Global Sensitivity Analyses for Test Planning with Black-Box Models for Mars Sample Return

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How to design tests with limited project sources?

OBJECTIVE

Design/plan experimental **tests** for: model validation, uncertainty quantification, digital twins, etc.

to support a project/mission **design** and **decision-making process** over the entire life cycle with **limited resources**

LIMITATIONS

- Constrained budget / schedule
- Computationally expensive models
- Black-box models
- Correlated model input parameters

SOLUTIONS

Design of experiments

- Use appropriate design of experiment to maximize value of information

Global sensitivity analyses (GSA)

- **Screen** uninfluential parameters and fix to nominal values
- **Prioritize** influential parameters to target through experiments

- Make practical through **multi-fidelity** simulation techniques
- Make informative through sensitivity indices that can uncover hidden effects and parameter interactions
- Use sensitivity indices that are agnostic about parameter dependencies

Outline

- What is global sensitivity analysis
- Application to Mars Sample Return
  - Overview
  - Case study
- Multi-fidelity simulation framework
- Design of experiments
- Global sensitivity analyses
  - Factor fixing
  - Factor prioritization
    - Univariate
    - Multivariate
  - Direction of change
  - Interactions
- Data assimilation and predictive models
- Conclusions

NOTE: All the results shown in this presentation are from the following reference:

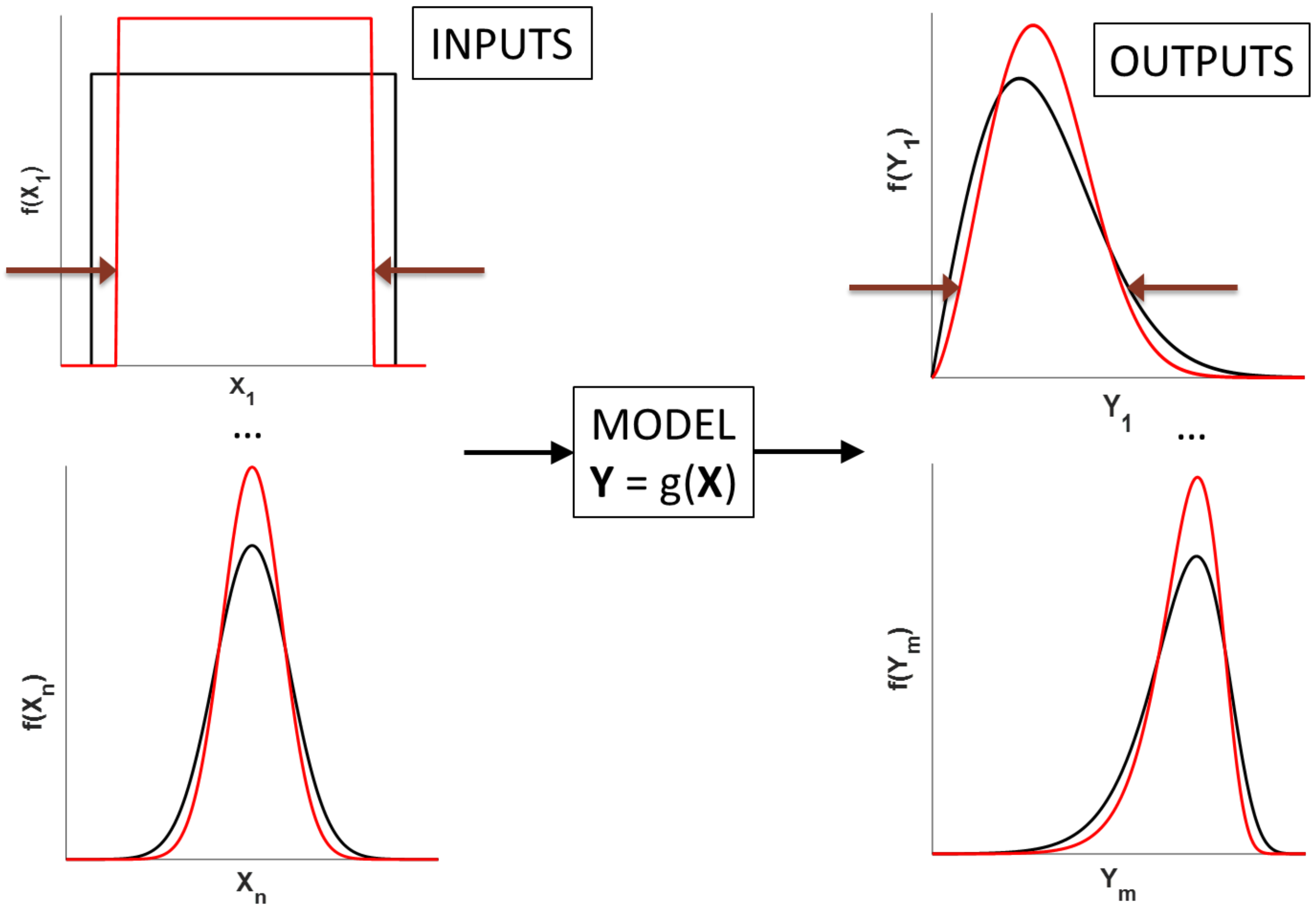
[1] Cataldo et al., "Global sensitivity analyses for test planning with black-boxes models for Mars Sample Return", *Operations Research*, submitted.

Global sensitivity analysis helps identify uncertainty drivers

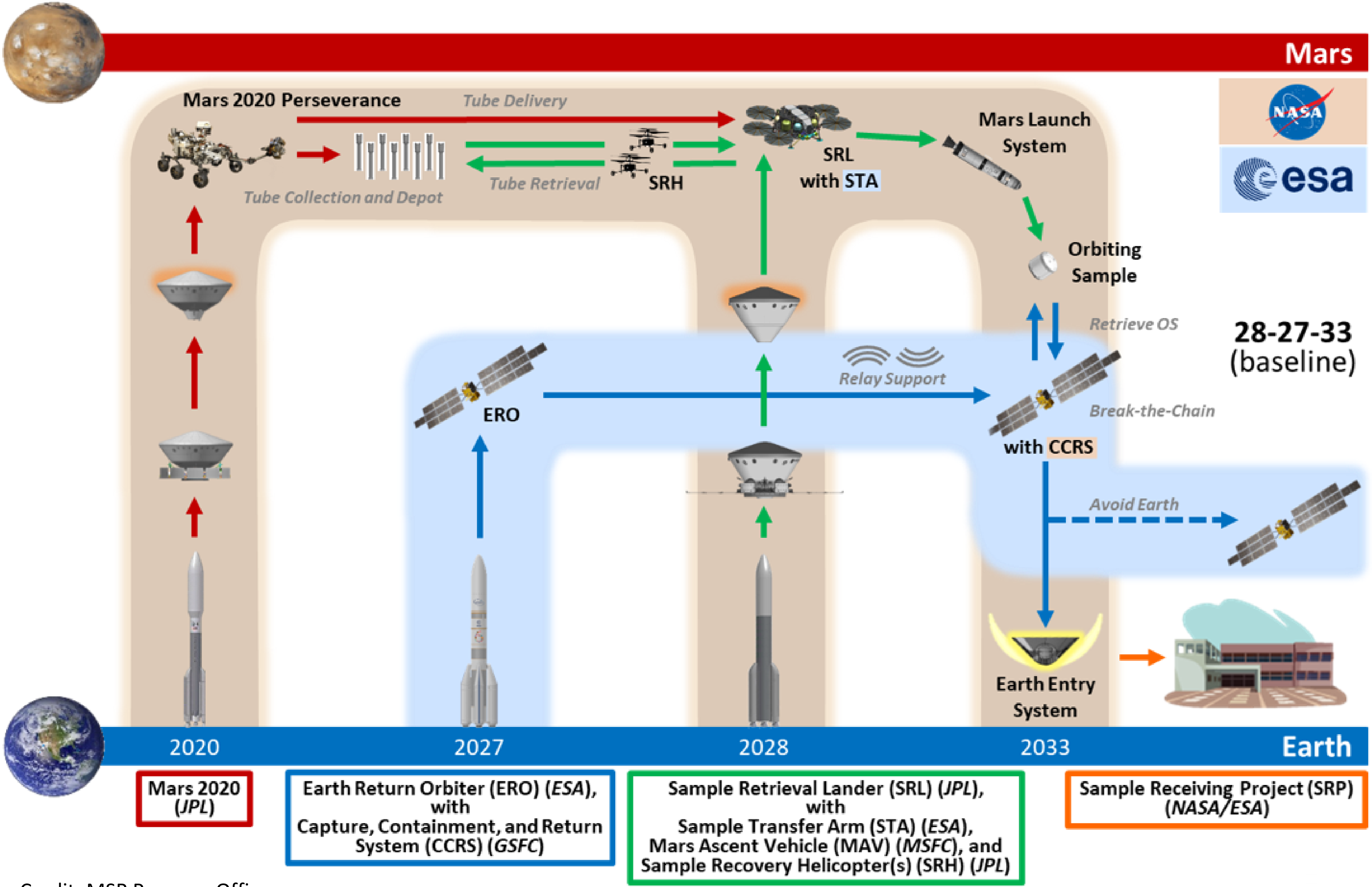
- **GOAL:** to determine the amount of uncertainty that would disappear in the outputs if one or more input parameters were known and fixed.

- Global sensitivity indices
  - Sobol' indices (main and total effects) [2]
  - Global importance measures [3]
  - Optimal transport-based measures [4]
  - Etc.

- Prioritize parameters based on the amount of reduction in the output uncertainty and target them through tests.



Mars Sample Return campaign architecture prior to 2024 re-architecture



Credit: MSR Program Office

As part of the NASA response to the September 2023 MSR Independent Review Board's report and in light of the current budget environment, the MSR Program is undergoing a consideration of changes in its mission architecture.

This work is based upon the previous baseline MSR architecture in which ERO-CCRS would return the OS to Earth within approximately five years of landing on Mars to retrieve samples collected by the Perseverance rover.

The CCRS project completed system development to a Preliminary Design Review level of maturity in mid-December 2023, after which it was stopped indefinitely pending the results of the re-architecting effort.

What are the drivers in the design of the Earth Entry System?

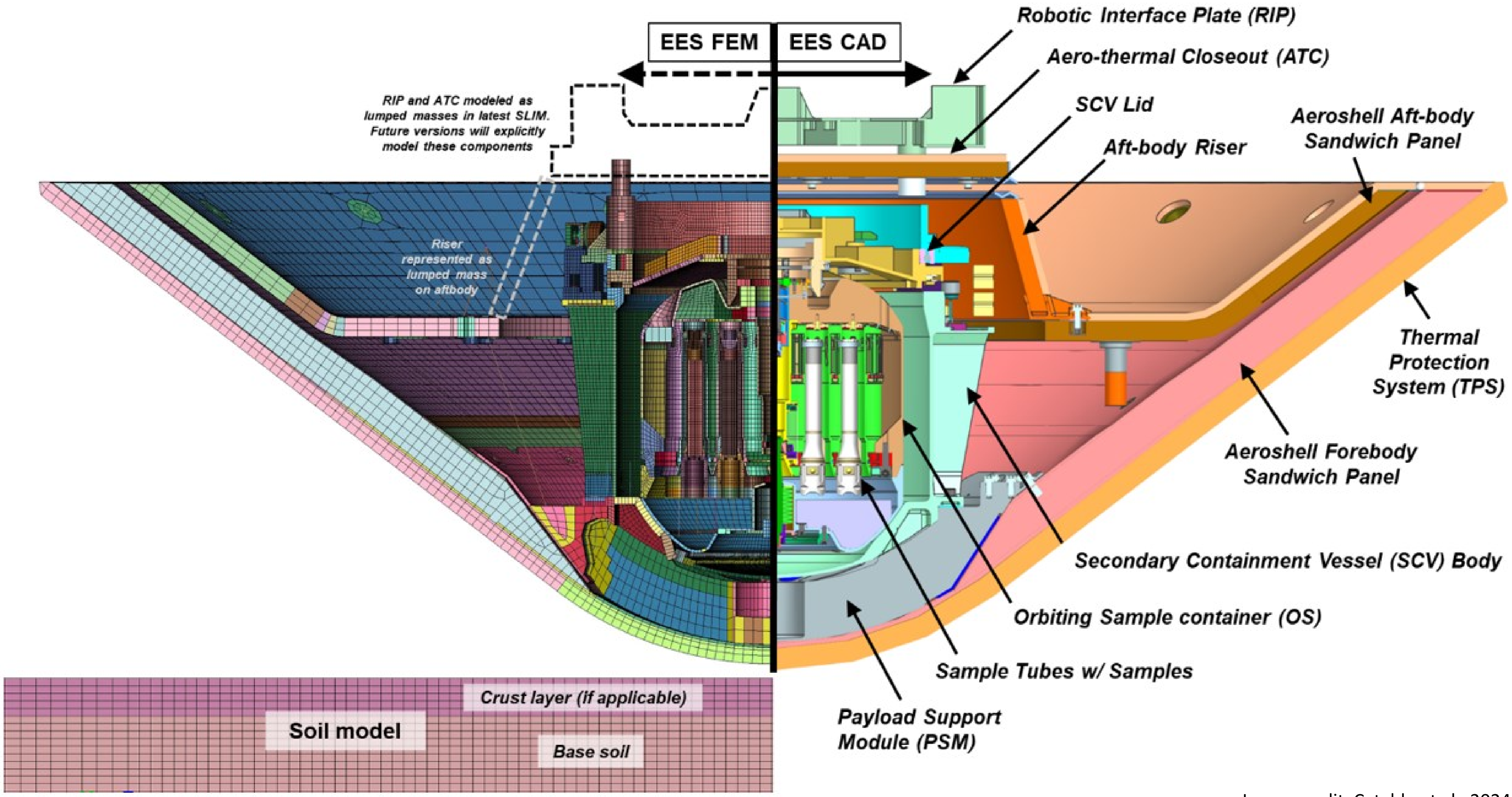


Image credit: Cataldo et al., 2024 [1]

The Earth Entry System model and study set-up

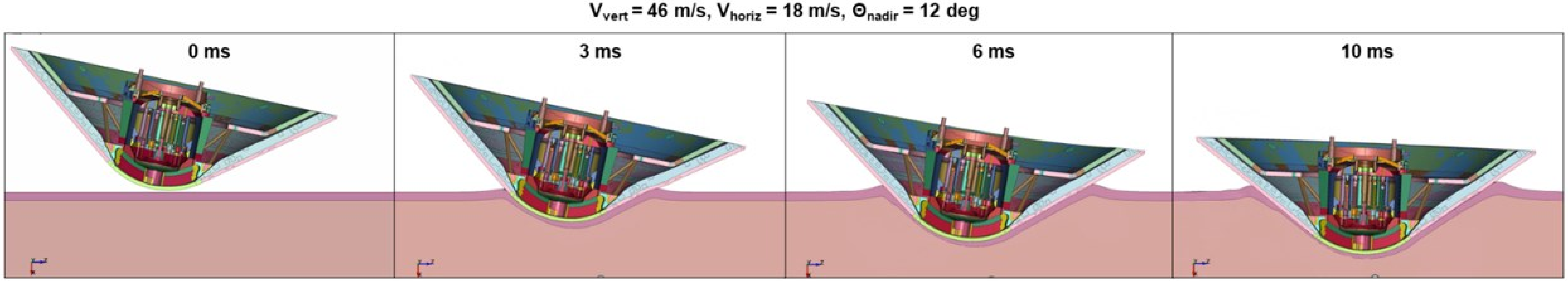


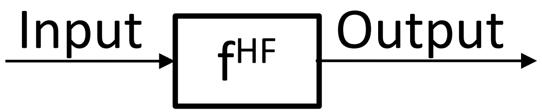
Image credit: Cataldo et al., 2024 [1]

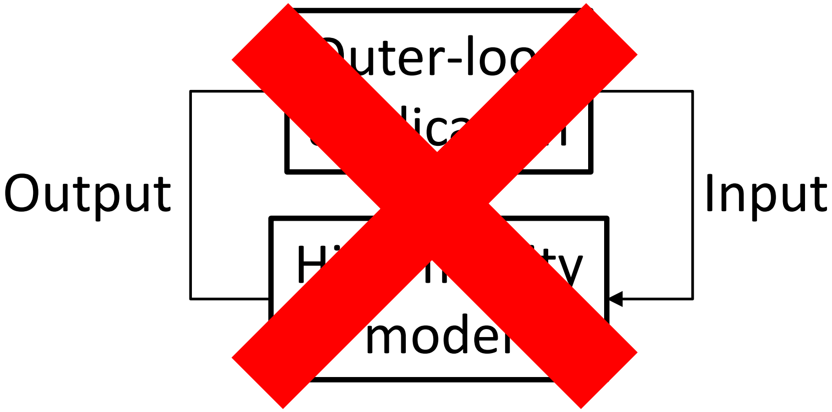
- System-Level Impact Model (SLIM)
  - LS-DYNA finite-element model of all key EES structural components and soil.
  - Can simulate full range of kinematic and soil conditions the EES is required to withstand.
- For the study presented here:
  - Varied 10 input parameters
  - Analyzed 8 output metrics
- GSA requires a large number of samples, e.g., *O*(1000) or more, to converge.
  - However, SLIM takes ~2.5 hours per run
  - In addition: license availability, queue time, code set-up, etc.

Resources become limited given the SLIM's overall large computational cost! **How to make GSA feasible?**

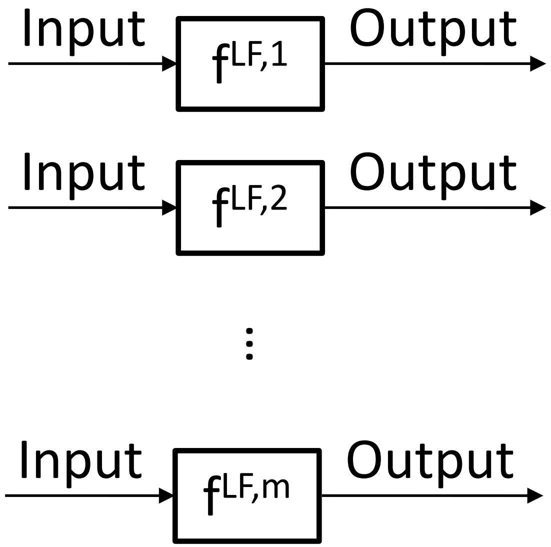
Multi-fidelity approach to computationally expensive models

High-fidelity (HF) model

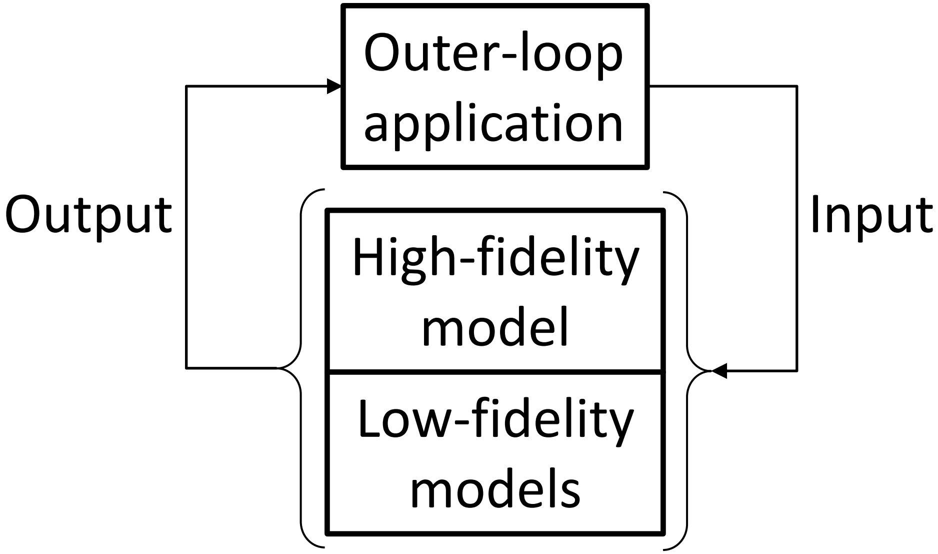




Low-fidelity (LF) models



- Invoke multiple models to reduce computational cost
- Maintain accuracy guarantees on outer-loop results



Samples are shared optimally among models

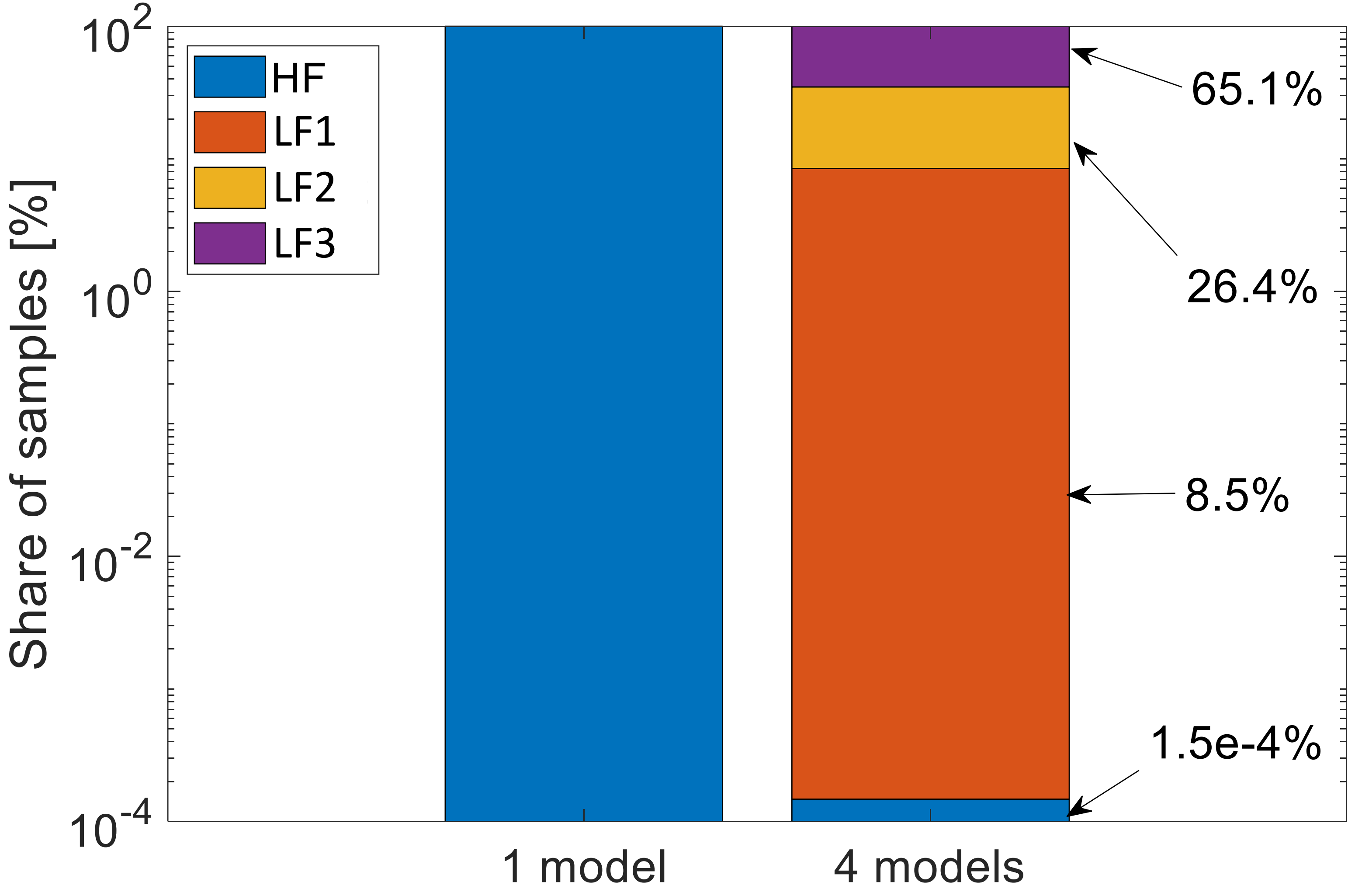


Image adapted from Cataldo et al., 2022 [5]

Allocation defined through an optimization process that trades LF models' correlation and cost

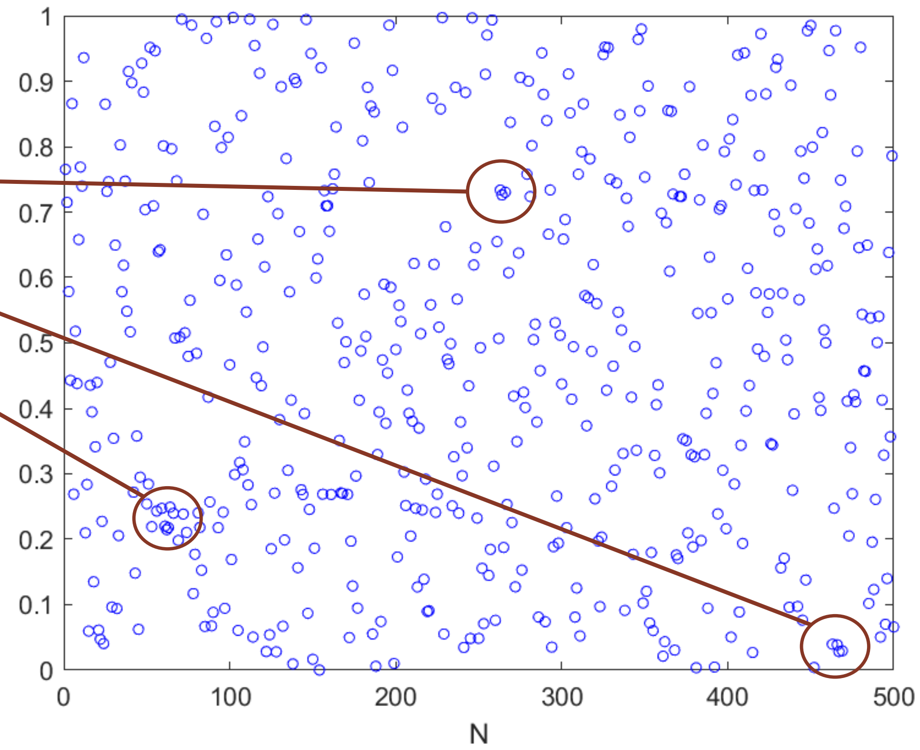
NOTE: the HF model is called only a handful times.

How to best choose the samples?

Select the best samples to maximize value of information from HF model

- Design of experiments with numerical models or test hardware
  - Monte Carlo

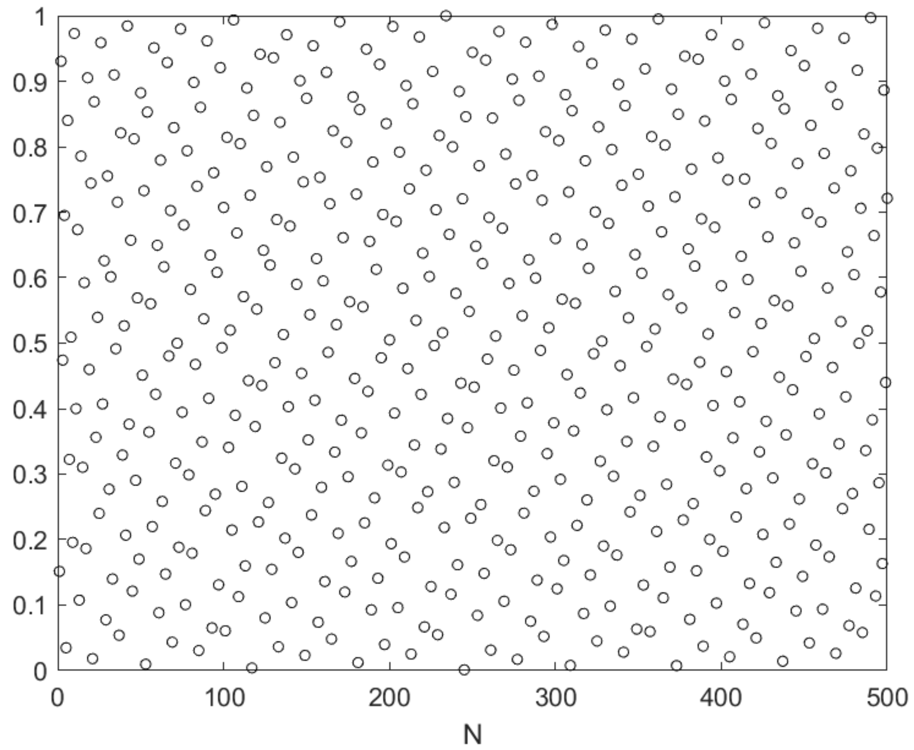
Clustered samples cause **low efficiency** due to **slow convergence**



Select the best samples to maximize value of information from HF model

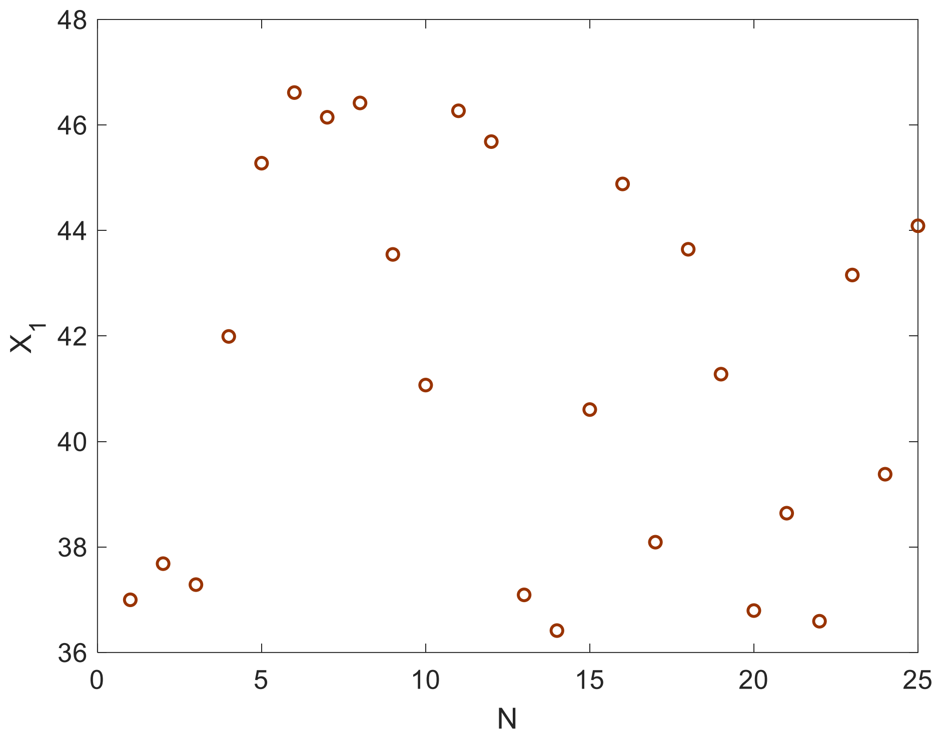
- Design of experiments with numerical models or test hardware
  - Monte Carlo
  - Latin Hypercube
  - Quasi-random
    - Halton
    - Sobol’

More uniformly spaced samples lead to **higher efficiency** due to **faster convergence**



Select the best samples to maximize value of information from HF model

- Design of experiments with numerical models or test hardware
  - Monte Carlo
  - Latin Hypercube
  - Quasi-random
    - Halton
    - Sobol’
  - Response surface
    - Box-Behnken
    - Central composite
  - D-Optimal
    - Seeks to minimize the covariance of the parameter estimates for a specified model
    - Good for non-linear models, constrained factors, correlated parameters
  - Maximum projection
    - Maximizes the product of the distances between potential design points with the goal of providing good **space-filling** properties on projections of factors [6].
  - Etc.



Selected for the application presented here, given the ability to run the SLIM only for 25 cases

Global sensitivity analysis settings used

FACTOR FIXING	
Morris' method	Morris, 1991 [7]

FACTOR PRIORITIZATION – UNIVARIATE	
Optimal transport-based	Borgonovo et al., 2024 [4]
δ–importance measure	Borgonovo, 2007 [8]
β^{KS}–importance measure	Baucells and Borgonovo, 2013 [9]
β^{Ku}–importance measure	Baucells and Borgonovo, 2013 [9]
Sobol' first-order main indices	Sobol', 1991 [2] and others

FACTOR PRIORITIZATION – MULTIVARIATE	
Optimal-transport based	Borgonovo et al., 2024 [4]

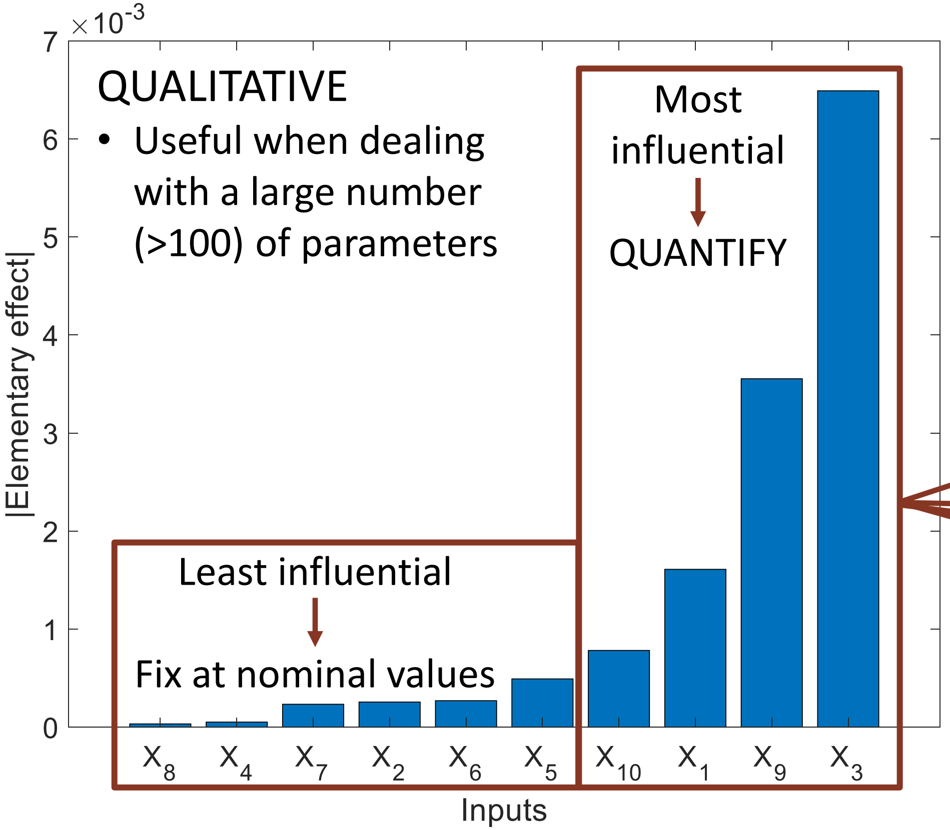
INTERACTION QUANTIFICATION	
Total indices	Sobol', 1991 [2]

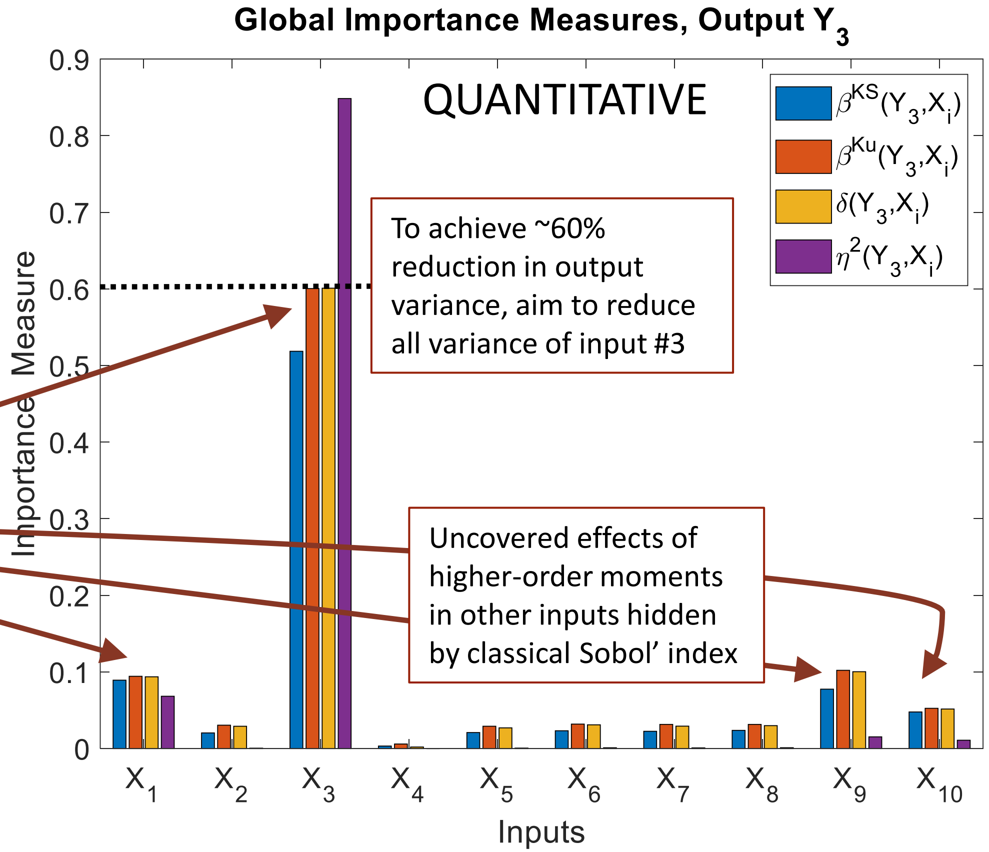
DIRECTION OF CHANGE	
Partial dependence functions Individual conditional expectation (ICE) plots	Friedman et al., 2001 [10] Goldstein et al., 2015 [11]
Discrepancy index	Baucells et al., 2021 [12]
Flatness index	Baucells et al., 2021 [12]

Factor fixing and prioritization: explore and quantify

- **Identify the least influential parameters,** which can confidently be fixed at their nominal value.
  - Use, for example, Morris' factor fixing method [7].

- **Quantify drivers' impact on model output**
  - Use sensitivity indices that:
    1. Can efficiently estimate parameter effects beyond variance through higher-order moments,
    2. Do not require independence among model inputs.

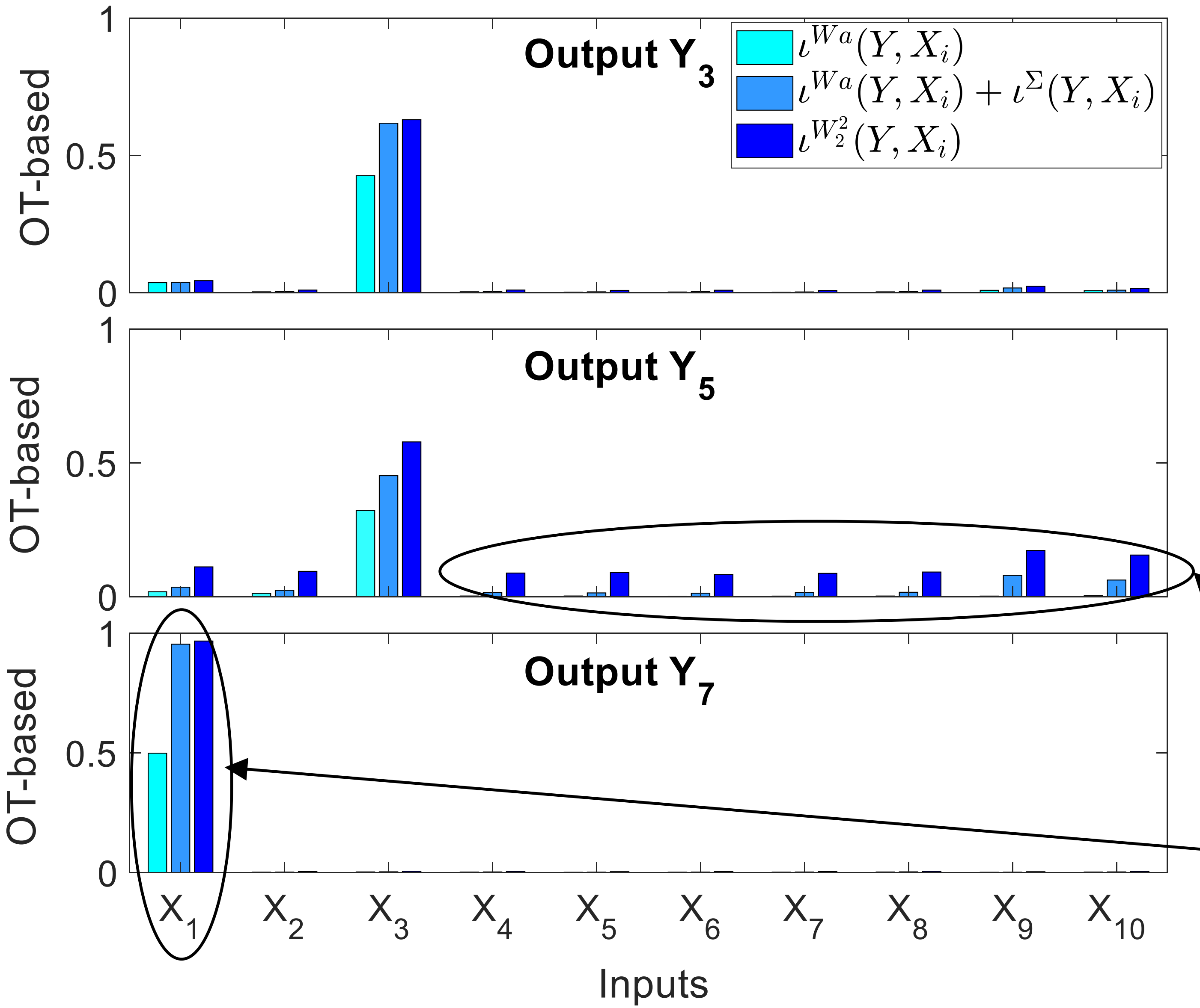




Images adapted from Cataldo et al., 2024 [1]

β^{KS}: Kolmogorov-Smirnov distance Beta [9], β^{Ku}: Kuiper distance Kappa [9]
δ: Borgonovo Delta (<u>Does not require independence among model inputs</u>) [8]
η^2: Pearson Correlation Ratio Eta = Sobol' main index [2]

Factor prioritization: optimal transport-based (univariate case)



$$\iota^{W_2^2}(Y, X_i) = \iota^{Wa}(Y, X_i) + \iota^{\Sigma}(Y, X_i) + \iota^{\Gamma}(Y, X_i)$$

First-order main effect (i.e., $1/2\ \eta^2$)

Second-order moment

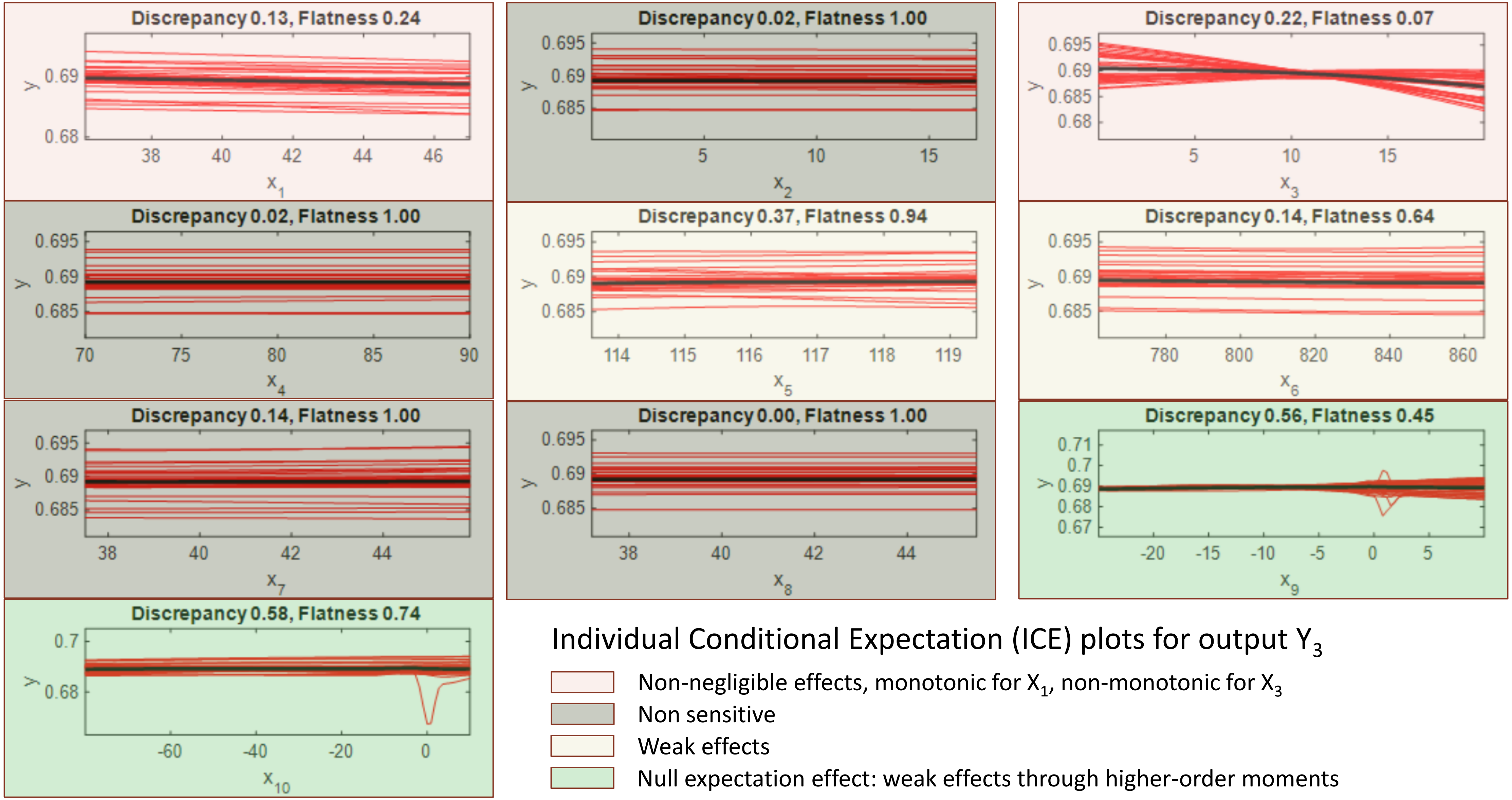
Higher-order moments

Main advantages:

1. Zero-independence
2. Max-functionality

Image adapted from Cataldo et al., 2024 [1]

Direction of change: opening the model’s black box

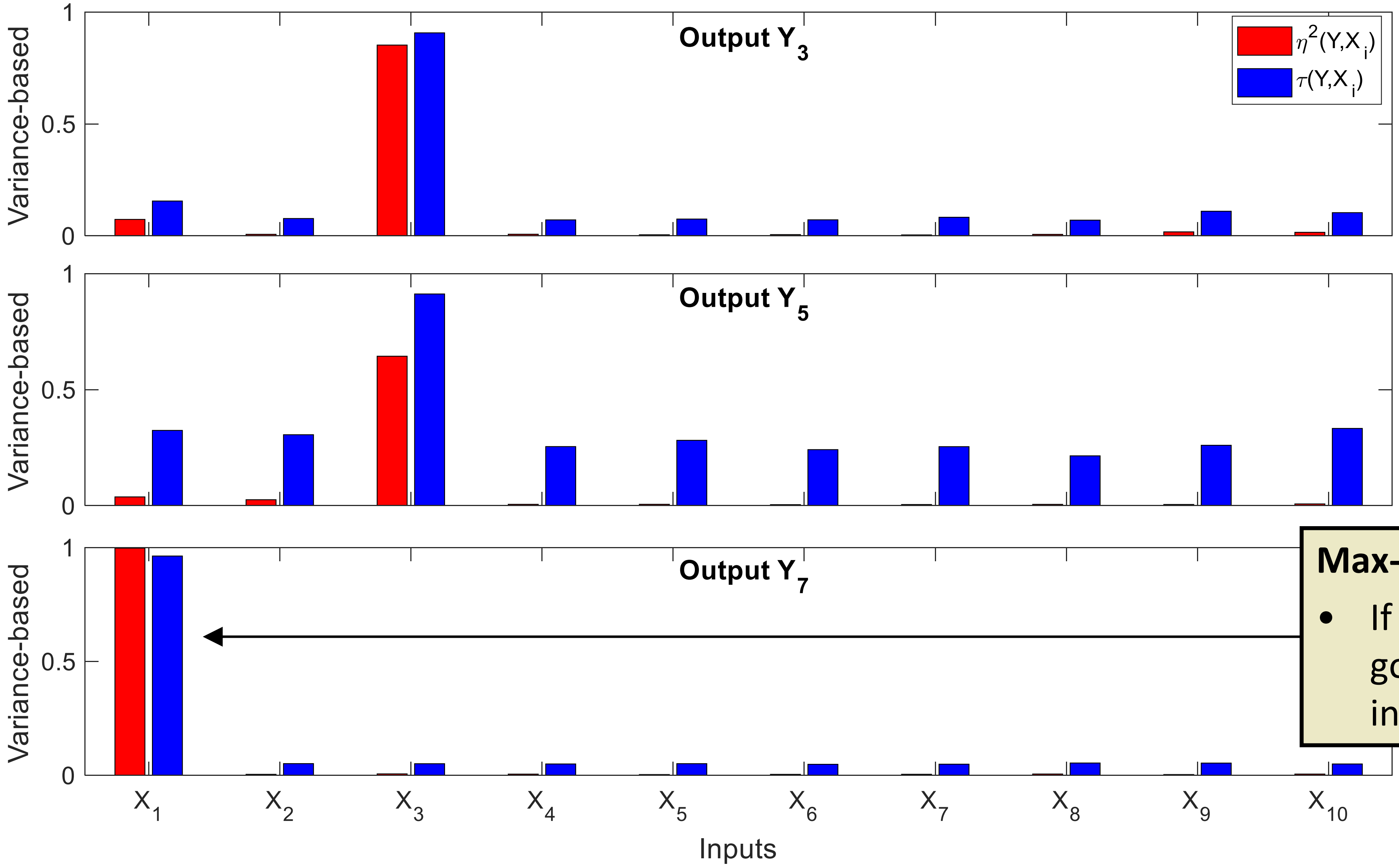


Individual Conditional Expectation (ICE) plots for output Y_3

- Non-negligible effects, monotonic for X_1, non-monotonic for X_3
- Non sensitive
- Weak effects
- Null expectation effect: weak effects through higher-order moments

Image adapted from Cataldo et al., 2024 [1]

Uncovering interactions



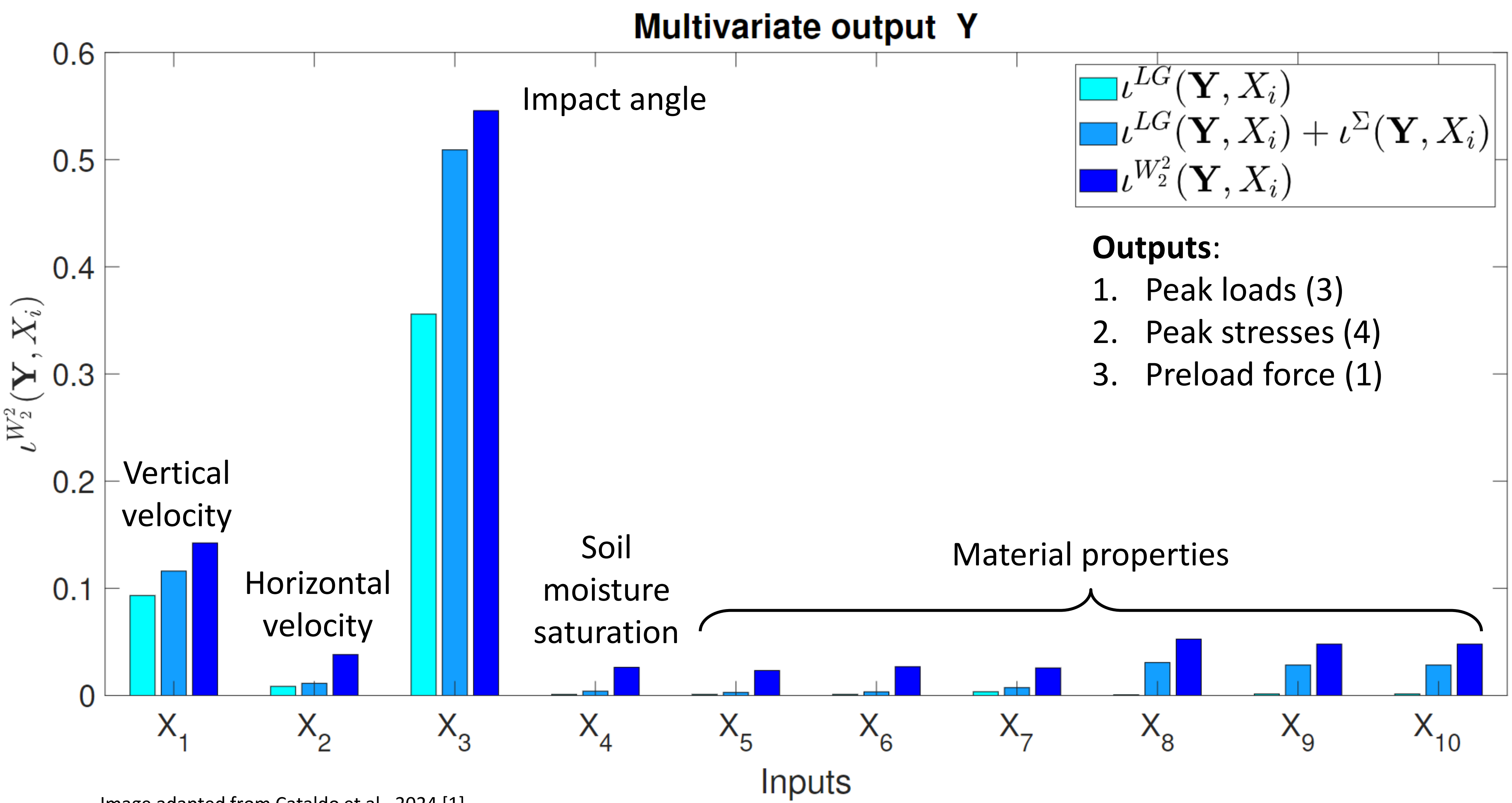
- Total effects τ computed through nearest-neighbor approach.
- Confirms insights from previous indices.

Max-functionality

- If all the uncertainty in X_1 goes away, the uncertainty in Y_7 also goes to zero.

Image credit: Cataldo et al., 2024 [1]

Factor prioritization: optimal transport-based (multivariate case)



Outputs:
1. Peak loads (3)
2. Peak stresses (4)
3. Preload force (1)

Image adapted from Cataldo et al., 2024 [1]

- Novel approach to identify overall drivers for all outputs.
- Kinematic factors are responsible for most uncertainty.
- Confirms findings from previous indices.

Proper data assimilation enables models to be dynamically updated

- **GOAL:** Leverage the power of properly designed experimental data to make the models predictive (e.g., digital twin) and increase our knowledge of the system under design early in the life cycle, bringing in noticeable improvements in the decision-making process and mission success.

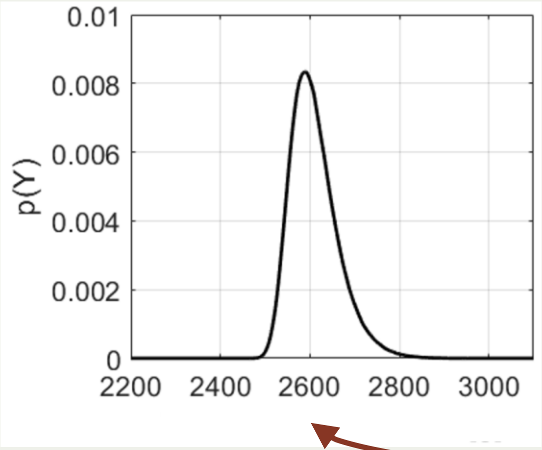
PRIOR

Uncertainty identification

Uncertainty characterization

Uncertainty propagation

Uncertainty analysis



Global Sensitivity Analyses

DATA

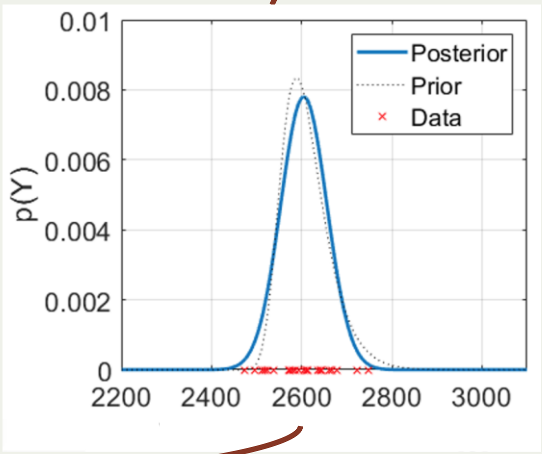
- Parameter inference experiments
- System-level tests

BAYES' THEOREM

POSTERIOR

Updated model

- Updated input parameters
- Validated model outputs (with ability to account for sensor / measurement error and model inadequacy)



- Repeat as needed

Use GSA to guide the decision-making process and optimize resources

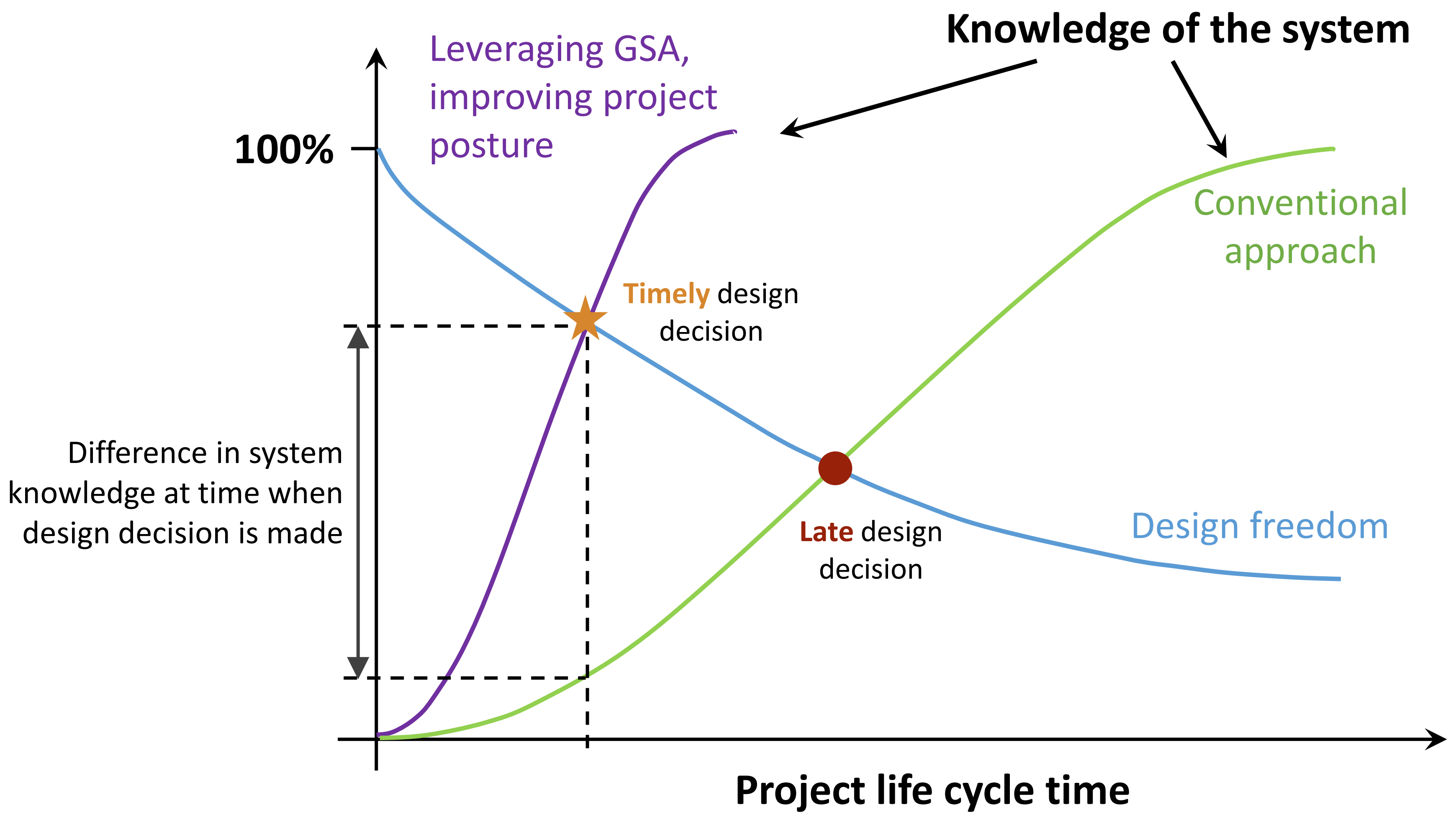


Image adapted from [13]

- Through these methodologies, **system knowledge is increased early in the life cycle** due to a systematic, rigorous approach to identifying and reducing important system uncertainties <u>prior to</u> system-level model validation experiments.

- This is ever more important considering that ~85% of a project's total life cycle cost is locked in by the end of preliminary design [14].

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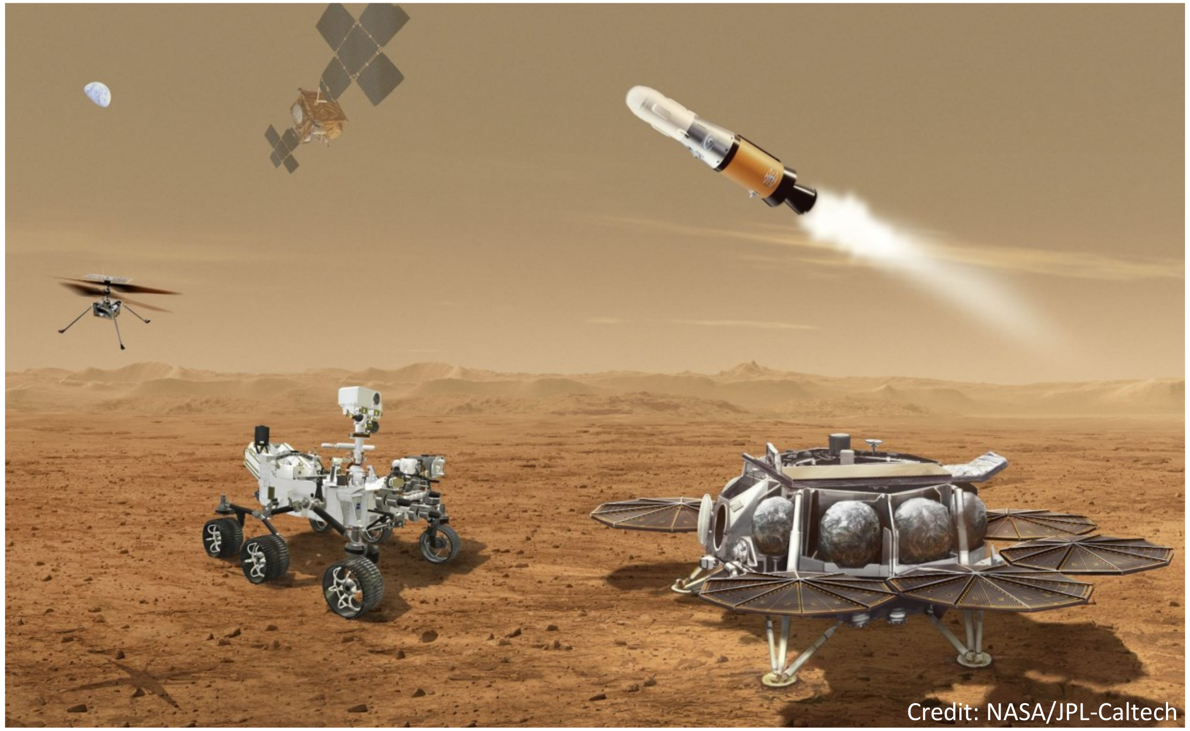
  - Mr. Kevin Carpenter — Jet Propulsion Laboratory
  - Prof. Emanuele Borgonovo — Bocconi University
  - Prof. Elmar Plischke — Clausthal University
  - Mr. Martin Nado — ISAE-SUPAERO (former)



QUESTIONS?

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Main references

- [1] G. Cataldo, E. Borgonovo, M. Nado, A. Siddens, K. Carpenter, E. Plischke, Global sensitivity analyses for test planning with black-boxes models for Mars Sample Return, *Oper. Res.*, submitted.
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- And references therein!