# Simulation-based Optimal Design under Uncertainty

Samy Missoum
Computational Optimal Design of Engineering Systems (CODES) Laboratory
University of Arizona

**SOTA presentation. WCSMO 15.**
**June 7, 2023. Cork, Ireland**

# Of the importance of uncertainties

Quantifying and propagating uncertainties is essential for

- The development of digital twins with good predictive capability

# Of the importance of uncertainties

Quantifying and propagating uncertainties is essential for

- The development of digital twins with good predictive capability
- Assessing the distribution and statistical moments of performance metrics

# Of the importance of uncertainties

Quantifying and propagating uncertainties is essential for

- The development of digital twins with good predictive capability
- Assessing the distribution and statistical moments of performance metrics
- Assessing reliability and robustness

# Of the importance of uncertainties

Quantifying and propagating uncertainties is essential for

- The development of digital twins with good predictive capability
- Assessing the distribution and statistical moments of performance metrics
- Assessing reliability and robustness
- Leveraging the power of design optimization techniques

# Optimization under uncertainty

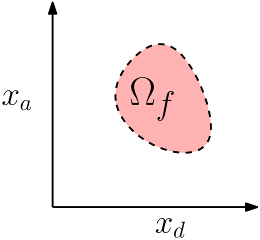
**Formulation #1. Reliability-based design optimization (RBDO).**

$$\begin{aligned} \min_{\boldsymbol{\mu}_d} \quad & F(\boldsymbol{\mu}_d) \\ s.t. \quad & \mathbb{P}((\mathbf{X}_d, \mathbf{X}_a) \in \Omega_f) \leq P_T \\ & \boldsymbol{\mu}_d^{min} \leq \boldsymbol{\mu}_d \leq \boldsymbol{\mu}_d^{max} \end{aligned}$$

# Optimization under uncertainty

**Formulation #1. Reliability-based design optimization (RBDO).**

$$\begin{aligned} \min_{\boldsymbol{\mu}_d} \quad & F(\boldsymbol{\mu}_d) \\ s.t. \quad & \mathbb{P}((\mathbf{X}_d, \mathbf{X}_a) \in \Omega_f) \leq P_T \\ & \boldsymbol{\mu}_d^{min} \leq \boldsymbol{\mu}_d \leq \boldsymbol{\mu}_d^{max} \end{aligned}$$

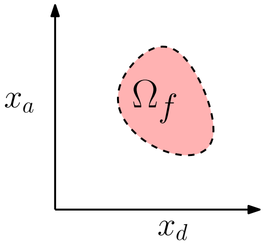



- $\Omega_f$: "Failure" domain. Defined through limit state functions $g_i$

# Optimization under uncertainty

**Formulation #1. Reliability-based design optimization (RBDO).**

$$\min_{\boldsymbol{\mu}_d} \quad F(\boldsymbol{\mu}_d)$$
$$s.t. \quad \mathbb{P}((\mathbf{X}_d, \mathbf{X}_a) \in \Omega_f) \leq P_T$$
$$\boldsymbol{\mu}_d^{min} \leq \boldsymbol{\mu}_d \leq \boldsymbol{\mu}_d^{max}$$

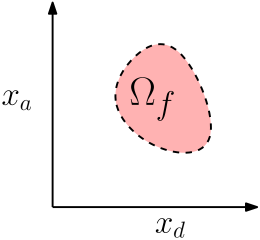



- $\Omega_f$: "Failure" domain. Defined through limit state functions $g_i$
- $\mathbf{X}_d$: Random design variables with hyperparameters $\boldsymbol{\mu}_d$ (e.g., mean)

# Optimization under uncertainty

**Formulation #1. Reliability-based design optimization (RBDO).**

$$\min_{\boldsymbol{\mu}_d} \quad F(\boldsymbol{\mu}_d)$$
$$s.t. \quad \mathbb{P}((\mathbf{X}_d, \mathbf{X}_a) \in \Omega_f) \leq P_T$$
$$\boldsymbol{\mu}_d^{min} \leq \boldsymbol{\mu}_d \leq \boldsymbol{\mu}_d^{max}$$




- $\Omega_f$: "Failure" domain. Defined through limit state functions $g_i$
- $\mathbf{X}_d$: Random design variables with hyperparameters $\boldsymbol{\mu}_d$ (e.g., mean)
- $\mathbf{X}_a$: Random parameters such as excitation amplitude (not "controllable").

# Optimization under uncertainty

**Formulation #2**. Introduce expectation $\mathbb{E}$ of QoI.

$$\begin{aligned} \min_{\boldsymbol{\mu}_d} \quad & \mathbb{E}(F(\mathbf{X}_d, \mathbf{X}_a)) \\ s.t. \quad & \mathbb{P}((\mathbf{X}_d, \mathbf{X}_a) \in \Omega_f) \leq P_T \\ & \boldsymbol{\mu}_d^{min} \leq \boldsymbol{\mu}_d \leq \boldsymbol{\mu}_d^{max} \end{aligned}$$

# Optimization under uncertainty

**Formulation #3**. Introduce standard deviation: $\Sigma$ for robust optimization. Multiobjective problem.

$$\begin{aligned} \min_{\boldsymbol{\mu}_d} \quad & \left(\mathbb{E}(F(\mathbf{X}_d,\mathbf{X}_a)), \Sigma(F(\mathbf{X}_d,\mathbf{X}_a))\right) \\ s.t. \quad & \mathbb{P}((\mathbf{X}_d,\mathbf{X}_a) \in \Omega_f) \leq P_T \\ & \boldsymbol{\mu}_d^{min} \leq \boldsymbol{\mu}_d \leq \boldsymbol{\mu}_d^{max} \end{aligned}$$

Simplest multiobjective formulation: weighted sum (in general not the true Pareto Front):

$$\min_{\boldsymbol{\mu}_d} \quad \alpha\mathbb{E}(F(\mathbf{X}_d,\mathbf{X}_a)) + (1-\alpha)\Sigma(F(\mathbf{X}_d,\mathbf{X}_a))$$

# Types of Uncertainties

- **Epistemic**: lack of knowledge, reducible (e.g., data sparsity, model form)
- **Aleatoric** (aka, aleatory): irreducible (e.g., wind speed distribution)

- **Random fields** (e.g., thickness distribution). Described using Karhunen-Loeve/POD.
- **Random processes (in time)** (e.g., random vibrations).

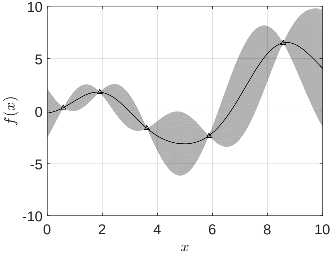
ARIZONA

# Example of epistemic uncertainty

Prediction of Gaussian Process (GP)/Kriging:

$$\tilde{f}(\mathbf{x}) = \underbrace{T(\mathbf{x})}_{\text{Trend}} \quad + \quad \underbrace{Z(\mathbf{x})}_{\text{Zero-mean GP}}$$

(Trend: from a constant to a Polynomial Chaos Expansion (PCE).)




**Prediction variance is readily available. Exists because of lack of data: epistemic uncertainty**

# Challenges

Some challenges are common to optimization

1. Curse of dimensionality
2. Computational time
3. Response non-smoothness (especially discontinuities)

# Challenges. Response Discontinuities.

## Consequence #1

Makes surrogate construction tedious

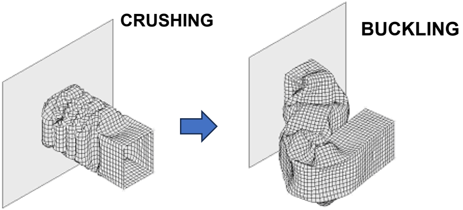
## Consequence #2

High sensitivity to uncertainty

## Consequence #3

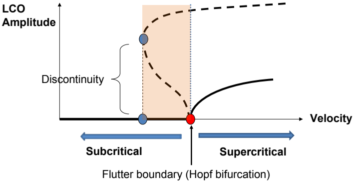
A major change in the physics of the problem might be happening!

# Challenges. Response Discontinuities.



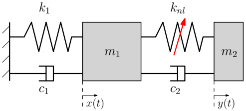

Structural Impact

# Challenges. Response Discontinuities.

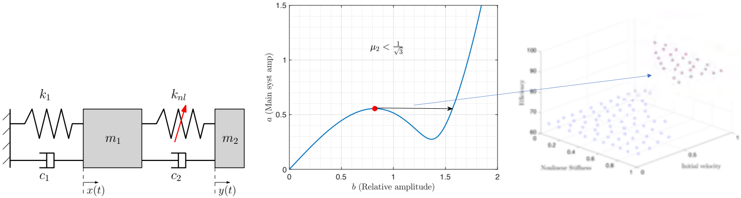



Sub-critical Limit Cycle Oscillations

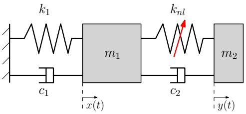
# Challenges. Response Discontinuities.

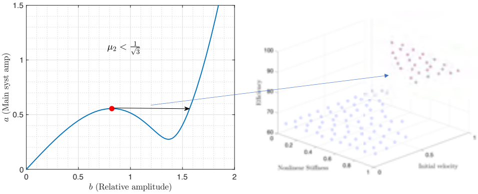


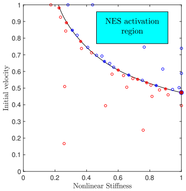
# Challenges. Response Discontinuities.



# Challenges. Response Discontinuities.




Nonlinear Energy Sinks

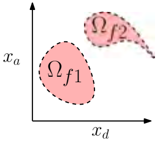
**Methological challenge**: detect the discontinuities and identify corresponding regions.

Some are specific to uncertainty quantification/reliability

- **Propagation** through multiple scales / through components of a system/ through disciplines (Bayesian networks) (Liang and Mahadevan, 2016)

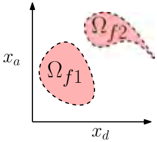
Some are specific to uncertainty quantification/reliability

- **Propagation** through multiple scales / through components of a system/ through disciplines (Bayesian networks) (Liang and Mahadevan, 2016)
- Complexity of failure domain



Some are specific to uncertainty quantification/reliability

- **Propagation** through multiple scales / through components of a system/ through disciplines (Bayesian networks) (Liang and Mahadevan, 2016)
- Complexity of failure domain




- **Rare event**: low probability (variance reduction: importance sampling, subset simulations (Au and Beck, 2001))

# Presentations at WCSMO 15

Two dedicated tracks

- Design under Uncertainty. 15 submissions.
- Robust Design and RBDO. 14 submissions.

Submissions to other tracks with words:" uncertainty, stochastic, robust": 16 .

Total number of uncertainty-related accepted submissions: 45 or about 8% of total submissions.

# Presentations at WCSMO 15

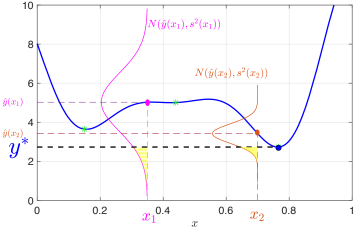
Out of the 45 submissions...

- 14 are methods/theory
- 31 are applications or "frameworks".
- 11 are related to topology optimization (about 5% of total TO track submission)
- 3 papers are related to AM

ARIZONA

# Gaussian Process-based methods. Bayesian Optimization with aleatory variance.

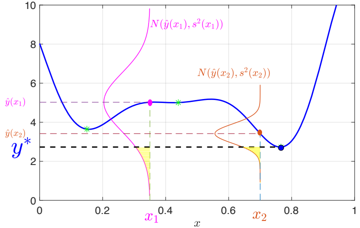
**“Basic” Bayesian Optimization**. Expected Improvement ($EI$).




Acquisition function: $EI(\mathbf{x}) = \mathbb{E}[max(y^* - Y, 0)]$

# Gaussian Process-based methods. Bayesian Optimization with aleatory variance.

**"Basic" Bayesian Optimization**. Expected Improvement (*EI*).

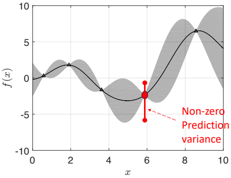



Acquisition function: $EI(\mathbf{x}) = \mathbb{E}[max(y^* - Y, 0)]$

**Extension to reliability**: Efficient Global Reliability Analysis.
From "expected improvement" to "expected feasibility" (Bichon *et* al. 2007).

# GP-based methods. Bayesian Opt. with aleatory variance.

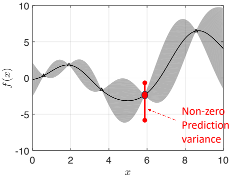
**Aleatory variance**: noise, random parameters...



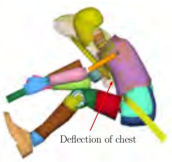

Aleatory variance

# GP-based methods. Bayesian Opt. with aleatory variance.

**Aleatory variance**: noise, random parameters...



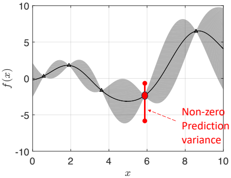

Aleatory variance

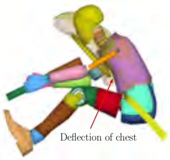


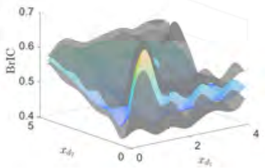

Occupant Restraining System

# GP-based methods. Bayesian Opt. with aleatory variance.

**Aleatory variance**: noise, random parameters...



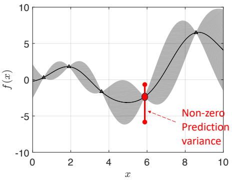



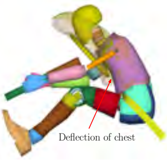



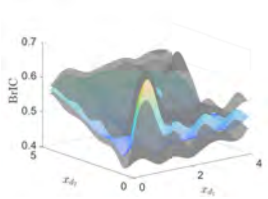

Aleatory variance | Occupant Restraining System | Brain Injury Criterion

# GP-based methods. Bayesian Opt. with aleatory variance.

**Aleatory variance**: noise, random parameters...



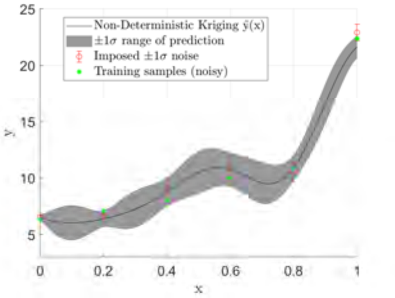




Aleatory variance | Occupant Restraining System | Brain Injury Criterion

The aleatory variance is a non-constant field (Heteroscedasticity). More than just a nugget term for the covariance matrix for regression!

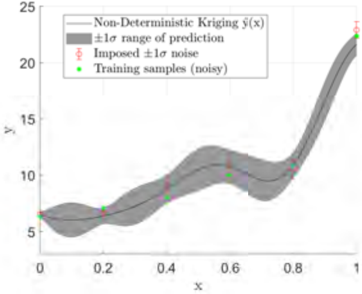
# GP-based methods. Bayesian Opt. with aleatory variance.

Fit Kriging with aleatory variance



# GP-based methods. Bayesian Opt. with aleatory variance.

Fit Kriging with aleatory variance




- Stochastic Kriging (Ankenman et al., 2010)
- Non-Deterministic Kriging (NDK) (sum of two GPs) (Bae et al., 2019)

# Bayesian Optimization with Aleatory Variance.

What changes for optimization?

- The aleatory variance is irreducible
- Reference optimum $T$ is no longer deterministic.
- Need for a updated expected improvement.

# Bayesian Optimization with Aleatory Variance.

What changes for optimization?

- The aleatory variance is irreducible
- Reference optimum $T$ is no longer deterministic.
- Need for a updated expected improvement.

$$EI_T(\mathbf{x}) = (T - \hat{y}(\mathbf{x}))\Phi\left(\frac{T - \hat{y}(\mathbf{x})}{\hat{\sigma}_{red}(\mathbf{x})}\right) + \hat{\sigma}_{red}(\mathbf{x})\phi\left(\frac{T - \hat{y}(\mathbf{x})}{\hat{\sigma}_{red}(\mathbf{x})}\right)$$

ARIZONA

# Bayesian Optimization with Aleatory Variance.

What changes for optimization?

- The aleatory variance is irreducible
- Reference optimum $T$ is no longer deterministic.
- Need for a updated expected improvement.

$$EI_T(\mathbf{x}) = (T - \hat{y}(\mathbf{x}))\Phi\left(\frac{T - \hat{y}(\mathbf{x})}{\hat{\sigma}_{red}(\mathbf{x})}\right) + \hat{\sigma}_{red}(\mathbf{x})\phi\left(\frac{T - \hat{y}(\mathbf{x})}{\hat{\sigma}_{red}(\mathbf{x})}\right)$$

Augmented $EI$, which account for aleatory variance $\hat{\sigma}_\epsilon$ (Ahmadisoleymani and Missoum, 2022):

$$AEI(\mathbf{x}) = EI_T\left(1 - \frac{\hat{\sigma}_\epsilon(\mathbf{x})}{\hat{\sigma}_{tot}(\mathbf{x})}\right)$$

# Multifidelity techniques for design under uncertainty

GPs are well known for data fusion : co-Kriging. Assume a dependence between fidelities (Kennedy and O'Hagan, 2000).

# Multifidelity techniques for design under uncertainty

GPs are well known for data fusion : co-Kriging. Assume a dependence between fidelities (Kennedy and O'Hagan, 2000). Auto-regressive formulation between the GPs

$$Z_i = \rho_{i-1}(\mathbf{x}) Z_{i-1} + Z_d(\mathbf{x})$$

$\rho_{i-1}$ can be constant or a function, even a GP (deep GPs) (Padriarkis, 2015).

# Multifidelity techniques for design under uncertainty

GPs are well known for data fusion : co-Kriging. Assume a dependence between fidelities (Kennedy and O'Hagan, 2000). Auto-regressive formulation between the GPs

$$Z_i = \rho_{i-1}(\mathbf{x}) Z_{i-1} + Z_d(\mathbf{x})$$

$\rho_{i-1}$ can be constant or a function, even a GP (deep GPs) (Padriarkis, 2015).

Several variations on the theme: (Xiao et al, 2018, Le Gratiet, 2013)

# Multifidelity techniques for design under uncertainty

Model management (choice of fidelity)

# Multifidelity techniques for design under uncertainty

Model management (choice of fidelity)

- Leverages the prediction variance information

# Multifidelity techniques for design under uncertainty

Model management (choice of fidelity)

- Leverages the prediction variance information
- Computation of information gain (e.g., cross-entropy, Kullback-Lieber). Application to reliability (mfEGRA): (Chauduri et al, 2021).

# Multifidelity techniques for design under uncertainty

Model management (choice of fidelity)

- Leverages the prediction variance information
- Computation of information gain (e.g., cross-entropy, Kullback-Lieber). Application to reliability (mfEGRA): (Chauduri et al, 2021).
- Possibility of "look-ahead" schemes (i.e., investigate scenarios without function evaluations (Picheny et al, 2010, Binois et al, 2019).

# Multifidelity techniques for design under uncertainty

Model management (choice of fidelity)

- Leverages the prediction variance information
- Computation of information gain (e.g., cross-entropy, Kullback-Lieber). Application to reliability (mfEGRA): (Chauduri et al, 2021).
- Possibility of "look-ahead" schemes (i.e., investigate scenarios without function evaluations (Picheny et al, 2010, Binois et al, 2019).

# Multifidelity techniques for design under uncertainty

Model management (choice of fidelity)

- Leverages the prediction variance information
- Computation of information gain (e.g., cross-entropy, Kullback-Lieber). Application to reliability (mfEGRA): (Chauduri et al, 2021).
- Possibility of "look-ahead" schemes (i.e., investigate scenarios without function evaluations (Picheny et al, 2010, Binois et al, 2019).

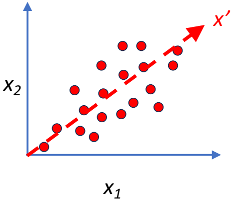
Note that there is a multifidelity version of Monte-Carlo sampling (MFMC) which has shown very good convergence properties. A key advantage: one can specify a budget. (Peherstorfer et al, 2018)

# Dimensionality reduction

**Dimensionality reduction**.
Is there a lower dimensional space that can explain most of the variance?

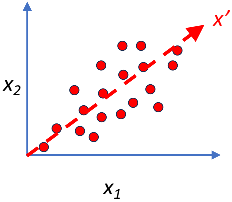
# Dimensionality reduction

**Dimensionality reduction**.
Is there a lower dimensional space that can explain most of the variance?
**The simplest**: Principal Component Analysis /Proper Orthogonal Decomposition



# Dimensionality reduction

**Dimensionality reduction**.
Is there a lower dimensional space that can explain most of the variance?
**The simplest**: Principal Component Analysis /Proper Orthogonal Decomposition

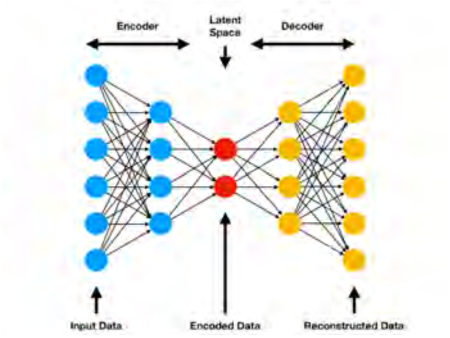



$y = \sum_{i=1}^{N} \alpha_i V_i$. Optim and/or reliability assessment can be performed in the space of coefficients $\alpha_i$ (Basudhar and Missoum, 2009).

# Dimensionality reduction

**Dimensionality reduction**. Nonlinear approaches. (Hou and Behdinan, 2022)

- Kernel PCA (nonlinear extension to PCA)
- Neural networks: Auto-encoders (D'Agostino et al. 2018, Li and Wang 2023)




(Credit image: neptune.ai)

# Dimensionality reduction

**Dimensionality reduction** and Sensitivity Analysis.
Use of Sobol indices: Provides the variance contribution of each variable to the total variance, including coupled effects.

# Dimensionality reduction

**Dimensionality reduction** and Sensitivity Analysis.
Use of Sobol indices: Provides the variance contribution of each variable to the total variance, including coupled effects.
For instance: first order indices:

$$S_i = \frac{\mathbb{V}_i(\mathbb{E}_{\sim i}(Y|X_i))}{\mathbb{V}(Y)}$$

Total indices enable the ranking and elimination of variables (Spagnol et al, 2019).

# High dimensional problem.

Other approaches? Examples from topology optimization. How to handle the large number of elements?

- Reduction through a field representation (Chen et al. 2011, Gao et al. 2022)

# High dimensional problem.

Other approaches? Examples from topology optimization. How to handle the large number of elements?

- Reduction through a field representation (Chen et al. 2011, Gao et al. 2022)
- Use of Stochastic Gradients. (De et al, 2023)

# High dimensional problem.

Other approaches? Examples from topology optimization. How to handle the large number of elements?

- Reduction through a field representation (Chen et al. 2011, Gao et al. 2022)
- Use of Stochastic Gradients. (De et al, 2023)

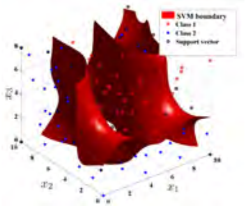

(Credit: De et al, SMO, 2023). Topology optimization with microstructure uncertainty. Use of stochastic gradients.

# Regression vs. classification

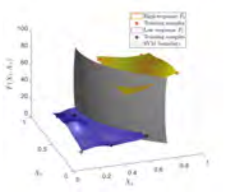
Classification useful for...

- discontinuous/binary problems.
- unsupervised space decomposition ( with clustering and adative sampling) (Basudhar and Missoum, 2010)

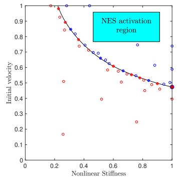
Support Vector Machines (SVM) has proven to be a tool of choice.




Example of SVM



Space decomposition




Adaptive boundary refinement

# Regression vs. classification

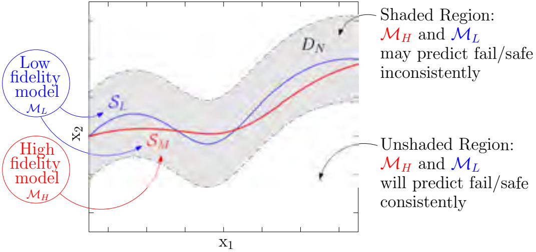
(Cont'd) Classification useful for...

- multifidelity reliability assessment (Pidaparthi and Missoum, 2023)

# Regression vs. classification

(Cont'd) Classification useful for...

- multifidelity reliability assessment (Pidaparthi and Missoum, 2023)
- reduction of function evaluations in series problems



# Directions

Technical areas that need more work:

- Dimensionality reduction/high dimensional problem/ manifold identification
- Propagation through multiple levels/scales
- Non-smooth responses
- Physics-Informed approaches and NN mapping.

# Directions

Technical areas that need more work:

- Dimensionality reduction/high dimensional problem/ manifold identification
- Propagation through multiple levels/scales
- Non-smooth responses
- Physics-Informed approaches and NN mapping.

On the non-technical side:

- Education
- Knowledge dissemination. Reduce the language gap.
- Still too much split between communities (UQ, MDO, Reliability)