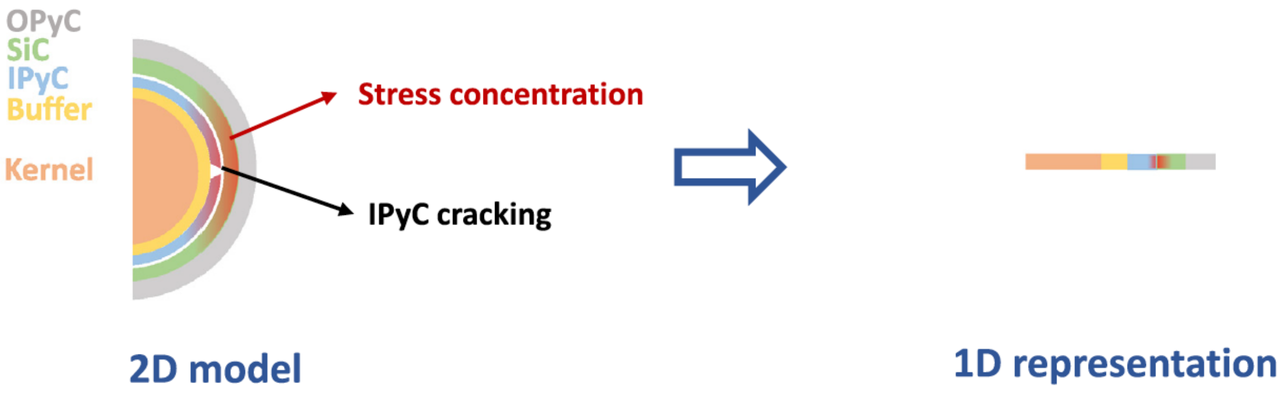
Momentum

$$\nabla \cdot \boldsymbol{\sigma} = 0$$

$$\boldsymbol{\sigma} = \mathcal{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_c - \boldsymbol{\varepsilon}_t - \boldsymbol{\varepsilon}_i)$$

MOOSE

Bison



(Jiang et al. 2021, Dhulipala et al. 2022)

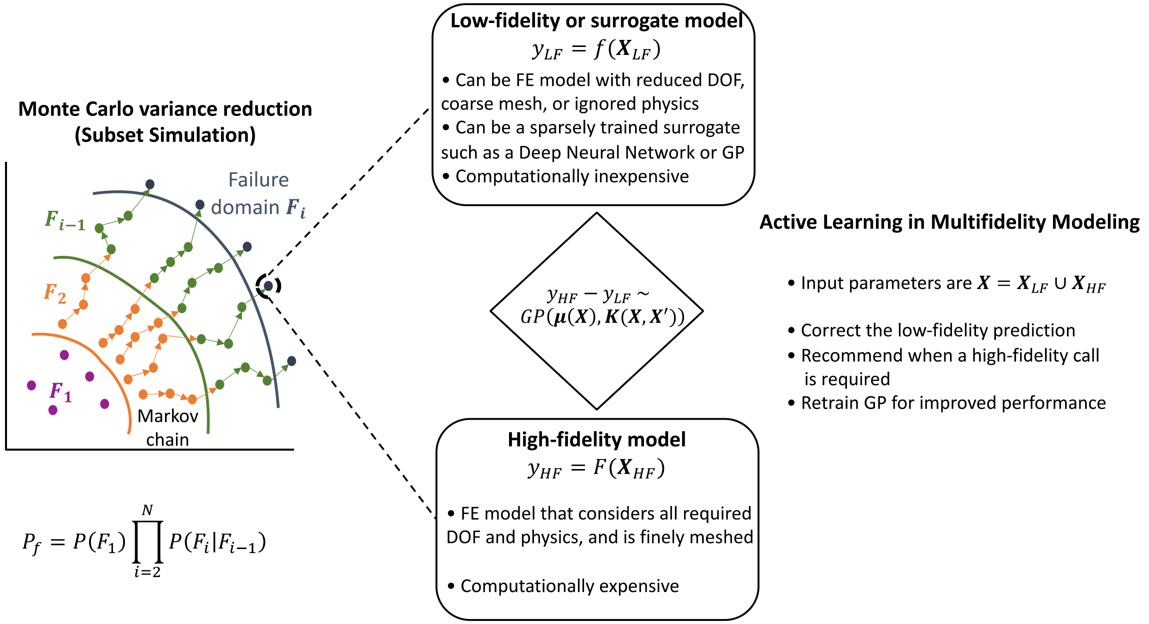
- Sophisticated material property relationships for the different protective layers in TRISO
- Numerically modeled using Bison fuel performance code based on MOOSE (Multiphysics Object Oriented Simulation Environment)
- **Failure mode:** SiC layer fracture most important. Caused by IPyC cracking induced stress conc.
- **1D model:** Fast (~ 11 seconds), approximates SiC stress conc. due to IPyC cracking
- **2D model:** Slow (~30 minutes), models SiC stress conc. using XFEM
- **Failure rates:** 1E-3 to 1E-7

Problem statement

$$P_f = \int_{\widetilde{F}(\boldsymbol{X})>\mathcal{F}} q(\boldsymbol{X})\, d\boldsymbol{X} \qquad P_f \approx \hat{P}_f = \frac{1}{N_m} \sum \mathbf{I}(\widetilde{F}(\boldsymbol{X}) > \mathcal{F})$$

(*F: Failure threshold; F(**X**): Model output; q(**X**): input distributions*)

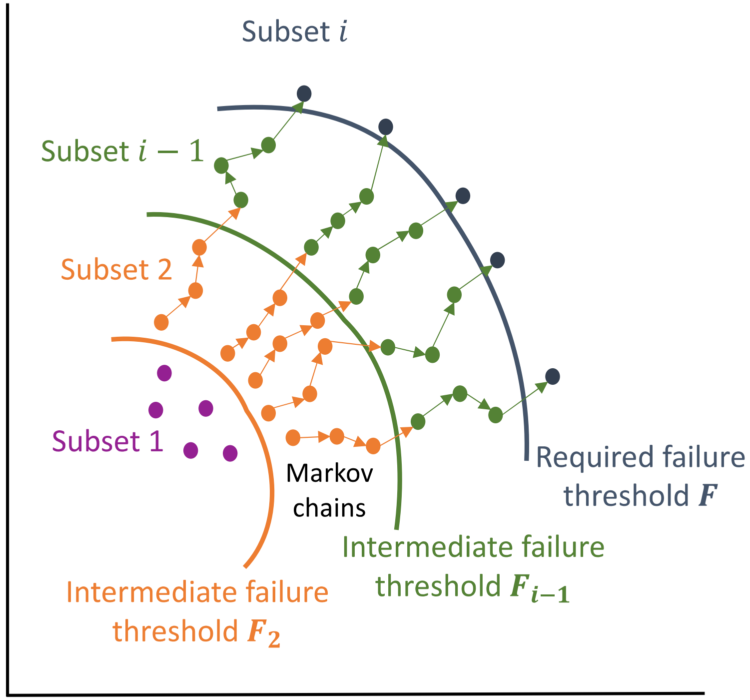
Proposed algorithm



Dhulipala et al. 2021

- Rare events estimation involves computing the multidimensional integral
- Monte Carlo and variance reduction methods require prohibitively large calls to the high-fidelity (HF) model
- **Multifidelity modeling:** Typically make assumptions about the modeling fidelities and/or require fixing the number of HF calls
- **Active learning:** Can breakdown for smaller failure probabilities (1E-4 or less) and/or require large number of Gaussian Process evaluations
- **Proposed: Active learning with multifidelity modeling**
  - Dynamically decides the HF calls
  - Flexibility over the LF model choice
  - Capable for Smaller failure probabilities
  - Doesn’t require large upfront GP evaluations

Background: Subset Simulation (variance reduction)

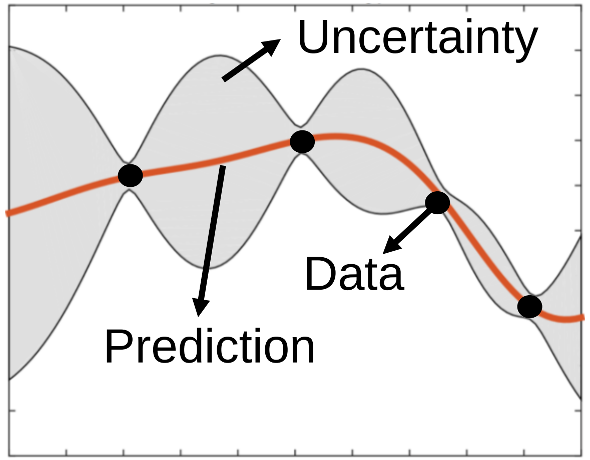


$$P_f = P(F_1)\prod_{i=2}^{N} P(F_i|F_{i-1})$$

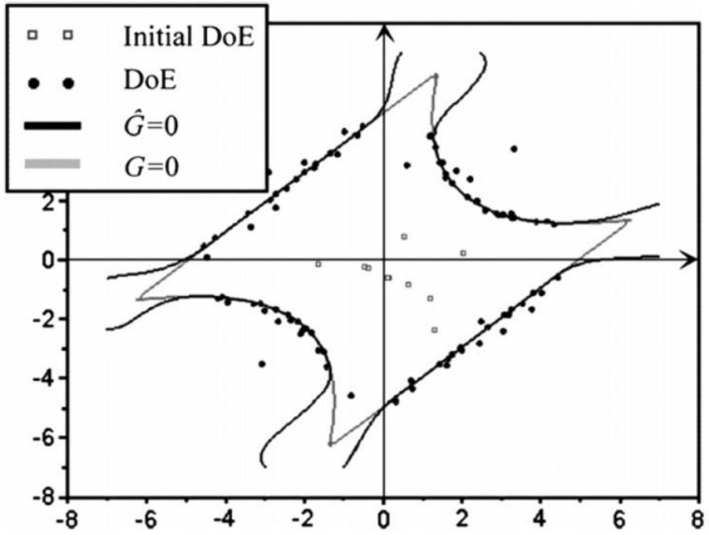
Proposed by Au and Beck (2001)

- Expresses small failure probabilities as a product of larger conditional probabilities (of the order 0.1)
- Creates intermediate failure thresholds before the required failure threshold
- An intermediate failure threshold is defined as the (1-x) percentile value of the samples in previous conditional level
- First conditional level: Direct Monte Carlo
- Subsequent conditional levels: Markov Chain Monte Carlo (Metropolis-Hastings or other variants)

Background: Active learning with Gaussian Process



(Credit: Cornell University)



(Echard et al. 2011)

- Posterior predictive distribution:

$$p(\boldsymbol{y}_* \mid \boldsymbol{X}, \boldsymbol{X}_*, \boldsymbol{y}) \sim \mathcal{N}\Big(k(\boldsymbol{X}_*, \boldsymbol{X})\, k(\boldsymbol{X}, \boldsymbol{X})^{-1}\, \boldsymbol{y},\; k(\boldsymbol{X}_*, \boldsymbol{X}_*) - k(\boldsymbol{X}_*, \boldsymbol{X})\, k(\boldsymbol{X}, \boldsymbol{X})^{-1}\, k(\boldsymbol{X}, \boldsymbol{X}_*) \Big)$$

- Both mean prediction and uncertainty quantification (quite robust under small training data)
- UQ enables the formulation of active learning functions: U-function (Echard et al. 2011), Expected Feasibility Function (Bichon et al. 2008)
- Active learning function decides when to call high-fidelity (HF) model in Monte Carlo schemes

Multifidelity active learning with Gaussian Process

Traditional U-function

GP prediction

Required failure threshold

$$U = \frac{|\mu_G(X) - F|}{\sigma_G(X)}$$

GP standard deviation

Multifidelity U-function

$y_{HF} = F(\boldsymbol{X}_{HF})$ High-fidelity model output

$y_{LF} = f(\boldsymbol{X}_{LF})$ Low-fidelity model output

$$\boldsymbol{X} = \boldsymbol{X}_{HF} \cup \boldsymbol{X}_{LF}$$

LF prediction

GP correction

$$U = \frac{|f(X_{LF}) + \bar{\epsilon}(X) - F|}{\sigma_\epsilon(X)}$$

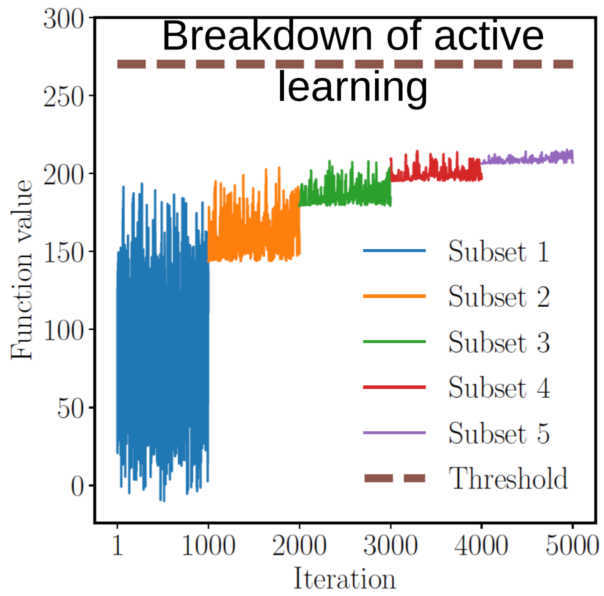
- Traditional active learning functions rely on Gaussian Process predictions entirely
- Performance of active learning schemes can be improved using multifidelity modeling
- U-function is extended to a multifidelity modeling setting owing to its simplicity
- A GP learns the differences between high-fidelity (HF) and low-fidelity (LF) predictions
- GP corrects the LF predictions for every test sample
- New multifidelity U-function to decide when to call the HF model

Coupled multifidelity active learning and Subset Simulation

Subset independent multifidelity U-function

Required failure threshold

$$U = \frac{|f(X_{LF}) + \bar{\epsilon}(X) - F|}{\sigma_\epsilon(X)}$$



Subset dependent multifidelity U-functions

Intermediate failure threshold

$$U^{MF}{}_s = \frac{|f(X_{LF}) + \bar{\epsilon}(X) - F_s|}{\sigma_\epsilon(X)}$$

(Intermediate conditional levels)

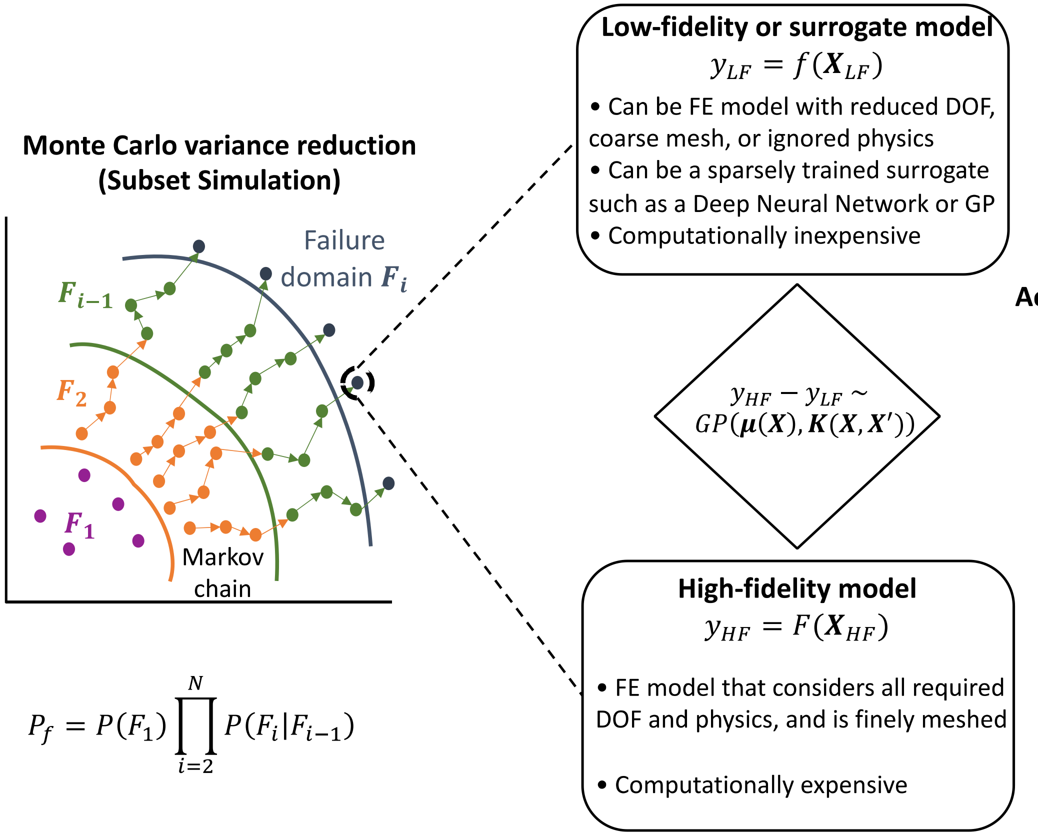
Required failure threshold

$$U^{MF}{}_s = \frac{|f(X_{LF}) + \bar{\epsilon}(X) - F|}{\sigma_\epsilon(X)}$$

(Final conditional level)

- Subset independent multifidelity U-function based on the required failure threshold
- Under smaller failure probabilities (~1E-5) differences between nominal model outputs and required failure threshold are large
- Active learning can breakdown as GP training is not triggered
- Subset dependent multifidelity U-functions are proposed
- Based on intermediate failure thresholds in Subset Simulation to trigger GP re-training
- Intermediate failure thresholds are estimated dynamically

Proposed active learning with multifidelity modeling



$$P_f = P(F_1) \prod_{i=2}^{N} P(F_i | F_{i-1})$$

Active Learning in Multifidelity Modeling

- Input parameters are $\boldsymbol{X} = \boldsymbol{X}_{LF} \cup \boldsymbol{X}_{HF}$
- Correct the low-fidelity prediction
- Recommend when a high-fidelity call is required
- Retrain GP for improved performance

- A GP is trained to learn the differences between HF and LF models (small number of samples)
- For each model evaluation in Subset Simulation, LF model is called
- LF model output is corrected using GP difference (HF-LF)
- Subset dependent U-function is computed to evaluate if HF call is required (threshold is 2)
- If HF call is made, the GP is retrained

Proposed algorithm: Statistical estimators

$$P_1 \approx \hat{P}_1 = \frac{1}{N}\sum_{i=1}^{N}\mathcal{P}_i \qquad \mathcal{P}_i = P(\mathbf{I}_i = 1) = \begin{cases} 1 \times \Phi_i + 0 \times (1-\Phi_i) = \Phi_i & \text{if } \mathbf{I}_{i,LF} = 1 \\ 0 \times \Phi_i + 1 \times (1-\Phi_i) = 1-\Phi_i & \text{if } \mathbf{I}_{i,LF} = 0 \end{cases}$$

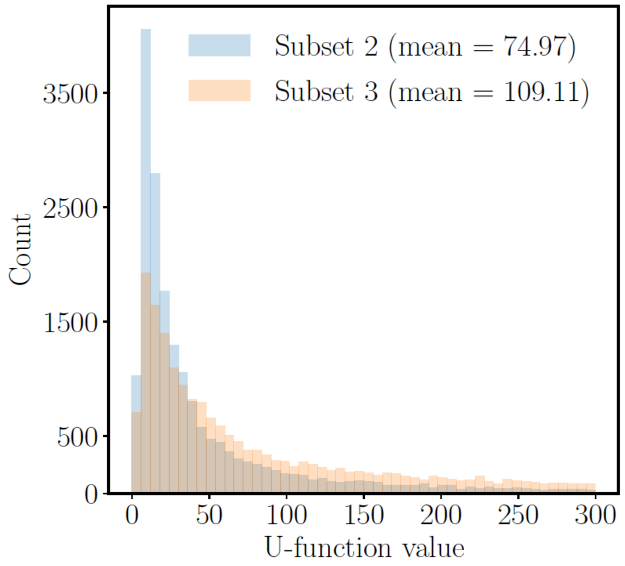
First conditional level

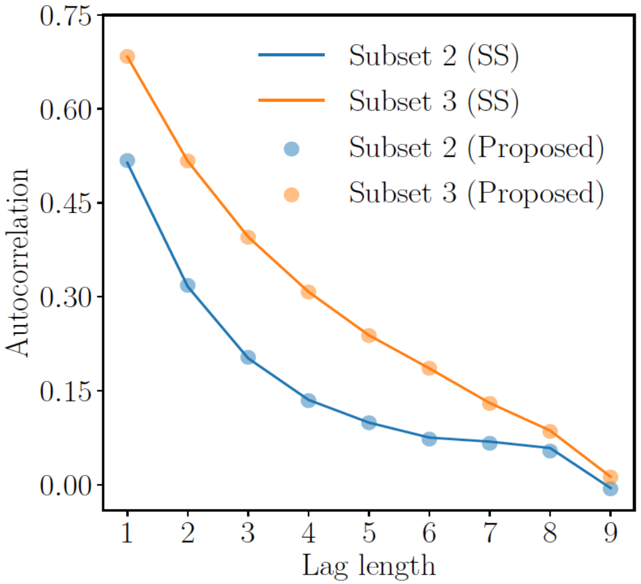
$$\gamma_1 \approx \hat{\gamma}_1 = \sqrt{\frac{1-\hat{P}_1}{\hat{P}_1\ N}}$$

$$P_{s|s-1} \approx \hat{P}_{s|s-1} = \frac{1}{N}\sum_{i=1}^{N_c}\sum_{k=1}^{N/N_c}\mathcal{P}^s_{ik} \quad \forall\, 1 < s \leq N_s,\ \mathcal{P}^s_{ik} = \begin{cases} 1 \times \Phi^s_{ik} + 0 \times (1-\Phi^s_{ik}) = \Phi^s_{ik} & \text{if } \mathbf{I}^s_{ik,LF} = 1 \\ 0 \times \Phi^s_{ik} + 1 \times (1-\Phi^s_{ik}) = 1-\Phi^s_{ik} & \text{if } \mathbf{I}^s_{ik,LF} = 0 \end{cases}$$

Subsequent conditional levels

$$\hat{\delta}_s = \sqrt{\frac{1-\hat{P}_{s|s-1}}{N\ \hat{P}_{s|s-1}}(1+\hat{\gamma}_s)} \qquad \hat{\gamma}_s = 2\sum_{k=1}^{N/N_c-1}\left(1-\frac{kN_c}{N}\ \hat{\rho}_s(k)\right)$$





- Traditional Subset Simulation estimators for conditional failure probabilities and coefficient of variations use indicator functions
- Due to reliance on a GP, these indicator functions change to probabilities because GP can have a slight error in mis-characterizing model failures (U-function threshold is 2)
- Updated statistical estimators are derived for the proposed algorithm
- For practical cases, U-function values are significantly greater than 2. Meaning, error in mis-characterizing model failures is negligible
- So, statistical estimators tend to Subset Simulation estimators

1D TRISO models failure analysis

Input parameters (7 and 11 uncertain)

Category	Parameter	Models 1 & 2	Models 3 & 4
Particle geometry	Kernel radius (μm)	$\mathcal{N}(213.35,\ 4.4)$	$\mathcal{N}(212.5,\ 5.0)$
	Buffer thickness (μm)	$\mathcal{N}(98.9,\ 8.4)$	$\mathcal{N}(100.0,\ 10.0)$
	IPyC thickness (μm)	$\mathcal{N}(40.4,\ 2.5)$	$\mathcal{N}(40.0,\ 3.0)$
	SiC thickness (μm)	$\mathcal{N}(35.2,\ 1.2)$	$\mathcal{N}(35.0,\ 2.0)$
	OPyC thickness (μm)	$\mathcal{N}(43.4,\ 2.9)$	$\mathcal{N}(40.0,\ 3.0)$
	Asphericity ratio	1.0	1.04
Fuel properties	Kernel density (gm/cm^3)	10.966	11.0
	Kernel theoretical density (gm/cm^3)	11.37	11.4
	Buffer density (gm/cm^3)	1.05	1.05
	Buffer theoretical density (gm/cm^3)	2.25	2.25
	IPyC density (gm/cm^3)	1.89	$\mathcal{N}(1.9,\ 0.02)$
	OPyC density (gm/cm^3)	1.907	$\mathcal{N}(1.9,\ 0.02)$
	IPyC anisotropy factor	1.0465	$\mathcal{N}(1.05,\ 0.005)$
	OPyC anisotropy factor	1.0429	$\mathcal{N}(1.05,\ 0.005)$
Layer strengths	IPyC strength	$\mathcal{W}(\sigma_{ms},\ 9.5)$	$\mathcal{W}(\sigma_{ms},\ 9.5)$
	SiC strength	$\mathcal{W}(\sigma_{ms},\ 6.0)$	$\mathcal{W}(\sigma_{ms},\ 6.0)$

uncertain

uncertain

uncertain

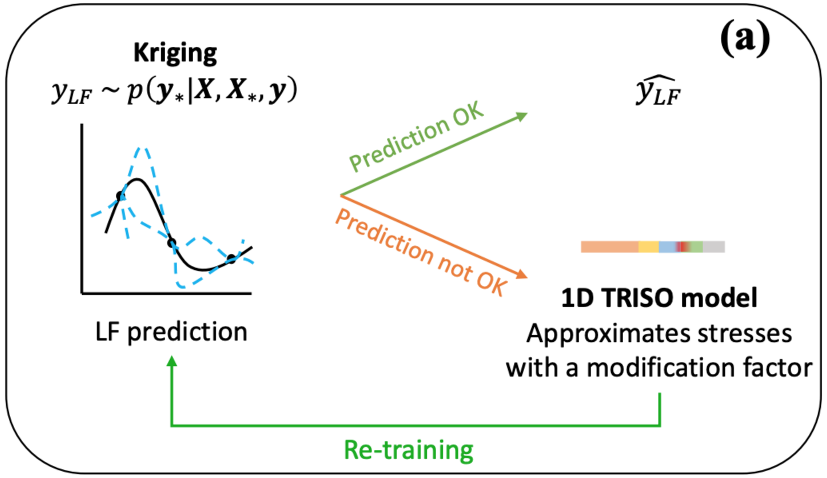
Output: SiC Stress – strength (> 0 is failure)

Irradiation temperatures

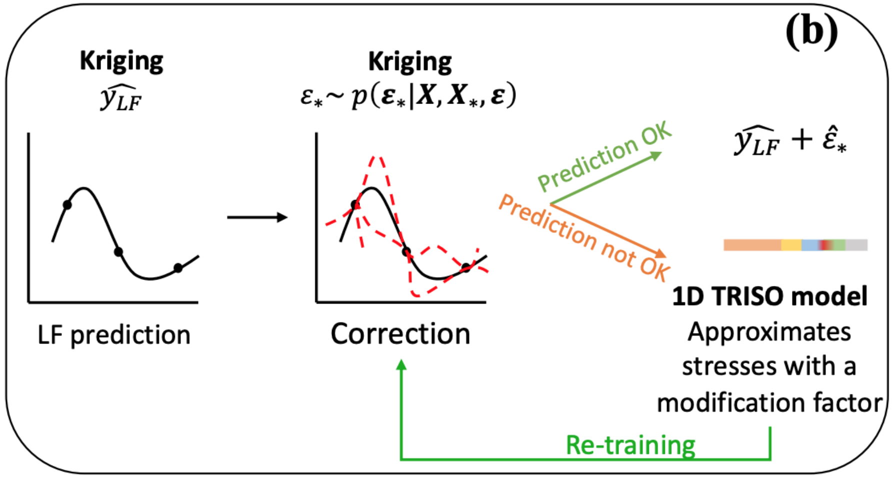
Model 1	Model 2	Model 3	Model 4
Type = Daily varying Max. = 1226.84°C Min. = 207.4°C	Type = Daily varying Max. = 1281.84°C Min. = 195.84°C	Type = Constant Value = 700.0°C	Type = Constant Value = 1000.0°C

1D TRISO models failure analysis

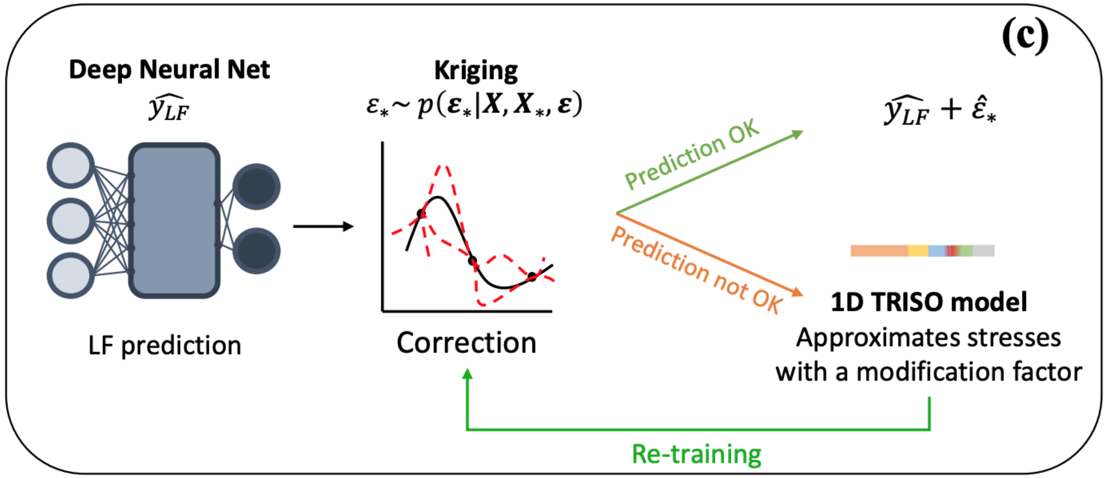
Only Kriging



Kriging (LF) + Kriging (correction)

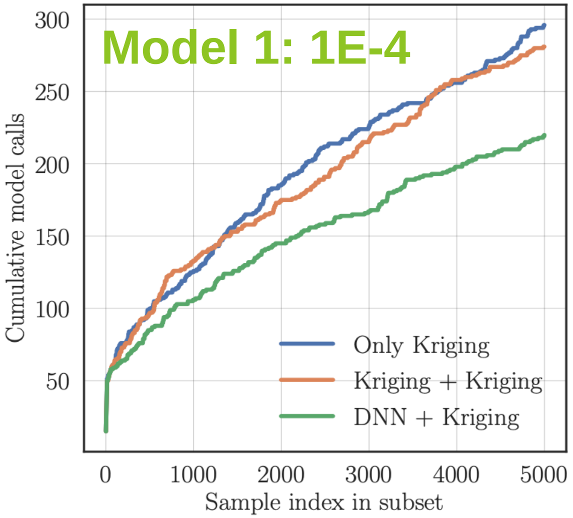


DNN (LF) + Kriging (correction)

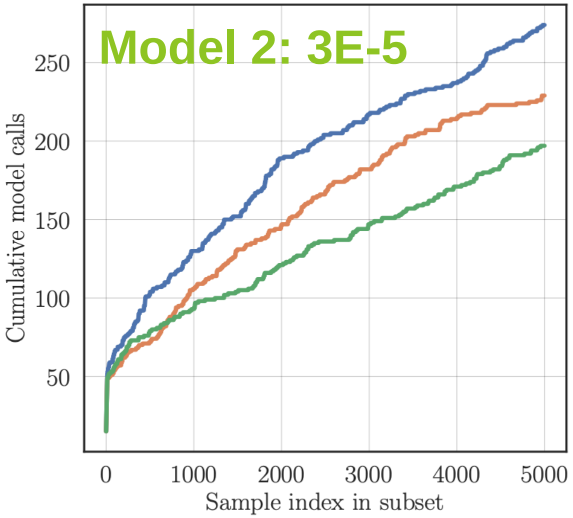


All surrogates trained on 12 evals of 1D TRISO output

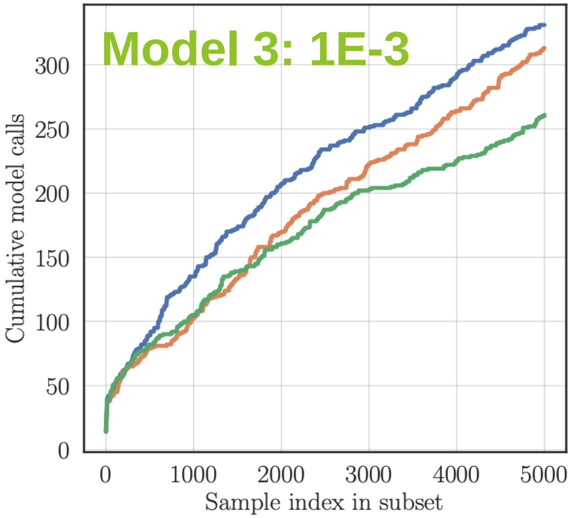
1D TRISO models failure analysis



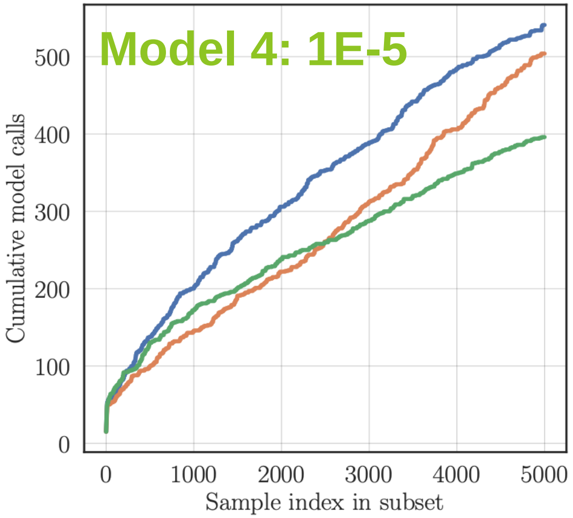
(a)



(b)



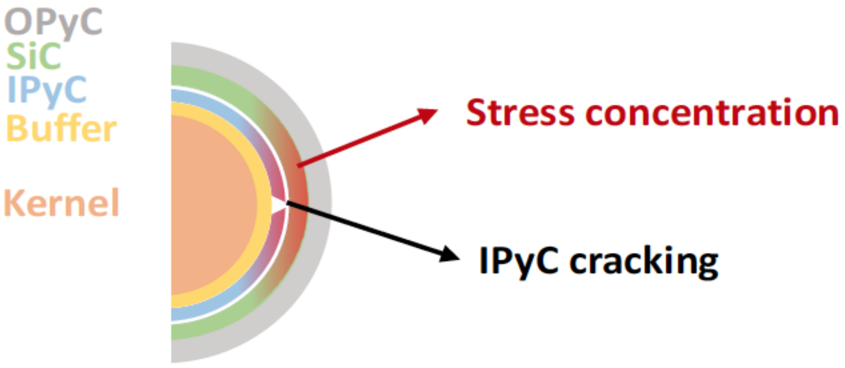
(c)

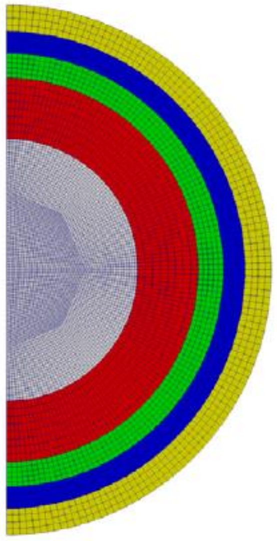


(d)

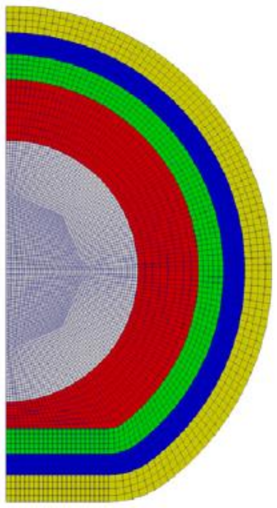
- All three strategies accurately predict the failure probabilities across the four models (COV ~0.08)
- Kriging + Kriging and DNN + Kriging require lesser calls to the 1D TRISO compared to Only Kriging
- DNN + Kriging 26% and 18% less calls than Kriging + Kriging and Only Kriging, respectively
- Possible reason for less calls: more information gain due to multifidelity models and better DNN regularization

2D TRISO models failure analysis





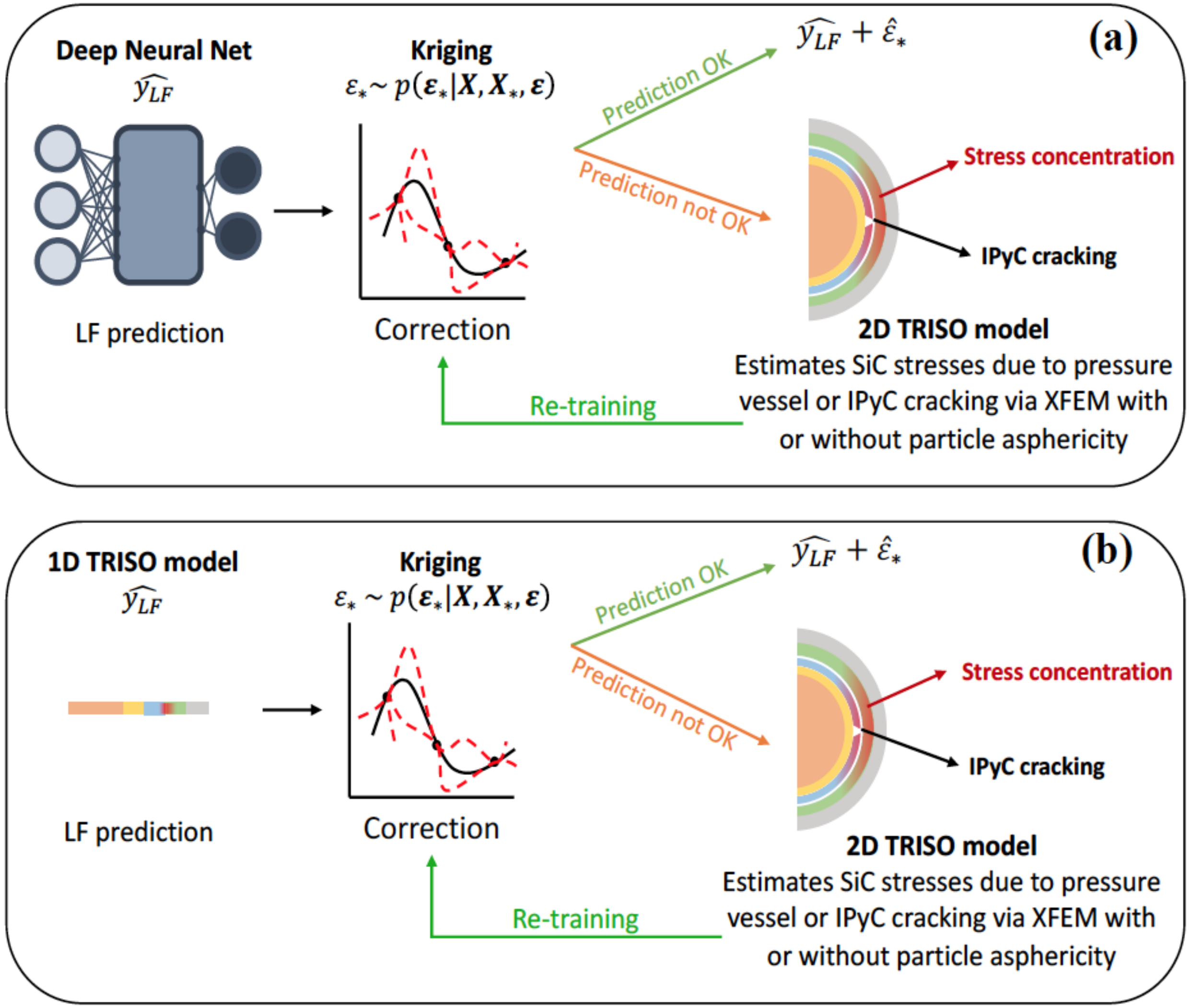
Spherical



Aspherical

- The 1-D models approximate stresses in the SiC layer based on modification factors
- These factors are calibrated by running evals of the 2-D model
- 2-D model explicitly models cracking in IPyC layer and stress conc. in SiC layer
- More accurate, but mesh density dependent. Therefore, computationally expensive (~30 mins)
- Same random input params: geometry, material props
- Same output: SiC stress – strength (> 0 failure)

2D TRISO models failure analysis

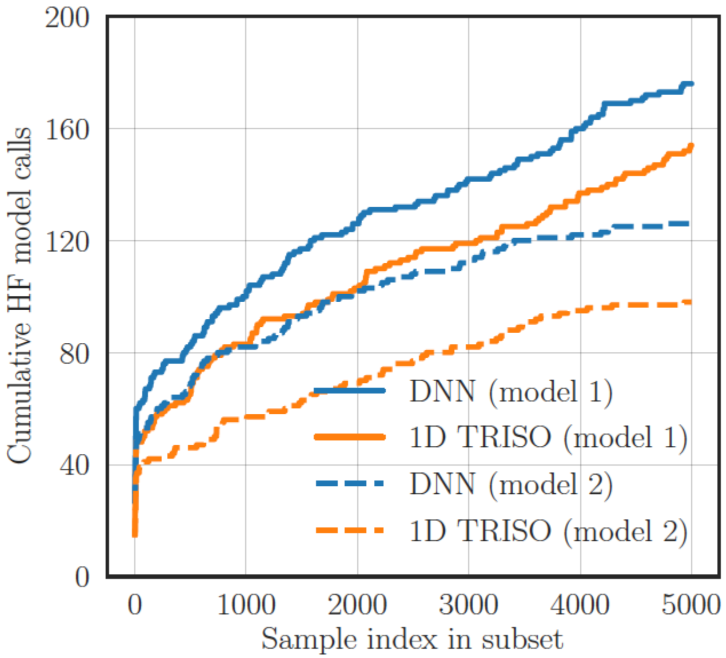


"Data-driven" strategy (DNN LF + Kriging correction)

"Physics-based" strategy (1D TRISO LF + Kriging correction)

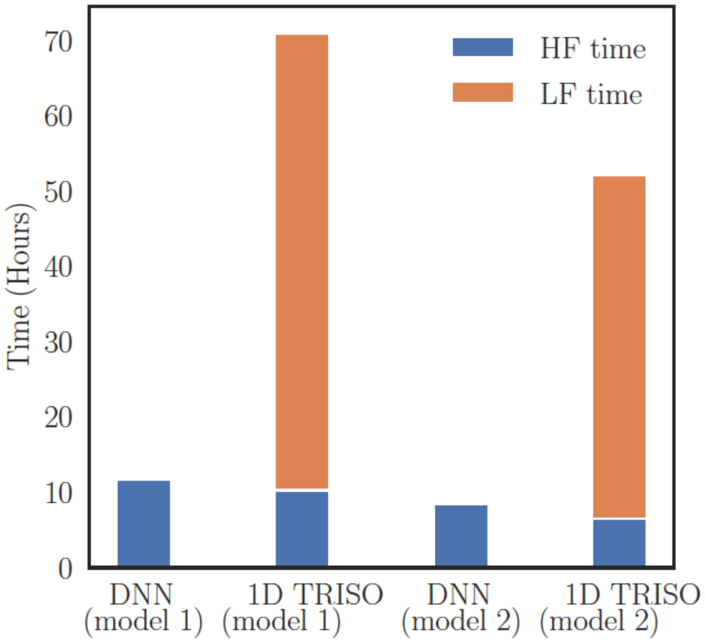
All surrogates trained on 12 evals of 2D TRISO output

2D TRISO models failure analysis



HF calls with sample index

Total simulation time

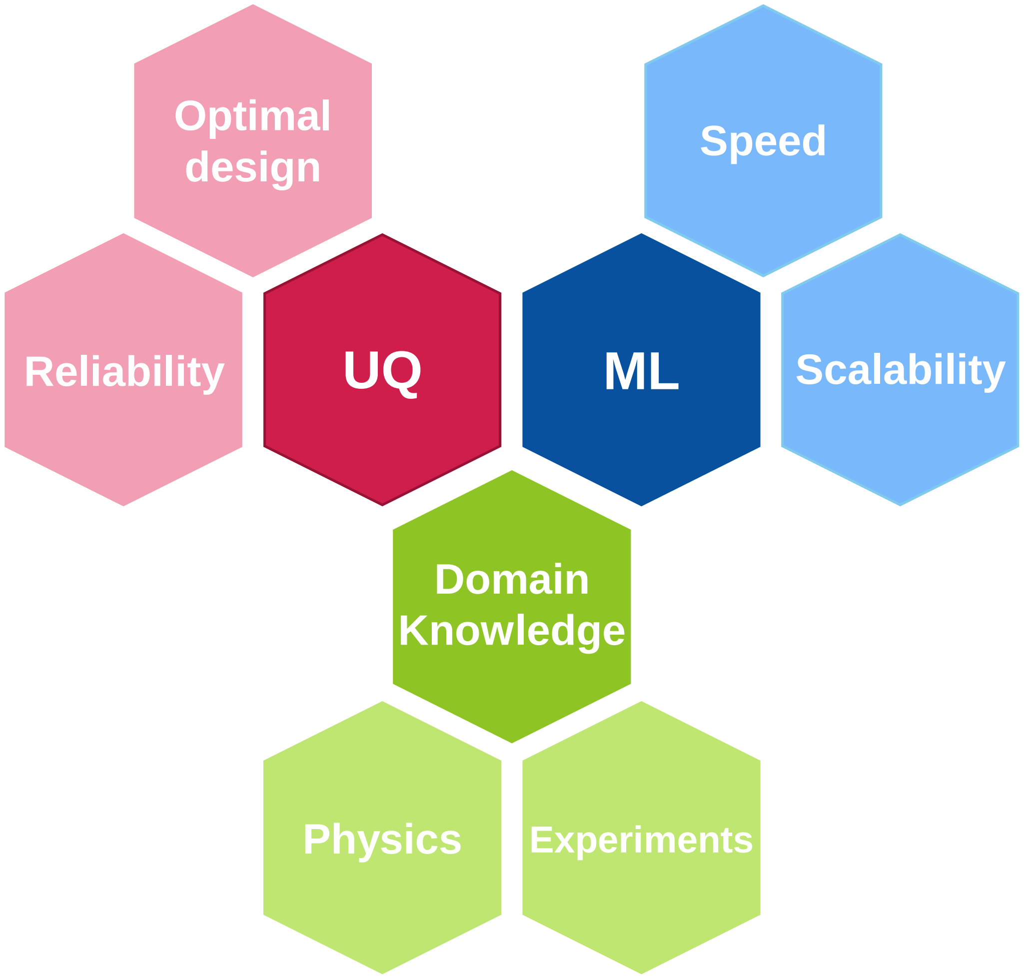


- Both “data-driven” and “physics-based” strategies accurately predict the failure probabilities for two models (COV ~ 0.08)
- “Physics-based” strategy which uses 1D TRISO LF requires 16% less calls to the 2D TRISO model
- “Data-driven” strategy has lesser overall simulation time because the DNN LF predictions are instantaneous
- 1D TRISO LF still requires 11 sec for each eval

IDAHO NATIONAL LABORATORY

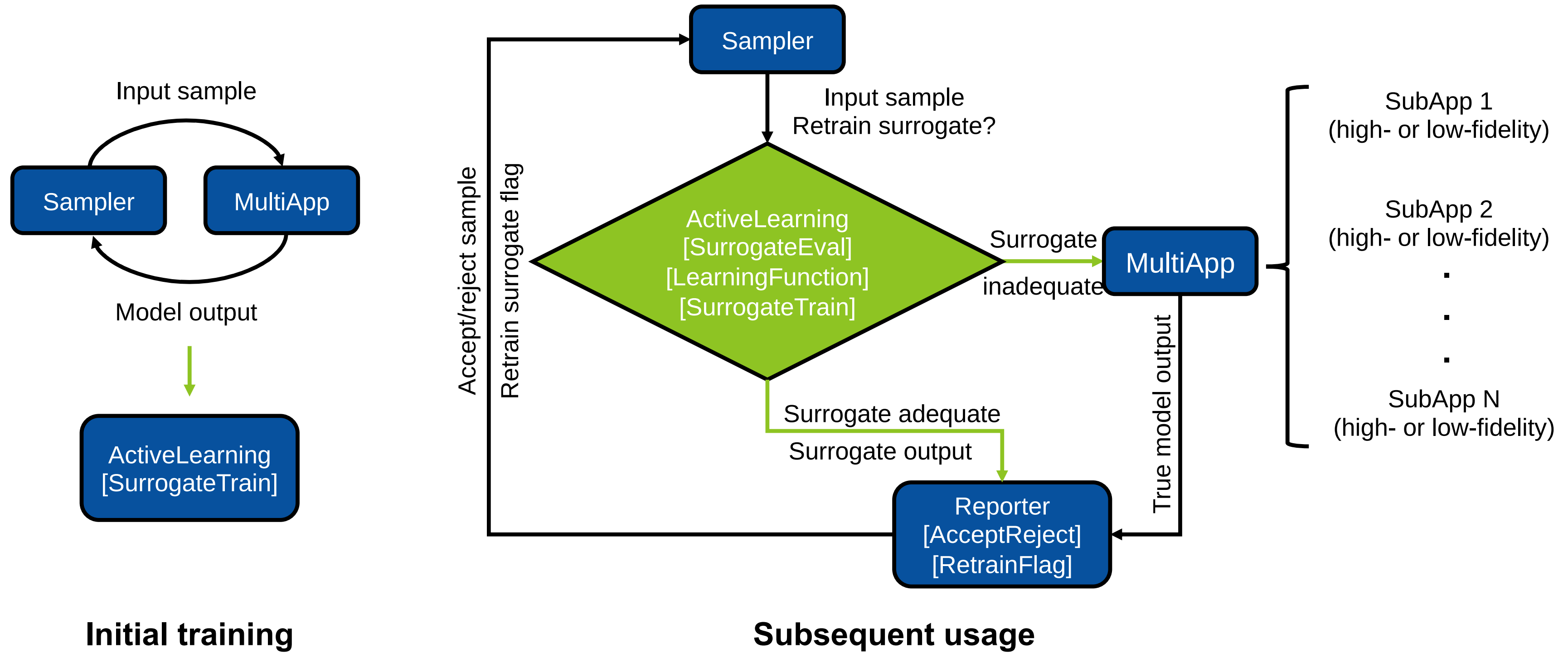
Outline

- **Prediction**
  - Deterministic and Bayesian predictions
  - A simple Bayesian surrogate: Gaussian Process
  - Beyond Gaussian Processes
- **Inference**
  - Sampling
  - Markov Chain Monte Carlo
  - Beyond MCMC: Hybrid MCMC and sampling as optimization
- **Active learning and Multifidelity modeling**
- **TRISO nuclear fuel failure analysis**
- **Ongoing work:**
  - **MOOSE stochastic tools module**
  - **Monte Carlo with Hamiltonian Neural Nets**



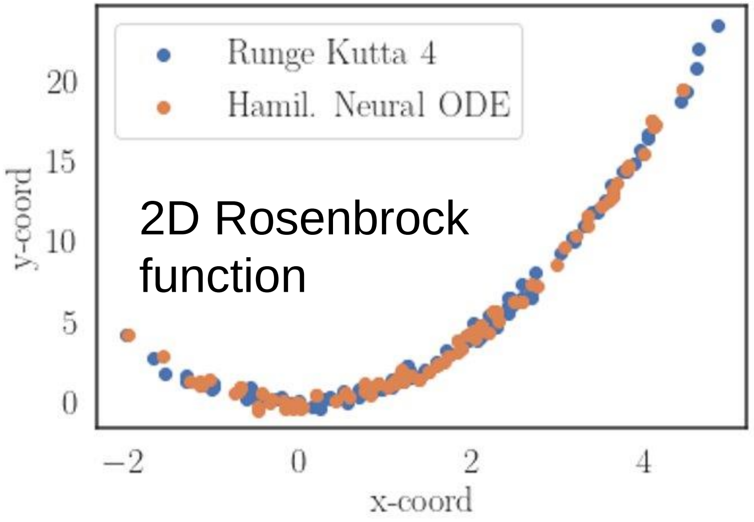
Combo of the above three benefits computational tasks

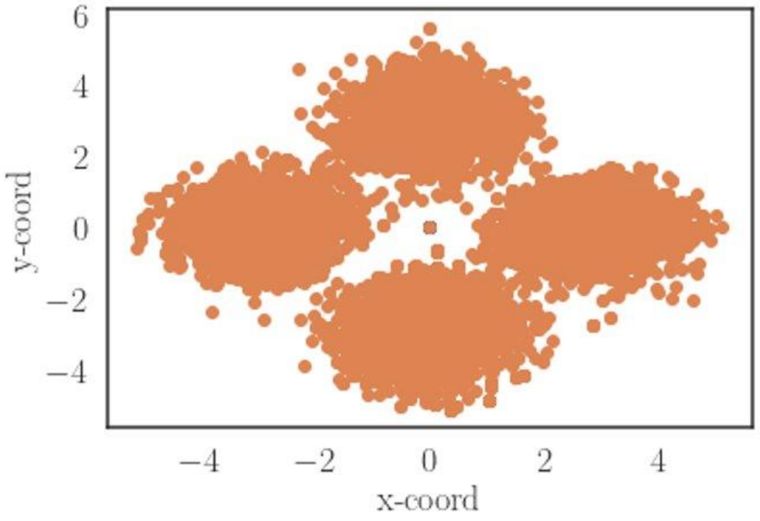
Adaptive sampling and active learning methods in MOOSE



- MOOSE: Multiphysics Object Oriented Simulation Environment (https://mooseframework.inl.gov/)
- Massively parallel, modular development, used for many applications
- Adaptive and active learning Monte Carlo algorithms in MOOSE Stochastic Tools Module

Monte Carlo with Hamiltonian Neural Networks





2D 4 Gaussian mixture

- Sampling from complex distributions can be performed more reliably with Hamiltonian Monte Carlo (HMC)

$$\boldsymbol{z}_1 = \boldsymbol{z}_0 + \int_{t_0}^{t_1} \boldsymbol{I}\ \nabla H(\boldsymbol{z})\ dt$$

- But gradient evaluations are computationally expensive!!

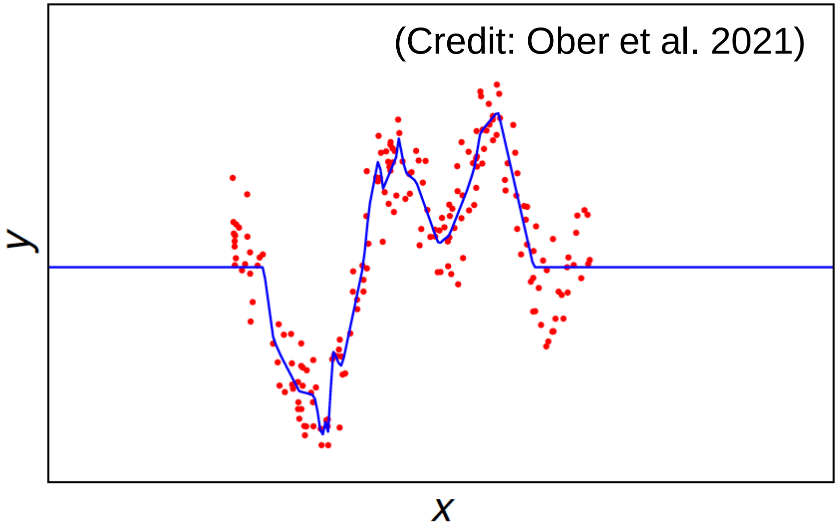
- Hamiltonian Neural ODEs learn the Hamiltonian dynamics and side-step gradient evaluations in HMC

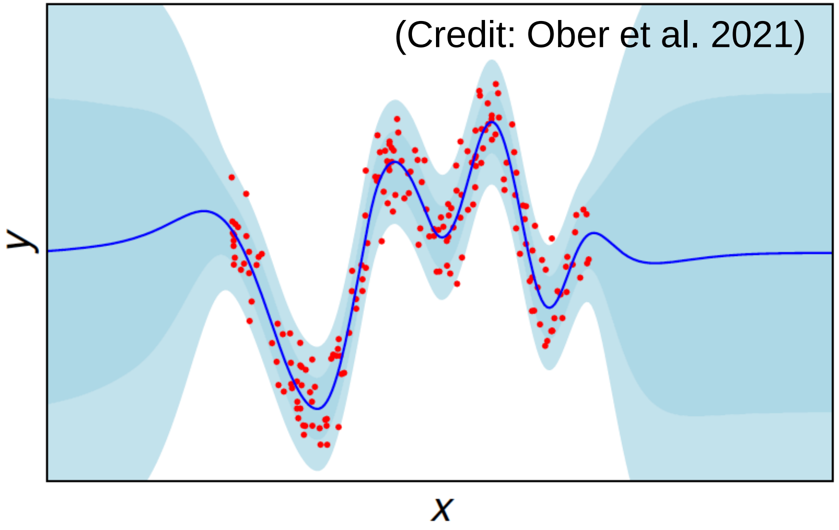
- In addition, they conserve the Hamiltonian

$$\mathcal{L}_{HNN} = \left\| \frac{\partial \mathcal{H}_\theta}{\partial \mathbf{p}} - \frac{\partial \mathbf{q}}{\partial t} \right\|_2 + \left\| - \frac{\partial \mathcal{H}_\theta}{\partial \mathbf{q}} - \frac{\partial \mathbf{p}}{\partial t} \right\|_2$$

- Useful for sampling from complex distributions efficiently

Thank you!
(Som.Dhulipala@inl.gov)





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