Quantification of Mixed Aleatory and Epistemic Uncertainties for Robust Design Optimization, in the Presence of Scarce and Functional Data

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New complex dynamic engineering systems (e.g., civil, nuclear, aerospace, chemical, ...) must operate under a wide range of uncertain conditions.

These are high-consequence safety-critical systems for which data is either very sparse or very expensive to collect.

Modeling and simulation standards (in particular, for government agencies) require the quantification of uncertainties and the evaluation of risk.

Uncertainty Classification in This Work

- **Aleatory uncertainty**
  - Caused by intrinsic variability (state of the system)
  - Irreducible
  - Modeled as a random vector
    \[ a \sim f_a \] (joint multi-dimensional PDF, \( n_a = 5, A = [0, 2]^{n_a} \))

- **Epistemic uncertainty**
  - Caused by ignorance (state of the modeler)
  - Reducible with additional experiments/simulations
  - Can take on any fixed value within a set
  - A refinement entails reducing the size of this set
    \[ e \sim E \] (hyper-rectangular set, \( n_e = 4, B = [0, 2]^{n_e} \))

Uncertainty Model (UM) \( \delta = (a, e) \sim \langle f_a, E \rangle \)
(Sub)-System Configuration

Disturbance $d$

Subsystem (model)

$y(a, e, t)$


(Crespo et al., 2022)
Integrated System Configuration

$y(a, e, t)$

Disturbance $d$

$r \rightarrow C(\theta) \rightarrow z_2(t)$

$(\theta = \text{design parameters, } n_\theta = 9)$

$z_1(t)$

$z_2(t)$


(Crespo et al., 2022)
Integrated System – Analysis Framework

\[ y(a, e, t) \]

Disturbance \( d \)

(\( \theta = \) design parameters, \( n_\theta = 9 \))

(random process)

https://uqtools.larc.nasa.gov/nasa-uq-challenge-problem-2020/ (Crespo et al., 2022)
There are **reliability requirements** \( g(a, e, \theta) < 0 \) that define conflicting objectives: stability \( (z_1 \text{ and } z_2 \text{ not to infinity}) \) \( (g_1) \), settling time \( (g_2) \), control effort/energy consumption \( (g_3) \)

- Epistemic uncertainty makes probabilistic metrics vary in a range

NASA Langley Uncertainty Quantification Challenge on Optimization Under Uncertainty – Tasks Considered in This Talk

A. Model Calibration & Uncertainty Quantification
(using **time series** from the **subsystem** and the **integrated system**)

Uncertainty Model (UM) \( \mathbf{\delta} = (\mathbf{a}, \mathbf{e}) \sim \langle \mathbf{f}_a, \mathbf{E} \rangle \)

B. Reliability-Based Design Optimization

Optimal design \( \mathbf{\theta}_{opt} \)

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A. Model Calibration & Uncertainty Quantification
(using **time series** from the **subsystem** and the **integrated system**)

Uncertainty Model (UM) $\delta = (a, e) \sim \langle f_a, E \rangle$

B. Reliability-Based Design Optimization

Optimal design $\theta_{opt}$
1. First stage (sub-step): functional (time-series) data from the real subsystem

(Fist stage) Uncertainty Model (UM-\(y\)) \(\delta(y) = (a, e) \sim \langle f_a, E \rangle\)

Real Subsystem

Subsystem model \(y(a, e, t)\)

Real sub-system observations \(D_1\)

\(D_1 = \{y^{(i)}(k)\}, i = 1, 2, \ldots, n_i = 100\)

\(k = 0, 1, \ldots, N_T = 5001\)
2. Second stage (sub-step) - Refinement: functional (time-series) data from the real integrated system (after a «round» of design optimization, from $\theta_{\text{baseline}}$ to $\theta_{\text{new}}$)

\[ D_2 = \{z_1^{(i)}(k), z_2^{(i)}(k)\}, \quad i = 1, 2, \ldots, n_2 = 100 \]
\[ k = 0, 1, \ldots, N_T = 5001 \]

Refined UM $\delta(yz)$

System model $z(a, e, \theta_{\text{new}}, t)$

(Refined) Uncertainty Model (UM-$yz$) $\delta(yz) = (a, e) \sim (f_a, E)$
A. Model Calibration & Uncertainty Quantification – Approaches Considered

1. Dimensionality reduction by Singular Value Decomposition (SVD)
2. Construction of SVD-based metamodels (Artificial Neural Networks-ANNS) to reduce the computational burden
3. Evaluation of the plausibility of the epistemic parameter values (→ refinement of the epistemic space) by a global, (average) Likelihood-based search (+ additional refinements based on model predictive capabilities)

Approach 1 (aleatory uncertainty):
4. Retrieval of the (unknown) input dataset by inverse optimization
5. Construction of a joint multivariate PDF for the aleatory input variables by fitting the retrieved input data with Sliced Normal (SN) distributions

Approach 2 (aleatory uncertainty):
4. Construction of a joint multivariate Likelihood by Sliced Normal (SN) distributions in the SVD space
5. Aleatory model calibration by Bayesian inverse uncertainty quantification
A. Model Calibration & Uncertainty Quantification

1. Dimensionality reduction by **Singular Value Decomposition (SVD)**

Real sub-system observations (time domain)

\[ D_1 = \{ y^{(i)}(k) \}, \quad i = 1, 2, \ldots, n_1 = 100 \]
\[ k = 0, 1, \ldots, N_T = 5001 \]

Singular Value decomposition (SVD)

- Centering: \( D_1^* = D_1 - \text{Mean}_{D_1} \)
- SVD: \( D_1^* = U \cdot S \cdot V' \)
- Projection: \( C_1 = D_1^* \cdot V[1 : n_B] \)

Projection of the dataset \( D_1 \) onto an orthonormal basis \( \mathcal{B} = \{ v_t, \quad t = 1, 2, \ldots, n_B(y) \} \), such that \( n_B(y) << N_T \) and at least \( \varepsilon \) (here 99%) of the total variance is retained (\( \rightarrow \) here \( n_B(y) = 10 \))

Real sub-system observations (projected space)

\[ C_1 = \{ c_{1, it} \}, \quad i = 1, 2, \ldots, n_1 = 100 \]
\[ t = 1, 2, \ldots, n_B(y) = 10 \]

Calibration and uncertainty quantification in the **(static multivariate) projected space** (i.e., in the space defined by the orthonormal basis \( \mathcal{B} \)) rather than in the **(dynamic multivariate) time domain**
A. Model Calibration & Uncertainty Quantification

2. Construction of SVD-based metamodels (Artificial Neural Networks-ANNs) to reduce the computational burden

Train $n_B$ metamodels to reproduce the coefficients of the SVD decomposition (only dependent on inputs $a,e$)

Given new inputs $a, e$ one can generate a “metamodel-based” transient:

$$\hat{y}(a, e, k) = \sum_{t=1}^{n_B} \hat{h}_t(a, e) \cdot v_t(k)$$
A. Model Calibration & Uncertainty Quantification

3. Evaluation of the **plausibility of the epistemic parameter values** (refinement of the epistemic space) by a **global, (average) Likelihood-based search**

- Fit PDFs $f_{h_y}(h_y), f_{h_z}(h_z)$ in the reduced SVD space on the data
  
  $C_1 = \{c_{1,i}\}, i = 1, 2, \ldots, n_1 = 100, \ t = 1, 2, \ldots, n_B(y) = 10$
  
  $C_2 = \{c_{2,i}\}, i = 1, 2, \ldots, n_2 = 100, \ t = 1, 2, \ldots, n_B(z_1) + n_B(z_2) = 17$

  
  For example: by (rough) **multivariate Kernel Density Estimation (KDE)**

  Notice: $f_{a|e}(a) \sim \frac{1}{K} f_h(h(a, e))$ ($f_h$ defines a likelihood for any $h(a, e)$ which we assign to $a$)

- For a point $e \in E$ to be plausible: it should be possible to find **at least some $a$** for which $f_h(h(a, e))$ is high
  
  - Sample several epistemic vectors $e_k, k = 1, 2, \ldots, N_e$
  - Sample many aleatory vectors $a_i, i = 1, 2, \ldots, N_a$
  - Evaluate the plausibility of each $e_k$ as its “average likelihood”:

  $$\mathcal{L}(e_k) \sim \sum_{i=1}^{N_a} f_{h_y}(h_y(a^{(i)}, e^{(k)})) \cdot f_{h_z}(h_z(a^{(i)}, e^{(k)}))$$

  $\mathcal{L}(e_1)$ $\mathcal{L}(e_3)$ $e_1$ $e_3$
A. Model Calibration & Uncertainty Quantification

3. Evaluation of the **plausibility** of the epistemic parameter **values** (refinement of the epistemic space) by a global, (average) Likelihood-based search

- Based on $L(e_k) \sim \sum_{i=1}^{N_a} f_{h_y}(h_y(a^{(i)}, e^{(k)})) \cdot f_{h_z}(h_z(a^{(i)}, e^{(k)}))$

  ✓ define the UM $E$ as the smallest hyper-rectangle enveloping the joint four-dimensional $\alpha$% Confidence Interval (CI) of $e$

  ➩ **Degree of confidence** and **robustness** in model calibration (in the presence of scarce data)

  ➩ **Degree of conservatism** in system design
A. Model Calibration & Uncertainty Quantification – Epistemic Space Plausibility (Refinement) – Results

Data from sub-system \((n_1 = 100)\)
\[ y(a, e, t) \]
UM-\(y\)

Additional data from integrated system \((n_2 = 100)\), \[ z(a, e, \theta_{\text{new}}, t) \]
UM-\(yz\)

**NOTE**: results in picture obtained without the refinements suggested by the challengers
A. Model Calibration & Uncertainty Quantification – Approaches Considered

1. Dimensionality reduction by Singular Value Decomposition (SVD)
2. Construction of SVD-based metamodels (Artificial Neural Networks-ANNs) to reduce the computational burden
3. Evaluation of the plausibility of the epistemic parameter values (→ refinement of the epistemic space) by a global, (average) Likelihood-based search (+ additional refinements based on model predictive capabilities)

Approach 1 (aleatory uncertainty):
4. Retrieval of the (unknown) input dataset by inverse optimization
5. Construction of a joint multivariate PDF for the aleatory input variables by fitting the retrieved input data with Sliced Normal (SN) distributions

Approach 2 (aleatory uncertainty):
4. Construction of a joint multivariate Likelihood by Sliced Normal (SN) distributions in the SVD space
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A. Model Calibration & Uncertainty Quantification

4. Retrieval of the (unknown) input dataset by inverse optimization

**Optimal** input aleatory vectors
- Select the value of $\boldsymbol{e}$ with maximum plausibility $\boldsymbol{e}^{\text{opt}}$
- Retrieve the input aleatory vectors $\boldsymbol{a}_i$, $i = 1, 2, \ldots, n_1+n_2$, corresponding to the output data (coming from the real system) projected in the SVD space:

$$
\boldsymbol{a}_i^{\text{opt}} = \arg \min_{\boldsymbol{a}_i} \{ \text{dist}(\mathbf{C}_1, \mathbf{C}_2), [\mathbf{h}_y(\boldsymbol{a}_i, \boldsymbol{e}^{\text{opt}}), \mathbf{h}_z(\boldsymbol{a}_i, \boldsymbol{e}^{\text{opt}})] \}
$$

Build robustness in the retrieval of the aleatory vectors
- Select different values $\boldsymbol{e}^{(k)}$ within the refined $\mathbf{E}$
- For each $\boldsymbol{e}^{(k)}$ repeat the optimization above to obtain different sets of aleatory vectors (corresponding to different plausible aleatory models)

$$
\boldsymbol{a}_i^{(1)} \quad \boldsymbol{a}_i^{(2)} \quad \ldots \quad \boldsymbol{a}_i^{(k)}
$$

$i = 1, 2, \ldots, n_1+n_2$
A. Model Calibration & Uncertainty Quantification

5. Construction of a **joint multivariate PDF** for the **aleatory input variables** by fitting the retrieved input data

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**Sliced Normal (SN) distributions**

- Parametric class of distributions
- Flexibility and versatility that allow accurate modelling of multivariate data
- Capability to capture very complex dependencies
- Relatively small modelling effort

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(Crespo et al., 2019)

(Colbert et al., 2019)
5. Construction of a **joint multivariate PDF** for the **aleatory input variables** by fitting the retrieved input data

**Sliced Normal (SN) distributions**

\[
f(\alpha; \mu, P, d) \sim \frac{\exp\left(-\frac{1}{2}\phi(\alpha; \mu, P, d)\right)}{(2\pi)^{nw/2}\sqrt{P^{-1}}} \quad (\mu, P, d) = \text{hyperparameters}
\]

Where:
- \( P = \text{positive semi-definite matrix} \)
- \( \phi(\alpha; \mu, P, d) = (W_d(\alpha) - \mu)^T \cdot P \cdot (W_d(\alpha) - \mu) \)
- \( W_d(\alpha) = \text{monomials of degree } d \text{ (or less) of } \alpha \text{ (in lexicographic order)} \)

Example: \( W_2(\alpha) = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = [a_1, a_2, a_1^2, a_1 \cdot a_2, a_2^2]^T \)

\[
\text{Dim}(W) = \text{Dim}(\mu) = n_W = \binom{n_a + d}{n_a} - 1
\]

\[
\text{Dim}(P) = n_W \cdot n_W
\]

For \( d > 1 \) SN PDFs can model complex, multi-modal distributions
5. Construction of a joint multivariate PDF for the aleatory input variables by fitting the retrieved input data

**Fitting Sliced Normal (SN) distributions**

(Maximum Likelihood Estimation in the polynomial space)

Retrieved input dataset \( A_a = \{a_i, i = 1, 2, \ldots, n_1 + n_2\} \)

Retrieved input dataset \( A_W = \{w_i, i = 1, 2, \ldots, n_1 + n_2\} \)

(polynomial space)

\[
\mathcal{L}(A_W; \mu, P, d) = \sum_{i=1}^{n_1+n_2} \log(f_W(w_i; \mu, P, d))
\]

\[
\langle \mu^*, P^* \rangle = \arg \max_{\mu, P} \left\{ \sum_{i=1}^{n_1+n_2} \log(f_W(w_i; \mu, P, d)) \right\} \quad \text{(Size: } n_w(n_w+3)/2) \]

(Bootstrap to limit overfitting)

\[
\mu^* = \frac{1}{n_1 + n_2} \sum_{i=1}^{n_1+n_2} w_i
\]

\[
P^* = \left( \frac{1}{n_1 + n_2} \sum_{i=1}^{n_1+n_2} (w_i - \mu^*) \cdot (w_i - \mu^*)^T \right)^{-1}
\]

(Crespo et al., 2019)
5. Construction of a joint multivariate PDF for the aleatory input variables by fitting the retrieved input data

**Fitting Sliced Normal (SN) distributions**

(Maximum Likelihood Estimation in the polynomial space)

\[
f(a; \mu, P, d) \sim \frac{\exp\left(-1/2\phi(a; \mu, P, d)\right)}{(2\pi)^{nw/2}\sqrt{P-1}}
\]

\[
\phi(a; \mu, P, d) = (W_d(a) - \mu)^T \cdot P \cdot (W_d(a) - \mu)
\]

Family of nested, closed, semi-algebraic confidence sets:

\[
S(\beta_\alpha) = \{a: (W_d(a) - \mu)^T \cdot P \cdot (W_d(a) - \mu) \leq \beta_\alpha\}
\]

- \(\alpha\) is the desired confidence (coverage) level
- \(\beta_\alpha\) to be determined (numerically) such that \(\alpha\)% of the data is enclosed in \(S(\beta_\alpha)\)
- Members of this family can be used to tightly enclose the data
- Polynomial structure \(\rightarrow\) simple treatment for rigorous uncertainty quantification

(Crespo et al., 2019)
5. Construction of a joint multivariate PDF for the aleatory input variables by fitting the retrieved input data

Ensure robustness in the joint multivariate PDF estimation

Option 1 (negligible discrepancies are observed in the models):
- Use the aleatory model obtained in correspondence of the epistemic vector \( \mathbf{e} \) with maximum plausibility \( \mathbf{e}^{opt} \)

\[
f_w(w; \mu^*, P^*, \mathbf{d}|\mathbf{e}^{opt}) \rightarrow f_a(\alpha|\mathbf{e}^{opt})
\]

Option 2 (discrepancies are observed in the model):
- Account for it by merging different aleatory models obtained for different values \( \mathbf{e}^{(k)} \) within the refined \( \mathbf{E} \)

\[
\sum_{k=1}^{N_e} b_k \cdot f_w(w; \mu^*, P^*, \mathbf{d}|\mathbf{e}^{(k)}) \rightarrow f_a(\alpha)
\]

(weight by the corresponding plausibility or consider equally plausible epistemic values in \( \mathbf{E} \))
A. Model Calibration & Uncertainty Quantification – Joint Multivariate Aleatory Models – Input Retrieval – Results

**Subsystem $y(t)$**

- **BEST** – $\text{dist} = 0.0759$
- **WORST** – $\text{dist} = 0.2330$

**Integrated system $z_1(t), z_2(t)$**

- **BEST** – $\text{dist} = 0.0962$
- **WORST** – $\text{dist} = 0.3344$
A. Model Calibration & Uncertainty Quantification – Joint Multivariate Aleatory Models – Input Retrieval and Fitting by Sliced Normals – Results

Data from integrated system \((n_2 = 100)\), \(z(a, e, \theta_{new}, t)\) + Data from subsystem \((n_1 = 100)\), \(y(a, e, t) \rightarrow UM-yz\)

- Input retrieval allows identifying (and treating) possible model discrepancies
- Optimization-based input retrieval is computationally convenient with scarce data
- SN: Accurate modelling of multivariate data and of complex dependencies
- SN: Data tightly enclosed by nested semi-algebraic sets of polynomial nature \((\rightarrow\) rigorous and simple treatment)
- SN: Parametric nature \(\rightarrow\) avoid kernels that perform poorly with scarce data
A. Model Calibration & Uncertainty Quantification – Joint Multivariate Aleatory Models – Input Retrieval and Fitting by Sliced Normals – Results

Data from integrated system \( (n_2 = 100), z(a, e, \theta_{\text{new}}, t) \) + Data from subsystem \( (n_1 = 100), y(a, e, t) \rightarrow \text{UM-yz} \)

- Sliced Normals of degree 4 (MLE) \( \rightarrow 119 \) parameters

- **Increase the degree** of the polynomial \( \rightarrow \) increase the capability to **tightly enclose the data** and capture complex patterns
- The analyst can «play» with the polynomial degree to obtain more or less **conservative/robust designs**, paying attention to **model generalization** capabilities (**overfitting**)
A. Model Calibration & Uncertainty Quantification – Approaches Considered

1. **Dimensionality reduction** by **Singular Value Decomposition (SVD)**
2. Construction of **SVD-based metamodels** (**Artificial Neural Networks-ANNS**) to reduce the **computational burden**
3. Evaluation of the **plausibility of the epistemic parameter values** (\(\rightarrow\) refinement of the **epistemic space**) by a **global, (average) Likelihood-based search**
   (+ additional refinements based on **model predictive capabilities**)

**Approach 1 (aleatory uncertainty):**

4. Retrieval of the **(unknown) input dataset** by **inverse optimization**
5. Construction of a **joint multivariate PDF** for the **aleatory input variables** by fitting the retrieved input data (in the physical space) with **Sliced Normal (SN) distributions**

**Approach 2 (aleatory uncertainty):**

4. Construction of a **joint multivariate Likelihood** by **Sliced Normal (SN) distributions** in the SVD space
5. **Aleatory model calibration** by **Bayesian inverse uncertainty quantification**
A. Model Calibration & Uncertainty Quantification

4. Construction of a **joint multivariate Likelihood** by **Sliced Normal (SN) distributions** in the SVD space (**maximum- and worst-case**)

- Fit PDFs $f_{h_y}(h_y)$, $f_{h_z}(h_z)$ in the reduced SVD space on the data
  \[ C_1 = \{ c_{1, it} \}, \quad i = 1, 2, ..., \quad n_1 = 100, \quad t = 1, 2, ..., \quad n_B(y) = 10 \]
  \[ C_2 = \{ c_{2, it} \}, \quad i = 1, 2, ..., \quad n_2 = 100, \quad t = 1, 2, ..., \quad n_B(z_1)+n_B(z_2) = 17 \]

Use **Sliced Normal (SN) distributions**

Precise modeling of **complex, nonlinear, multi-modal distributions and dependencies**

Desirable to obtain an **accurate and robust aleatory model** by **Bayesian inversion**
A. Model Calibration & Uncertainty Quantification

5. Aleatory model calibration by Bayesian inverse uncertainty quantification

- Use non-informative priors for $\mathbf{a}$ ($A = [0, 2]^n_a$, $\rho_a(\mathbf{a})$)

- For a given epistemic vector $\mathbf{e}^{(k)}$, evaluate the posterior PDF of $\mathbf{a}$:

  $f_{\mathbf{a}|\mathbf{e}^{(k)}}(\mathbf{a}) \sim \frac{1}{K} f_h(h(\mathbf{a}, \mathbf{e}^{(k)}))$

  (Notice: $f_h$ defines a likelihood for any $h(\mathbf{a}, \mathbf{e})$ which we assign to $\mathbf{a}$)

  \[ f_{\mathbf{a}|\mathbf{e}^{(k)}}(\mathbf{a}) = \frac{1}{K} f_h(h(\mathbf{a}, \mathbf{e}^{(k)})) \cdot \rho_a(\mathbf{a}) \]

  (non-parametric estimation: sample the posterior by MCMC)

- Repeat for different epistemic vectors $\mathbf{e}^{(k)}$, to increase robustness in the PDF estimation (if computational burden acceptable)
Data from integrated system \( (n_2 = 100) \), \( z(a, e, \theta_{\text{new}}, t) \) + Data from subsystem \( (n_1 = 100) \), \( y(a, e, t) \rightarrow \text{UM-}yz \)

500000 samples by MCMC
Affine-invariant ensemble sampler (AIES)

Comparison with Sliced Normals:
- Similar marginals (even if Bayesian inversion seems to underestimate spread)
- Completely different dependence structure!
- Higher computational cost for Bayesian inversion (input retrieval + SN is more convenient with scarce data)
- MCMC can “skip” areas of the search space with small likelihood or “isolated” modes
- Reflection about the relation \( f_{\text{ale}}(a) = \frac{1}{K} f_h(h(a, e^k)) \cdot p_a(a) \) and the optimization-based input retrieval adopted before (if any)…
A. Model Calibration & Uncertainty Quantification – Joint Multivariate Aleatory Models – Results

Model comparison → Energy score:
Multivariate generalization of the Continuous Rank Predictive Score (CRPS)

\[
ES((f_a, E), C) = \frac{1}{n_1+n_2} \sum_{i=1}^{n_1+n_2} ES((f_a, E), c_i) = \frac{1}{n_1+n_2} \sum_{i=1}^{n_1+n_2} \left( \frac{1}{N_q} \sum_{q=1}^{N_q} \|h_q\| c_i - \frac{1}{2N_a^2} \sum_{i=1}^{N_o} \sum_{j=1}^{N_o} \|h_q - h_j\| \right)
\]

Projected model outputs  Projected data

Models  ES
Input retrieval-SN 3  15.3
Input retrieval-SN 4  18.2
Bayesian inversion  23.8
NASA Langley Uncertainty Quantification Challenge on Optimization Under Uncertainty – Tasks Considered in This Talk

A. Model Calibration & Uncertainty Quantification
(Using time series from the subsystem and the integrated system)

Uncertainty Model (UM) $\delta = (\alpha, e) \sim \langle f_{\alpha}, E \rangle$

B. Reliability-Based Design Optimization

Optimal design $\theta_{opt}$
B. Reliability Analysis of Baseline Design

Refined Uncertainty Model (UM) $\delta$

$\alpha \sim f_{\alpha}$

$\delta$

$g_1(a, e, \theta_{\text{baseline}})$ (stability)

$g_2(a, e, \theta_{\text{baseline}})$ (settling time)

$g_3(a, e, \theta_{\text{baseline}})$ (energy consumption)

$w(a, e, \theta_{\text{baseline}}) = \max_{i=1,\ldots,n_g=3} g_i(a, e, \theta_{\text{baseline}})$

Failure probability (epistemic) bounds

$R_i(\theta) = \left[ \min_{e \in E} \mathbb{P}[g_i(a, e, \theta) \geq 0], \max_{e \in E} \mathbb{P}[g_i(a, e, \theta) \geq 0] \right] \quad i = 1, \ldots, n_g$

$R(\theta) = \left[ \min_{e \in E} \mathbb{P}[w(a, e, \theta) \geq 0], \max_{e \in E} \mathbb{P}[w(a, e, \theta) \geq 0] \right]$

Maximum severity of requirements violation

$s_i(\theta) = \max_{e \in E} \left\{ \mathbb{E} \left[ g_i(a, e, \theta) \mid g_i(a, e, \theta) \geq 0 \right] \mathbb{P}[g_i(a, e, \theta) \geq 0] \right\} \quad i = 1, \ldots, n_g$
Conceptual steps and methods employed:

A. **Double-loop simulation** to calculate failure probability bounds:
   1. **Genetic Algorithms (GAs)** to thoroughly *explore the epistemic parameter ranges* and *find extreme (upper and lower) bounds* of the failure probabilities
      ➔ Evaluate bounds of the epistemic box $E!$
   2. **Monte Carlo Simulation (MCS)** to propagate *aleatory uncertainty*

B. **Artificial Neural Network (ANN) metamodels** to *reduce the computational burden*
   ➔ Possibility to perform several «batch» model evaluations at reasonable cost
B. Reliability-Based Design Optimization

**Refined Uncertainty Model (UM) δ**

\[
\delta \sim f_{\delta}
\]

\[
a \sim f_a
\]

\[
e \sim E
\]

\[
\begin{align*}
g_1(a, e, \theta_{\text{new}}) \\
g_2(a, e, \theta_{\text{new}}) \\
g_3(a, e, \theta_{\text{new}}) \\
w(a, e, \theta_{\text{new}}) = \max_{i=1,\ldots,n_g=3} g_i(a, e, \theta_{\text{new}})
\end{align*}
\]

**Requirements model**

\[
g(a, e, \theta_{\text{new}})
\]

**New design** \(\theta_{\text{new}}\)

**Optimality criterion**

**Robust Design:** minimize the (epistemic) upper bound of the the failure probability for the worst-case performance function \(w(a, e, \theta)\)

\[
\theta_{\text{new}} = \arg \min_{\theta} \left\{ \max_{e \in E} P[w(a, e, \theta) \geq 0] \right\}
\]

\[
P_{\text{fail}}(\theta_{\text{new}}) < P_{\text{fail}}
\]
B. Reliability-Based Design Optimization

Conceptual steps and methods employed:
1. Genetic Algorithms (GAs) to explore the design space
2. Double-loop simulation (GA + MCS) & ANNs to evaluate the upper bound of the worst-case requirement failure probability

Iterative Optimization Algorithm

\[
\begin{align*}
\theta_{new}^{\text{curr}} &= \theta_{baseline} \\
\text{Set } \theta_{new}^{\text{curr}} &= \theta_{new}^{\text{updated}} \\
[\theta, \theta] &= \theta_{new}^{\text{curr}} \pm k \cdot |\theta_{new}^{\text{curr}}| \\
&= (a, e, \theta) \rightarrow w(a, e, \theta) \\
\theta_{new}^{\text{updated}} &= \arg \min_{[\theta, \theta]} \left\{ \max\ P[w(a, e, \theta) \geq 0] \right\} \\
\theta_{i,new}^{\text{updated}} &= \theta_i \text{ or } \theta_{i,new}^{\text{updated}} = \bar{\theta}_i \\
\theta_{new}^{\text{updated}} &= \theta_{new} \\
\end{align*}
\]
B. Reliability-Based Design Optimization – Results

**Failure probabilities**

\[ \alpha \sim f_a \quad e \sim E \quad \theta_{\text{final}} \]

- Strong reduction in \( R_1(\theta) \) (2-3 orders of magnitude)
- Reduction in \( R_2(\theta), R_3(\theta), R(\theta) \) by factors 3.4-8.3
- Violation severity reduced by factors 450 (\( g_1 \)), 21 (\( g_2 \)), 52 (\( g_3 \))
Conclusions

- The NASA Langley Uncertainty Quantification (UQ) Challenge on Optimization Under Uncertainty – Technical solutions:

  ✓ A. Model Calibration & Uncertainty Quantification:
    - Functional data (Time series) ➔ Calibration in high-dimensional spaces ➔ dimensionality reduction by SVD
    - Repeated model evaluations ➔ high computational cost ➔ SVD-based ANN metamodels
    - Uncertainties of different nature and representation ➔ joint calibration
      - Epistemic (sets) plausibility ➔ global (average) Likelihood-based exploration
      - Aleatory uncertainty (joint multivariate PDFs):
        - Nonlinear, complex, multimodal dependencies + few data ➔ Sliced Normal distributions
        - Optimization-based inverse input data identification (and fitting)
        - (Non-parametric) Bayesian inversion
        - Possible overfitting ➔ bootstrap-based parameter estimation
        - Robustness in the face of uncertainties
          - Mixing multiple plausible aleatory models
          - Regulate “tightness” of confidence regions (data enclosing sets)
          - (Maximum- VS Worst Case-Likelihood Estimation)
Conclusions

- The NASA Langley Uncertainty Quantification (UQ) Challenge on Optimization Under Uncertainty – **Technical solutions**:

  ✓ **B. Reliability-Based Design Optimization:**
  - Robust Design: minimize the (epistemic) upper bound of the failure probability for the worst-case performance function
  - Double-loop simulation to calculate failure probability bounds
    - Genetic Algorithms (GAs) to thoroughly (globally) explore the epistemic parameter ranges and find extreme (upper and lower) bounds of the failure probabilities (in abrupt, multimodal, disconnected search spaces)
    - Monte Carlo Simulation to propagate aleatory uncertainty
  - Repeated model evaluations ➔ high computational cost ➔ (iteratively trained) ANN metamodels
Current Issues and Possible Future Developments

Current issues:
- Model inaccuracies (“discrepancies”) or just poor calibration strategy and/or poor description of multivariate dependence structures?
- Sampling-based strategies ➞ high flexibility but low “computational efficiency”
- Check ANN metamodel accuracy in mapping high-dimensional spaces and estimating small failure probabilities
- Robust designs satisfactory even in the presence of poorly calibrated models, but possibly overly conservative

Possible future developments:
- Rigorous quantification of model overfitting (in particular, for SN distributions)
- Assess the proposed calibration approaches by comparison with other sound methods (e.g., purely non-parametric/moment matching): bias? under/over-estimation of uncertainty?
- Rigorous assessment of model discrepancies (if any)
- More efficient (sampling?) methods for estimating small failure probabilities (e.g., bounds of $R_1$)
- Other rigorous approaches for robust design: non-parametric distributionally-robust methods and or Scenario Theory to optimally control, select and possibly discard outliers
References

N. Pedroni, “Computational methods for the robust optimization of the design of a dynamic aerospace system in the presence of aleatory and epistemic uncertainties”, Mechanical Systems and Signal Processing (Special Issue NASA Langley Challenge on Optimization under Uncertainty), Volume 164, 1 February 2022, paper 108206, ISSN 0888-3270.
THANK YOU!

QUESTIONS?