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

UQSay #44 – Uncertainty Quantification @Paris-Saclay, 17/03/2022

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NASA Langley Uncertainty Quantification Challenge on Optimization Under Uncertainty – Motivation

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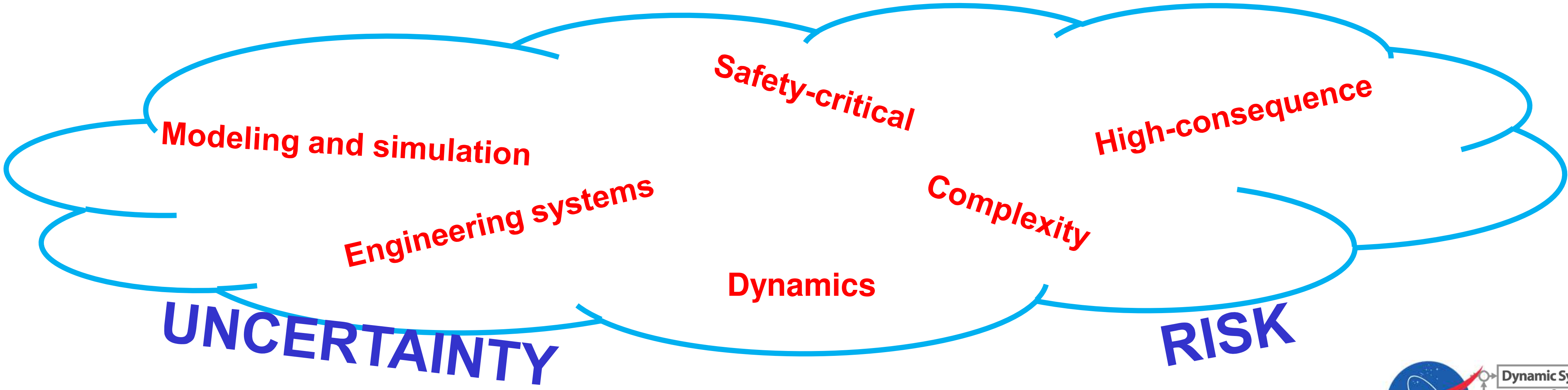
- New complex dynamic engineering systems (e.g., civil, nuclear, *aerospace*, chemical, …) must operate under a wide range of uncertain conditions
- These are high-consequence safety-critical systems for which data is either very sparse or very expensive to collect
- Modeling and simulation standards (in particular, for government agencies) require the quantification of uncertainties and the evaluation of risk



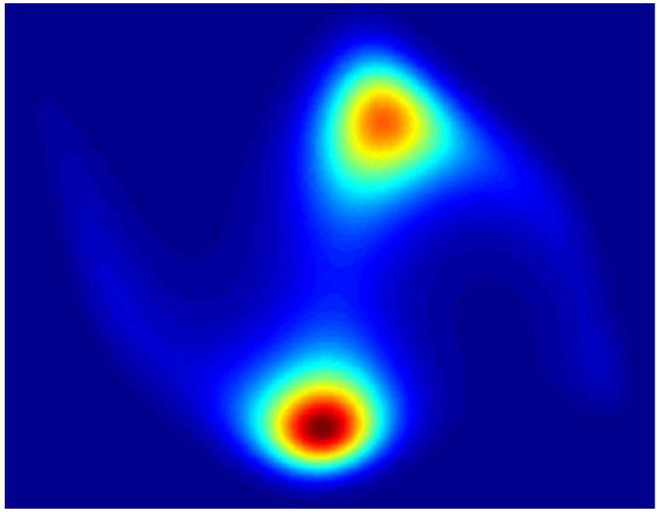
https://uqtools.larc.nasa.gov/nasa-uq-challenge-problem-2020/

Dynamic Systems & Control Branch

Uncertainty Classification in This Work

- **Aleatory uncertainty**
  - Caused by intrinsic variability (state of the system)
  - Irreducible
  - Modeled as a **random vector**

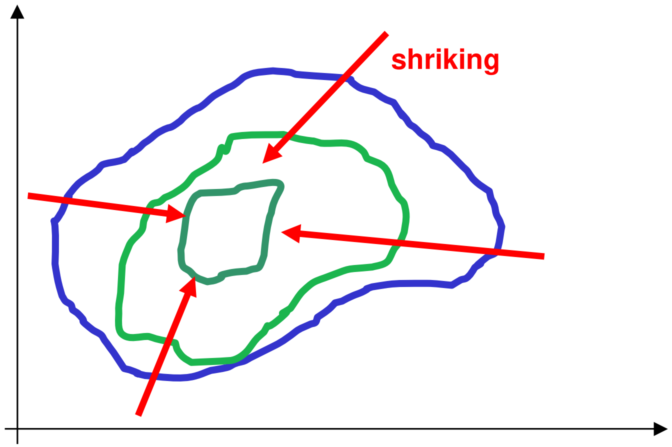
    $\boldsymbol{a} \sim f_{\boldsymbol{a}}$ (joint multi-dimensional PDF, $n_a = 5$, $A = [0, 2]^{na}$)



(Crespo et al., 2019)

- **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

    $\boldsymbol{e} \sim \boldsymbol{E}$ (hyper-rectangular set, $n_e = 4$, $B = [0, 2]^{ne}$)



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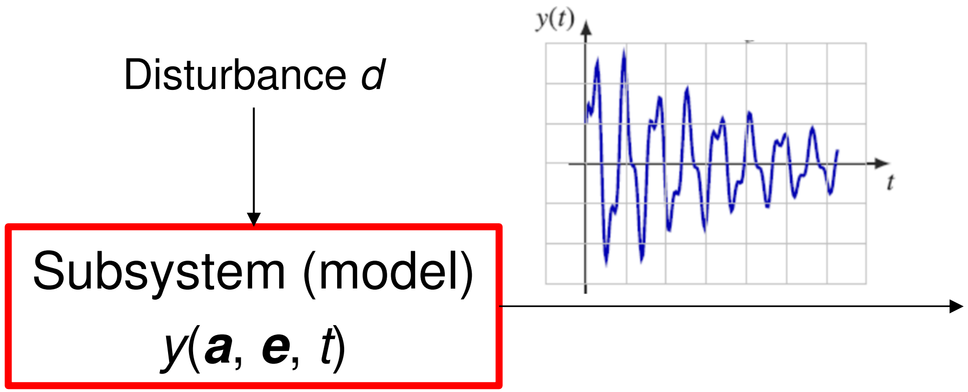
Uncertainty Model (UM) $\boldsymbol{\delta} = (\boldsymbol{a}, \boldsymbol{e}) \sim \langle f_{\boldsymbol{a}}, \boldsymbol{E} \rangle$

(Sub)-System Configuration



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(Crespo et al., 2022)

Integrated System Configuration

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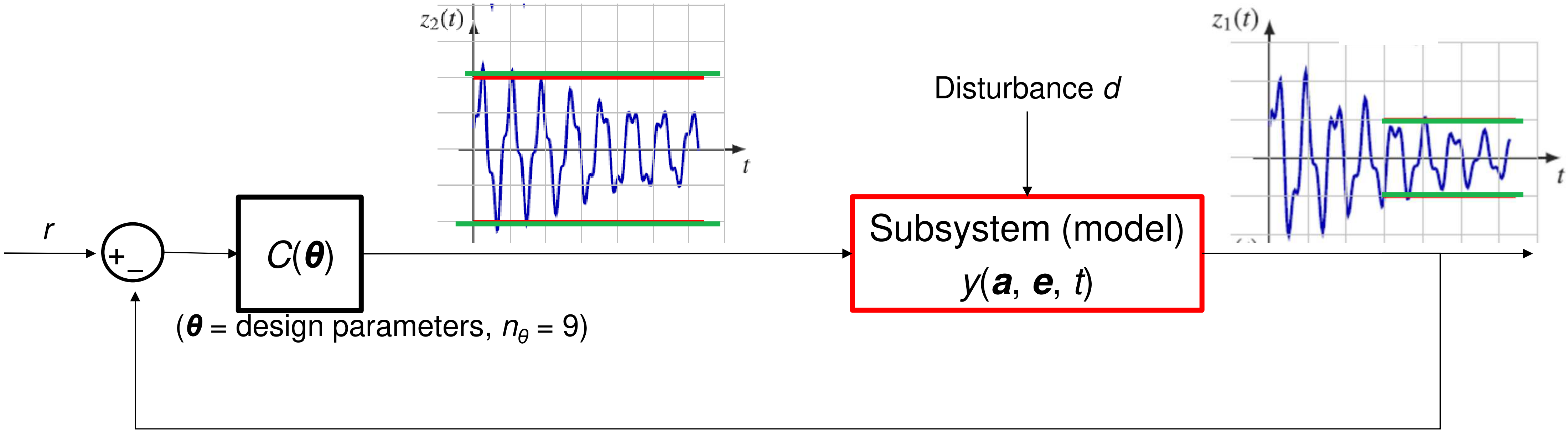

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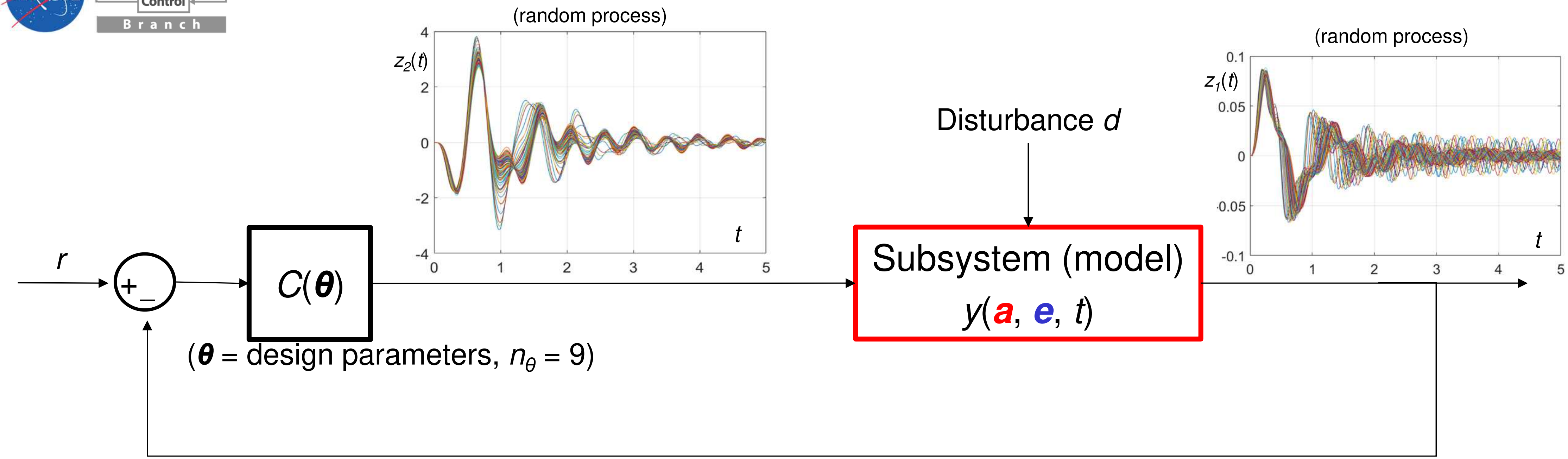
(Crespo et al., 2022)

Integrated System – Analysis Framework



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(Crespo et al., 2022)

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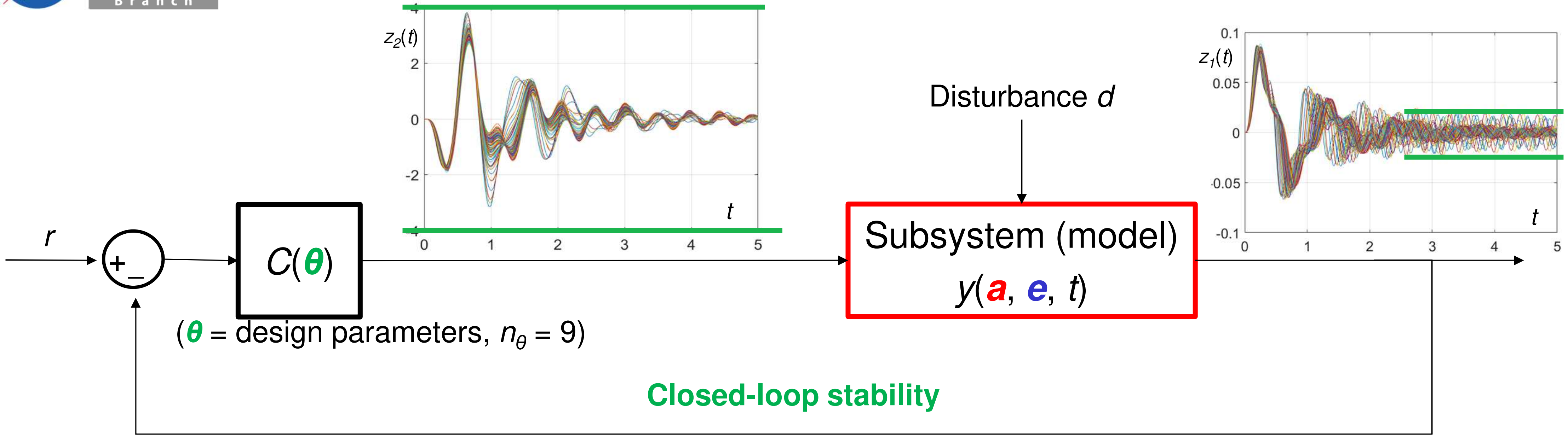
$$g_3 = \max_{t \in [0,T]} |z_2(a, e, \theta, t)| - 4$$

$$g_2 = \max_{t \in [T/2,T]} |z_1(a, e, \theta, t)| - 0.02$$

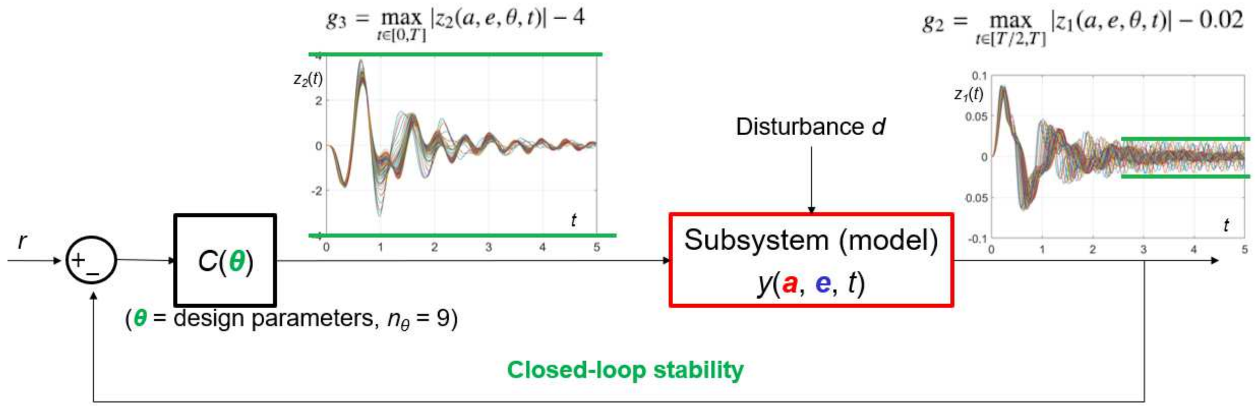


- There are **reliability requirements** $\boldsymbol{g}(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}) < 0$ that define conflicting objectives: stability (z_1 and z_2 not to infinity) (g_1), settling time (g_2), control effort/energy consumption (g_3)
- Epistemic uncertainty makes probabilistic metrics vary in a range

https://uqtools.larc.nasa.gov/nasa-uq-challenge-problem-2020/

(Crespo et al., 2022)

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) $\delta = (\boldsymbol{a}, \boldsymbol{e}) \sim \langle \boldsymbol{f_a}, \boldsymbol{E} \rangle$?

B. Reliability-Based Design Optimization

Optimal design $\boldsymbol{\theta}_{opt}$?

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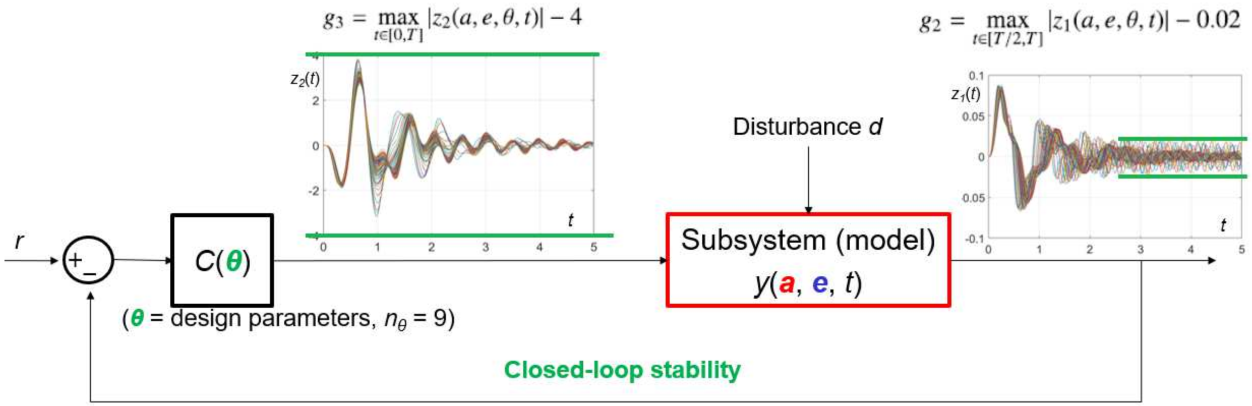

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B. Reliability-Based Design Optimization

Optimal design $\boldsymbol{\theta}_{opt}$?

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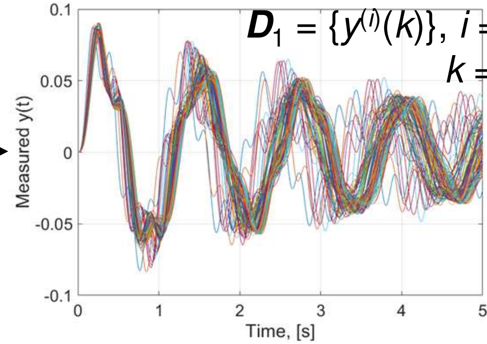
1. First stage (sub-step): functional (time-series) data from the **real subsystem**

Real sub-system observations D_1



$\boldsymbol{D}_1 = \{y^{(i)}(k)\}$, $i = 1, 2, \ldots, n_1 = 100$
$k = 0, 1, \ldots, N_T = 5001$

Real Subsystem

Uncertainty Model (UM-y) $\delta(y)$

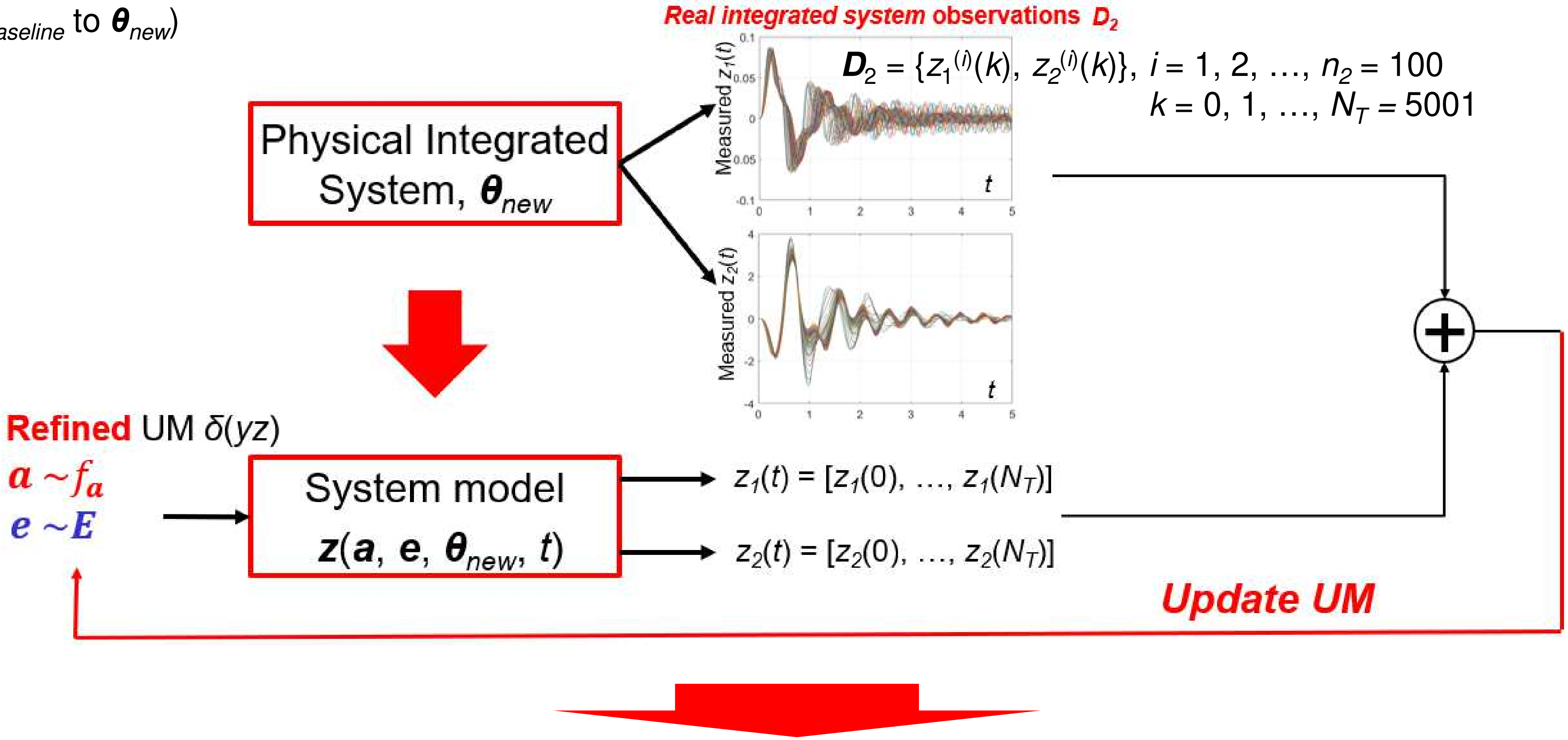
$(\boldsymbol{a}, \boldsymbol{e}) \sim \langle f_{\boldsymbol{a}}, E \rangle$

Subsystem model $y(\boldsymbol{a}, \boldsymbol{e}, t)$

$y(t) = [y(0), \ldots, y(N_T)]$
(discrete time history)

(Fist stage) Uncertainty Model (UM-y) $\delta(y)$ = $(\boldsymbol{a}, \boldsymbol{e}) \sim \langle \boldsymbol{f}_{\boldsymbol{a}}, \boldsymbol{E} \rangle$

2. Second stage (sub-step) - Refinement: functional (time-series) data from the **real integrated system**
(after a «round» of design optimization,
from $\boldsymbol{\theta}_{baseline}$ to $\boldsymbol{\theta}_{new}$)



(Refined) Uncertainty Model (UM-yz) $\delta(yz) = (\boldsymbol{a}, \boldsymbol{e}) \sim \langle \boldsymbol{f_a}, \boldsymbol{E} \rangle$

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):

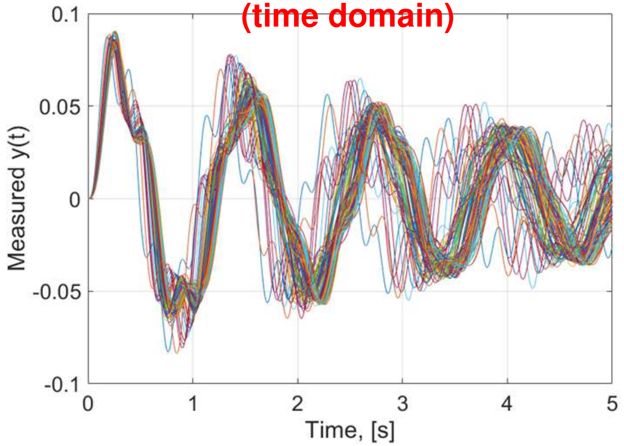
4. Retrieval of the **(unknown) input dataset** by **inverse optimization**
5. Construction of a **joint multivariate PDF** for the **aleatory input variables** by fitting the retrieved input data with **Sliced Normal (SN) distributions**

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**

1. Dimensionality reduction by Singular Value Decomposition (SVD)

Real sub-system **observations (time domain)**



$\boldsymbol{D}_1 = \{y^{(i)}(k)\}$, $i = 1, 2, \ldots, n_1 = 100$

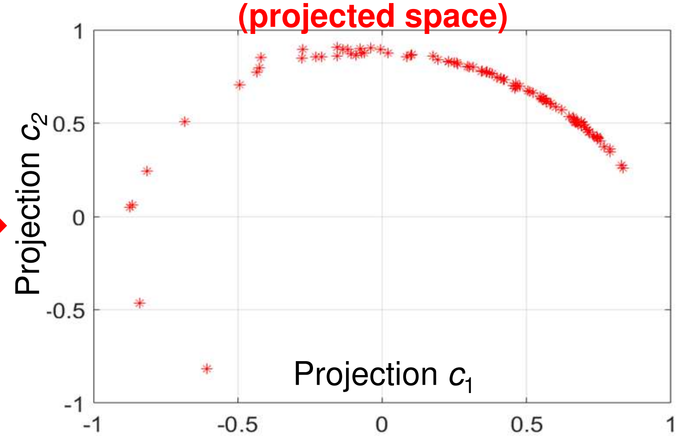
$k = 0, 1, \ldots, N_T = 5001$

Singular Value decomposition (SVD)

- Centering: $\boldsymbol{D}_1^* = \boldsymbol{D}_1 - \boldsymbol{Mean}_{\boldsymbol{D1}}$
- SVD: $\boldsymbol{D}_1^* = \boldsymbol{U} \cdot \boldsymbol{S} \cdot \boldsymbol{V}'$
- Projection: $\boldsymbol{C}_1 = \boldsymbol{D}_1^* \cdot \boldsymbol{V}[1{:}n_B]$

$$c_{it}\left(\boldsymbol{a}^{(i)}\right) = \sum_{k=1}^{N_T} y^{(i)}(k) \cdot v_t(k)$$

Real sub-system **observations (projected space)**



$\boldsymbol{C}_1 = \{c_{1,it}\}$, $i = 1, 2, \ldots, n_1 = 100$

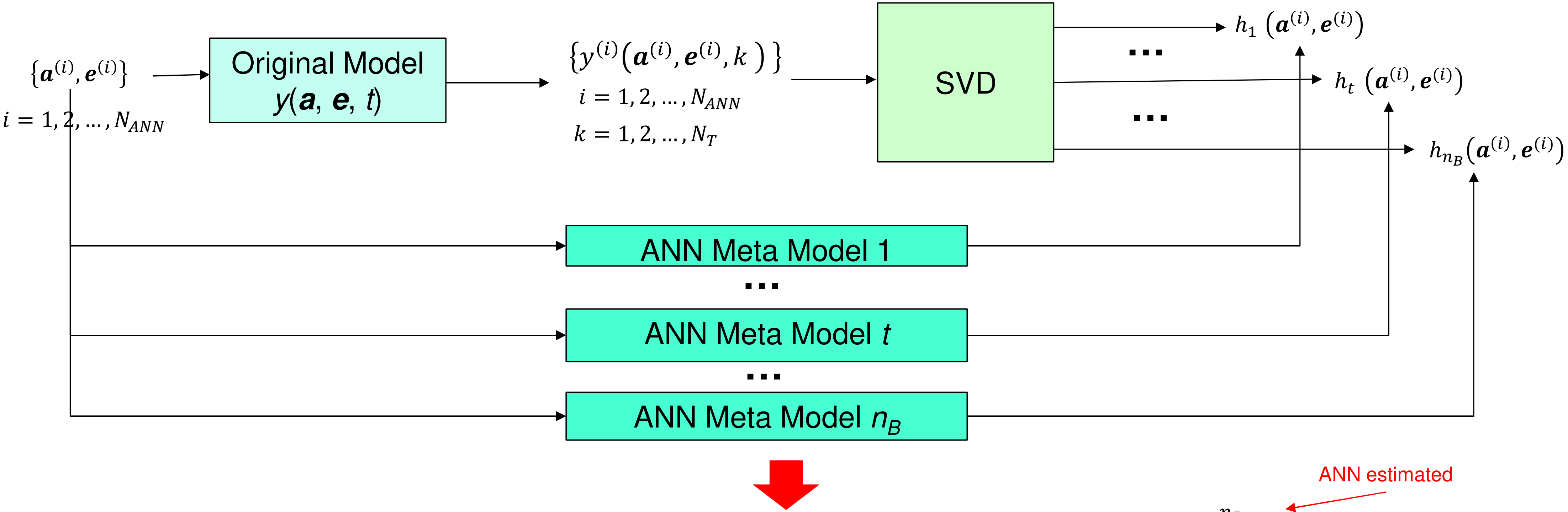
$t = 1, 2, \ldots, n_B(y) = 10$

Projection of the dataset $\boldsymbol{D}_1$ onto an orthonormal basis $\beta = \{\boldsymbol{v}_t, t = 1, 2, \ldots, n_B(y)\}$, such that $n_B(y) << N_T$ and at least ε (here 99%) of the total variance is retained (→ here $n_B(y) = 10$)

Calibration and uncertainty quantification in the **(static multivariate) *projected* space** (i.e., in the space defined by the orthonormal basis β) **rather than in the (dynamic multivariate) time domain**

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***)



ANN estimated

Given new inputs ***a***, ***e*** one can generate a "metamodel-based" transient: $\hat{y}(\boldsymbol{a}, \boldsymbol{e}, k) = \sum_{t=1}^{n_B} \hat{h}_t(\boldsymbol{a}, \boldsymbol{e}) \cdot v_t(k)$

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

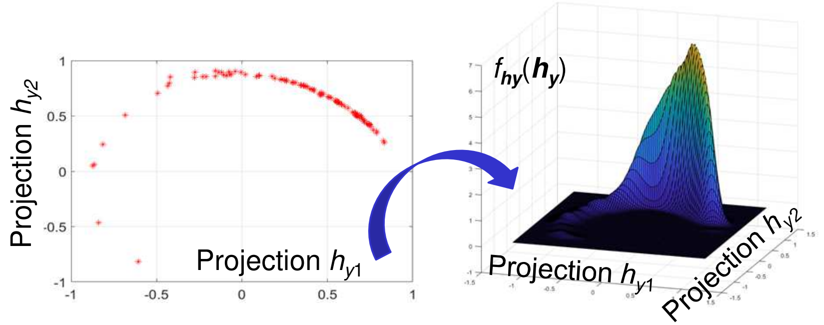
- Fit PDFs $f_{hy}(\boldsymbol{h_y})$, $f_{hz}(\boldsymbol{h_z})$ in the reduced SVD space on the data

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

  $\boldsymbol{C_2} = \{c_{2,it}\}$, $i = 1, 2, \ldots, n_2 = 100$, $t = 1, 2, \ldots, n_B(z_1)+n_B(z_2) = 17$

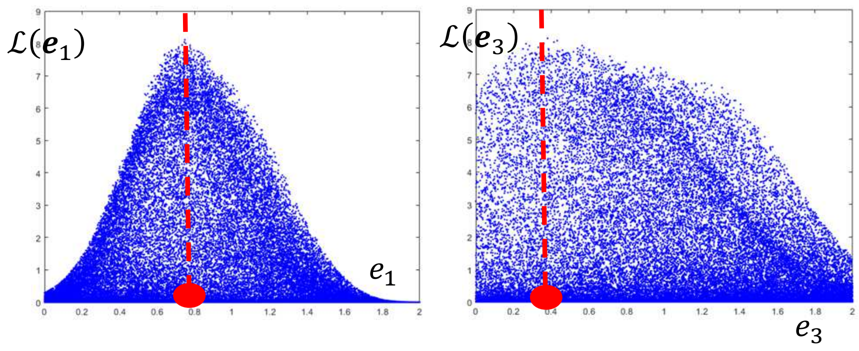
  For example: by (rough) **multivariate Kernel Density Estimation (KDE)**

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



- For a point $\boldsymbol{e} \in \boldsymbol{E}$ to be plausible: it should be possible to find *at least some* $\boldsymbol{a}$ for which $f_{\boldsymbol{h}}\big(\boldsymbol{h}(\boldsymbol{a}, \boldsymbol{e})\big)$ is high
  - ✓ Sample several epistemic vectors $\boldsymbol{e}_k$, $k = 1, 2, \ldots, N_e$
  - ✓ Sample many aleatory vectors $\boldsymbol{a}_i$, $i = 1, 2, \ldots, N_a$
  - ✓ Evaluate the plausibility of *each* $\boldsymbol{e}_k$ as its "average likelihood":

$$\mathcal{L}(\boldsymbol{e}_k) \sim \sum_{i=1}^{N_a} f_{\boldsymbol{hy}}\left(\boldsymbol{h}_y\left(\boldsymbol{a}^{(i)}, \boldsymbol{e}^{(k)}\right)\right) \cdot f_{\boldsymbol{hz}}\left(\boldsymbol{h}_z\left(\boldsymbol{a}^{(i)}, \boldsymbol{e}^{(k)}\right)\right)$$



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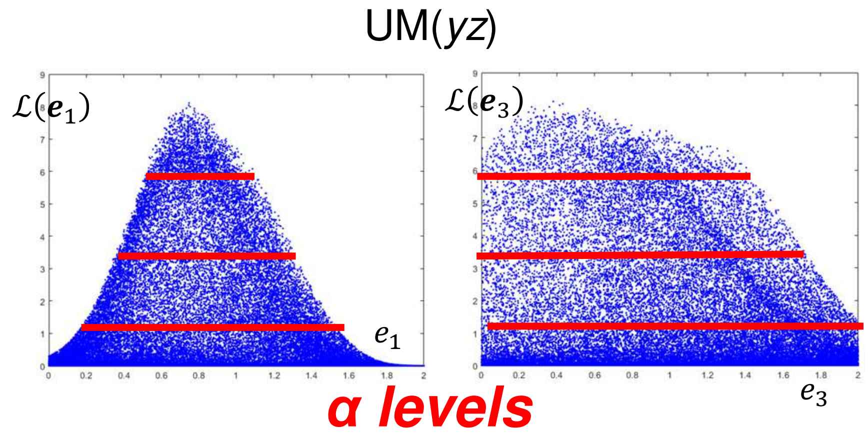
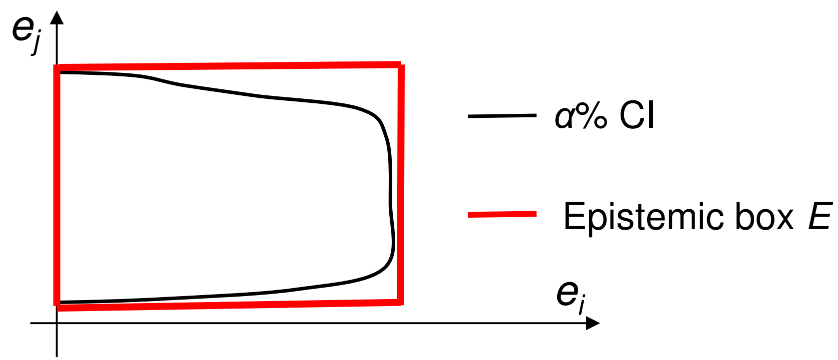


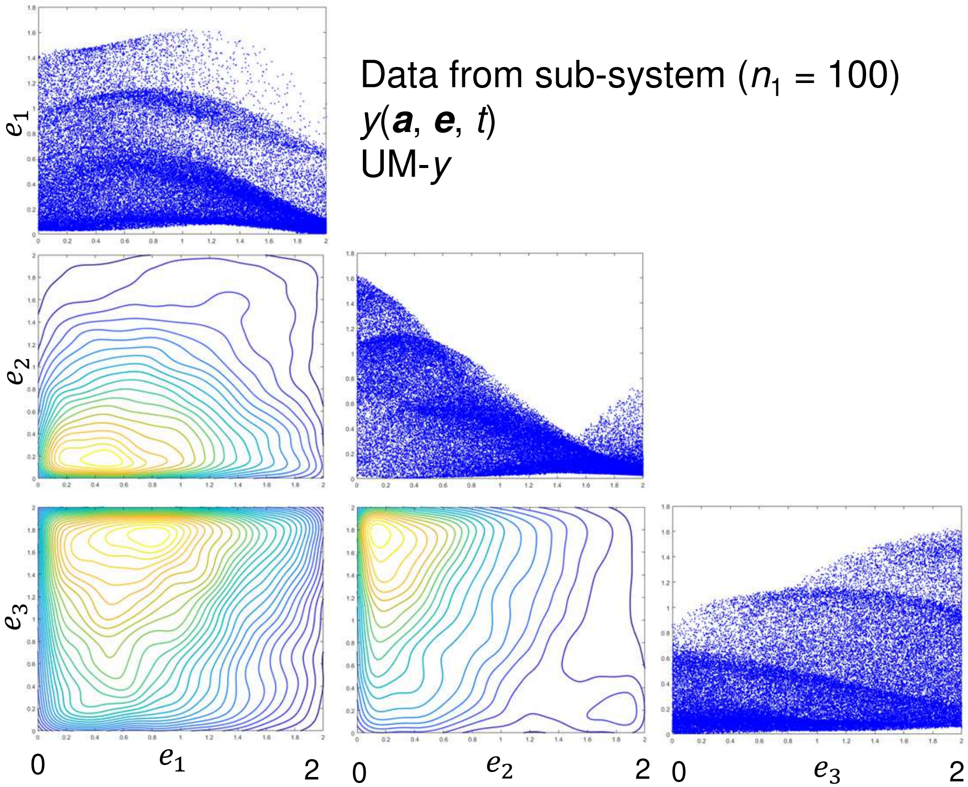
- Based on $\mathcal{L}(\boldsymbol{e}_k) \sim \sum_{i=1}^{N_a} f_{\boldsymbol{hy}}\left(\boldsymbol{h}_y\left(\boldsymbol{a}^{(i)}, \boldsymbol{e}^{(k)}\right)\right) \cdot f_{\boldsymbol{hz}}\left(\boldsymbol{h}_z\left(\boldsymbol{a}^{(i)}, \boldsymbol{e}^{(k)}\right)\right)$
  - ✓ define the UM *E* as the smallest hyper-rectangle enveloping the joint four-dimensional α% Confidence Interval (CI) of ***e***

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

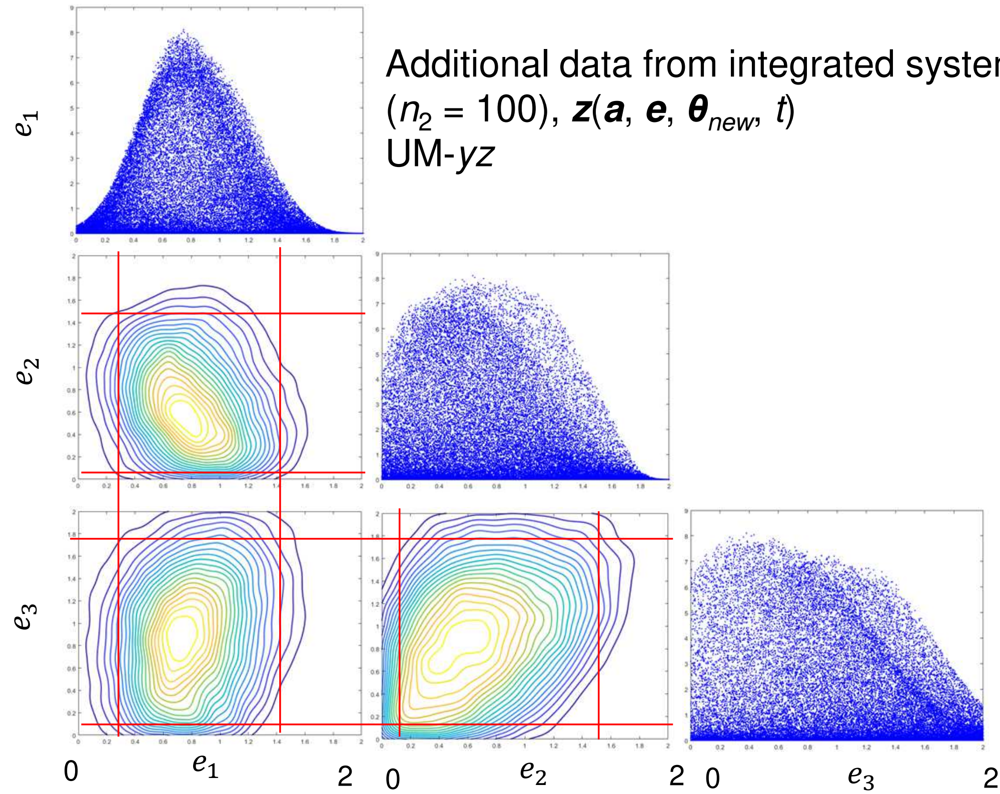
➡ **Degree of conservatism** in system design



A. Model Calibration & Uncertainty Quantification – Epistemic Space Plausibility (Refinement) – Results



Data from sub-system (n_1 = 100)
$y(\boldsymbol{a}, \boldsymbol{e}, t)$
UM-y



Additional data from integrated system (n_2 = 100), $\boldsymbol{z}(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{new}, t)$
UM-yz

Epistemic box of the joint 95% Confidence Interval

NOTE: results in picture obtained without the refinements suggested by the challengers

A. Model Calibration & Uncertainty Quantification – Approaches Considered

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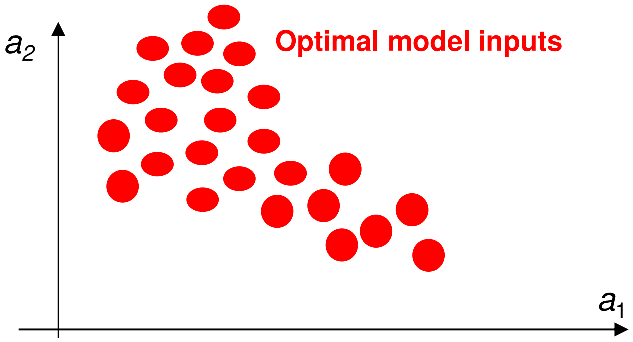
4. Retrieval of the **(unknown) input dataset** by **inverse optimization**



«Optimal» input aleatory vectors

- Select the value of $\boldsymbol{e}$ with maximum plausibility $\boldsymbol{e}^{opt}$
- 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:

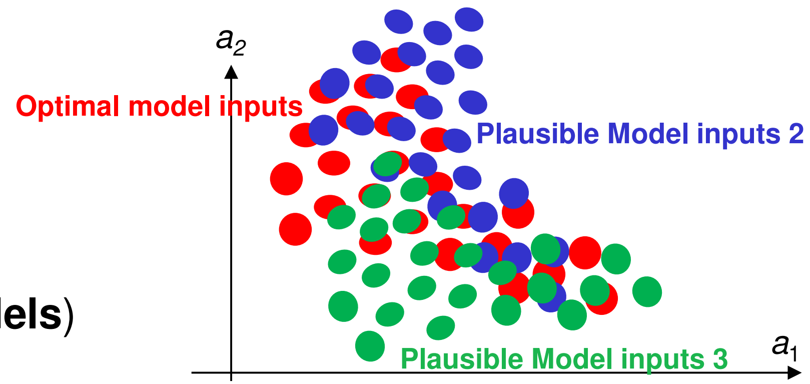
$$\boldsymbol{a}_i^{\,opt} = \arg\min_{\boldsymbol{a}_i}\left\{dist\left(\underbrace{[\boldsymbol{C}_1, \boldsymbol{C}_2]}_{\text{Projected data}}, \underbrace{\left[\boldsymbol{h}_y(\boldsymbol{a}_i, \boldsymbol{e}^{opt}), \boldsymbol{h}_z(\boldsymbol{a}_i, \boldsymbol{e}^{opt})\right]}_{\text{Projected model outputs}}\right)\right\}$$

Build robustness in the retrieval of the aleatory vectors

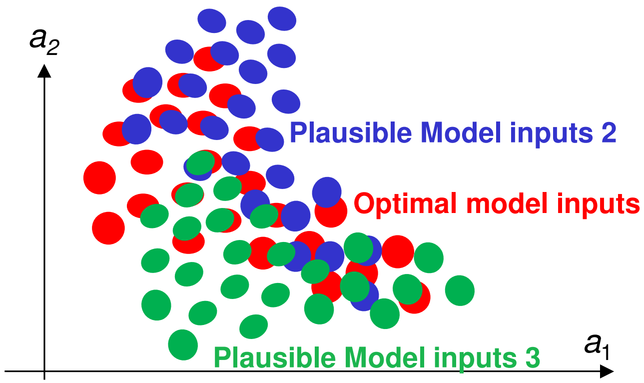
- Select different values $\boldsymbol{e}^{(k)}$ within the refined $\boldsymbol{E}$
- For each $\boldsymbol{e}^{(k)}$ repeat the optimization above to obtain different sets of aleatory vectors (corresponding to **different plausible aleatory models**)

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

$i = 1, 2, \ldots, n_1+n_2$

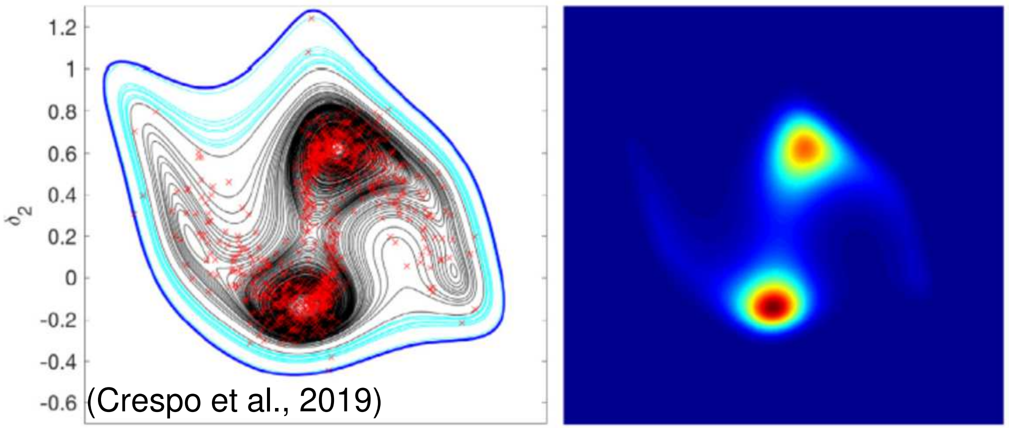


5. Construction of a **joint multivariate PDF** for the **aleatory input variables** by fitting the retrieved input data

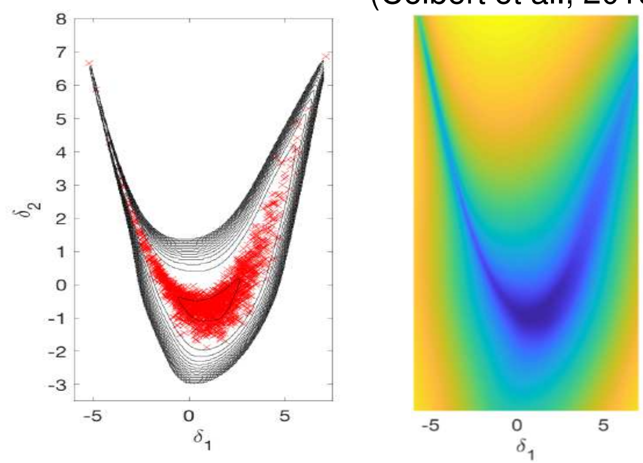


Sliced Normal (SN) distributions

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



(Crespo et al., 2019)



(Colbert et al., 2019)

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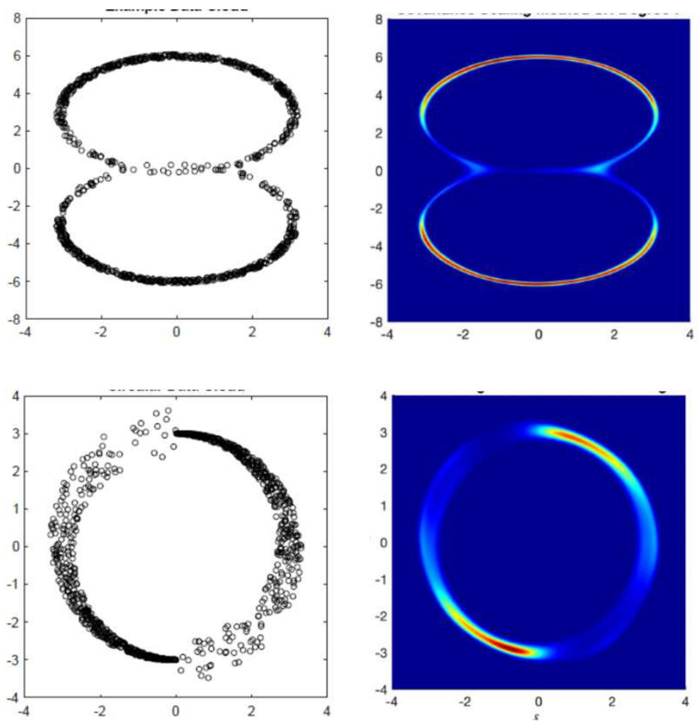
Sliced Normal (SN) distributions

(Colbert et al., 2020)



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

Where:

$\boldsymbol{P}$ = positive semi-definite matrix

$\phi(\boldsymbol{a}; \boldsymbol{\mu}, \boldsymbol{P}, d) = (\boldsymbol{W}_d(\boldsymbol{a}) - \boldsymbol{\mu})^T \cdot \boldsymbol{P} \cdot (\boldsymbol{W}_d(\boldsymbol{a}) - \boldsymbol{\mu})$

$\boldsymbol{W}_d(\boldsymbol{a})$ = monomials of degree *d* (or less) of ***a*** (in lexicographic order)

Example: $\boldsymbol{W}_2(\boldsymbol{a}) = \left(\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}\right) = [a_1, a_2, a_1^2, a_1 \cdot a_2, a_2^2]^T$

Dim($\boldsymbol{W}$) = Dim($\boldsymbol{\mu}$) = $n_W = \binom{n_a + d}{n_a} - 1$

Dim($\boldsymbol{P}$) = $n_W * n_W$

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 $A_{\boldsymbol{a}} = \{\boldsymbol{a}_i, i = 1, 2, \dots, n_1 + n_2\}$

Retrieved input dataset $A_W = \{\boldsymbol{w}_i, i = 1, 2, \dots, n_1 + n_2\}$
(polynomial space)

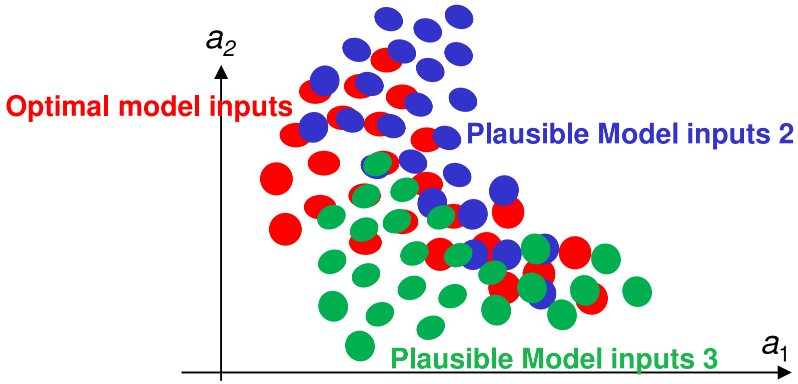
$$\mathcal{L}(A_W; \boldsymbol{\mu}, \boldsymbol{P}, d) = \sum_{i=1}^{n_1+n_2} log\left(f_W(\boldsymbol{w}_i; \boldsymbol{\mu}, \boldsymbol{P}, d)\right)$$

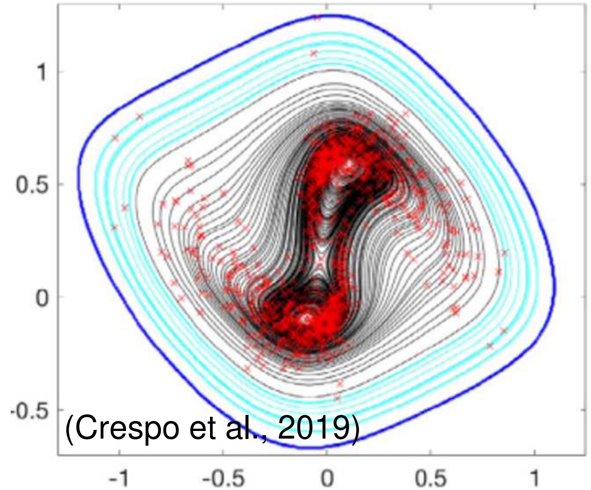
$$\langle \boldsymbol{\mu}^{\star}, \boldsymbol{P}^{\star} \rangle = \arg \max_{\boldsymbol{\mu}, \boldsymbol{P}} \left\{ \sum_{i=1}^{n_1+n_2} log\left(f_W(\boldsymbol{w}_i; \boldsymbol{\mu}, \boldsymbol{P}, d)\right) \right\}$$ (Size: $n_w*(n_w+3)/2$)

(Bootstrap to limit overfitting)

$$\boldsymbol{\mu}^{\star} = \frac{1}{n_1+n_2} \sum_{i=1}^{n_1+n_2} \boldsymbol{w}_i$$

$$\boldsymbol{P}^{\star} = \left(\frac{1}{n_1+n_2} \sum_{i=1}^{n_1+n_2} (\boldsymbol{w}_i - \boldsymbol{\mu}^{\star}) \cdot (\boldsymbol{w}_i - \boldsymbol{\mu}^{\star})^T \right)^{-1}$$





(Crespo et al., 2019)

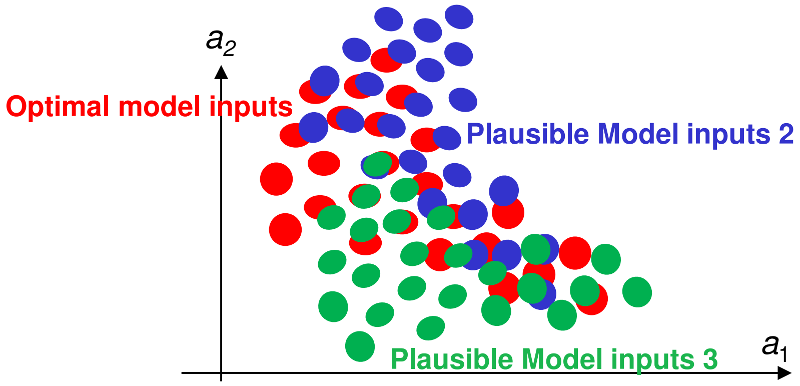
5. Construction of a **joint multivariate PDF** for the **aleatory input variables** by fitting the retrieved input data

Fitting Sliced Normal (SN) distributions

(Maximum Likelihood Estimation in the polynomial space)

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

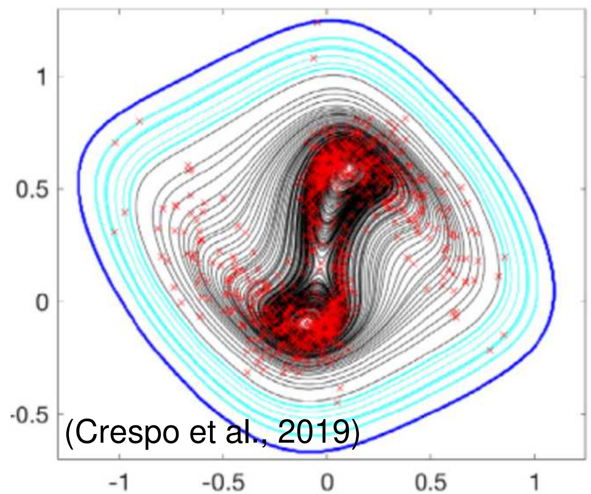
$$\phi(\boldsymbol{a};\boldsymbol{\mu},\boldsymbol{P},d)=(\boldsymbol{W}_d(\boldsymbol{a})-\boldsymbol{\mu})^T\cdot\boldsymbol{P}\cdot(\boldsymbol{W}_d(\boldsymbol{a})-\boldsymbol{\mu})$$



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

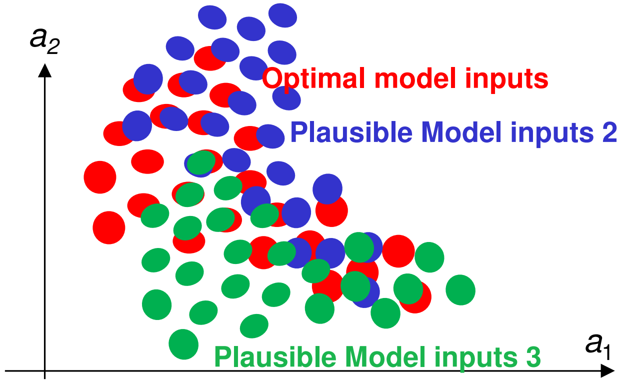
$$S(\beta_\alpha)=\{\boldsymbol{a}:(\boldsymbol{W}_d(\boldsymbol{a})-\boldsymbol{\mu})^T\cdot\boldsymbol{P}\cdot(\boldsymbol{W}_d(\boldsymbol{a})-\boldsymbol{\mu})\leq\beta_\alpha\}$$

- α is the desired confidence (coverage) level
- β_α to be determined (numerically) such that α% of the data is enclosed in $S(\beta_\alpha)$
- Members of this family can be used to tightly enclose the data
- Polynomial structure → 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 ***e*** with maximum plausibility $\boldsymbol{e}^{opt}$

$$f_W(\boldsymbol{w}; \boldsymbol{\mu}\star, \boldsymbol{P}\star, d|\boldsymbol{e}^{opt}) \longrightarrow f_{\boldsymbol{a}}(\boldsymbol{a}|\boldsymbol{e}^{opt})$$

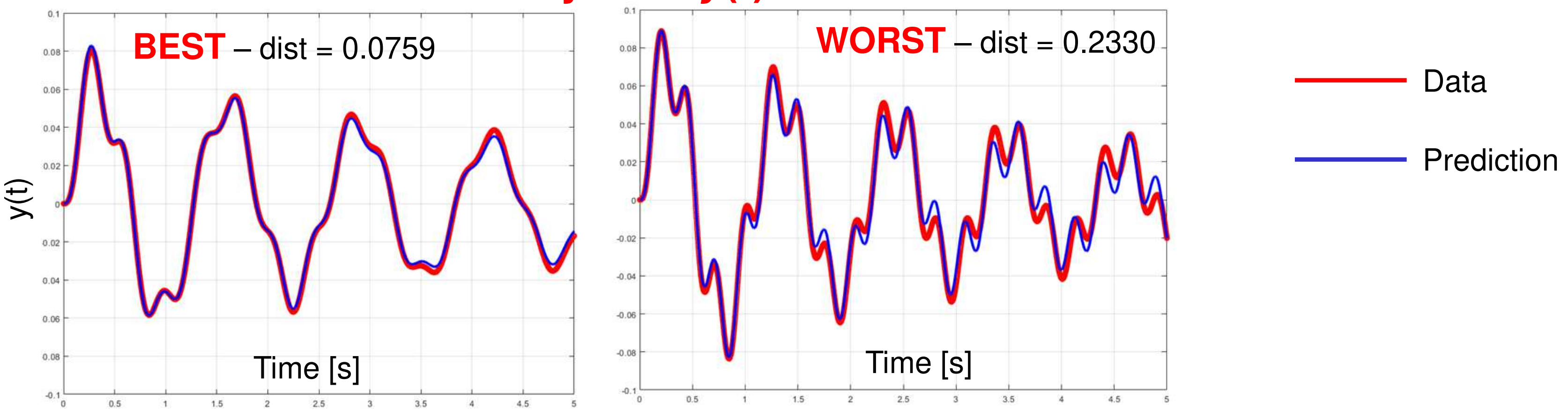
Option 2 (discrepancies are observed in the model):

- Account for it by merging different aleatory models obtained for different values $\boldsymbol{e}^{(k)}$ within the refined ***E***

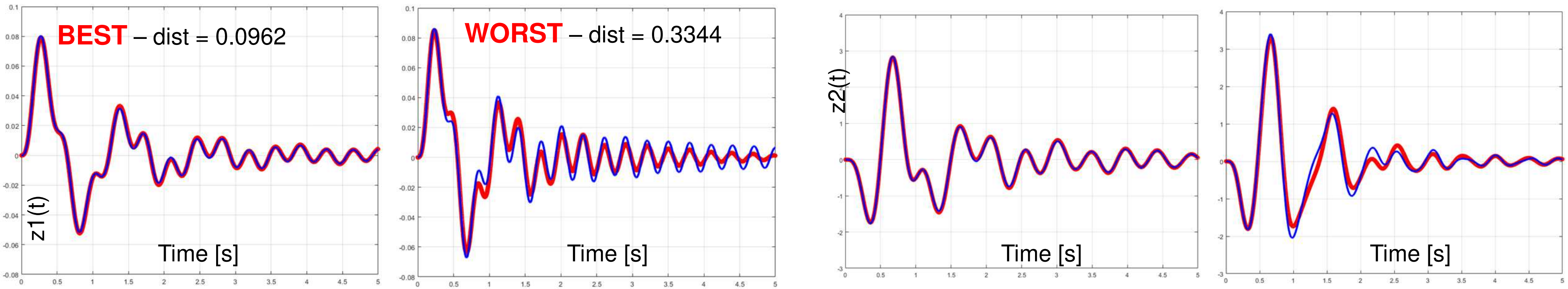
$$\sum_{k=1}^{N_e} b_{\boldsymbol{e}^k} \cdot f_W(\boldsymbol{w}; \boldsymbol{\mu}\star, \boldsymbol{P}\star, d|\boldsymbol{e}^{(k)}) \longrightarrow f_{\boldsymbol{a}}(\boldsymbol{a})$$

(weight by the corresponding plausibility or consider *equally plausible* epistemic values in ***E***)

Subsystem $y(t)$



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



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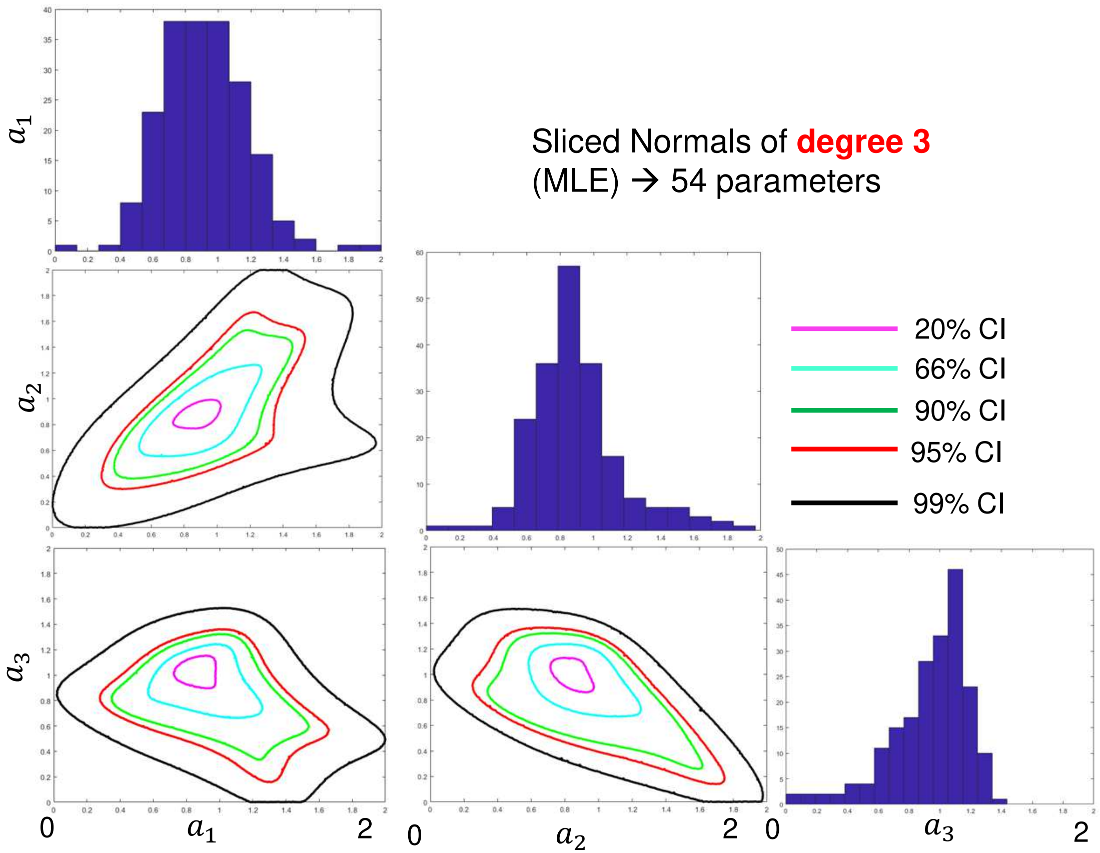
Data from integrated system (n_2 = 100), $\boldsymbol{z}(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{new}, t)$ + Data from subsystem (n_1 = 100), $y(\boldsymbol{a}, \boldsymbol{e}, t)$ → **UM-*yz***



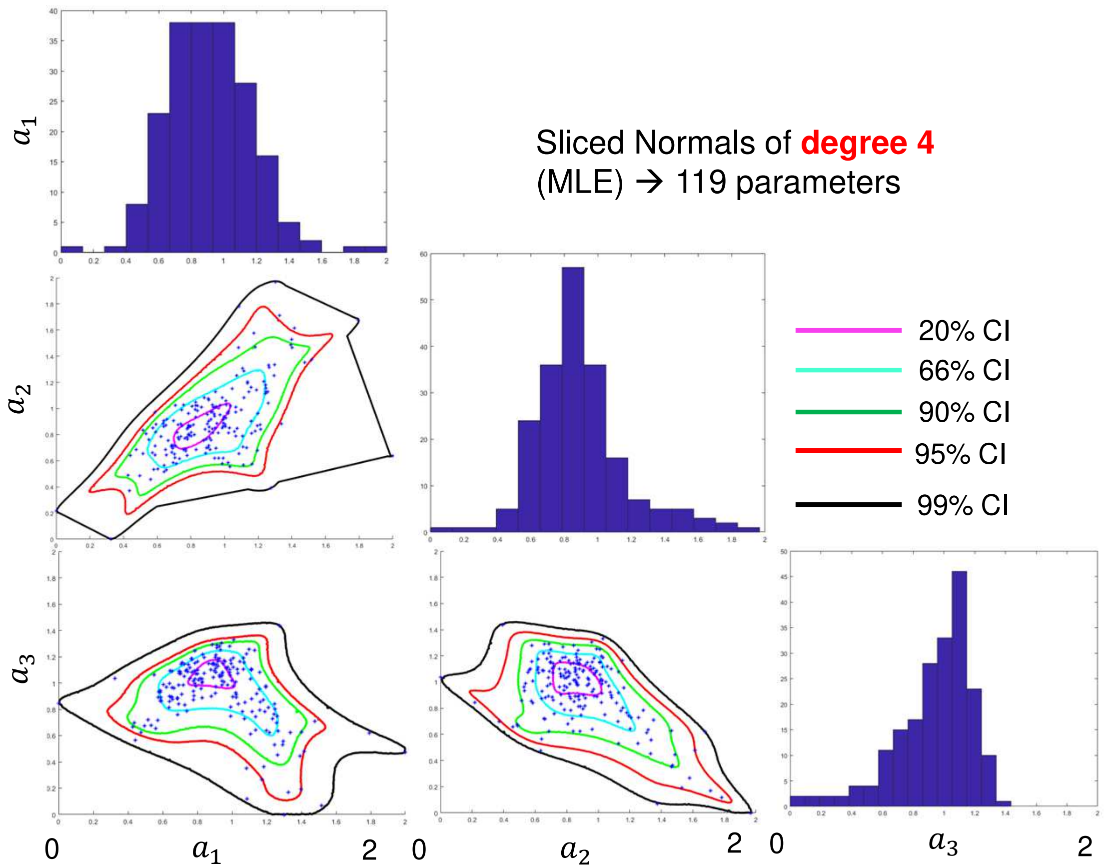
- Input retrieval allows identifying (and treating) possible **model discrepancies**

Larger epistemic sets or multiple (mixed) aleatory models

- 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 (→ rigorous and simple treatment)
- **SN: Parametric nature** → 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), $\boldsymbol{z}(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{new}, t)$ + Data from subsystem (n_1 = 100), $y(\boldsymbol{a}, \boldsymbol{e}, t)$ → **UM-*yz***



- **Increase the degree** of the polynomial → 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** (→ **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**

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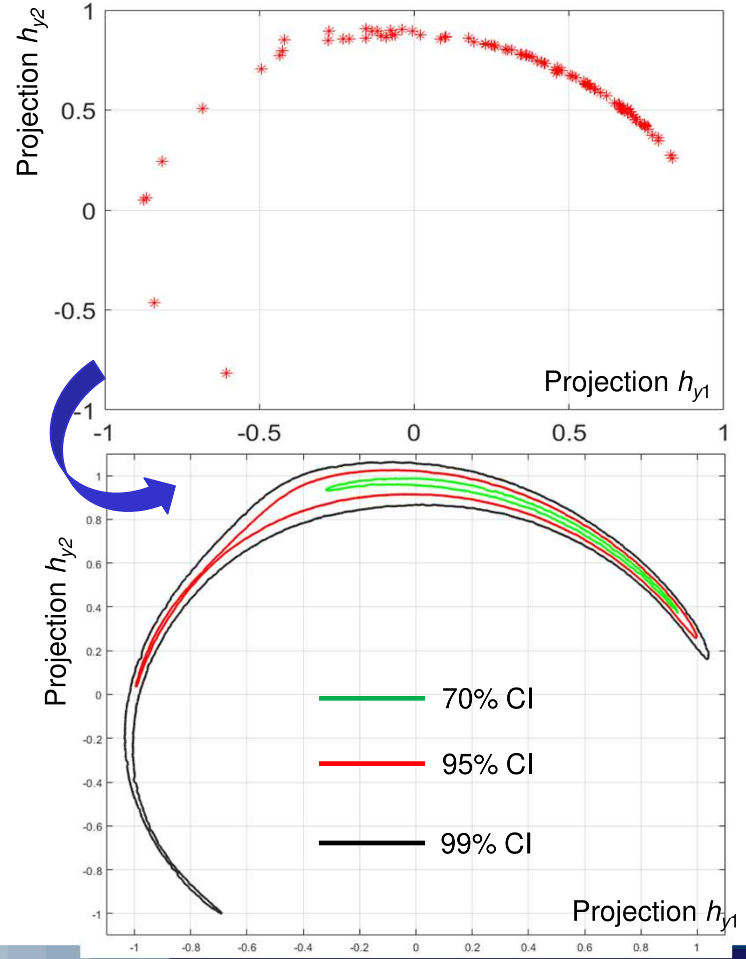
4. Construction of a **joint multivariate Likelihood** by **Sliced Normal (SN) distributions** in the SVD space **(maximum- and worst-case)**

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



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**

5. Aleatory model calibration by Bayesian inverse uncertainty quantification

- Use non-informative priors for $\boldsymbol{a}$ ($A = [0, 2]^{na}$), $p_{\boldsymbol{a}}(\boldsymbol{a})$
- For a given epistemic vector $\boldsymbol{e}^{(k)}$, evaluate the posterior PDF of $\boldsymbol{a}$:

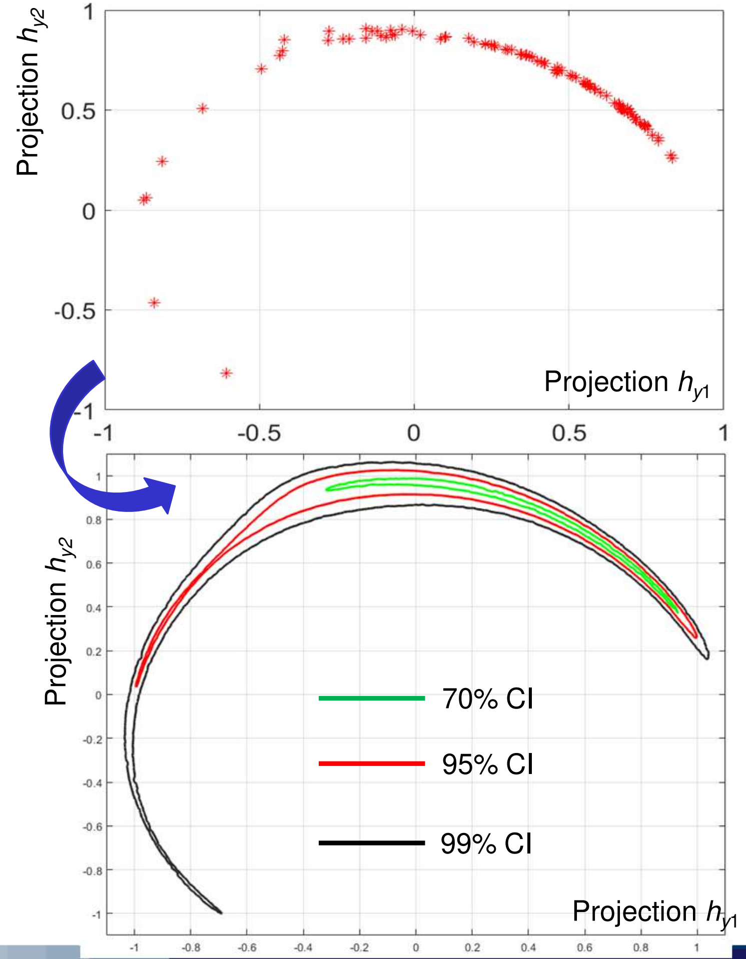
Notice: $f_{\boldsymbol{a}|\boldsymbol{e}^k}(\boldsymbol{a}) \sim \frac{1}{K} f_{\boldsymbol{h}}\left(\boldsymbol{h}(\boldsymbol{a}, \boldsymbol{e}^k)\right)$

($f_{\boldsymbol{h}}$ defines a likelihood for any $\boldsymbol{h}(\boldsymbol{a}, \boldsymbol{e})$ which we assign to $\boldsymbol{a}$)

$$f_{\boldsymbol{a}|\boldsymbol{e}^k}(\boldsymbol{a}) = \frac{1}{K} f_{\boldsymbol{h}}\left(\boldsymbol{h}(\boldsymbol{a}, \boldsymbol{e}^k)\right) \cdot p_{\boldsymbol{a}}(\boldsymbol{a})$$

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

- Repeat for different epistemic vectors $\boldsymbol{e}^{(k)}$, to increase robustness in the PDF estimation (if computational burden accaptable)



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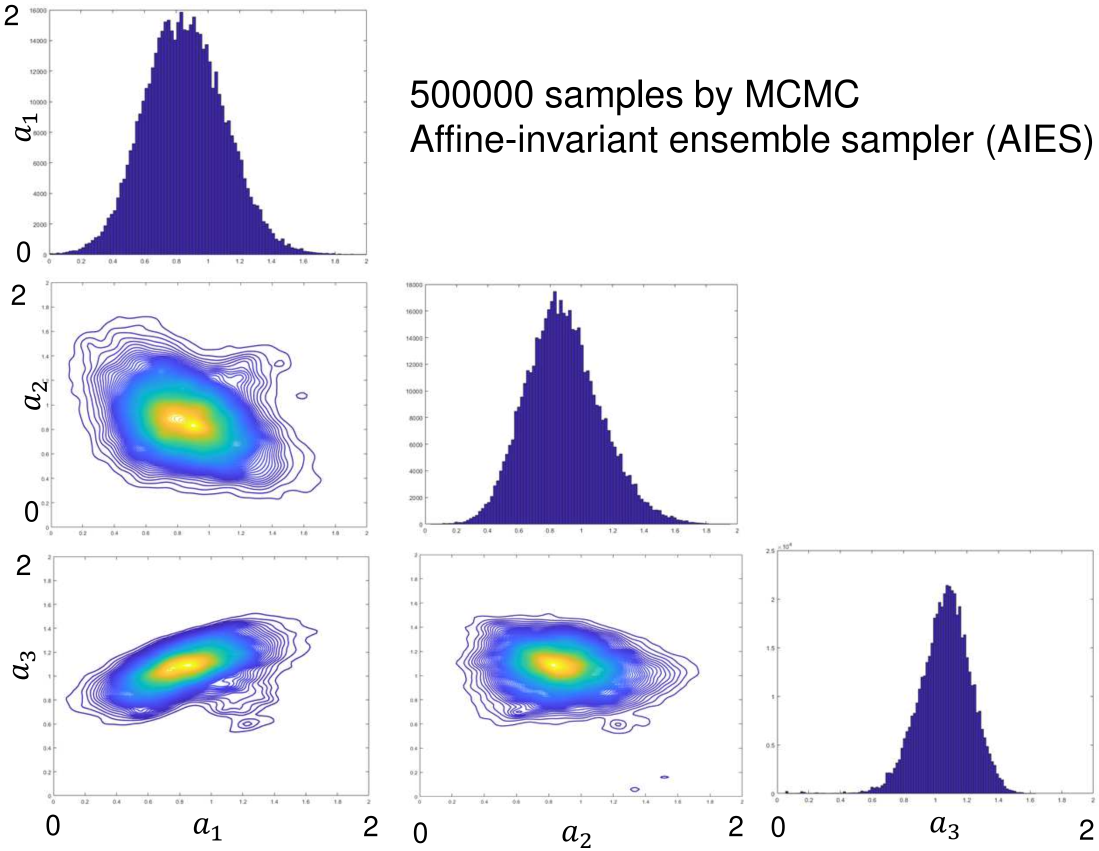
Data from integrated system (n_2 = 100), $\boldsymbol{z}(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{new}, t)$ + Data from subsystem (n_1 = 100), $y(\boldsymbol{a}, \boldsymbol{e}, t)$ → **UM-*yz***



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 $f_{\boldsymbol{a}|\boldsymbol{e}^k}(\boldsymbol{a}) = \frac{1}{K} f_h\left(\boldsymbol{h}(\boldsymbol{a}, \boldsymbol{e}^k)\right) \cdot p_{\boldsymbol{a}}(\boldsymbol{a})$ and the optimization-based input retrieval adopted before (if any)…

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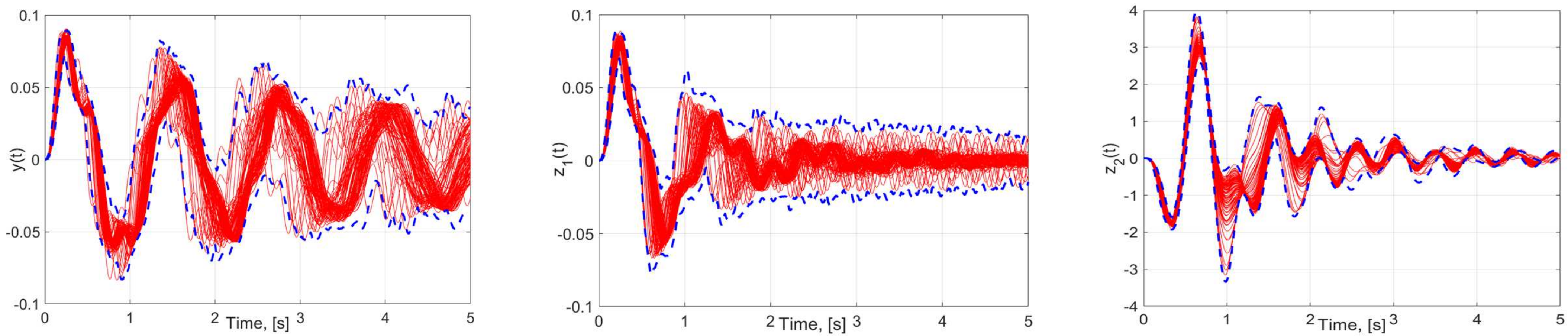
Model comparison → **Energy score:**

Multivariate generalization of the Continuous Rank Predictive Score (CRPS)

$$ES(\langle f_{\boldsymbol{a}}, E\rangle, \boldsymbol{C}) = \frac{1}{n_{1+}n_2}\sum_{i=1}^{n_{1+}n_2} ES(\langle f_{\boldsymbol{a}}, E\rangle, \boldsymbol{c}_i) = \frac{1}{n_{1+}n_2}\sum_{i=1}^{n_{1+}n_2}\left(\frac{1}{N_a}\sum_{q=1}^{N_s}\|\boldsymbol{h}_q - \boldsymbol{c}_i\| - \frac{1}{2N_a^2}\sum_{q=1}^{N_a}\sum_{j=1}^{N_a}\|\boldsymbol{h}_q - \boldsymbol{h}_j\|\right)$$

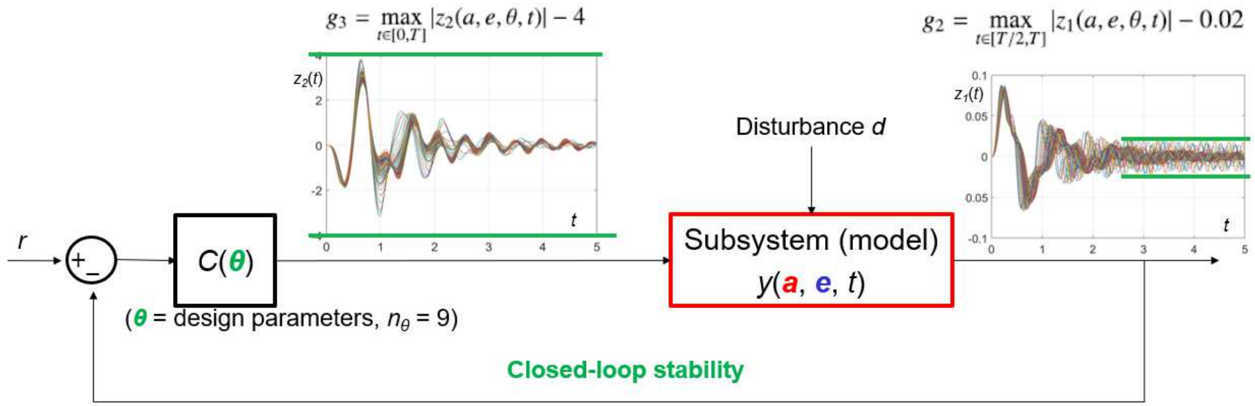
Projected model outputs Projected data

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

Dynamic Systems & Control Branch



A. Model Calibration & Uncertainty Quantification

(using **time series** from the *subsystem* and the *integrated system*)

?

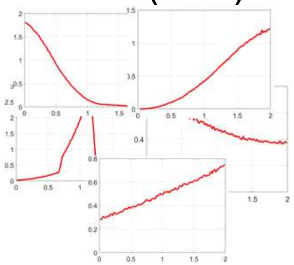
Uncertainty Model (UM) $\delta = (\boldsymbol{a}, \boldsymbol{e}) \sim \langle \boldsymbol{f_a}, \boldsymbol{E} \rangle$

B. Reliability-Based Design Optimization

?

Optimal design $\boldsymbol{\theta}_{opt}$

Refined Uncertainty Model (UM) δ



$\boldsymbol{a} \sim f_{\boldsymbol{a}}$

e_1
e_2
e_3
e_4

$\boldsymbol{e} \sim \boldsymbol{E}$

Requirements model
$\boldsymbol{g}(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{baseline})$

$g_1(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{baseline})$ (stability)

$g_2(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{baseline})$ (settling time)

$g_3(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{baseline})$ (energy consumption)

$$w(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{baseline}) = \max_{i=1,\dots,n_g=3} g_i(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{baseline})$$

P_{fail}?

Failure probability (epistemic) bounds

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

$R_i(\theta)$

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

$R(\theta)$

Maximum severity of requirements violation

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

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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

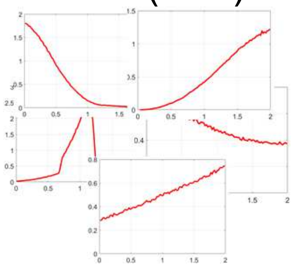
   → Evaluate bounds of the epistemic box *E*!

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

Refined Uncertainty Model (UM) δ



$\boldsymbol{a} \sim f_{\boldsymbol{a}}$

e_1
e_2
e_3
e_4

$\boldsymbol{e} \sim \boldsymbol{E}$

Requirements model
$\boldsymbol{g}(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{new})$

New design $\boldsymbol{\theta}_{new}$

$g_1(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{new})$

$g_2(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{new})$

$g_3(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{new})$

$$w(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{new}) = \max_{i=1,\ldots,n_g=3} g_i(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}_{new})$$

$$P_{\text{fail}}(\boldsymbol{\theta}_{new}) < P_{\text{fail}}$$

Optimality criterion

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

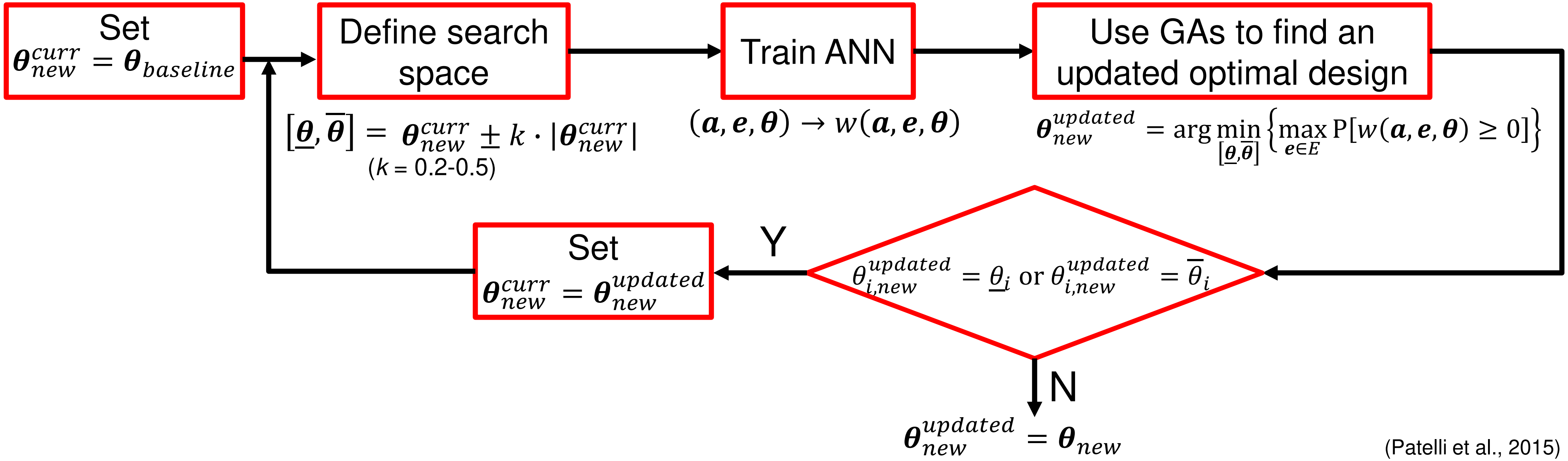
$$\boxed{\boldsymbol{\theta}_{new} = \arg\min_{\boldsymbol{\theta}} \left\{ \max_{\boldsymbol{e}\in E} P[w(\boldsymbol{a}, \boldsymbol{e}, \boldsymbol{\theta}) \geq 0] \right\}}$$

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**

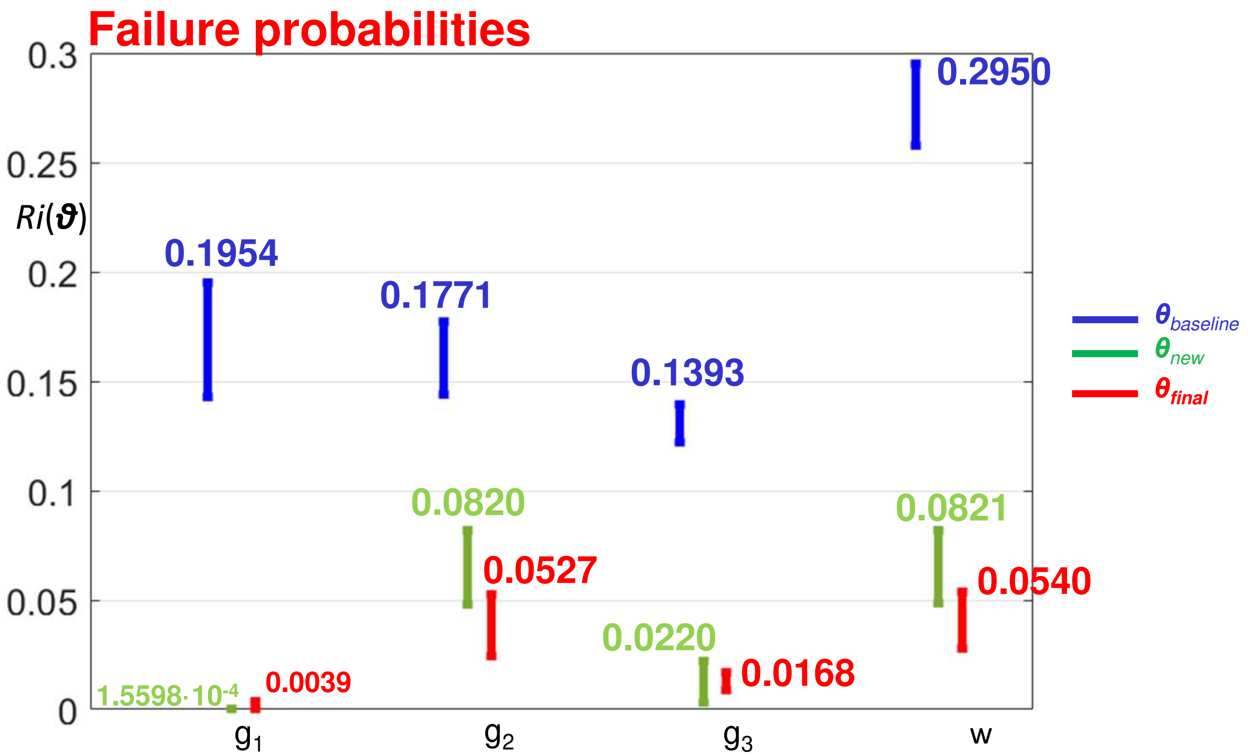
Iterative Optimization Algorithm

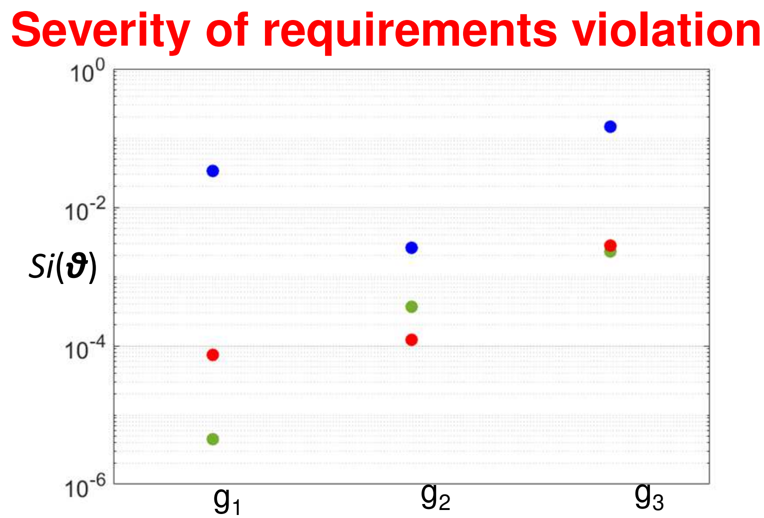


(Patelli et al., 2015)

B. Reliability-Based Design Optimization – Results

$\boldsymbol{a} \sim f_{\boldsymbol{a}}$ $\boldsymbol{e} \sim E$ ➡ $\boldsymbol{\theta}_{final}$





- Strong reduction in $R_1(\boldsymbol{\theta})$ (2-3 orders of magnitude)
- Reduction in $R_2(\boldsymbol{\theta})$, $R_3(\boldsymbol{\theta})$, $R(\boldsymbol{\theta})$ 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)

- 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

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THANK YOU!

QUESTIONS?