



Representing the Unknown in Computer Simulations: From Reduced-Order to Generative Models

James Warner

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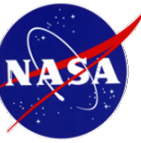
Department of Mechanical Engineering Research Seminar Series

University of Texas at San Antonio

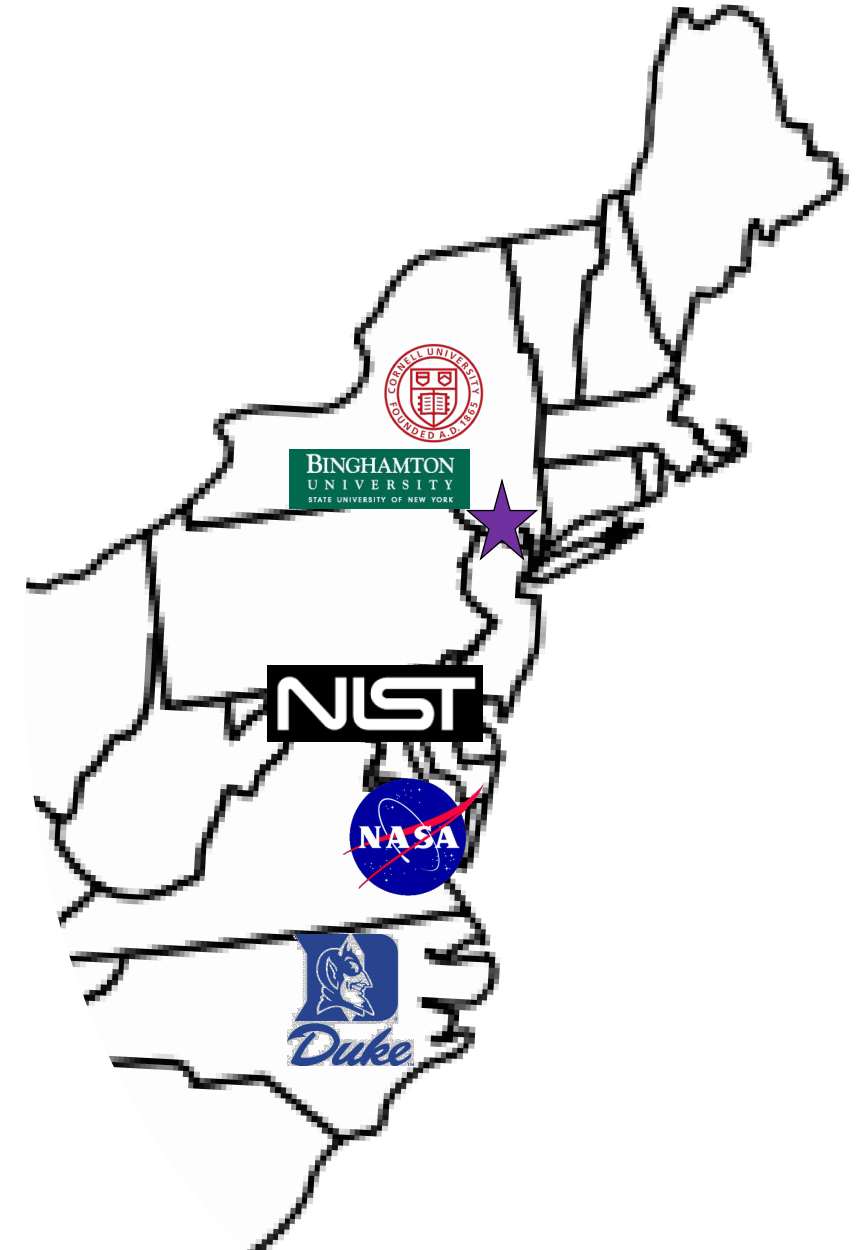
September 13th, 2024

Team Members: Geoffrey Bomarito, Patrick Leser, Paul Leser, Michael Stanley, Tristan Shah

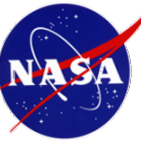
About Me – Academic/Professional Bio



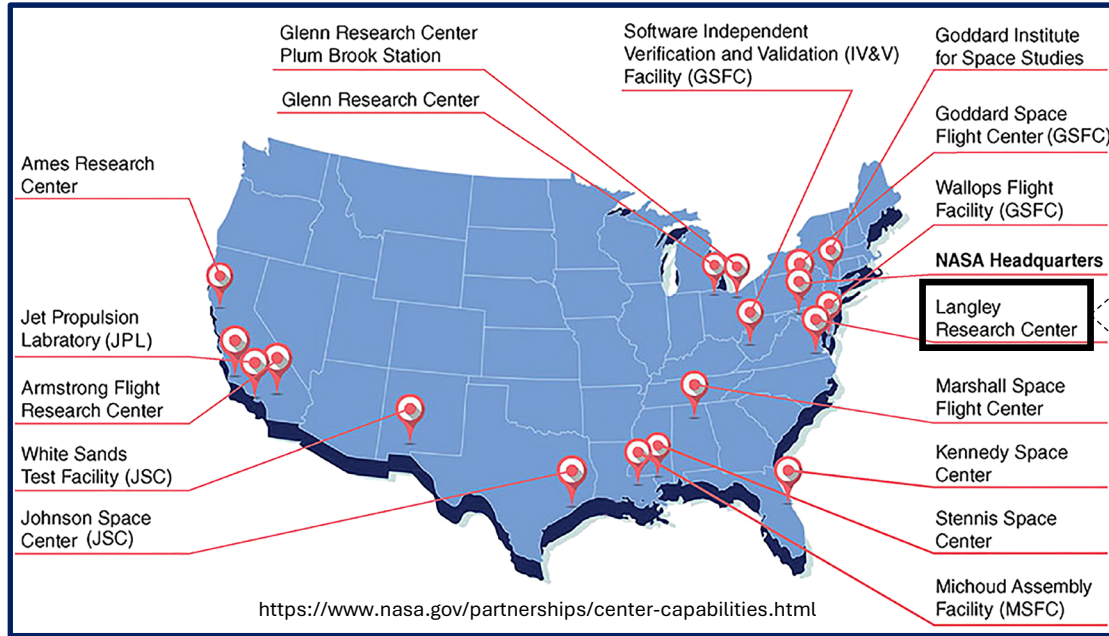
- **Hometown:** Warwick, NY
- **Binghamton University** *B.S. Mechanical Engineering*
- **N.I.S.T** *Undergraduate Researcher*
- **Cornell University** *MS/PhD Civil Engineering*
- **Duke University** *Research Associate / Visiting Student*
- **NASA** *Senior Computational Scientist*
 - Langley Research Center, Hampton, VA
 - Durability, Damage Tolerance, and Reliability Branch
 - 2013 – Present
 - Research focus: uncertainty quantification & scientific machine learning



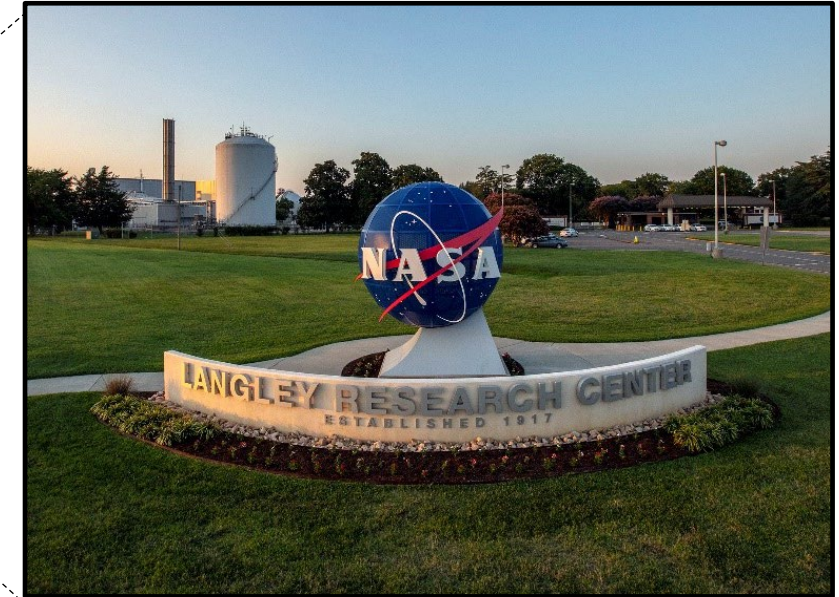
NASA Langley Research Center



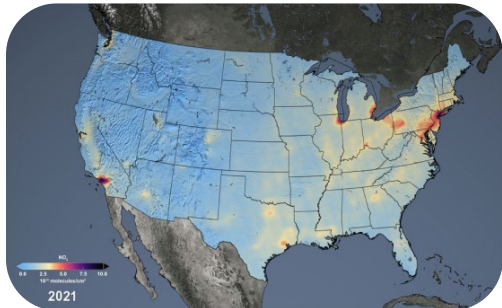
NASA Facilities and Centers Across the US



Langley Research Center, Hampton, VA



Earth's Atmospheric Composition



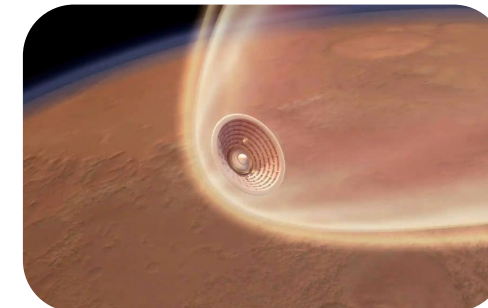
On-Demand Mobility Technologies



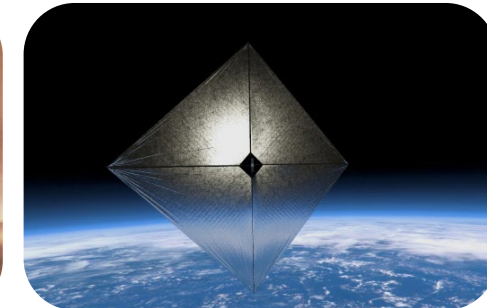
Commercial Air Transport Technologies



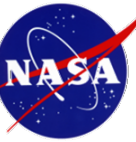
Entry, Descent & Landing Systems



Advanced Space Structures



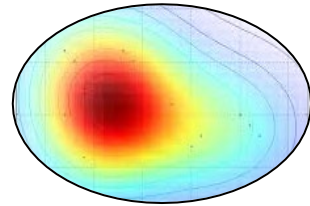
Research Group Overview



Skills

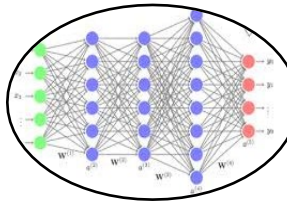
Applied Mathematics
Software Development
Probability
Statistics
Applied Physics
Mechanical Testing
Aerospace Engineering
Numerical Methods
Solid Mechanics

Research Areas



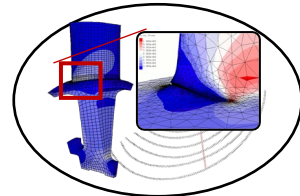
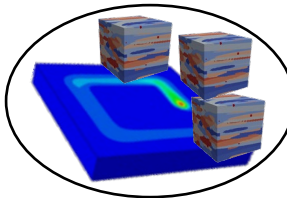
Uncertainty quantification

Machine Learning



High Performance Computing

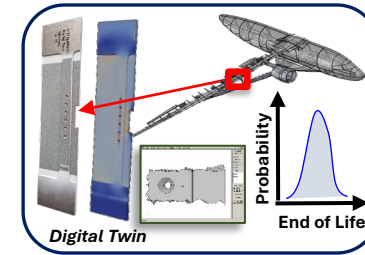
Damage Science



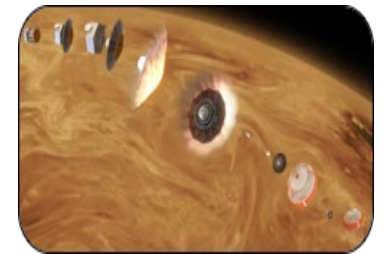
Fatigue and Fracture

Applications

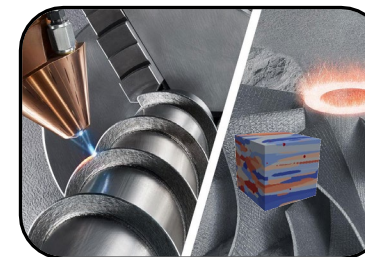
Certification by
Analysis



Entry, Descent,
and Landing



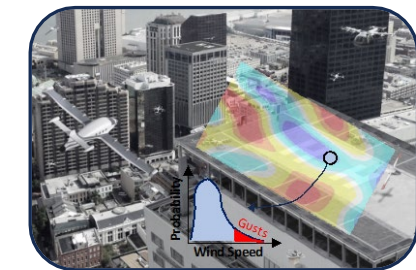
Additive
Manufacturing



Space Hardware
Reliability

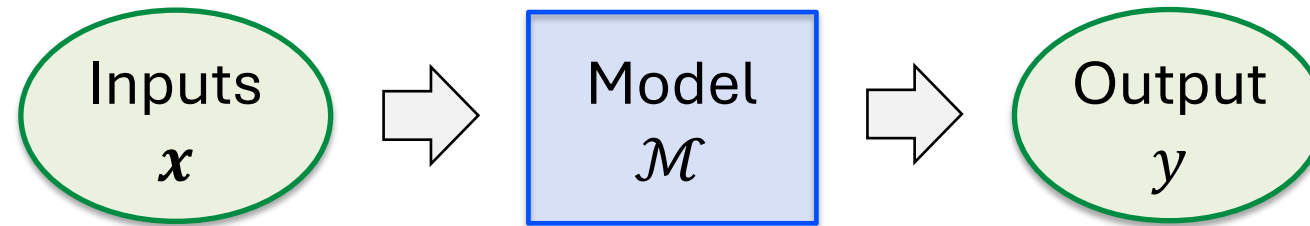


Weather-Tolerant Urban
Air Mobility (UAM)

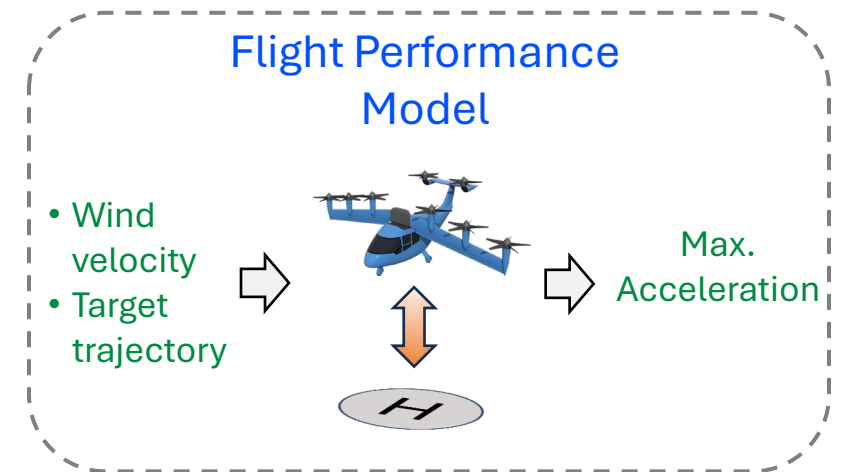
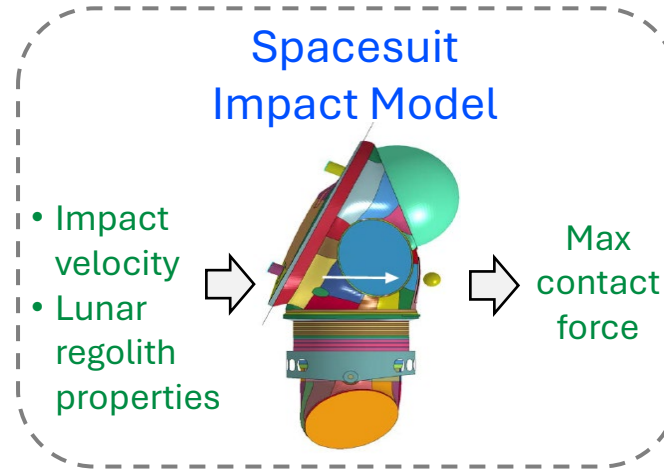
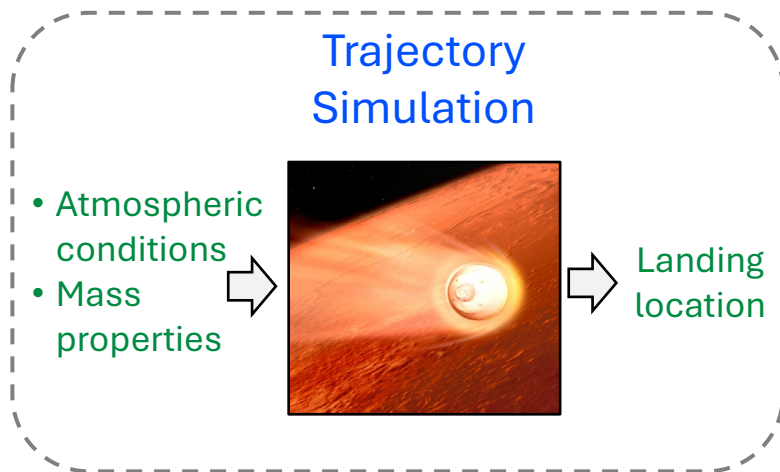
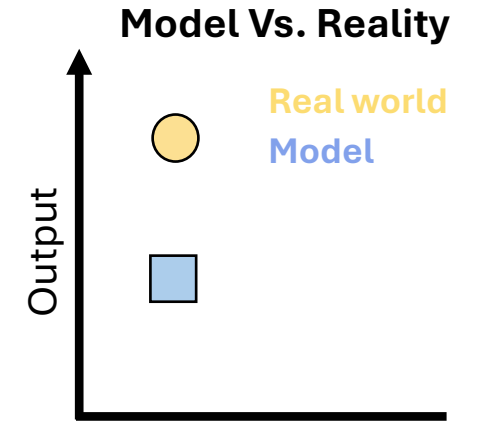
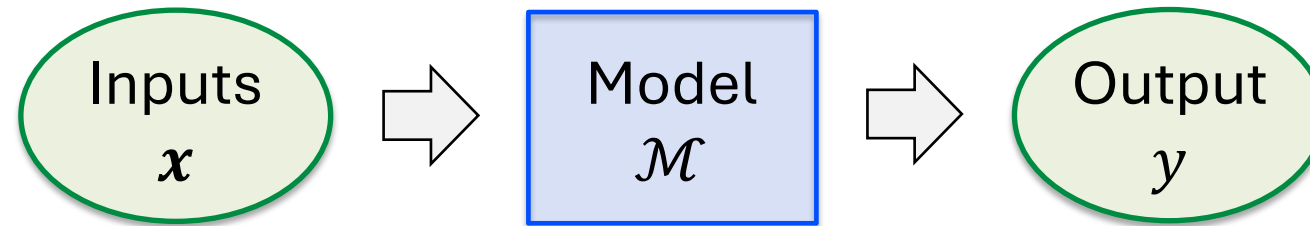
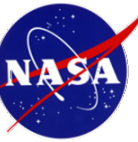


1. Uncertainty Quantification (UQ) Overview
2. Stochastic Reduced Order Models (SROMs)
 - Increasing UQ efficiency
3. Deep Generative Models
 - Modeling complex, high-dimensional probability distributions
4. Summary

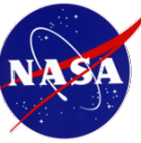
Modeling and Simulation



Modeling and Simulation

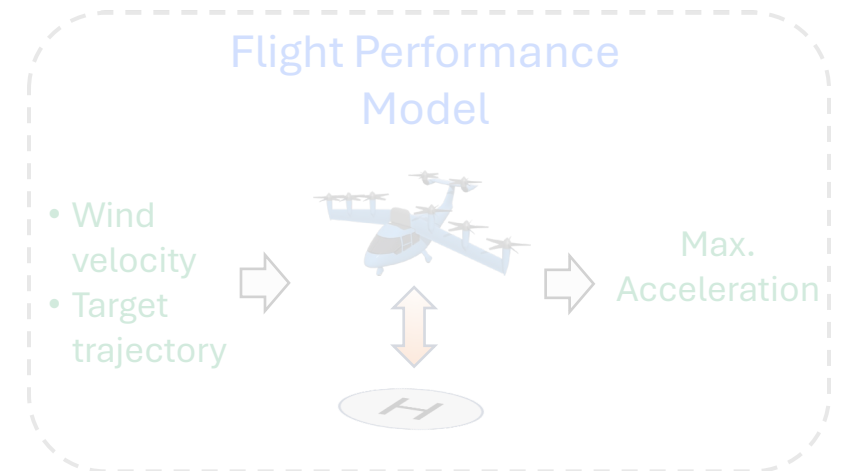
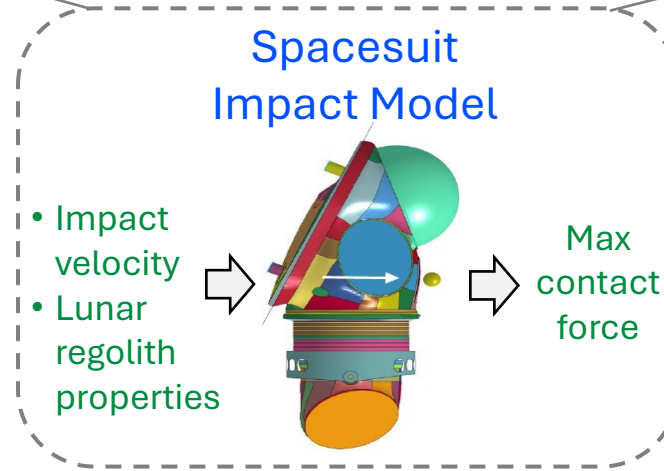
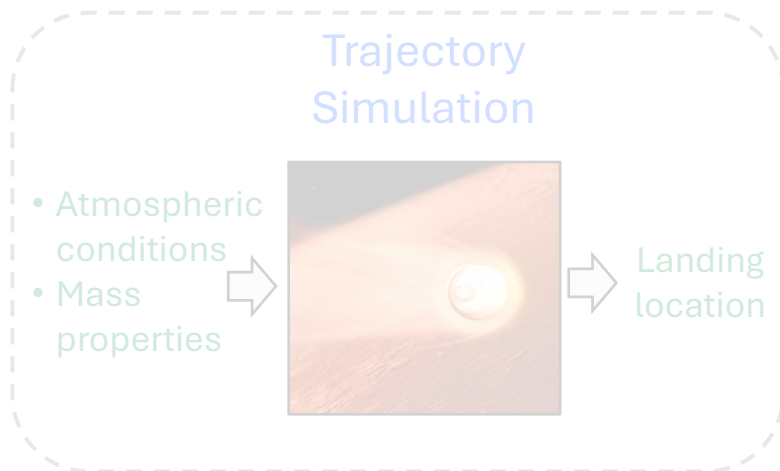
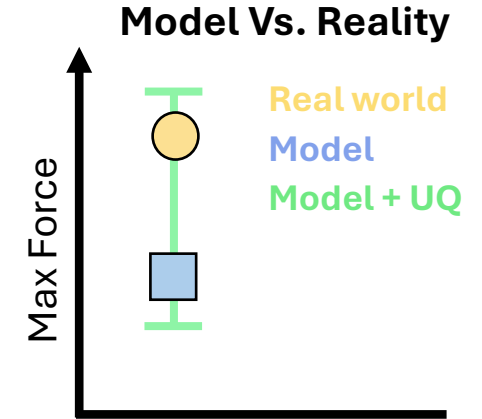
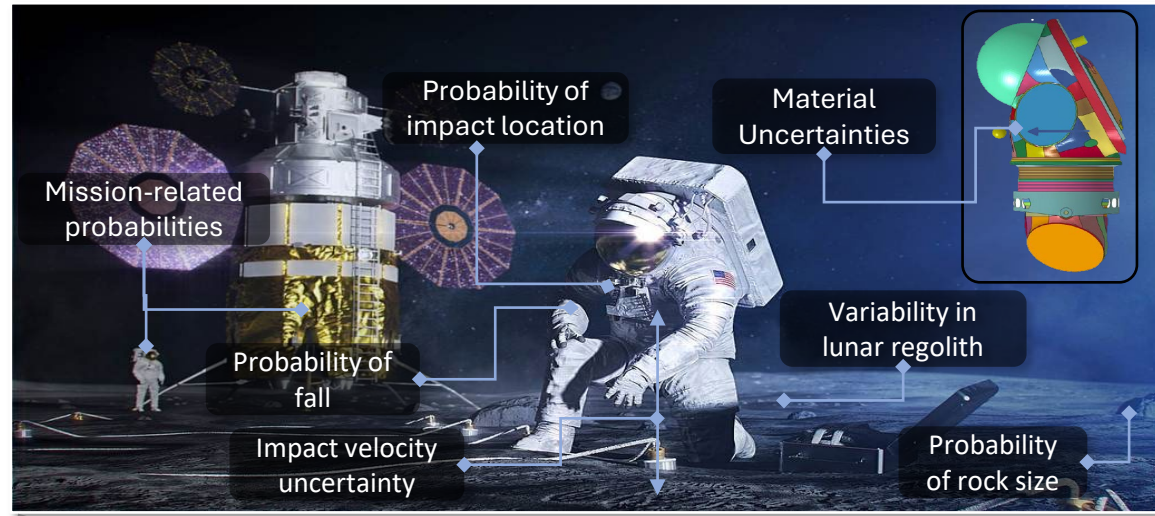


Uncertainty in Computer Simulations

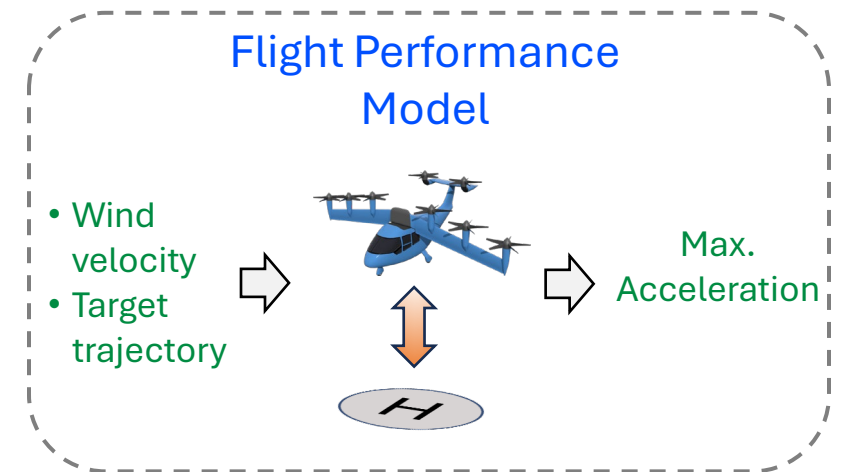
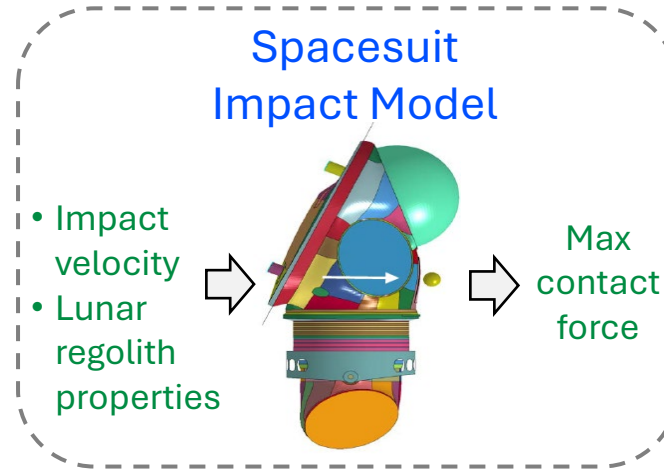
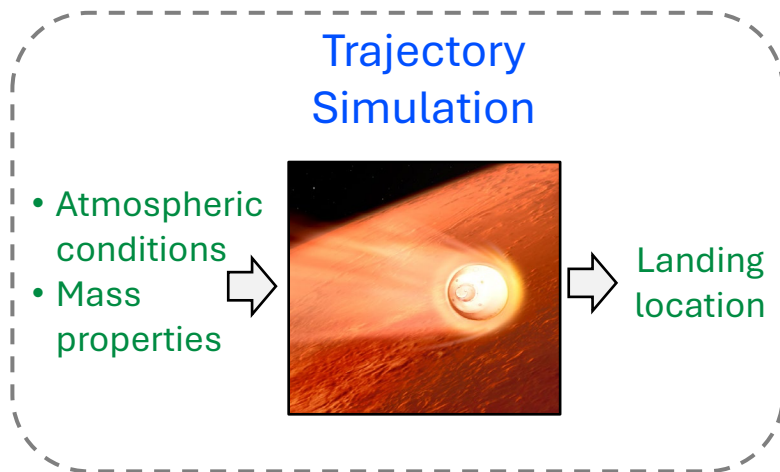
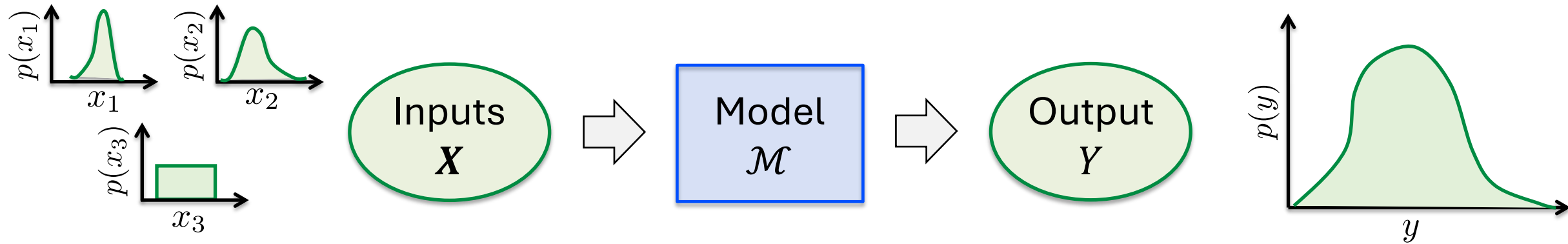
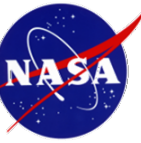


Sources of Uncertainty:

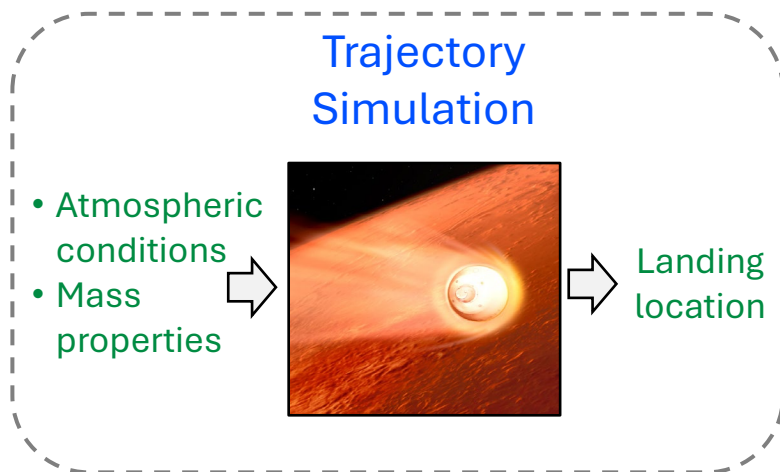
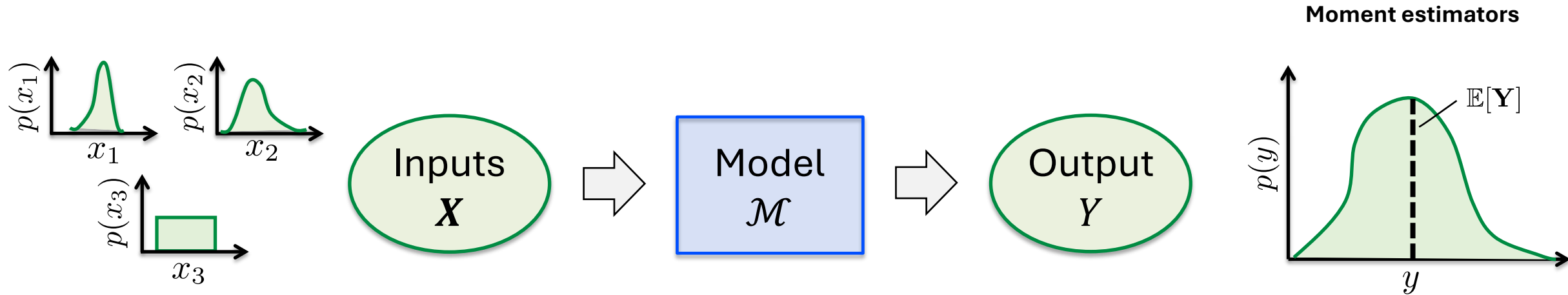
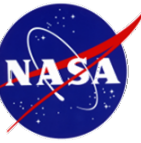
- **Input parameters**
- Model form error
- Numerical errors



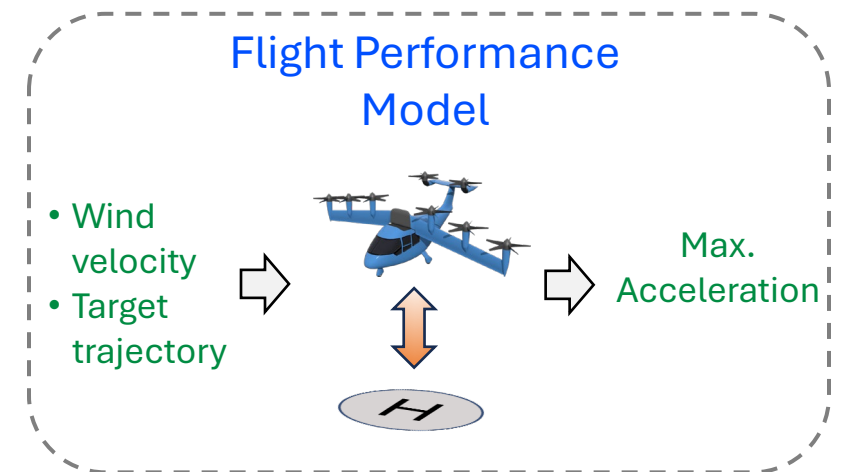
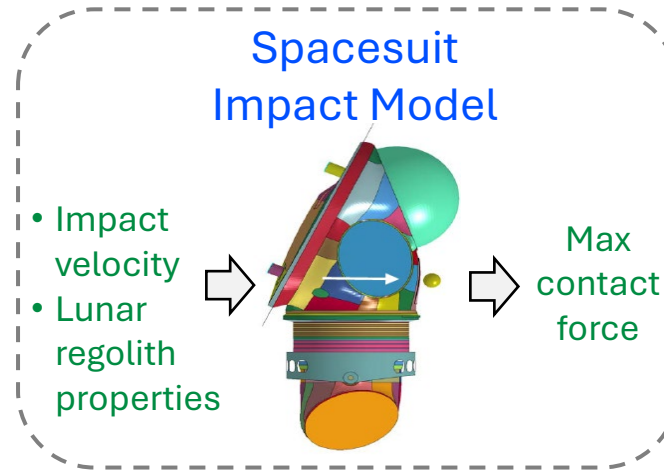
Uncertainty Quantification (UQ)



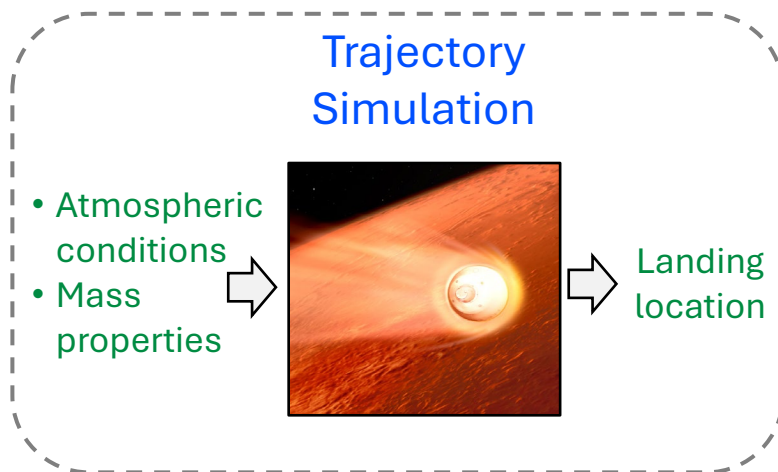
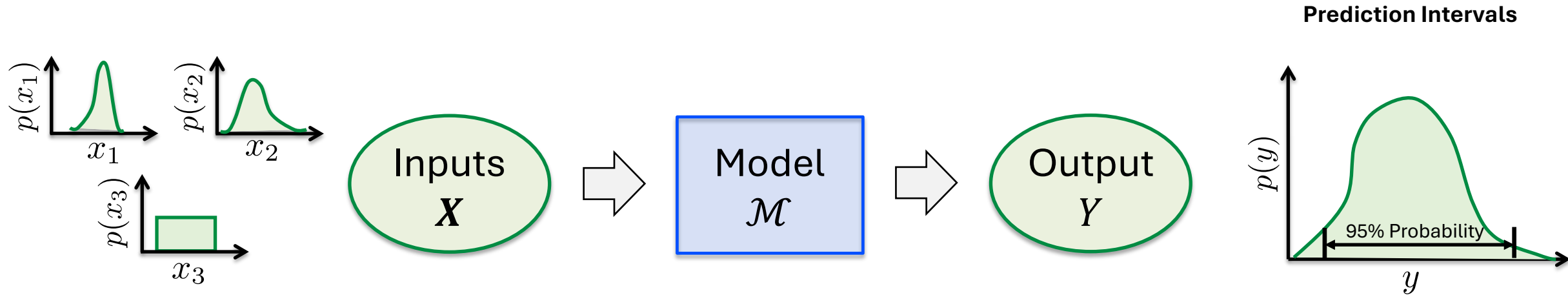
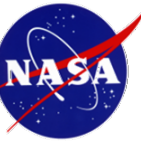
Uncertainty Quantification (UQ)



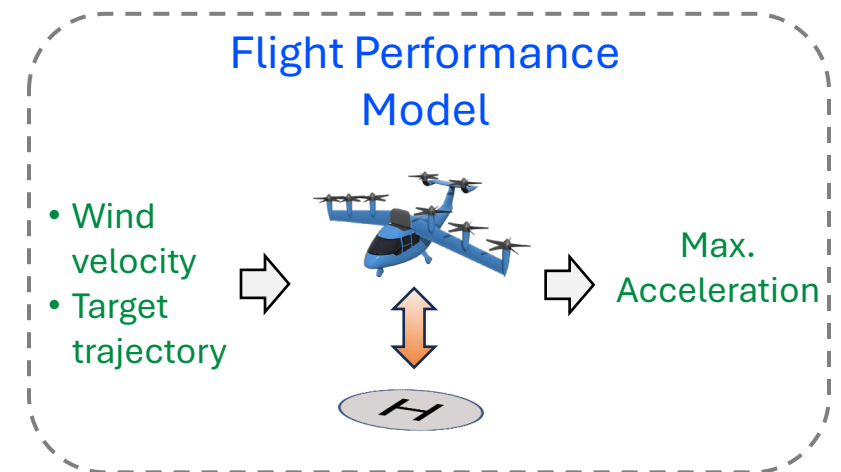
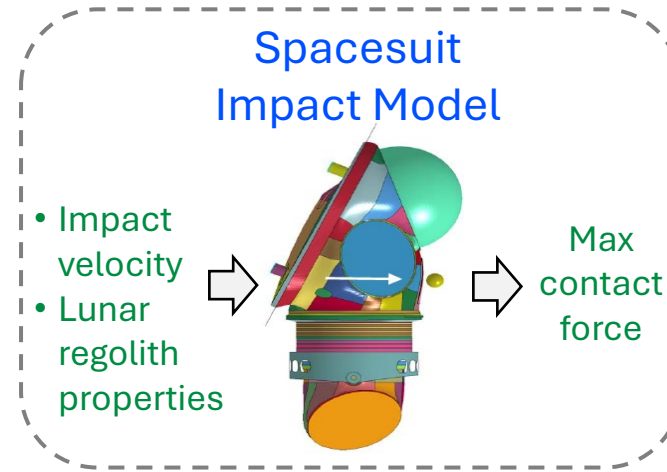
➤ Expected landing location



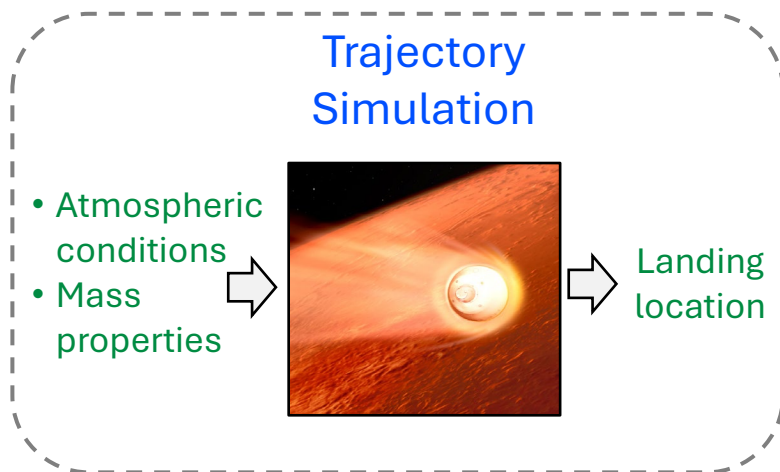
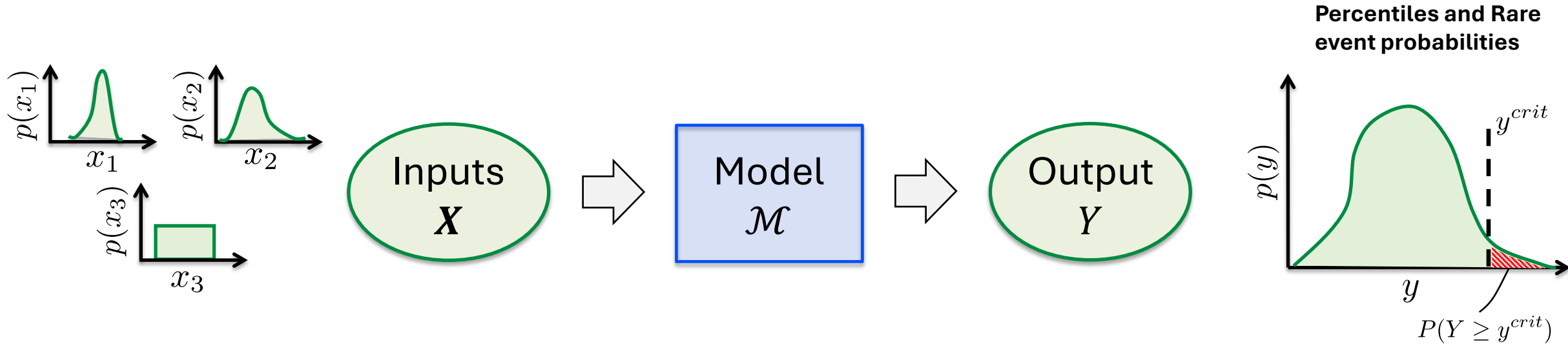
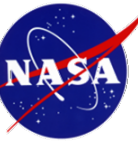
Uncertainty Quantification (UQ)



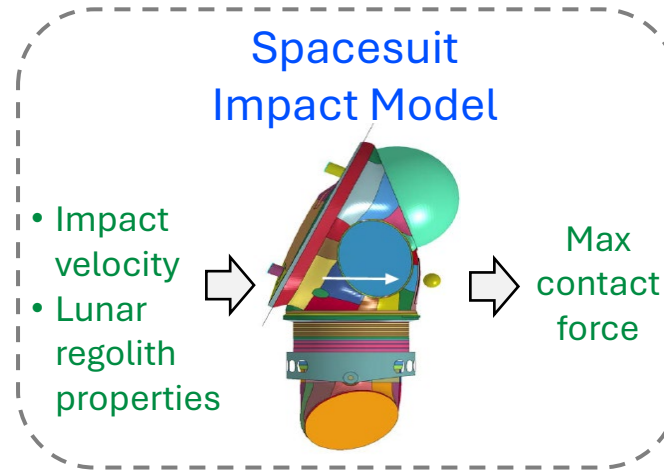
- Expected landing location
- **95% confidence landing ellipse**



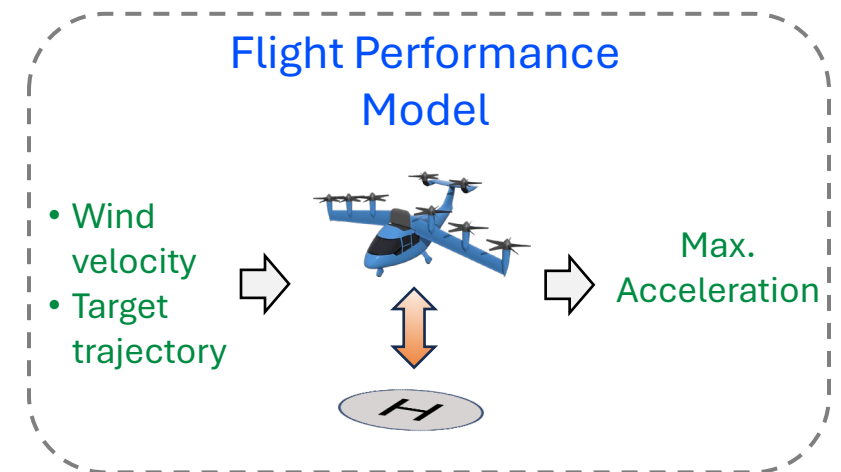
Uncertainty Quantification (UQ)



- Expected landing location
- 95% confidence landing ellipse

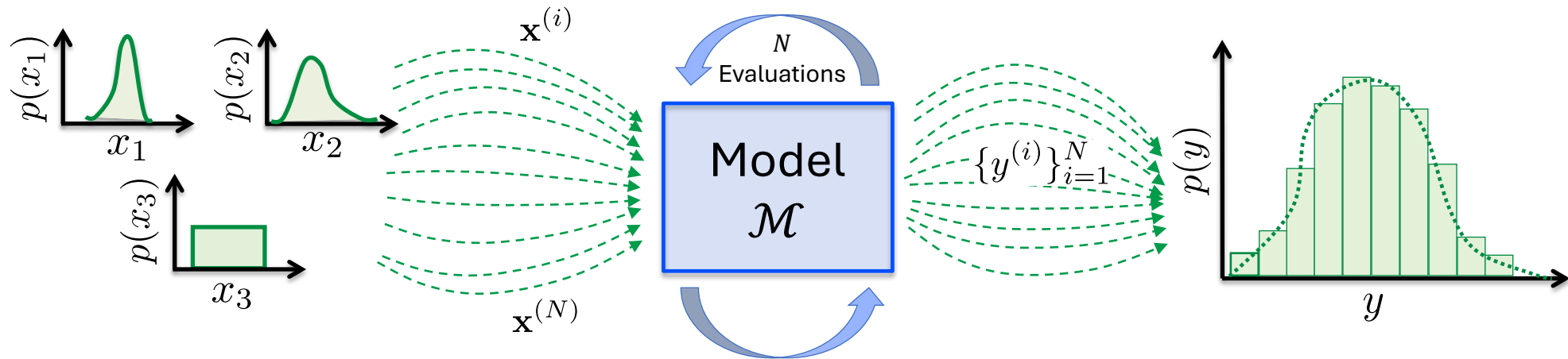
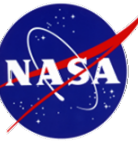


- **Probability of failure**



- **Probability of failure**

Monte Carlo Simulation (MCS)



MCS Procedure

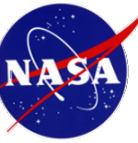
Repeat for N iterations:

- Generate random input sample, $\mathbf{x}^{(i)} \sim p(\mathbf{x})$
- Evaluate model and store output, $y^{(i)} = \mathcal{M}(\mathbf{x}^{(i)})$

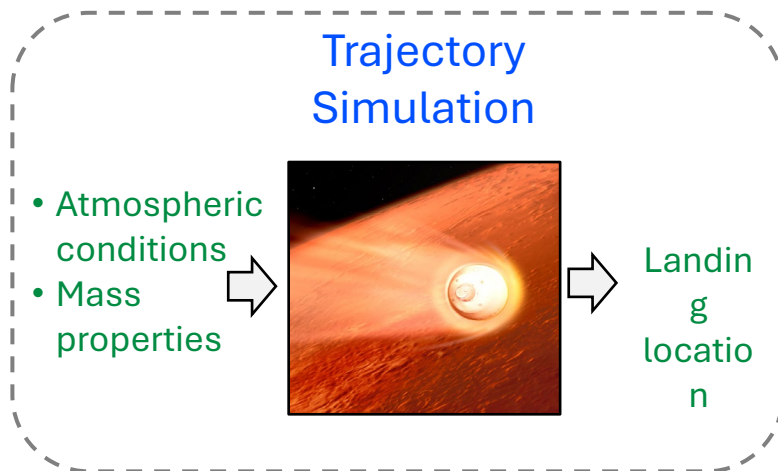
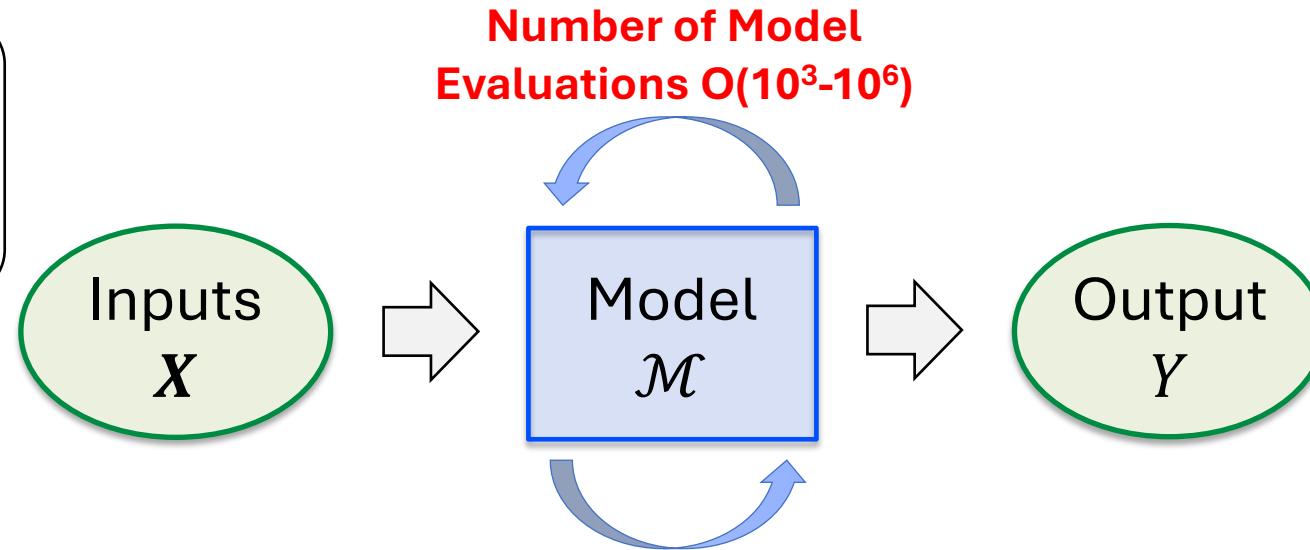
Postprocess output samples, $\{y^{(i)}\}_{i=1}^N$, to estimate:

- $p(y)$ (use histogram or kernel density estimate)
- $\mathbb{E}[Y] \approx \frac{1}{N} \sum_{i=1}^N y^{(i)}$ (expected value $\approx$ sample average)
- $P(Y \geq y^{crit}) \approx \frac{1}{N} \sum_{i=1}^N \mathbf{1}(y^i \geq y^{crit})$ (failure probability $\approx$ proportion of samples that failed)

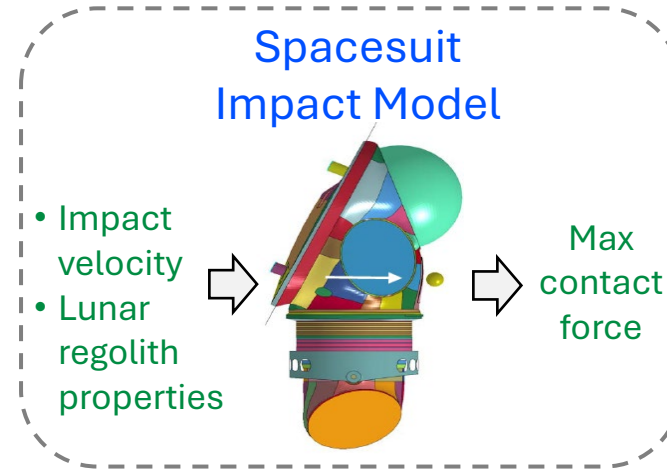
Challenge 1: Computational Expense



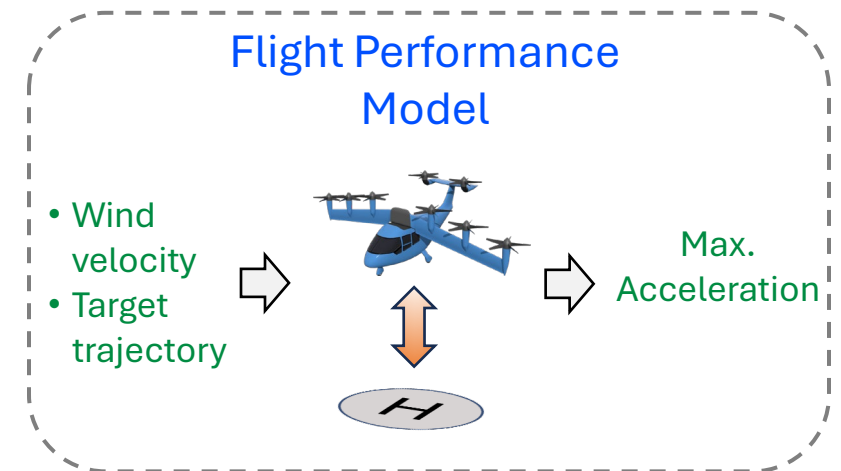
UQ with high-fidelity physics-based models can be computationally intractable



Computation Time:
 $O(\text{mins-hours})$

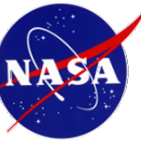


Computation Time:
 $O(\text{hours-days})$

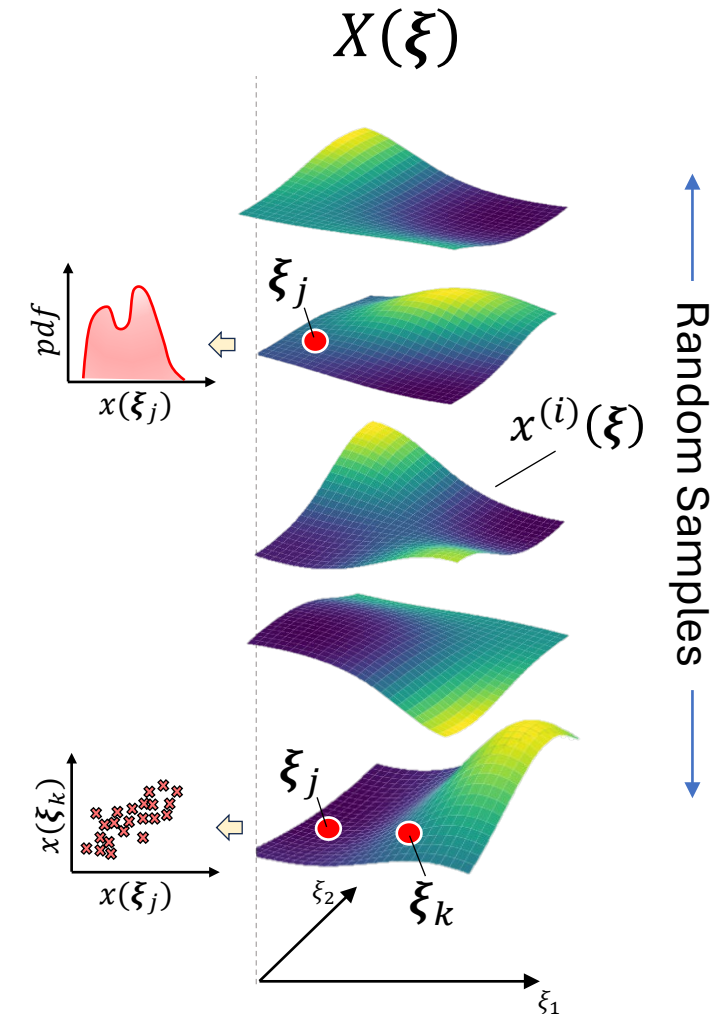


Computation Time:
 $O(\text{mins-hours})$

Challenge 2: High-Dimensional Uncertainties



- Inputs to simulations are often *random fields*, $X(\xi)$, that must be discretized
 - E.g., heterogenous material properties
- Representing $X(\xi)$ can be difficult
 - Non-Gaussian behavior
 - Complex correlation structure
 - Lack of closed-form expression (access to samples only)
 - Limited/sparse data
 - Inability to measure directly



1. Uncertainty Quantification (UQ) Overview

2. **Stochastic Reduced Order Models (SROMs)**

- Increasing UQ efficiency

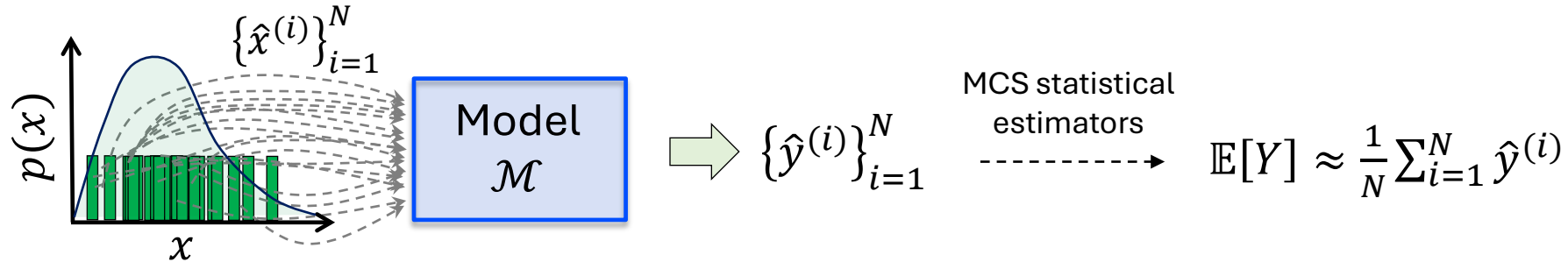
3. Deep Generative Models

- Modeling complex, high-dimensional probability distributions

4. Summary

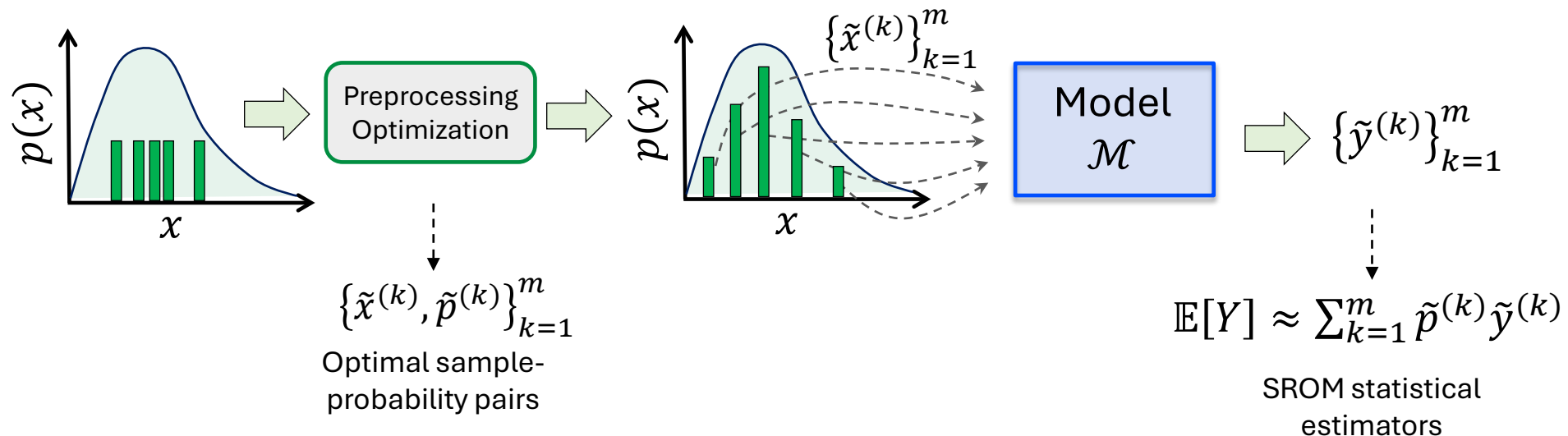
Stochastic Reduced Order Models (SROMs)

- **MCS** – a (potentially) huge number, N , of random, equally-likely samples



- **SROMs** – a small number, m , of optimally selected/weighted samples

$$m \ll N$$



SRROM Optimization

Construct SRROM, $\tilde{\mathbf{X}}$, to minimize statistical errors with respect to target, $\mathbf{X} \in \Gamma \subset \mathbb{R}^d$:

$$\begin{aligned} \tilde{\mathbf{X}} &\equiv \operatorname{argmin}_{\{\tilde{\mathbf{x}}\}, \tilde{\mathbf{p}}} \left(\sum_{i=1}^3 \alpha_i e_i(\{\tilde{\mathbf{x}}\}, \tilde{\mathbf{p}}) \right) \\ \text{s.t. } &\sum_{k=1}^m \tilde{p}^{(k)} = 1 \text{ and } \tilde{p}^{(k)} \geq 0, \forall k \end{aligned}$$

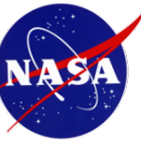
$$\begin{aligned} e_1(\{\tilde{\mathbf{x}}\}, \tilde{\mathbf{p}}) &= \frac{1}{2} \sum_{i=1}^d \int_{I_i} \left| \tilde{F}_i(x_i) - F_i(x_i) \right| dx_i \quad (\text{Distributions}) \\ e_2(\{\tilde{\mathbf{x}}\}, \tilde{\mathbf{p}}) &= \frac{1}{2} \sum_{i=1}^d \sum_{q=1}^{\bar{q}} \left| \tilde{\mu}_i(q) - \mu_i(q) \right| \quad (\text{Moments}) \\ e_3(\{\tilde{\mathbf{x}}\}, \tilde{\mathbf{p}}) &= \frac{1}{2} \sum_{i,j=1; j>i}^d \left| \tilde{r}(i,j) - r(i,j) \right| \quad (\text{Correlations}) \end{aligned}$$

SRROM

Target

- SRROM size, m , chosen based on computation budget
- $\mathbf{X}$ can be characterized by closed-form distribution, $p(\mathbf{x})$, or samples $\{\hat{x}^{(i)}\}_{i=1}^N$

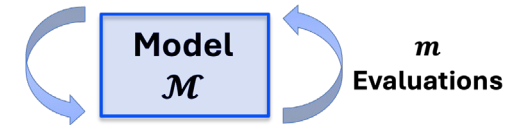
Uncertainty Propagation via SROMs



1) Construct SROM, $\tilde{X} = \{\tilde{x}^{(k)}, \tilde{p}^{(k)}\}_{k=1}^m$, via optimization



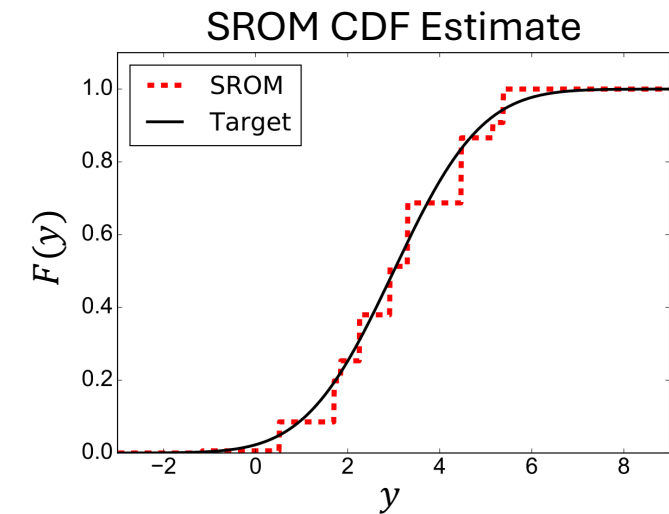
2) Evaluate model for each SROM sample, $\tilde{y}^{(k)} = \mathcal{M}(\tilde{x}^{(k)}) \forall k$



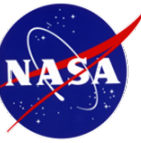
3) Form estimators using $\tilde{Y} = \{\tilde{y}^{(k)}, \tilde{p}^{(k)}\}_{k=1}^m$

- Moments: $\mathbb{E}[Y^q] \approx \sum_{k=1}^m \tilde{p}^{(k)} (\tilde{y}^{(k)})^q$
- CDF: $F(y) \approx \sum_{k=1}^m \tilde{p}^{(k)} \mathbf{1}(\tilde{y}^{(k)} \leq y)$

- 👍 Conceptually simple
- 👍 Efficient (requires $m \ll N$ simulations)
- 👎 Low resolution CDF estimates
- 👎 Inaccurate tail probability estimates



SROMs as Local Surrogate Models (1/2)



- The SROM approximation can equivalently be viewed as a piecewise constant surrogate model, $\tilde{y}_C(\mathbf{X}) \approx \mathcal{M}(\mathbf{X})$:

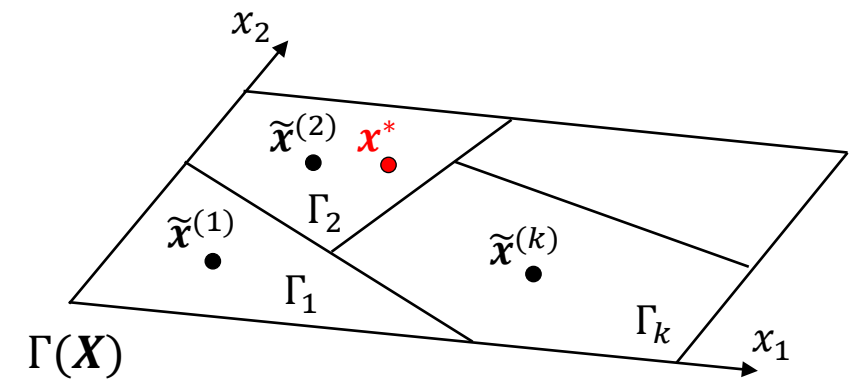
$$\tilde{y}_C(\mathbf{X}) = \sum_{k=1}^m \mathbf{1}(\mathbf{X} \in \Gamma_k) \tilde{y}^{(k)}$$

- Γ_k is a Voronoi partition of Γ with centers at $\tilde{\mathbf{x}}^{(k)}$
- $P(\mathbf{X} \in \Gamma_k) \approx \tilde{p}^{(k)}$

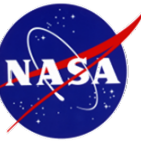
Example: making prediction for new input, $\mathbf{x}^* \sim p(\mathbf{x})$

$$\begin{aligned} \tilde{y}_C(\mathbf{x}^*) &= \sum_{k=1}^m \mathbf{1}(\mathbf{X} \in \Gamma_k) \tilde{y}^{(k)} \\ &= \mathbf{1}(\mathbf{x}^* \in \Gamma_1) \tilde{y}^{(1)} + \mathbf{1}(\mathbf{x}^* \in \Gamma_k) \tilde{y}^{(2)} + \dots \\ &= \tilde{y}^{(2)} \end{aligned}$$

Note: In the original image, arrows indicate that the first term is 0 and the last term is 0, leaving the middle term.



SROMs as Local Surrogate Models (2/2)

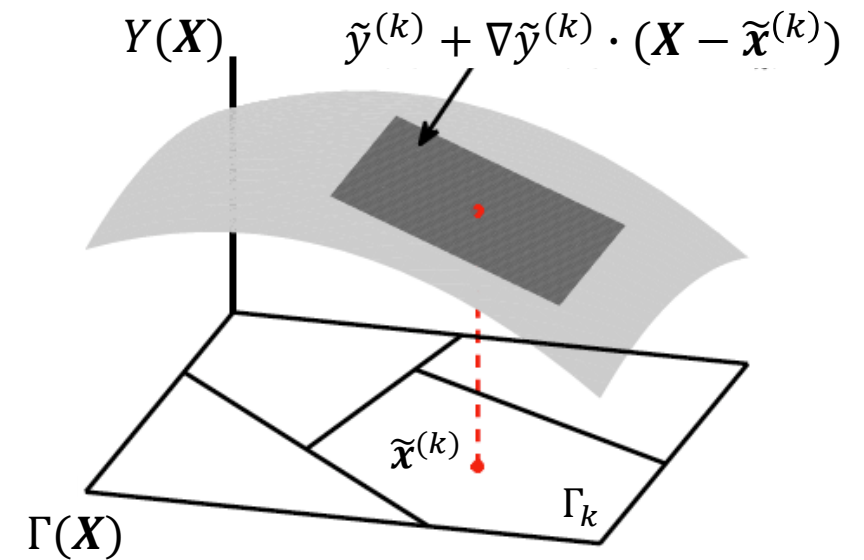


- Can incorporate gradient information to obtain piecewise-linear surrogate model:

$$\tilde{y}_L(\mathbf{X}) = \sum_{k=1}^m \mathbf{1}(\mathbf{X} \in \Gamma_k) [\tilde{y}^{(k)} + \nabla \tilde{y}^{(k)} \cdot (\mathbf{X} - \tilde{\mathbf{x}}^{(k)})]$$

$$\text{Where } \nabla \tilde{y}^{(k)} = \left(\frac{\partial y(\mathbf{X})}{\partial x_1}, \dots, \frac{\partial y(\mathbf{X})}{\partial x_d} \right)^T \bigg|_{\mathbf{X}=\tilde{\mathbf{x}}^{(k)}}$$

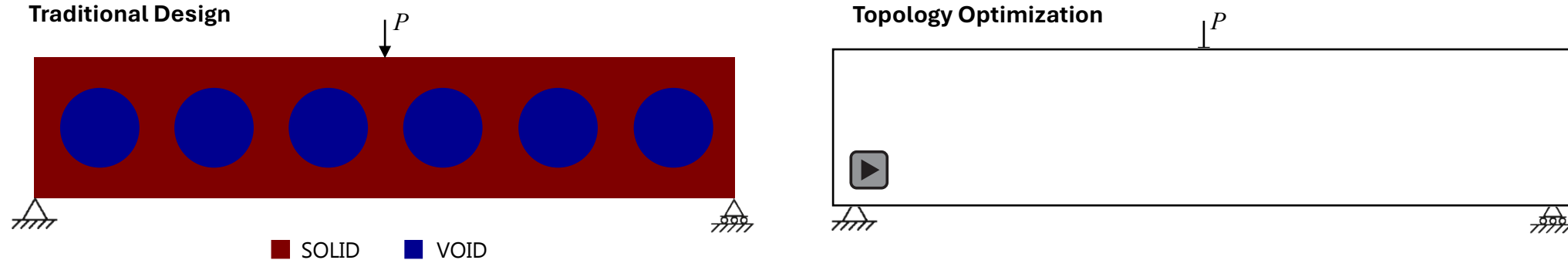
- 👍 Higher resolution distribution estimates
- 👍 More accurate tail probability estimates
- 👎 Requires finite difference derivatives
- 👎 More expensive: $m(d + 1)$ simulations



J. M. Emery et al. *Int. J. Numer. Meth. Engng.* 2015.

Application: Topology Optimization

- **Goal:** Obtain optimal distribution of material within a domain



- **Formulation:** Compute element densities, $\phi \in [0,1]$, through optimization

$$\min_{\phi} \mathbf{C}(\phi) = \mathbf{F}^T \mathbf{U}(\phi) \quad \text{-----} \rightarrow \quad \text{Minimize structural compliance}$$

$$\text{s. t.} \quad \mathbf{K}(\phi) \mathbf{U}(\phi) = \mathbf{F} \quad \text{-----} \rightarrow \quad \text{Satisfy governing equations}$$

$$V(\phi) \leq V_{max} \quad \text{-----} \rightarrow \quad \text{Satisfy volume/weight constraint}$$

- How does the optimal design change if there are uncertainties in loads, materials, etc.?

Topology Optimization Under Uncertainty

- Introduce loading uncertainties represented by random vector, $\mathbf{X}$
- Robust design optimization (RDO) formulation:

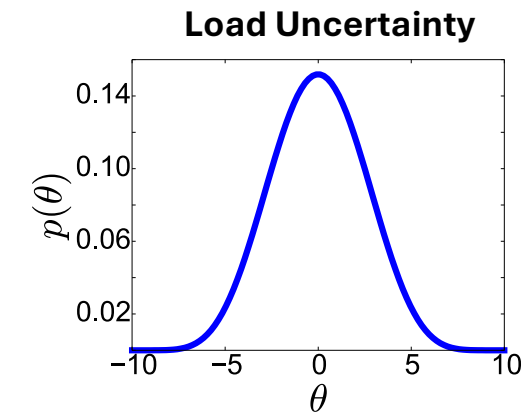
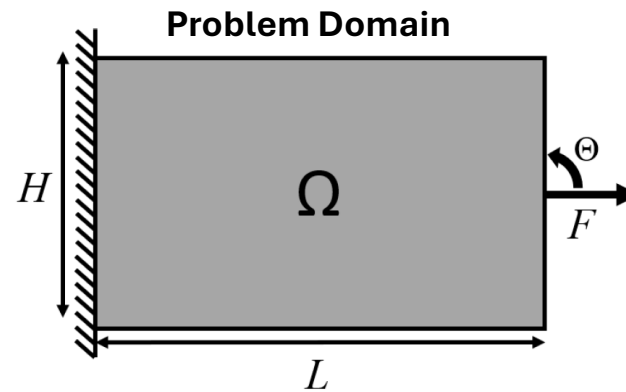
$$\begin{aligned} \min_{\phi} \quad & \mathbb{E}[\mathbf{C}(\phi; \mathbf{X})] + k\text{Std}[\mathbf{C}(\phi; \mathbf{X})] \longrightarrow \text{Encourages designs that are robust to uncertainty} \\ \text{s. t.} \quad & \boxed{\mathbf{K}(\phi)\mathbf{U}(\phi; \mathbf{X}) = \mathbf{F}(\phi; \mathbf{X})} \longrightarrow \text{UQ at each optimization iteration to solve:} \\ & V(\phi) \leq V_{max} \qquad \qquad \qquad \mathbf{U} = \mathcal{M}(\mathbf{X}) = \mathbf{K}^{-1}\mathbf{F}(\mathbf{X}) \end{aligned}$$

- **Approach:** use SROMs to efficiently evaluate RDO objective*
 - Opportunity for significant computational savings
 - Simpler piecewise-constant SROM works well for $\mathbb{E}[\mathbf{C}]$ and $\text{Std}[\mathbf{C}]$
 - SROM-RDO is drop-in replacement for MCS-RDO after initial SROM construction

*A. Torres et. al. Robust topology optimization under loading uncertainties via stochastic reduced order models. 2021.

Example: Benchmark Tension Bar (1/2)

- **Goal:** Determine optimal design under randomly oriented load with 25% volume constraint

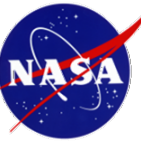


Deterministic vs. Robust Tension Bar Designs (SRM size, $m = 30$)

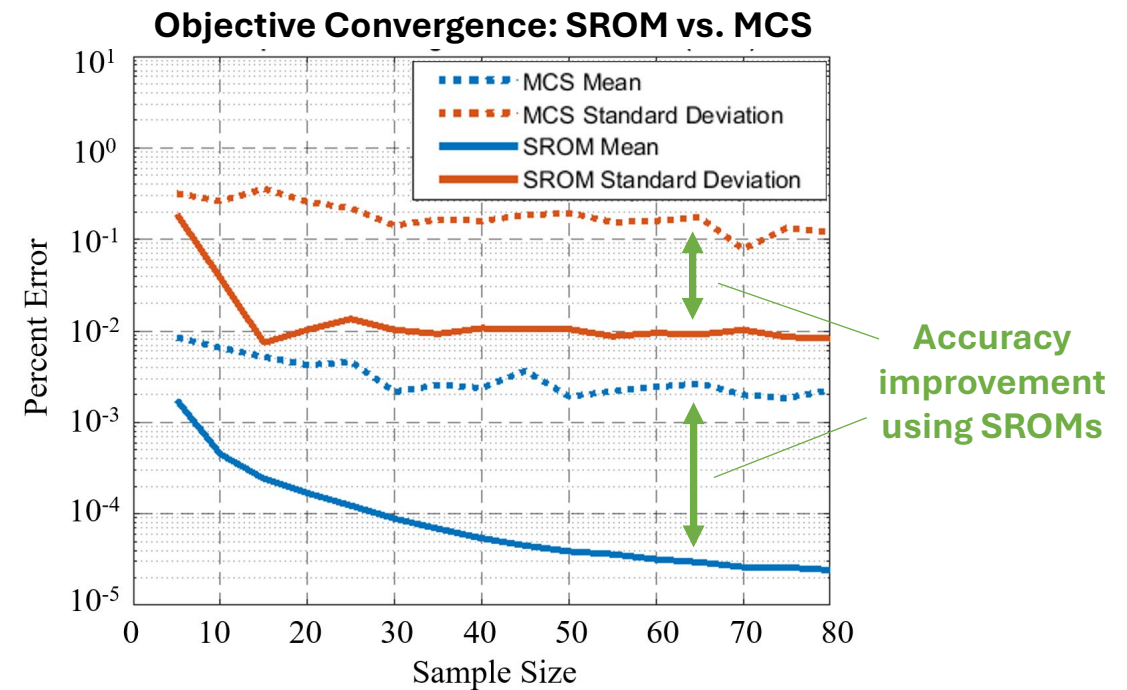
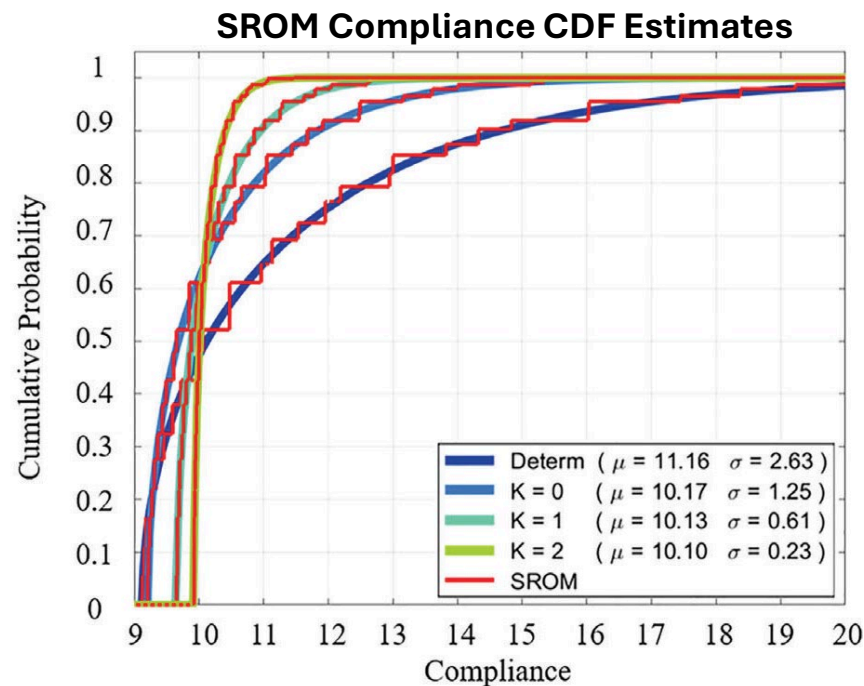
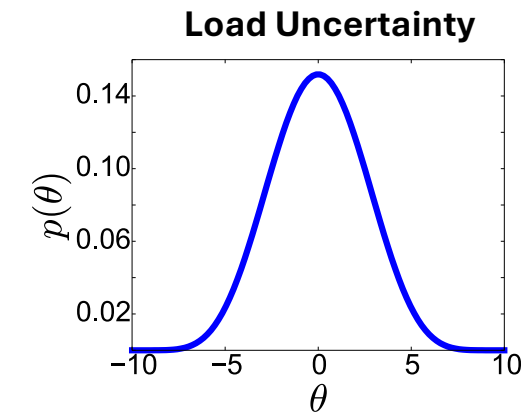
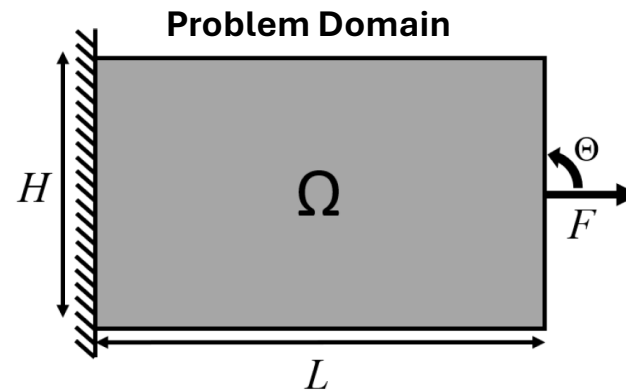
k	Deterministic	0	1	2
Final Design				
$E[C]$	11.16	10.17	10.13	10.10
$std(C)$	2.63	1.23	0.61	0.23

Increasing Robustness

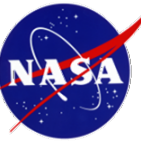
Example: Benchmark Tension Bar (1/2)



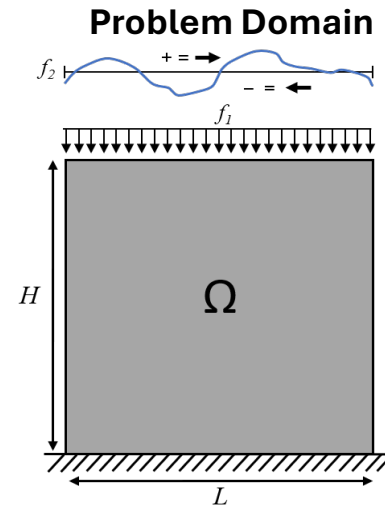
- **Goal:** Determine optimal design under randomly oriented load with 25% volume constraint



Example: Carrier Plate



- **Goal:** Determine optimal design under random horizontally distributed load with 40% volume constraint
- 200x200 mesh (40k unknowns)



Load Uncertainty

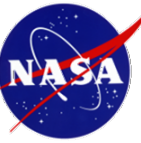
- Deterministic vertical component
- Uncertain horizontal component (zero mean Gaussian Process)
- Modeled with Karhunen-Loève expansion using **nine** independent random variables

Deterministic vs. Robust Tension Bar Designs (SRM size, $m = 200$)

k	Deterministic	0	1	2	3
Final Design					
$E[C]$	384.21	339.75	344.42	343.50	349.83
$std(C)$	132.35	45.33	35.49	29.61	28.77

SRM provided
~20X
computational
speedup versus
MCS

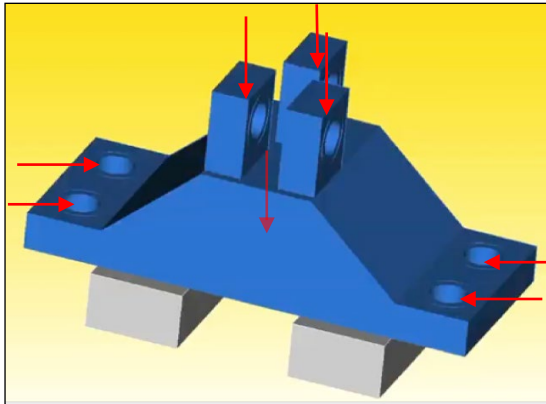
SROMs in Production Design Software



- Robust topology optimization using SROMs was implemented in Sandia's *PLATO* software for large scale 3D design under uncertainty



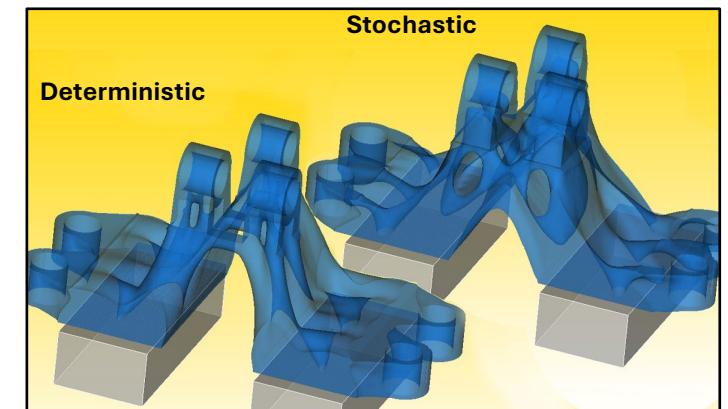
Randomly oriented loading



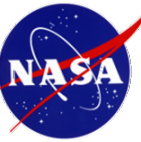
Optimization progression



Final design comparison

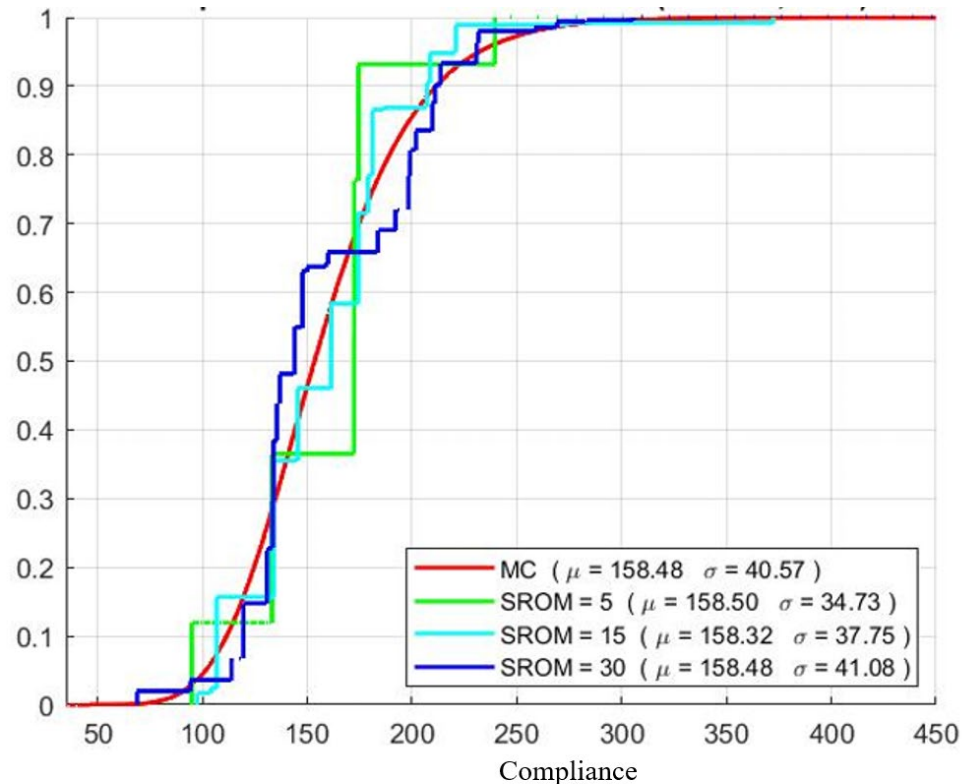


Piecewise Constant vs. Linear SROM

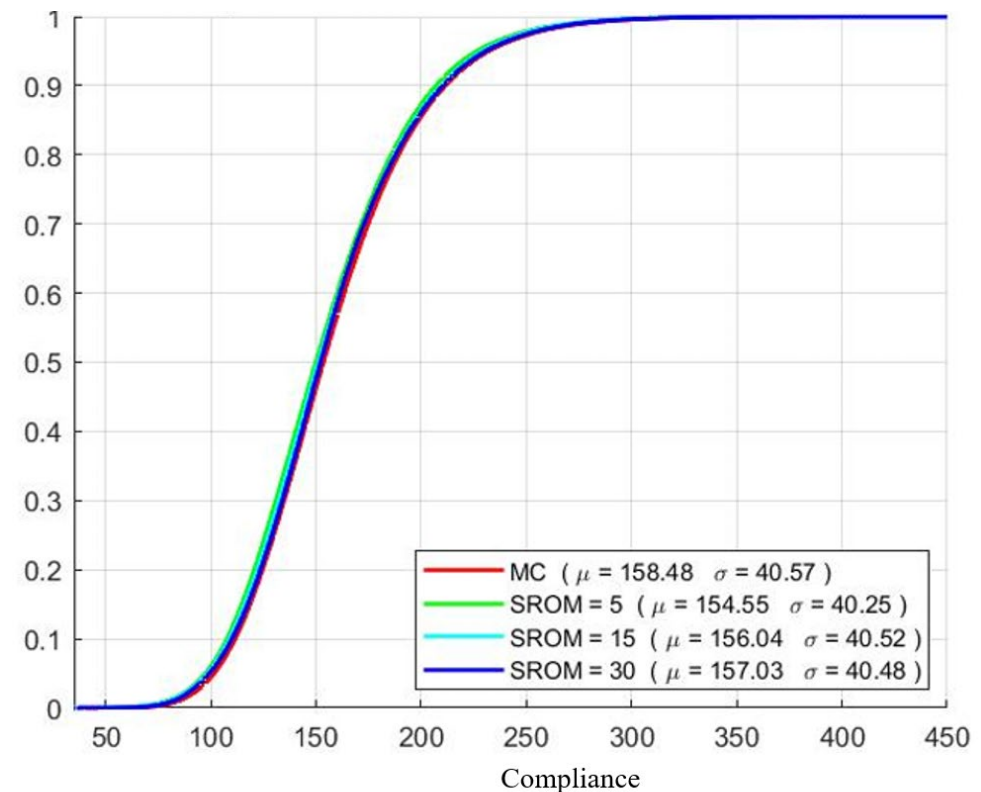


- The piecewise linear SROM approach has been explored in the context of reliability-based topology optimization

Compliance CDF: Piecewise Constant SROM



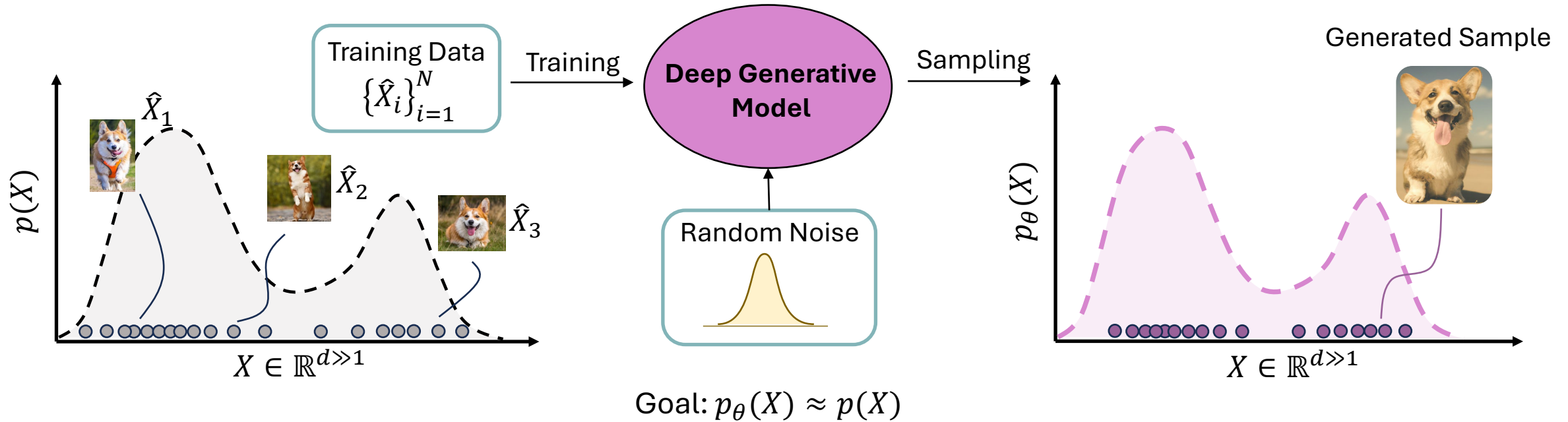
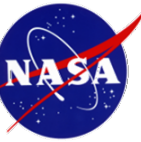
Compliance CDF: Piecewise Linear SROM



➤ More accurate CDFs and tail probabilities at the cost of extra model evaluations

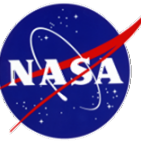
1. Uncertainty Quantification (UQ) Overview
2. Stochastic Reduced Order Models (SROMs)
 - Increasing UQ efficiency
- 3. Deep Generative Models**
 - Modeling complex, high-dimensional probability distributions
4. Summary

Deep Generative Modeling Overview



Training Data	Generative Model Architectures/Algorithms	Examples
Images	Generative adversarial networks (GANs), variational autoencoders (VAEs), diffusion models	DALL-E, Midjourney
Text, Audio, Video	Recurrent neural networks (RNNs), long short term memory (LSTM) networks, transformers	ChatGPT, Gemini, Jukebox

Generative Models for UQ



Inverse Material Identification [2]

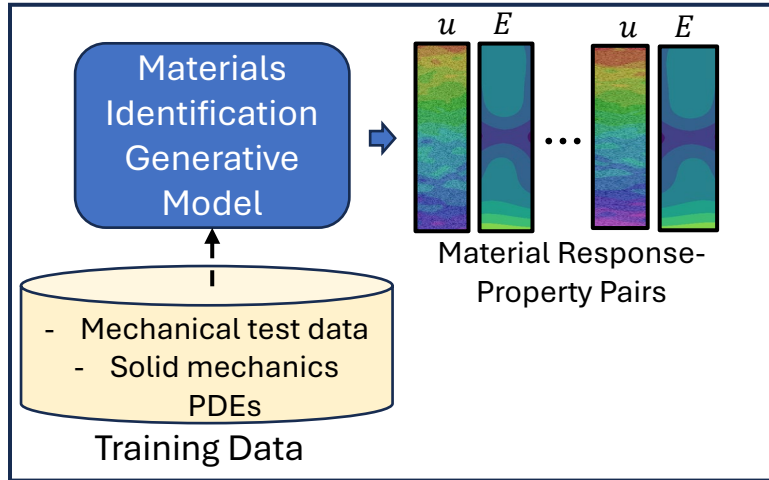
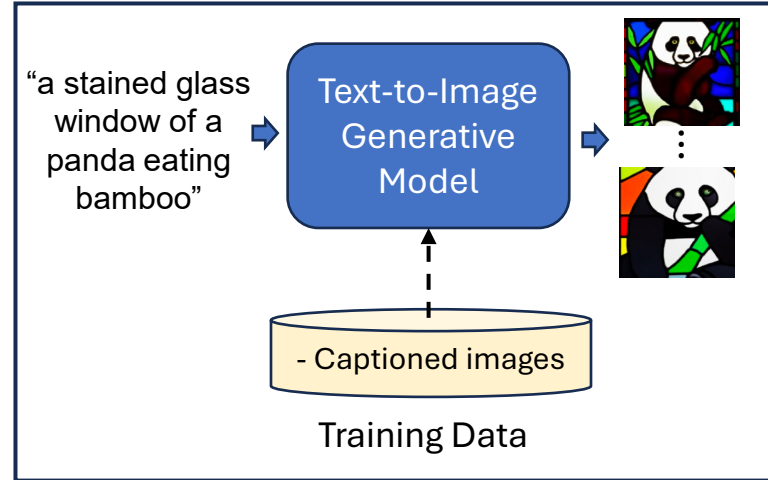
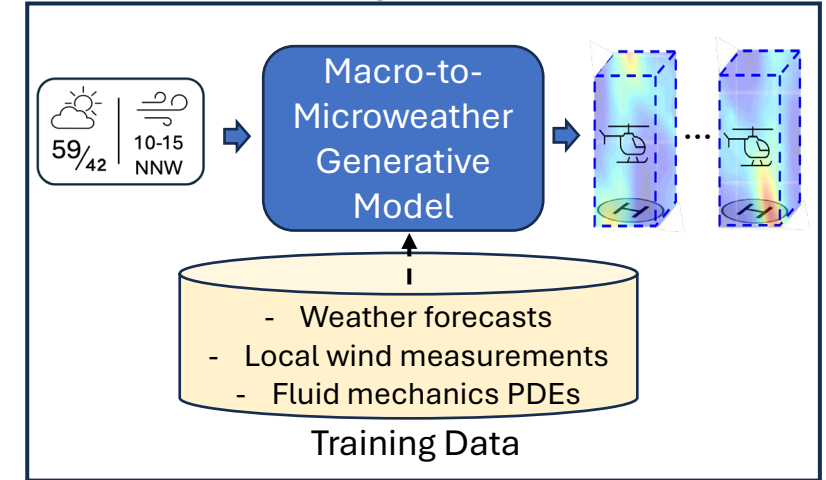


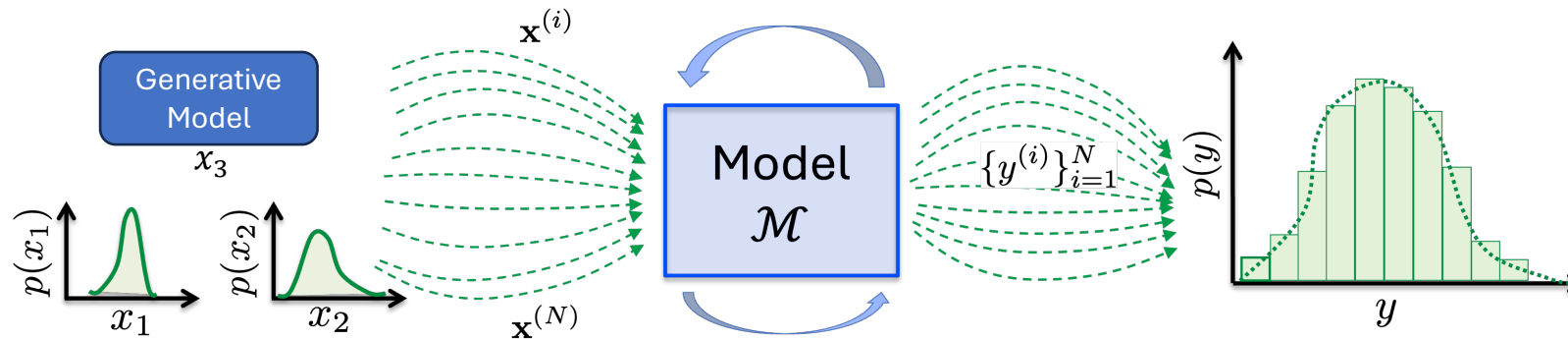
Photo Generation [1]



Wind Velocity Field Estimation



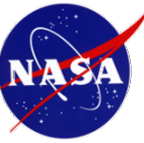
Generative Models as Random Inputs for UQ



[1] Nichol et. al. GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models. 2021.

[2] Warner et. al. Inverse Estimation of Elastic Modulus Using Physics-Informed Generative Adversarial Networks. 2020.

Application: Urban Air Mobility (UAM)

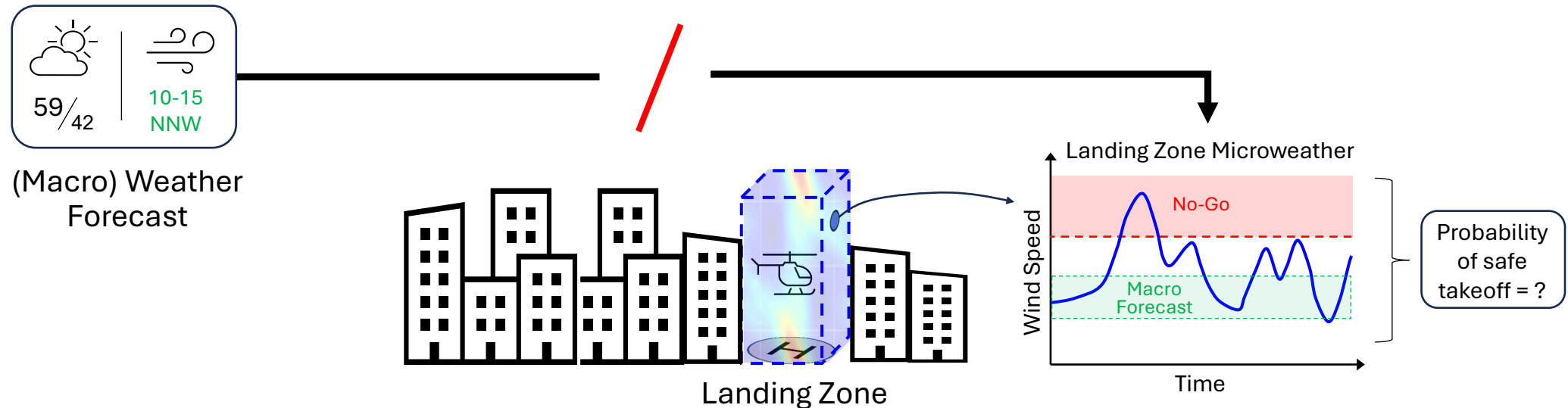


- UAM will not be widely adopted until it is perceived to be as safe, reliable, and convenient as existing urban transportation modes



Problem: Microweather Nowcasting

- Assess local wind velocities (*microweather*) over short time horizons (*nowcasting*)

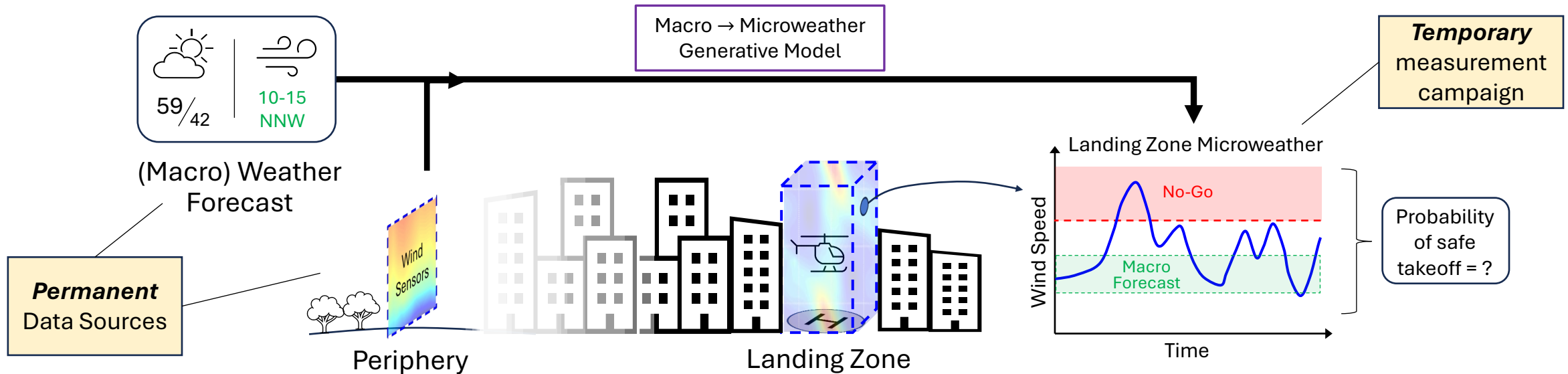


Challenges:

- Mild macro weather conditions can yield unsafe urban microweather conditions
- Microweather conditions vary rapidly and randomly across space and time
- Traditional physics-based predictions are not computationally tractable

Approach: Conditional Generative AI

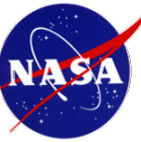
- Enable accurate, efficient, and **probabilistic** wind velocity predictions



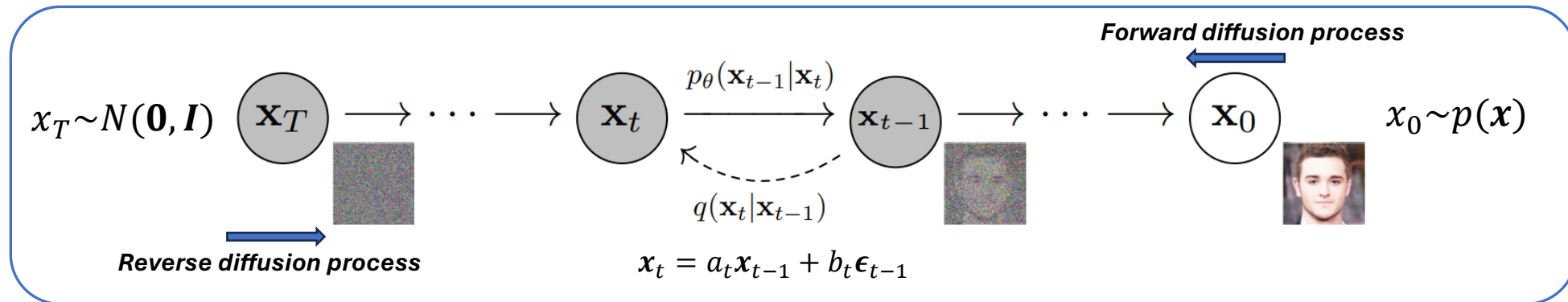
Requirements:

- Captures random variability in wind fields
- Does not require permanent wind profiling system installation
- Updates predictions based on real-time weather conditions
- Makes predictions continuously in space and time

Denoising Diffusion Probabilistic Models (DDPMs)



- DDPMs progressively add noise to dataset then learn to reverse the process [1]



- Often implemented by training a neural network, ϵ_θ , to model the noise [2]

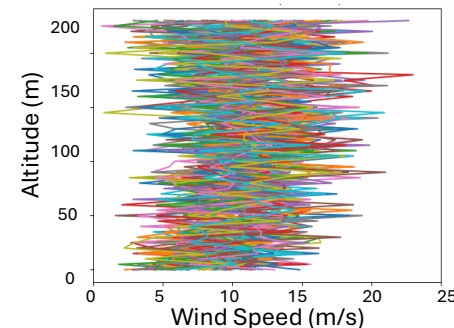
$$\theta^* = \underset{\theta}{\operatorname{argmin}} \mathbb{E}_{t, x_0, \epsilon} [\|\epsilon - \epsilon_\theta(x_t, t)\|^2]$$

- Sample by starting from Gaussian noise and iteratively denoising with ϵ_θ

Noise $\rightarrow$ Cat Image [3]

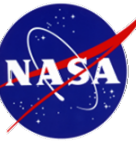


Noise $\rightarrow$ Wind vs. Altitude



- [1] Ho, J. et al. Denoising diffusion probabilistic models. 2020.
- [2] Nichol et al. Improved denoising diffusion probabilistic models. 2021.
- [3] Intro to Diffusion Model. dzdata.medium.com. 2023.

Proof of Concept Example



- **Goal**

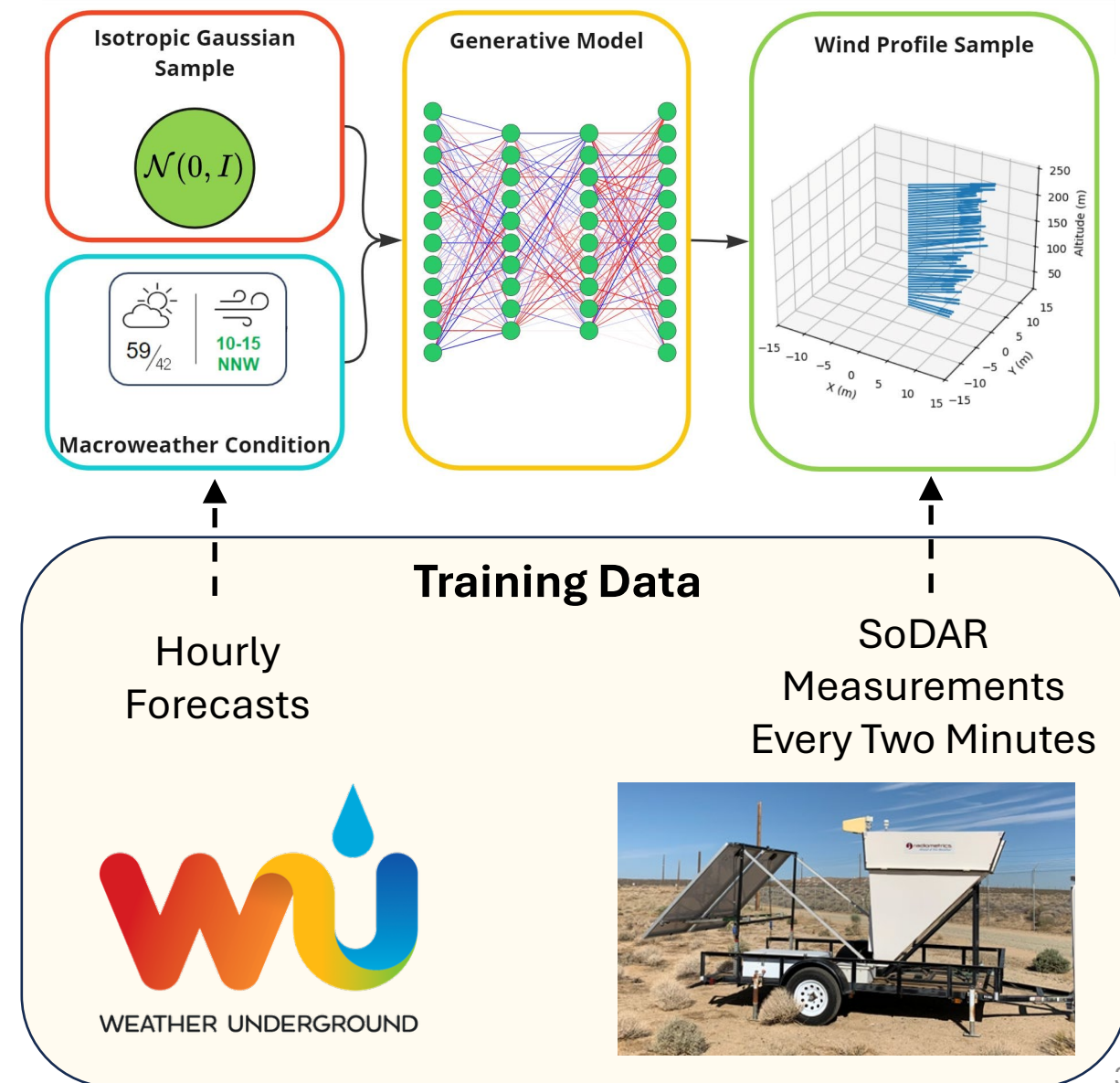
- Demonstrate probabilistic map from macro->microweather wind velocities using DDPMs

- **Microweather Data**

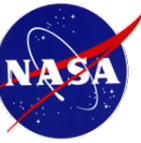
- Velocity vs. altitude from Sonic Detection and Ranging (SoDAR)
- 10 day measurement campaign at NASA Armstrong Flight Research Center (~6500 samples)

- **Macroweather Data**

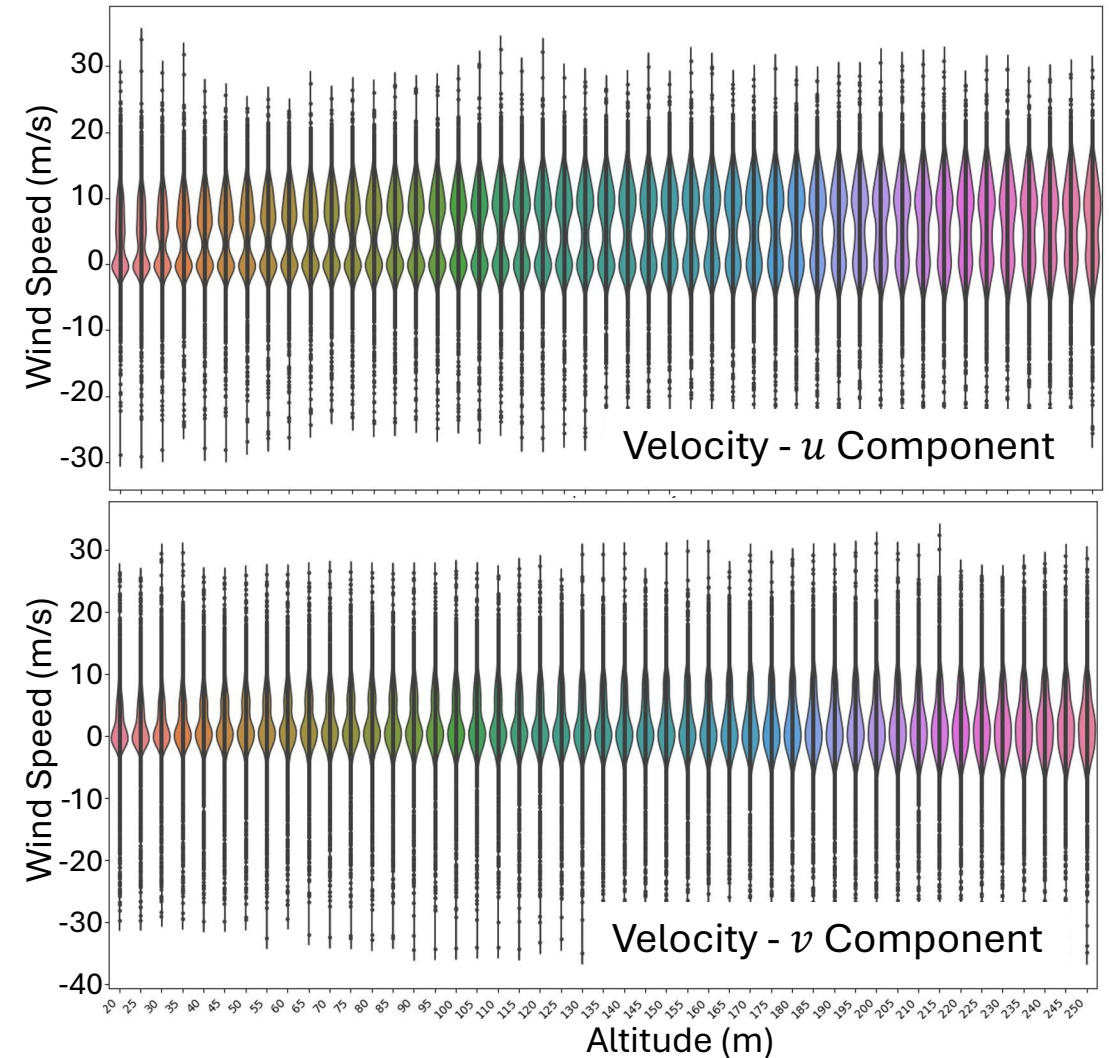
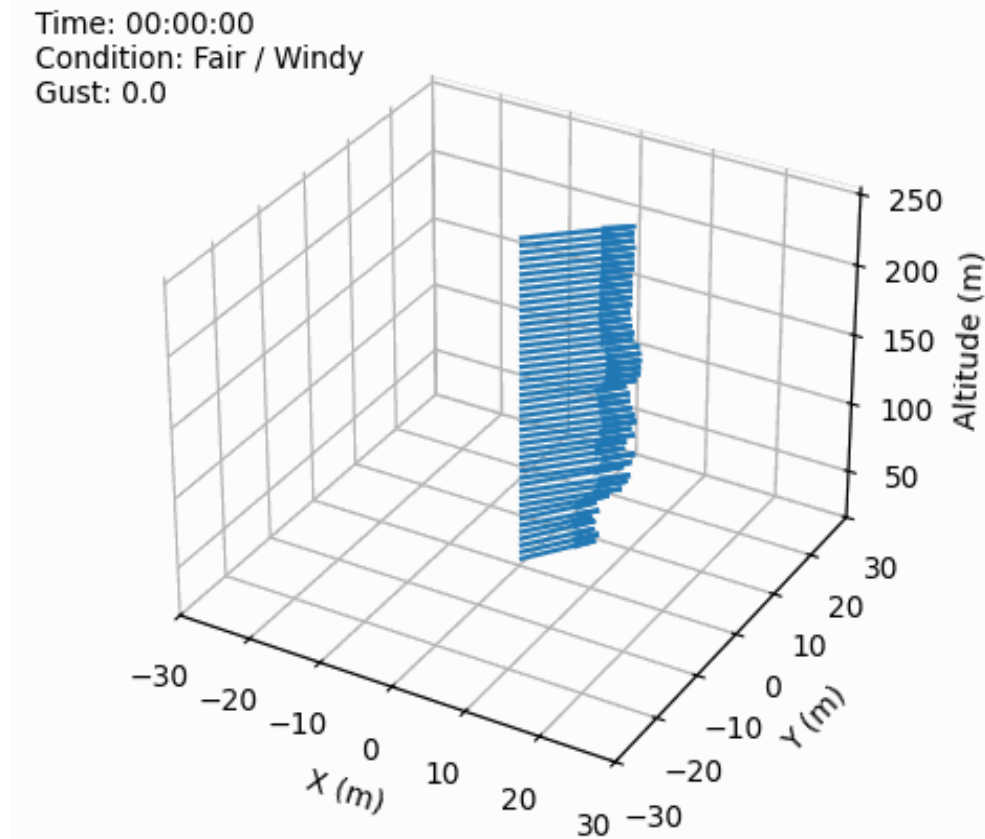
- Hourly forecasts from wunderground.com



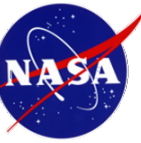
SoDAR Wind Measurement Data



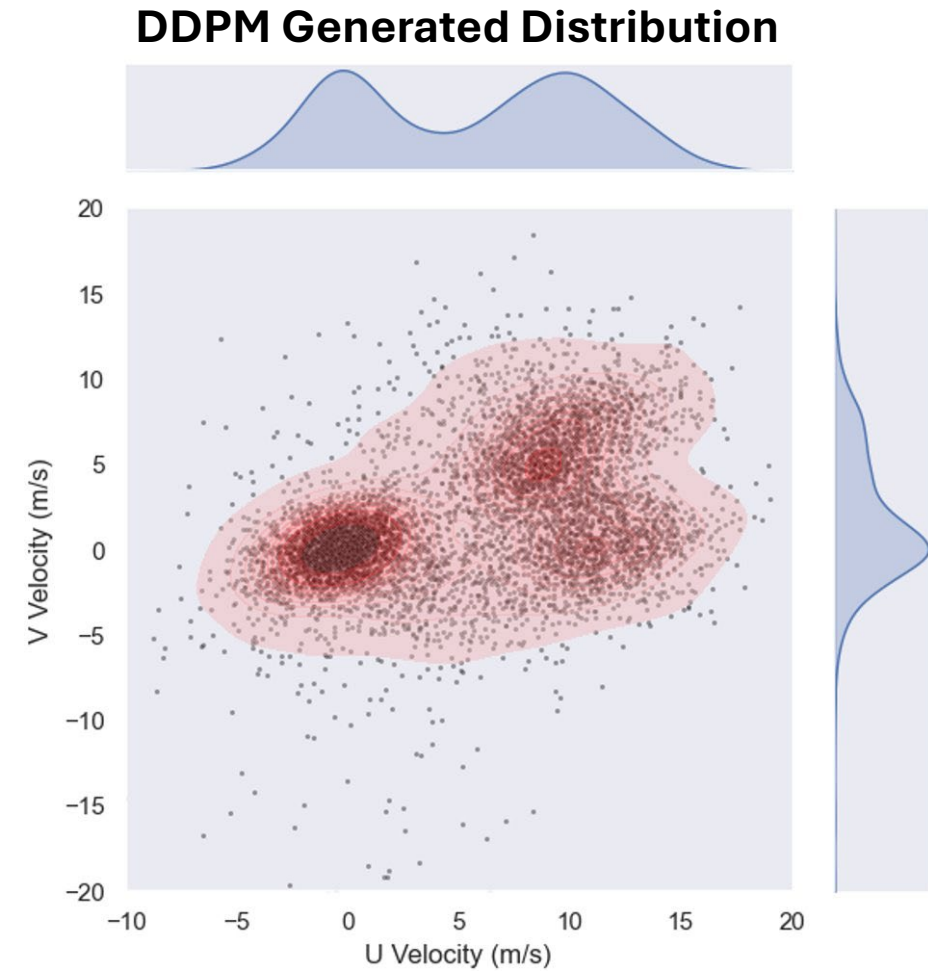
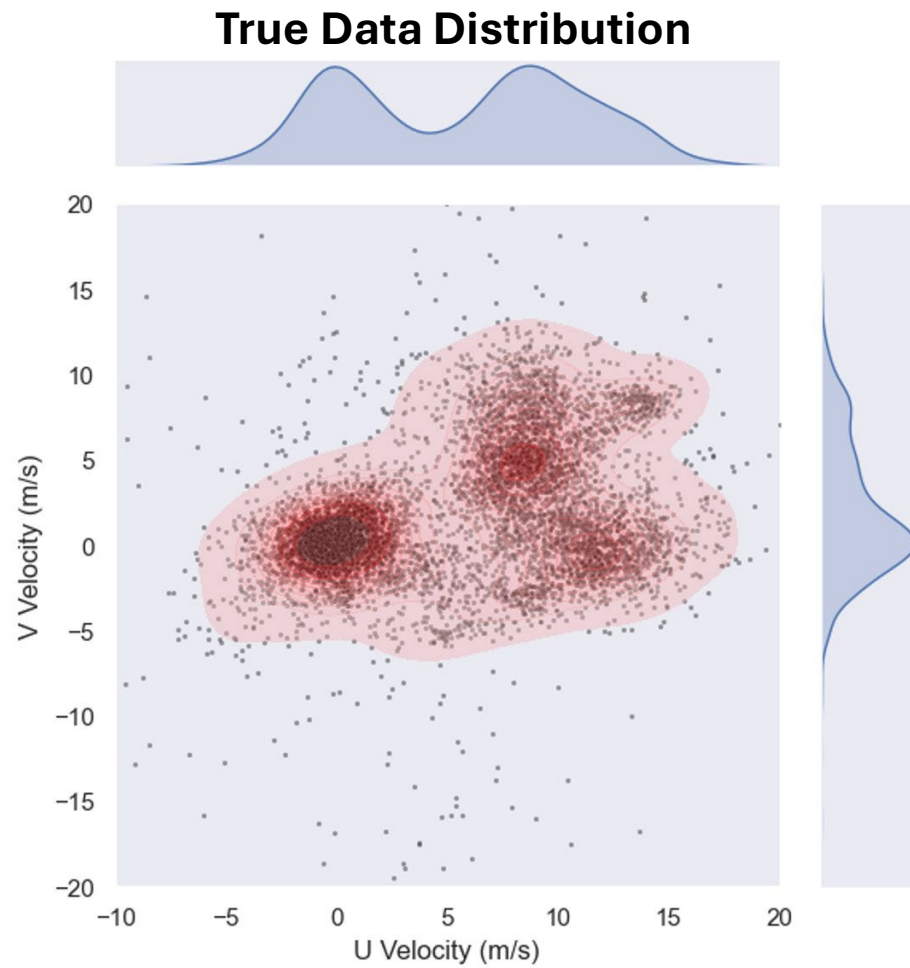
- Wind velocity samples as a function of time (left) and altitude (right)



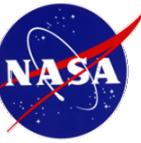
Unconditional Wind Generation



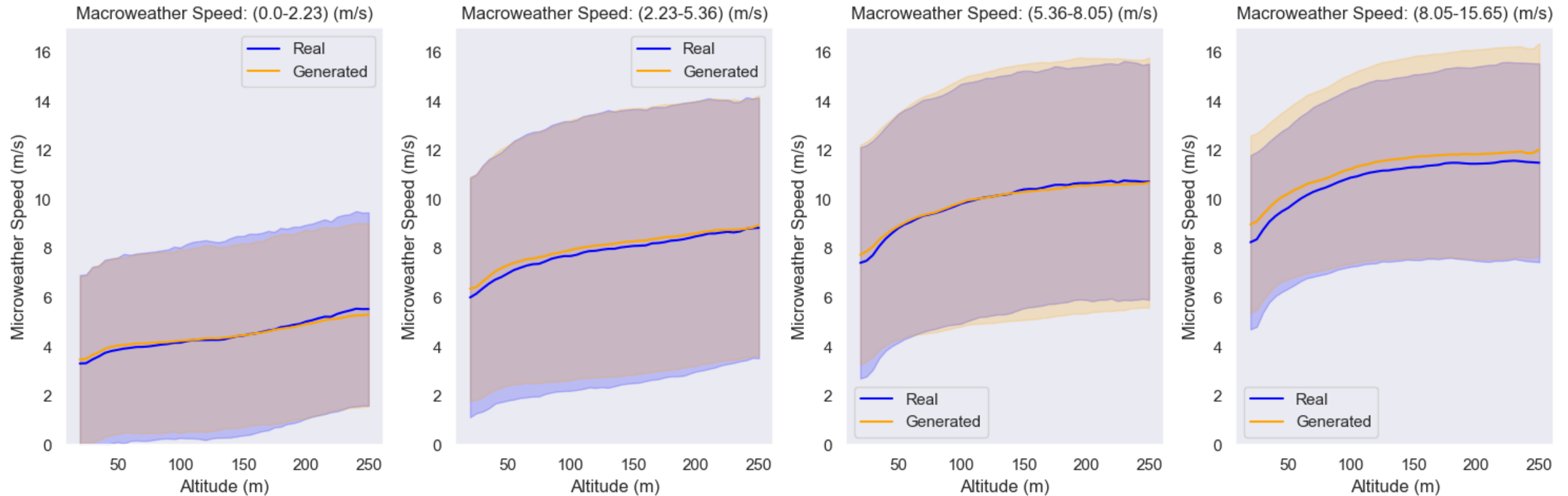
- Wind velocity samples averaged over altitude (no macro wind conditioning)



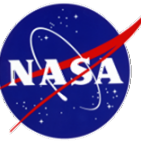
Macro → Micro Conditional Wind Generation



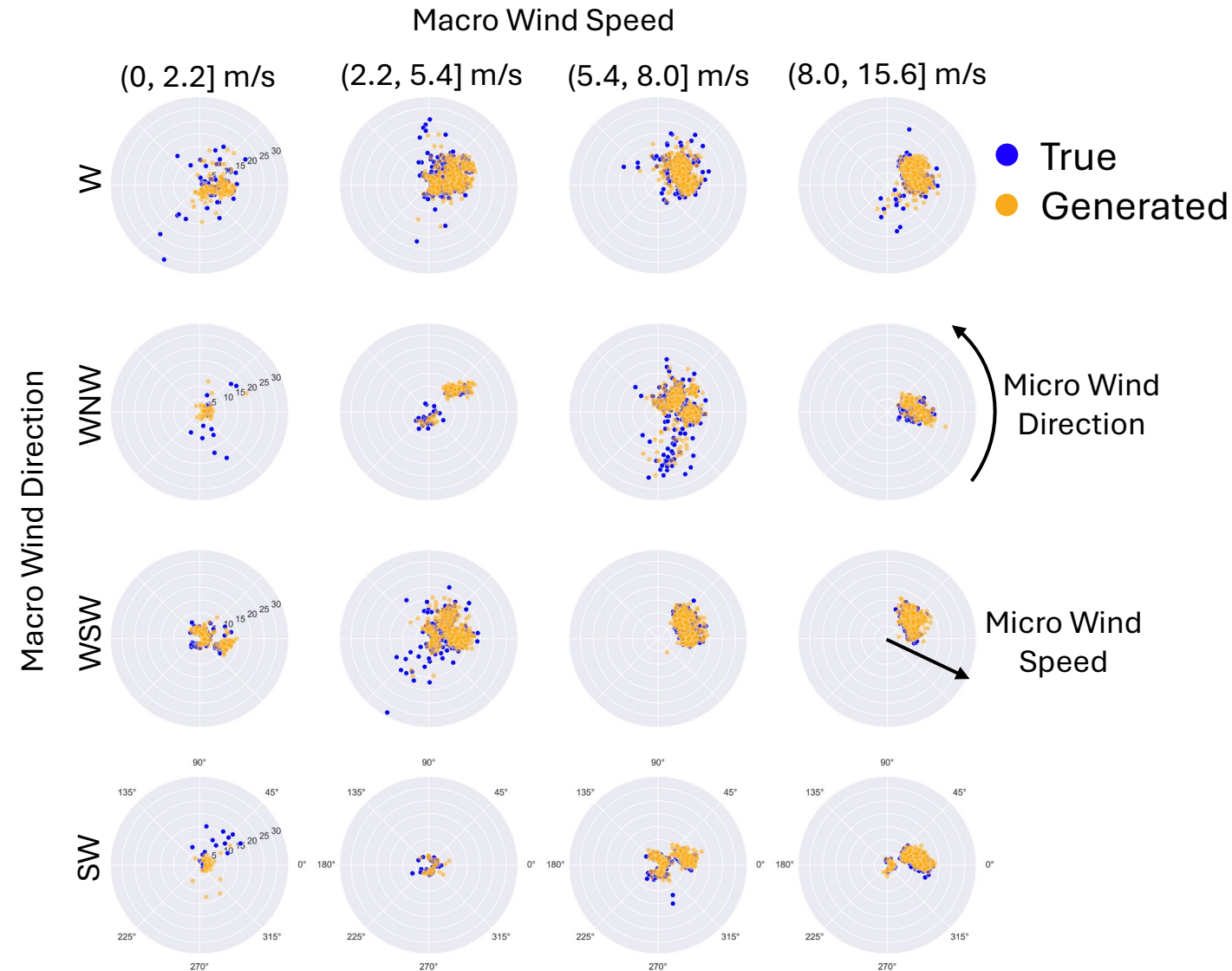
- Mean/STD of wind velocity vs. altitude samples conditioned on macro wind speed



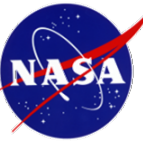
Macro → Micro Conditional Wind Generation



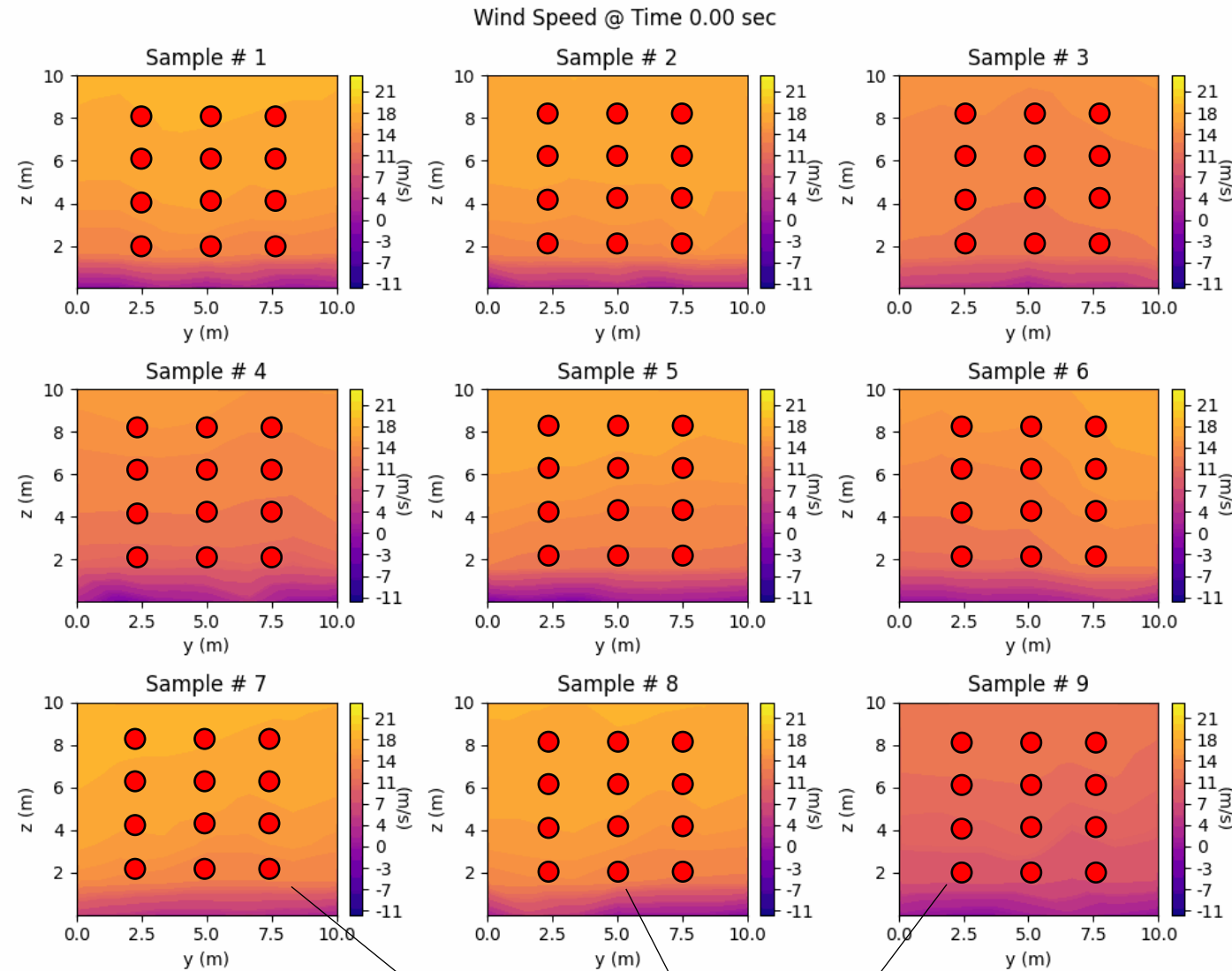
- Conditioning on macro wind speed & direction pairs
- K-fold cross validation used to leave out one condition pair at a time for testing
- Samples averaged over altitude for plotting



Extrapolating Beyond Sensor Measurements

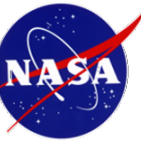


- Existing proof of concept is limited to predictions at sensor locations
- Current/future work is exploring **functional** DDPMs that can generate **continuous** wind velocity fields from sparse sensors that are **physically and/or statistically consistent**
- Related work
 - Physics-informed neural networks; Raissi et. al.
 - Physics-Informed Diffusion Models; Bastek et. al
 - Enforcing statistical constraints in generative adversarial networks for modeling chaotic dynamical systems; Wu et. al

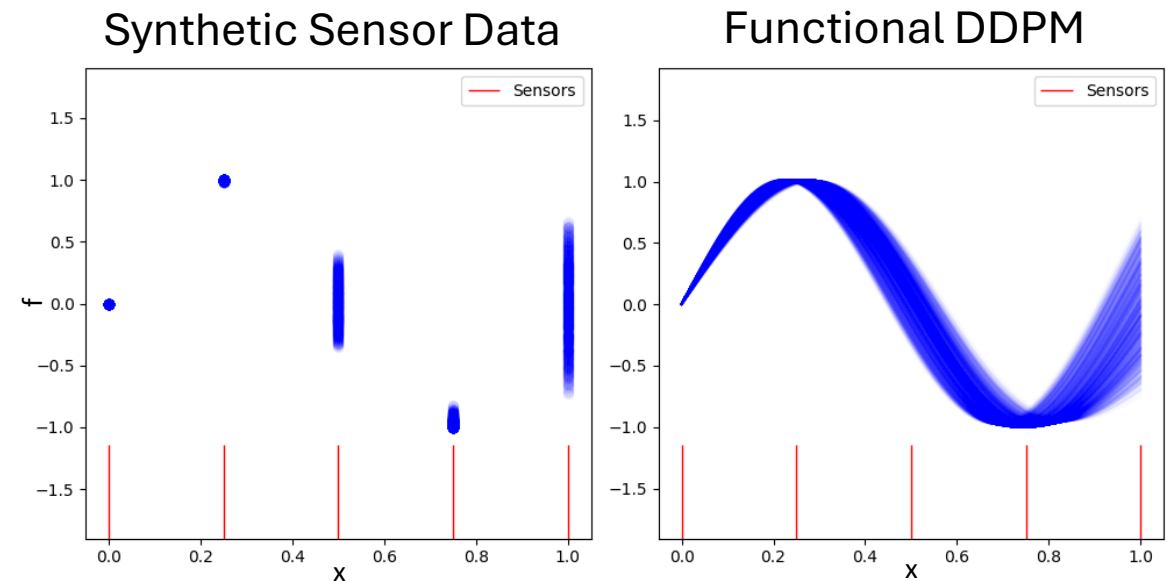
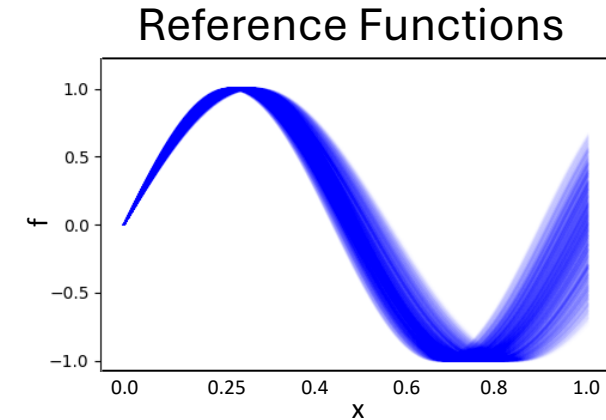


Measurement Locations

Simple Synthetic Example

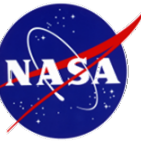


- Goal - learn random functions:
 - $f(x) = \sin(Bx)$
 - $B \sim \text{Beta}(2, 2)$
- DDPM trained to reproduce sparse data while satisfying differential equation constraint
 - $R(x) = f''(x) + B^2 f(x) = 0$
- DDPM uses functional neural network inspired by Deep Operator Networks (DeepONets)*



*DeepONet: Learning nonlinear operators ...; Lu et al. 2020

Summary



- Uncertainty Quantification (UQ) helps represent the unknown in computer simulations, yielding probabilistic predictions and enabling risk-informed decision making
- Common UQ challenges include overcoming the associated computational expense and modeling high-dimensional sources of uncertainty
- Stochastic reduced order models (SROMs) are a conceptually simple approach to speed up UQ analyses
 - Applied for computationally-efficient robust design optimization
- Generative models are a promising approach for representing model inputs that are complex and high-dimensional for UQ
 - Applied to probabilistic estimation of microweather wind velocity fields

Questions



- Email: james.e.warner@nasa.gov