# Multifidelity Uncertainty Quantification (UQ) at NASA

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# Outline

- Entry, Descent, and Landing (EDL) & the ADEPT Mission
- Monte Carlo simulation for EDL
- Multifidelity methods for EDL statistics
  - Multi-level Monte Carlo (MLMC)
  - Approximate control variates (ACVs)
  - Multifidelity Monte Carlo (MFMC)
- Estimating Rare Events with Multifidelity Importance Sampling (MFIS)
- Conclusions

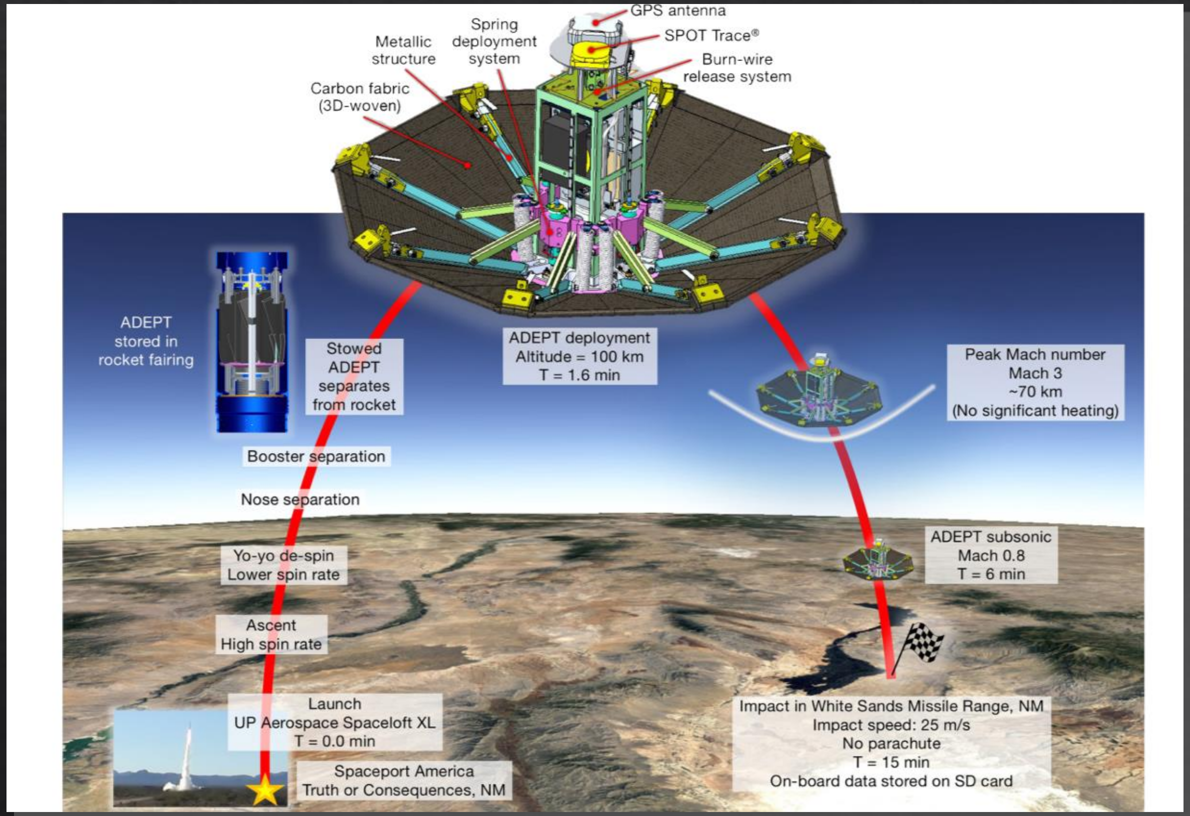
# Entry, Descent, and Landing (EDL)

- Goal: Conceive, design, assess, and optimize vehicle systems for EDL at the Earth as well as the other planetary bodies of the solar system

- Primary flight mechanics tool used is the Program to Optimize Simulated Trajectories II (POST2)
  - Simulates vehicle trajectory
  - Used for many Mars and Lunar missions

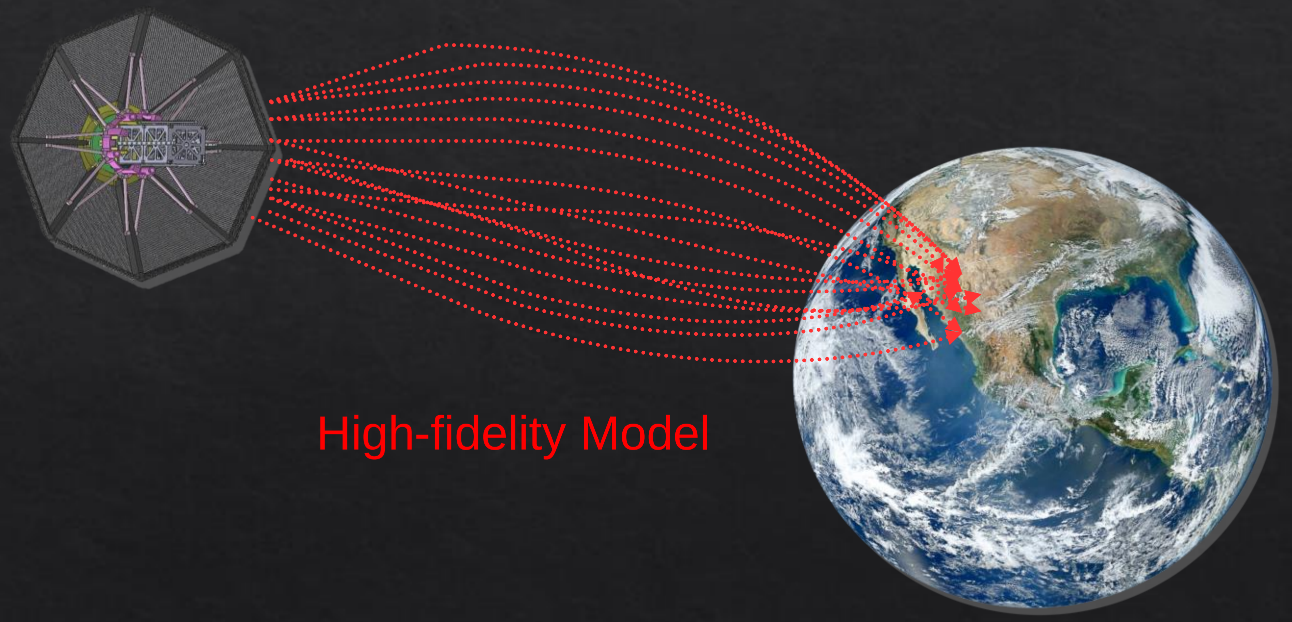
# The ADEPT Mission

- Launched Sept. 2018
- Test of a new heat shield technology for EDL
- Uncertainties:
  - initial state, atmospheric conditions, noisy data from onboard measurements, etc.
- POST2 was used to model the flight path
- Goal: Identify landing location with given confidence

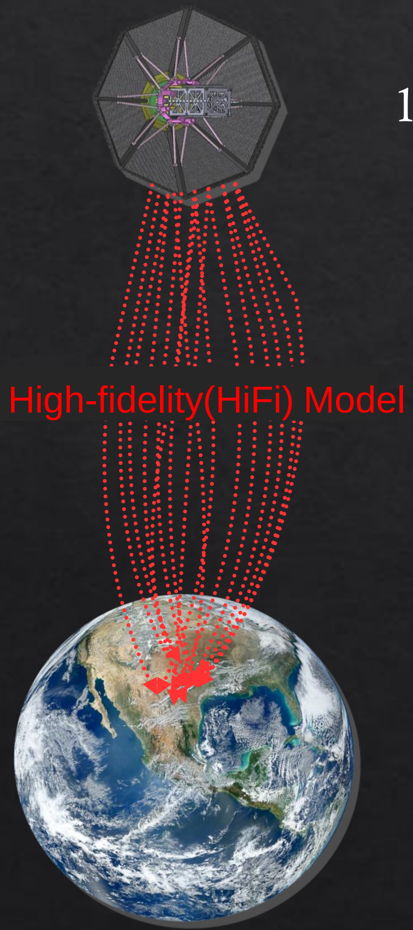


# Monte Carlo Simulation

- Current state involves using Monte Carlo simulations to propagate uncertainty
  - Depending on desired statistics, can involve thousands or even millions of simulations
  - Can be very time-consuming



# Monte Carlo Simulation




1) Draw random inputs

$N$ samples

$\{X^{(i)}\}$

2) Evaluate model

**HiFi Model**

$Y^{(i)} = \mathcal{M}(X^{(i)})$

$i = 1, \ldots, N$

$\{Y^{(i)}\}$

3) Form estimator

$$\mathbb{E}[Y] \approx \hat{Y} = \frac{1}{N}\sum_{i=1}^{N} Y^{(i)}$$

Unbiased: $\mathbb{E}[\hat{Y}] = \mathbb{E}[Y]$

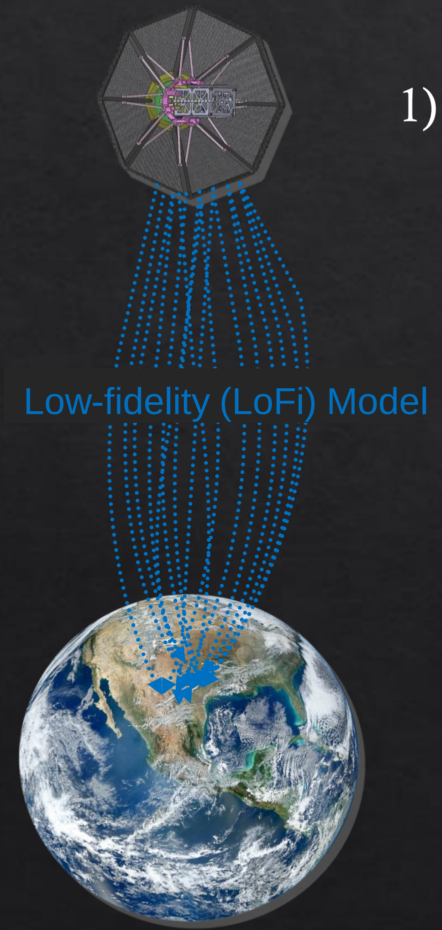
Total Solution Time: $C^{\text{tot}} = N \times C$

$N \sim O(10^4)$

HiFi model cost

# Monte Carlo Simulation with Surrogate

- Use a low-fidelity model to speed up estimate

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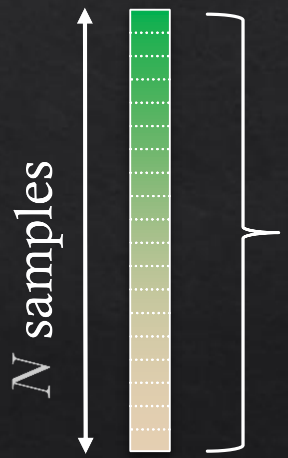



$\{X^{(i)}\}$

2) Evaluate model

**LoFi Model**

$$\widetilde{Y}^{(i)} = \widetilde{\mathcal{M}}(X^{(i)})$$

$i = 1, \dots, N$

$\{\widetilde{Y}^{(i)}\}$

3) Form estimator

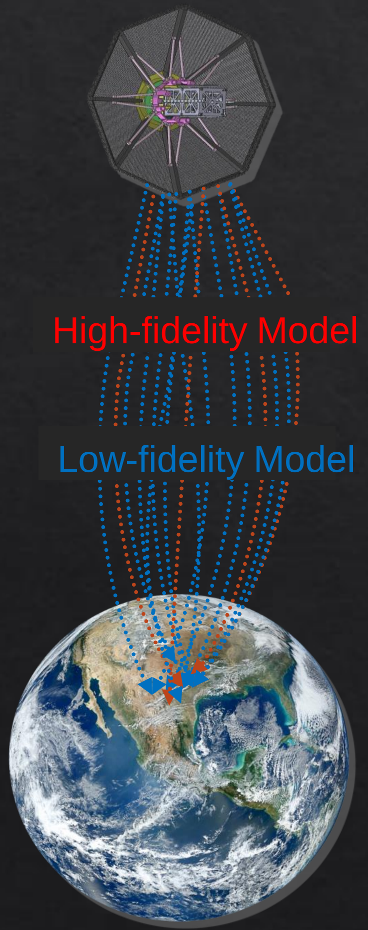
$$\mathbb{E}[Y] \approx \hat{\widetilde{Y}} = \frac{1}{N}\sum_{i=1}^{N} \widetilde{Y}^{(i)}$$

**Biased:** $\mathbb{E}[\hat{\widetilde{Y}}] \neq \mathbb{E}[Y]$

Total Solution Time: $C^{\mathrm{tot}} = \underbrace{N}_{N \sim O(10^4)} \times \underbrace{\widetilde{C}}_{\text{LoFi model cost}}$

# Multi-level Monte Carlo (MLMC) Simulation

- Use a low-fidelity model and correct with high-fidelity model




1) Draw random inputs

$N$ samples

$\tilde{N}$ samples

2) Evaluate model

**HiFi Model**

$$Y^{(i)} = \mathcal{M}(X^{(i)})$$

**LoFi Model**

$$\widetilde{Y}^{(i)} = \widetilde{\mathcal{M}}(X^{(i)})$$

3) Form estimator

$$\mathbb{E}[Y] \approx f\left(\{Y^i\}, \{\widetilde{Y}^i\}, N, \widetilde{N}\right)$$

# MLMC Simulation

- Use a low-fidelity model and correct with high-fidelity model

$$\boxed{\mathbb{E}[Y] \approx f\left(\{Y^i\}, \{\tilde{Y}^i\}, N, \tilde{N}\right)}$$

$$\hat{Y}_{\text{MLMC}} = E[\tilde{Y}] + E[Y - \tilde{Y}]$$

$$\frac{1}{\tilde{N}}\sum_{i=1}^{\tilde{N}} \tilde{Y}^i + \frac{1}{N}\sum_{i=1}^{N}(Y^i - \tilde{Y}^i)$$

Unbiased

$$\mathbb{E}[\hat{Y}_{\text{MLMC}}] = E[Y]$$

Total Solution Time:

$$C^{\text{tot}} = NC + (N + \tilde{N})\tilde{C}$$

Can Extend to More Models

Variance of difference of successive models should be decreasing

# ADEPT Results: Landing Site Prediction

**Predicting Satellite Landing Location with Target Precision ($10^{-2}$)**

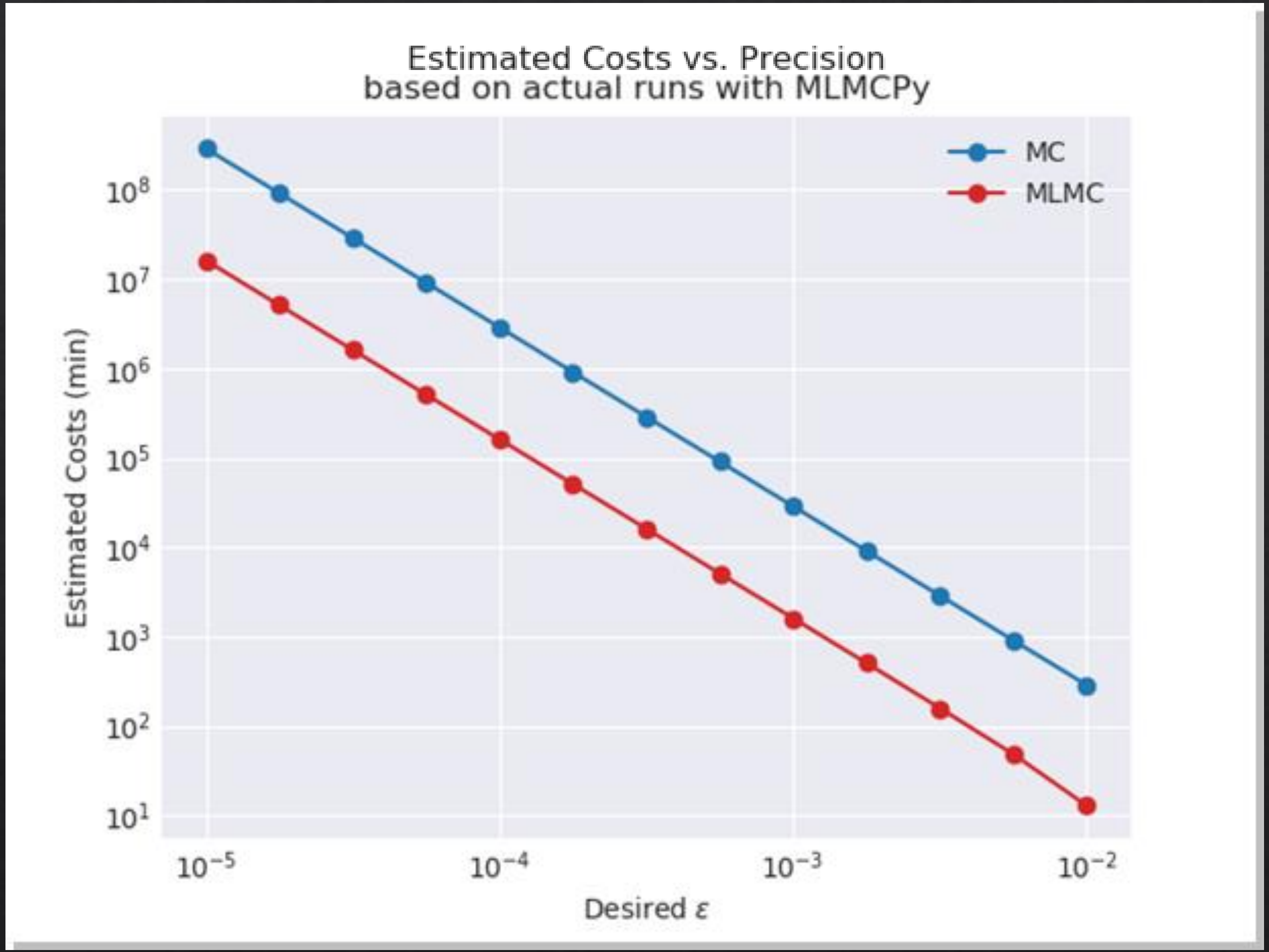
**Access to three POST2 models:**

| Model | Time Step | Run Time |
|---|---|---|
| Level 0 | $10^{-1}$ | 3 sec |
| Level 1 | $10^{-2}$ | 23 sec |
| Level 2 | $10^{-3}$ | 227 sec |

- **Monte Carlo simulation:**
  - 3000 x level 2 simulations → 189 hours
- **MLMC with three levels:**
  - 6982 x level 0 simulations
  - 248 x level 1 simulations
  - 60 x level 2 simulations

  → 11 hours

# ADEPT Results: Landing Site Prediction



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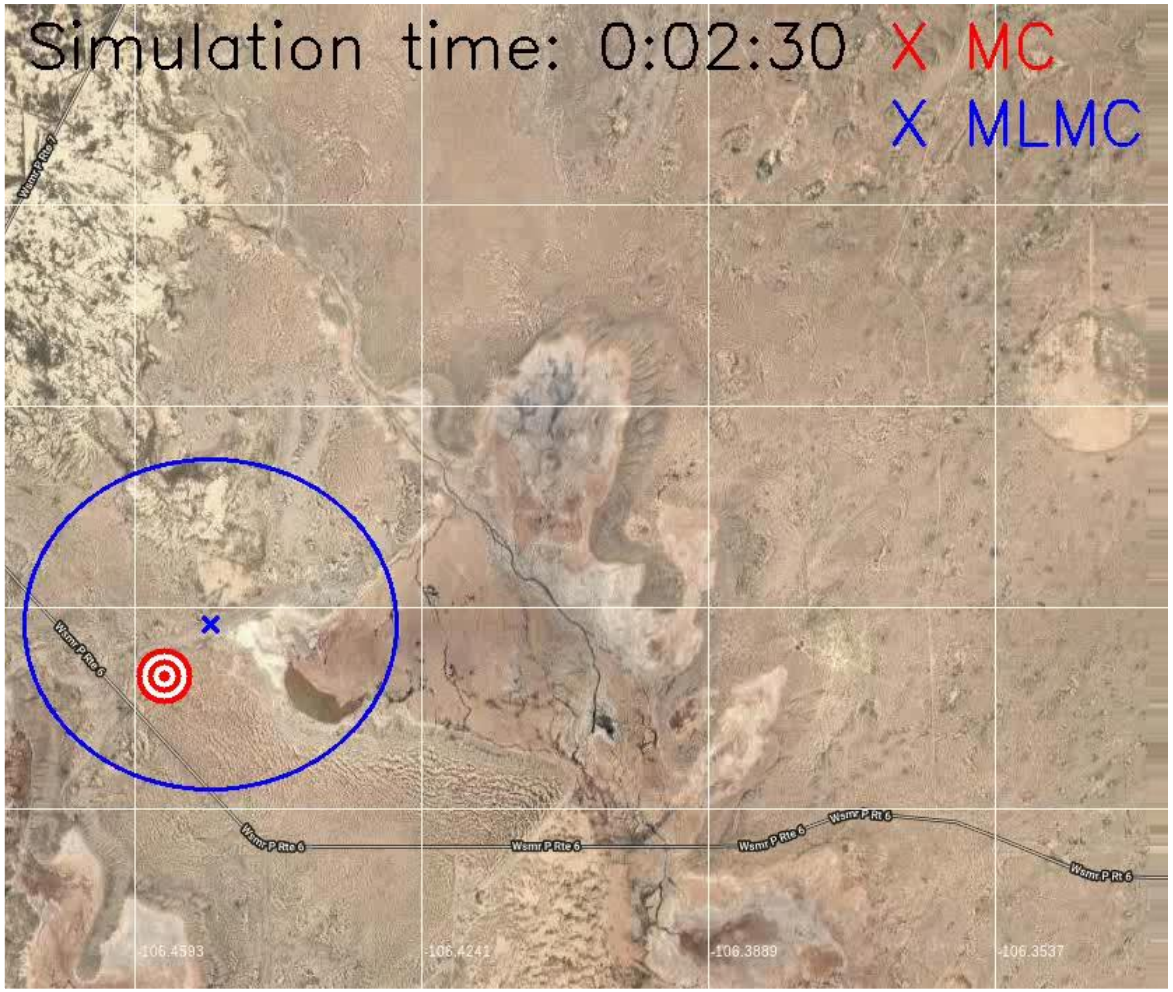



*More confidence with less time/resources*

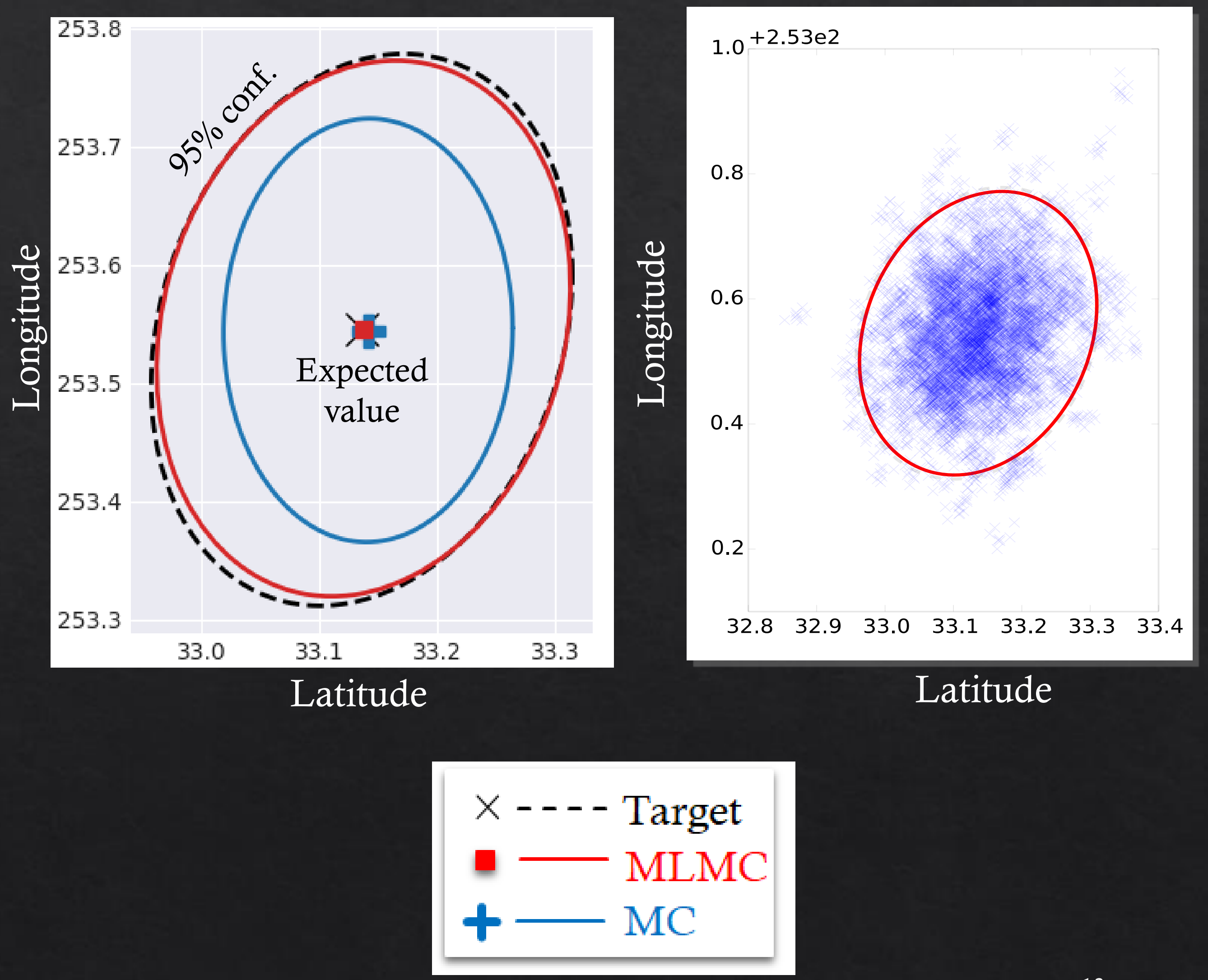
# Beyond Expected Values

## Confidence Ellipse

- We want 95% confidence of where ADEPT's touchdown would occur
- ~8,000 high-fidelity touchdown positions used for reference
- Note: It would take ~18.7 days for MC to run all 8,000 cases in serial
- So if given 250 min, MC can only run ~75 cases

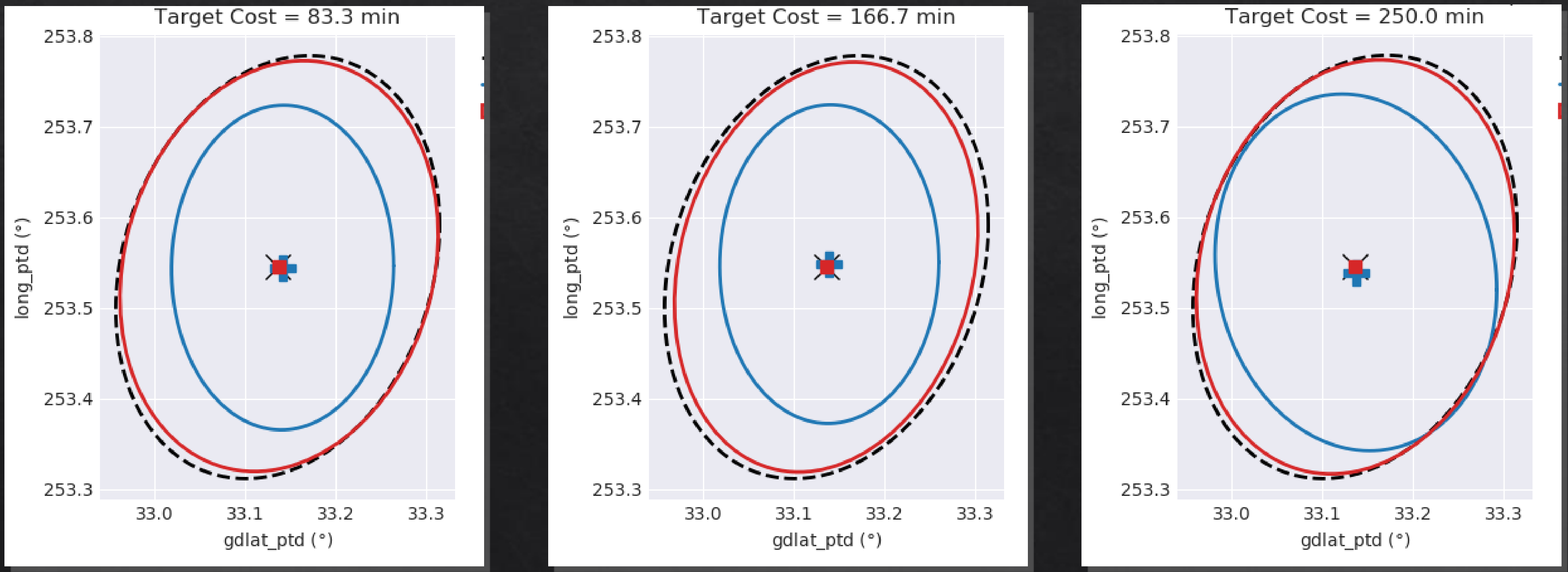
## Gaussian Assumption

- Confidence Ellipses were calculated based on the mean and covariance matrix of the sample data using a Gaussian assumption
- Shows good agreement with the general case for the ADEPT model



# MC vs. MLMC


>>>>>>> Desired Target Cost Increasing >>>>>>>



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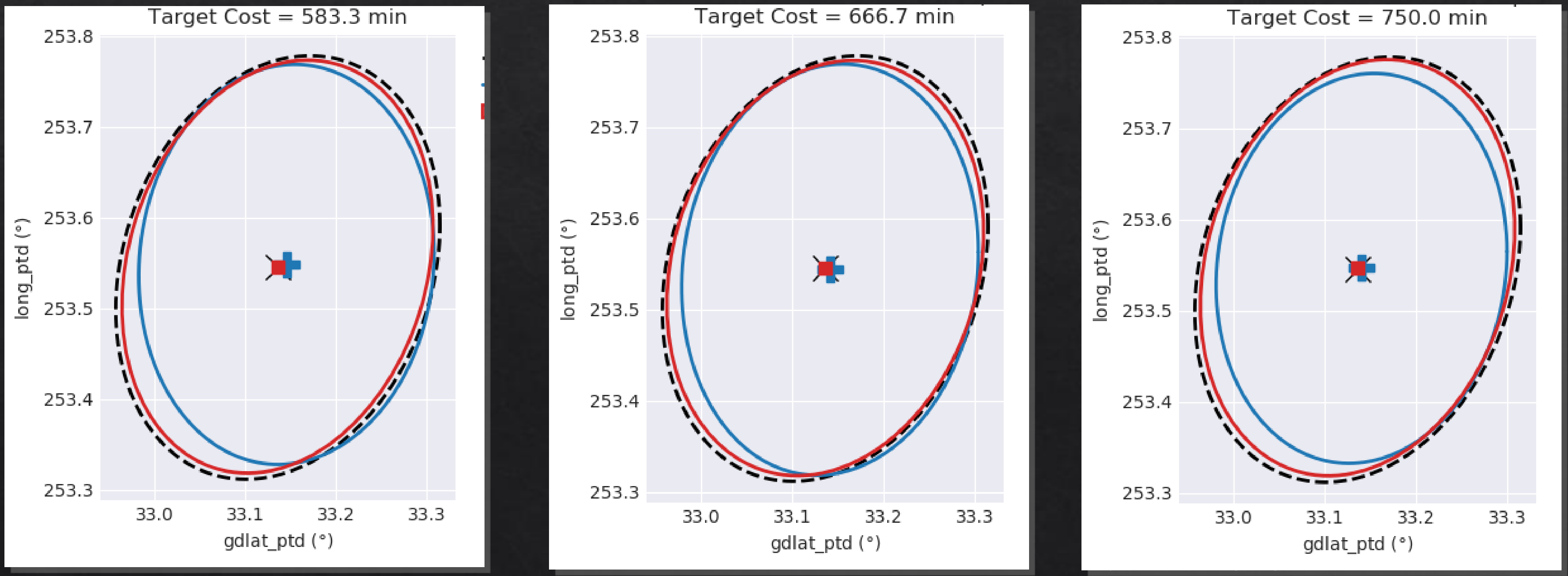
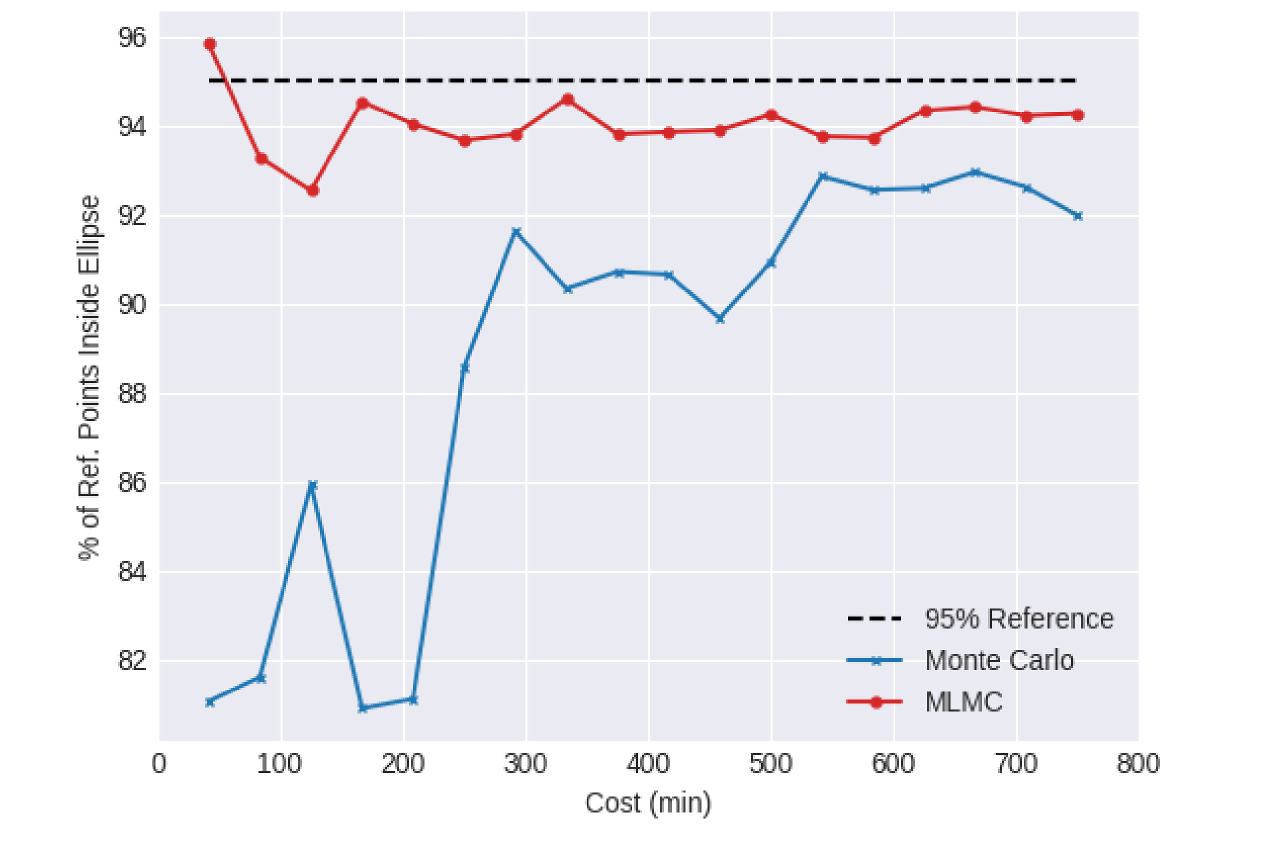


# Confidence Ellipse Summary

- MLMC's 95% Confidence Ellipse was consistently closer to the 95% Reference Ellipse than was Traditional MC's

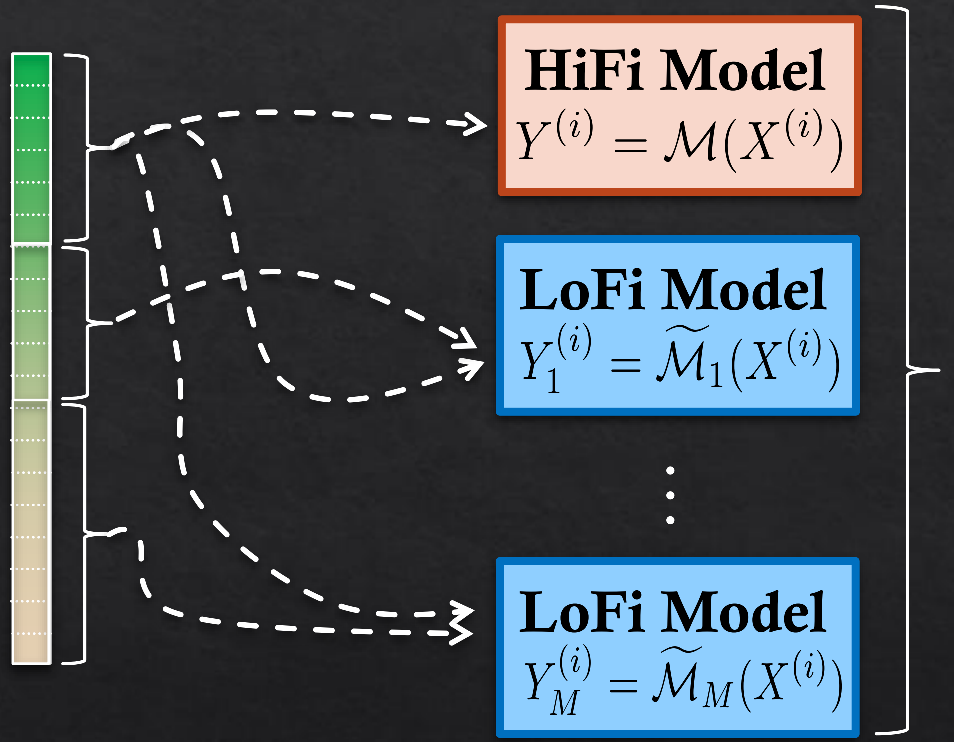


# Multi-Model MC

1) Draw random inputs

2) Evaluate model

3) Form estimator




$$\mathbb{E}[Y] \approx f\left(\{Y^i\}, N, \{\tilde{Y}_1^i\}, \ldots \{\tilde{Y}_M^i\}, \{\tilde{N}_j\}\right)$$

Find best estimator (smallest error/variance)

- How many samples for each model?
- How are samples shared between models?
- How model outputs are combined?
- Which models are used?

# Approximate Control Variates (ACV)

$$E[Y] = \widehat{Q_0}(X_0^1) + \sum_{i=1}^{M} \alpha_i \left( \widehat{Q_i}(X_i^1) - \widehat{Q_i}(X_i^2) \right)$$

- $\widehat{Q_i}(X_i)$ is the MC estimator for model $i$ using input samples $X_i$
- $\alpha_i$ are the control variate coefficients
  - Optimal $\alpha_i$ can be calculated
- MLMC is an example of an ACV with $\alpha_i = 1$
  - This is in general sub-optimal
- ACVs have no constraint on converging "levels" of models

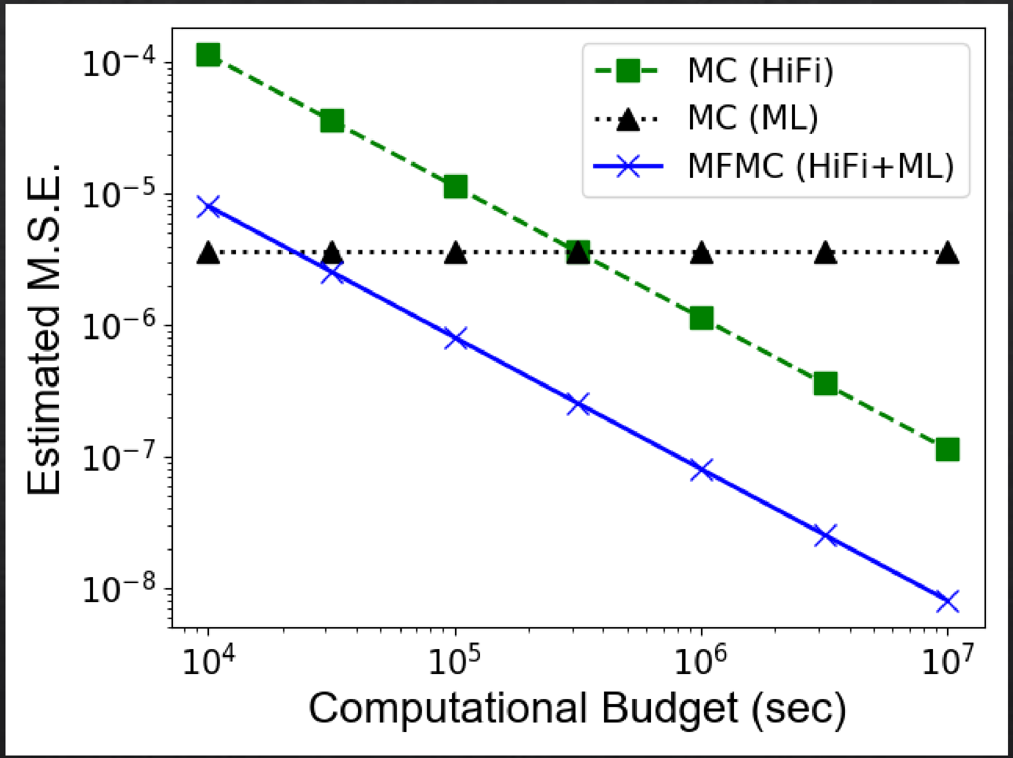
# Multifidelity Monte Carlo (MFMC)

$$E[Y] = \widehat{Q_0}(X_0^1) + \sum_{i=1}^{M} \alpha_i \left( \widehat{Q_i}(X_i^1) - \widehat{Q_i}(X_i^2) \right)$$

- Specific instance of ACV
- Nested recursion of input samples: $X_i^2 = X_{i-1}^1$ and $X_{i-1}^1 \subset X_i^1$
    - Lower fidelity models use all the same inputs as the high fidelity models plus some extra
- Has analytical solution for optimal sizes of input sample groups, $X_i^1$ and control variate coefficients $\alpha$

# Results: MFMC vs. Surrogate Modeling

- Significantly increased precision when combining the high-fidelity model with machine learning using MFMC rather than using one or the other with MC




- Recall: Mean Squared Error (M.S.E) $= \text{Bias}^2(\hat{Y}_{MXMC}) + \text{Var}[\hat{Y}_{MXMC}]$
  - The bias of the ML model cannot be reduced with more evaluations

# Effect of Model Choice

- Start with 4 models
- Choose which models are included
- See what the effect is on variance

| Models Used | Type | Correlation to Hi-Fi |
|---|---|---|
| High-Fidelity POST2 | Timestep 0.001 | 1.0 |
| Low-Fidelity POST2 | Timestep 0.1 | 0.9958 |
| Support Vector | Machine Learning | 0.9676 |
| K-Nearest Neighbors | Machine Learning | 0.9135 |

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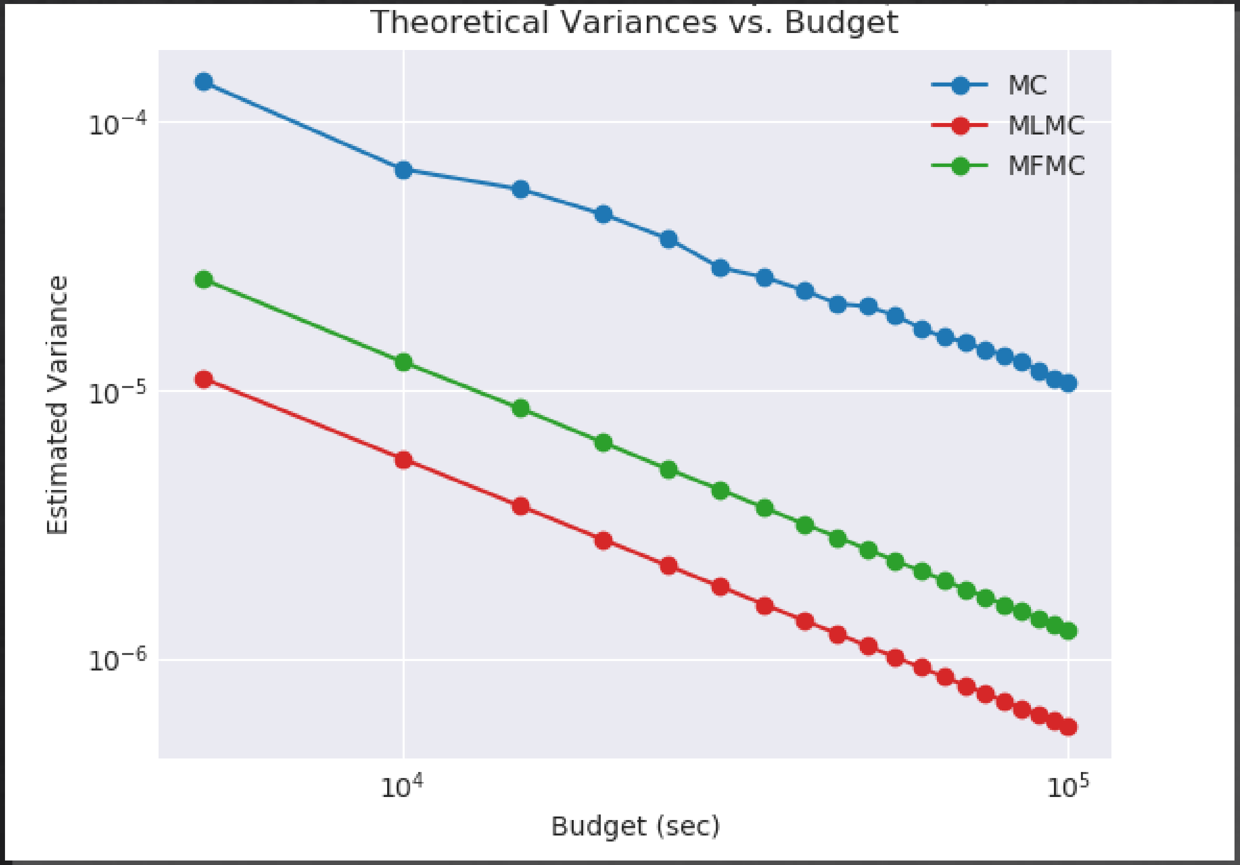

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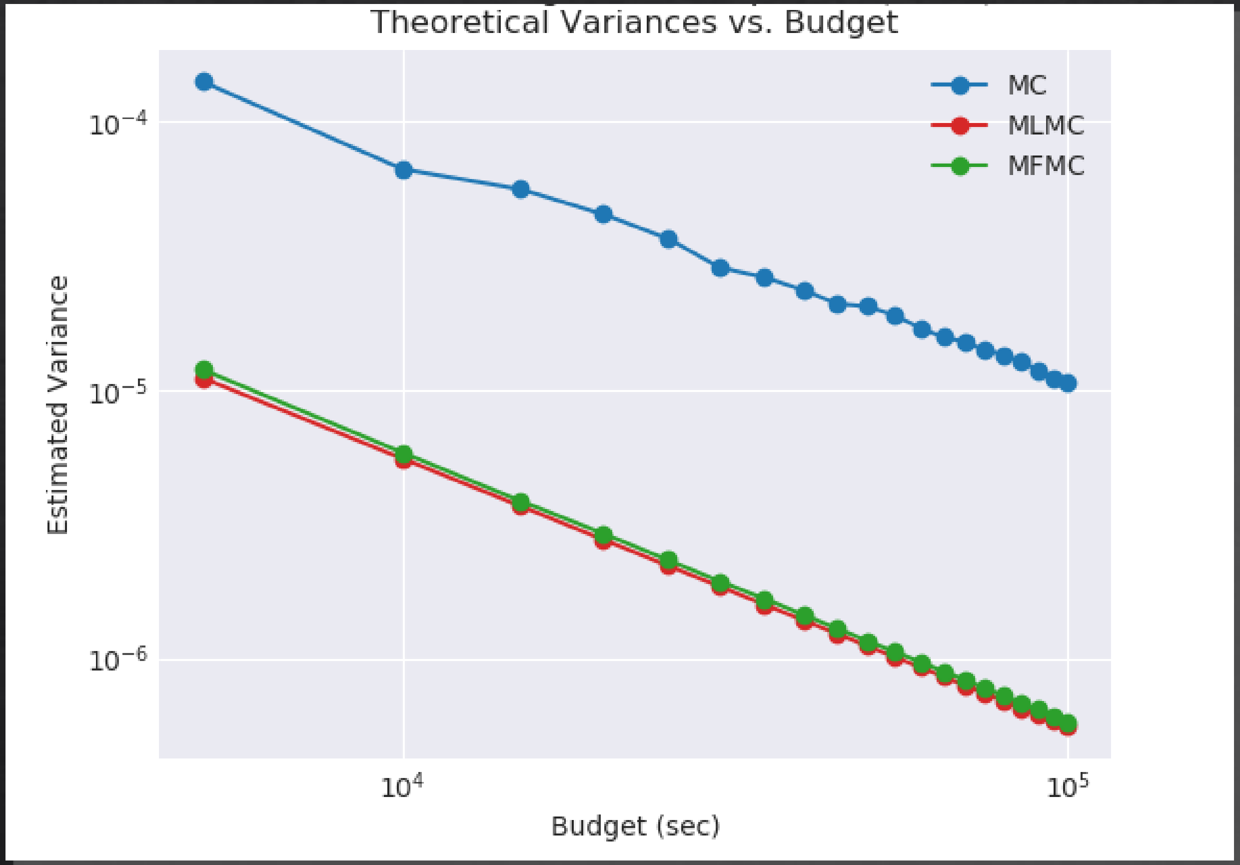

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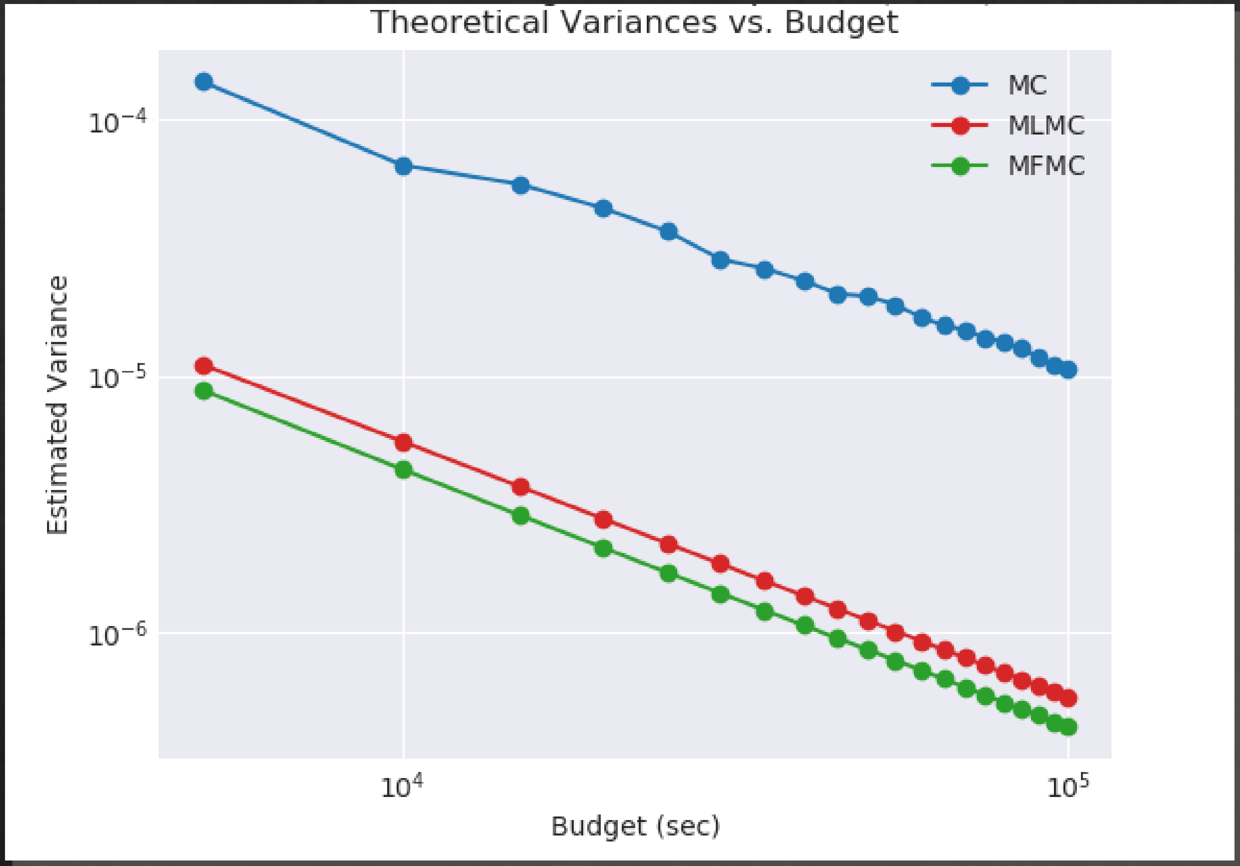

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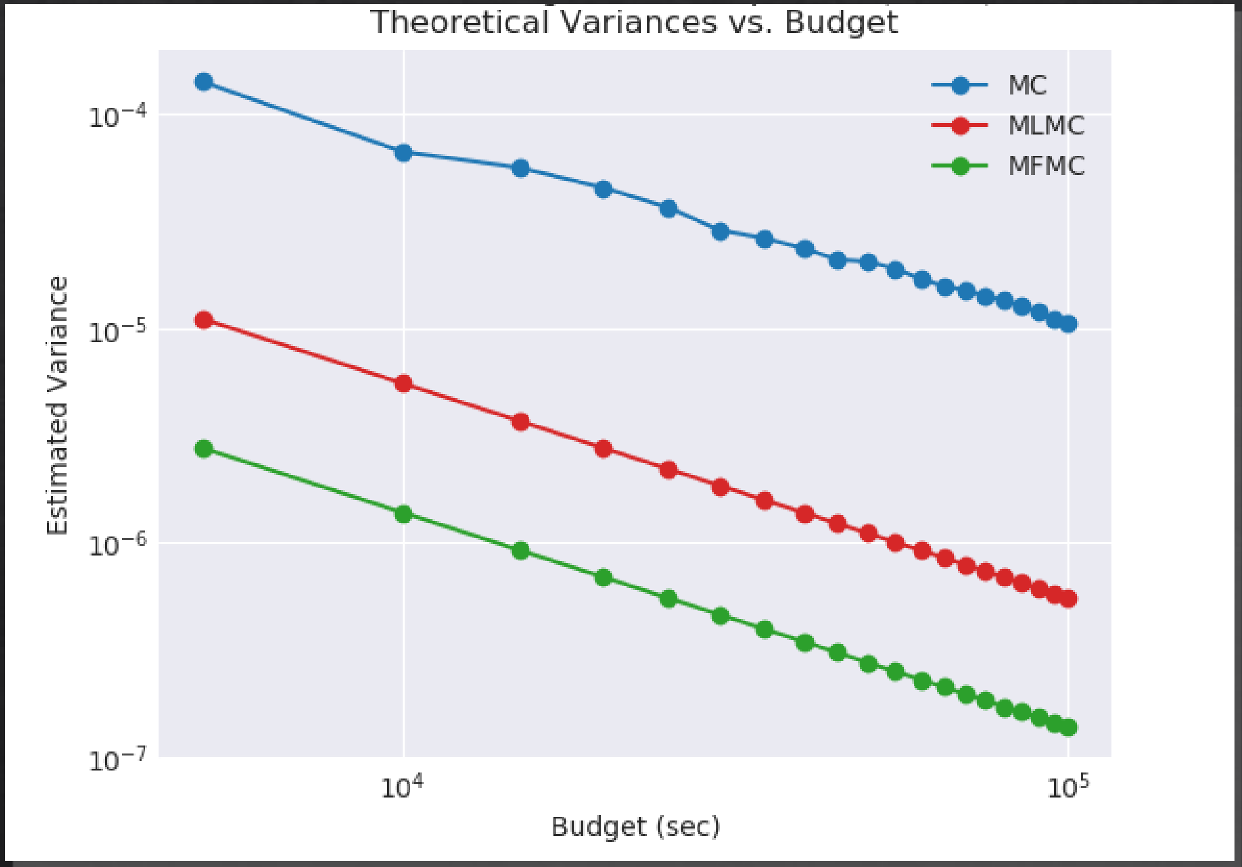
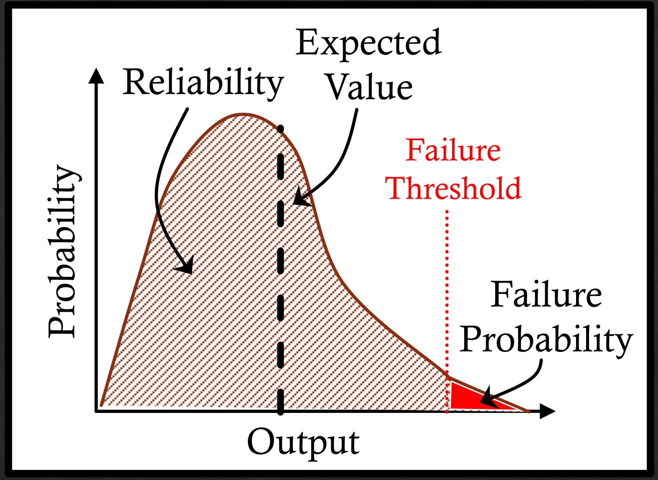
→ Combining all four models, we find roughly 4x improvement over MLMC



# Simulating Rare Events with Multifidelity UQ

- The multifidelity methods discussed so far have been aimed at estimators for the expected value of a model output

$$E[Y] \approx \frac{1}{N}\sum_{i=1}^{N} y^{(i)} \qquad y^{(i)} = \mathcal{M}(x^{(i)}) \qquad x^{(i)} \sim p(x)$$




- We are often interested in estimating the probability of rare events, e.g., failure probability:

$$P(y_{crit} \leq Y) \approx \frac{1}{N}\sum_{i=1}^{N} \mathbb{I}(y_{crit} \leq y^{(i)})$$

$y_{crit}$ : failure threshold

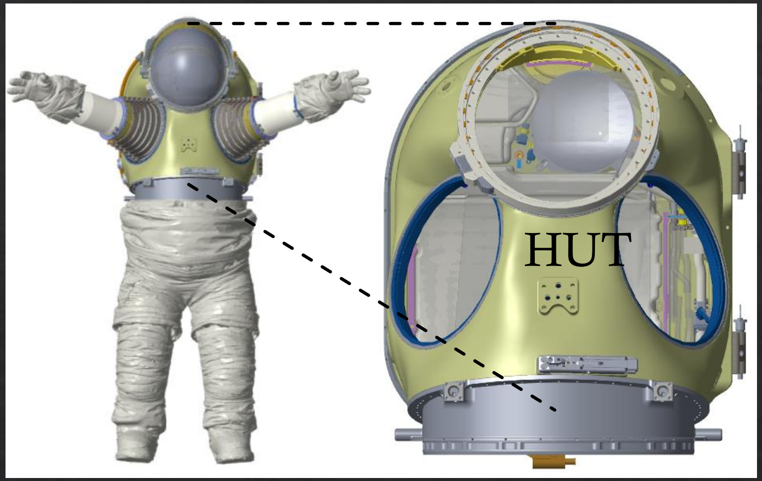
$$\mathbb{I}(A) = \begin{cases} 1, & \text{if A is true} \\ 0, & \text{otherwise} \end{cases}$$

$P(y_{crit} \geq Y)$ : reliability

- Estimating failure probability with Monte Carlo can be infeasible
  - Example:
    - If $P(y_{crit} \leq Y)$ = $10^{-3}$ , then N ≈ $10^5$ for a Monte Carlo estimate with 10% margin of error.

# Reliability Estimation at NASA

- NASA is designing a new space suit, the *Exploration Extravehicular Mobility Unit* (xEMU), for future lunar missions
- In order to certify the Hard Upper Torso (HUT) portion of the suit, we need to show that the design results in a probability of no impact failure (i.e. reliability) of 0.997 or better while supporting lunar surface activities
- **Sources of Uncertainty:**
  - **Impact loads** (lunar terrain/rock characteristics, fall risk profile, likely impact locations on suit, etc.)
  - **Structural model for suit impact** (material properties, modeling assumptions/discrepancies, etc.)
  - **Experimental uncertainties** (measurement errors)
- **Failure:** impact damage causes a leak rate in the suit above a critical value




xEMU Spacesuit

# Reliability Estimation at NASA

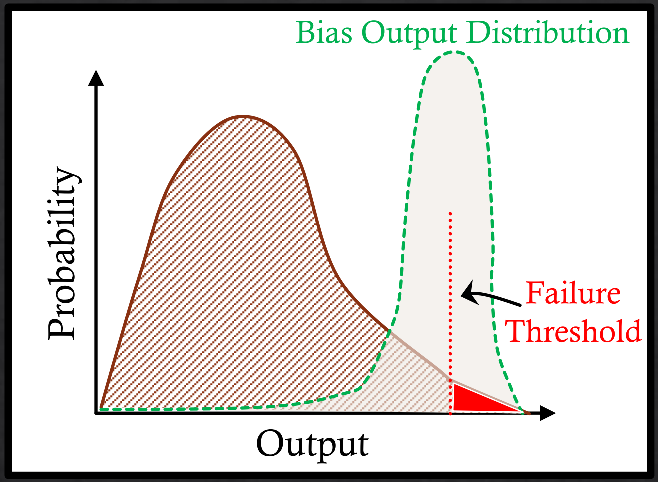
- *Frangible joints* are used to separate launch vehicle stages and payloads by detonating a controlled explosive
- The design of frangible joint must be strong enough to withstand normal launch and flight loads, yet weak enough to fracture when stage separation is required
- **Sources of Uncertainty:**
  - **Manufacturing variability** (FJ geometry parameters)
  - **Material variability** (Johnson-Cook plasticity model parameters)
  - **Environmental factors** (temperature, blast load parameters)

Frangible Joint Separation Mechanism

- **Failure:** the frangible joint does not cause separation upon charge detonation

# Importance Sampling (IS)

$$\alpha \equiv P(y_{crit} \leq Y) \approx \frac{1}{N}\sum_{i=1}^{N} \mathbb{I}(y_{crit} \leq y^{(i)}) \quad \begin{cases} y^{(i)} = \mathcal{M}(x^{(i)}) \\ x^{(i)} \sim p(x) \end{cases}$$




- **Original problem**: it can take a huge number of samples to yield enough failures to get an accurate failure probability estimate with Monte Carlo sampling
- **Solution:** Importance sampling

$$\hat{\alpha}_{IS} \approx \frac{1}{N}\sum_{i=1}^{N} \mathbb{I}(y_{crit} \leq y^{(i)}) \frac{p(x^{(i)})}{q(x^{(i)})} \qquad \text{where } x^{(i)} \sim q(x)$$

$q(x)$ : bias distribution

$w(x) \equiv \frac{p(x)}{q(x)}$ : importance weight

➢ Unbiased estimator for failure probability

- **New problem**: how do we construct a bias distribution for our inputs that results in a significantly higher percentage of failure outputs?

# Multifidelity Importance Sampling (MFIS)

- Use a low-fidelity model to construct a bias distribution then use a high-fidelity model to generate an *unbiased* importance sampling estimator for failure probability
- Procedure:
  1) Perform Monte Carlo simulation using the low-fidelity model to produce a collection of inputs that cause failure
  2) Construct bias distribution by fitting a Gaussian mixture model to the collection of failed inputs
  3) Draw samples from the bias distribution and evaluate the high-fidelity model
  4) Generate importance sampling estimator from high fidelity outputs and importance weights
- If the low-fidelity model is accurate *near the failure region*, MFIS can yield substantial computational speedup versus Monte Carlo simulation

# Example: Ishigami Function

- Contains three inputs, each independently uniformly distributed in $[-\boldsymbol{\pi}, \boldsymbol{\pi}]$
- High fidelity equation:

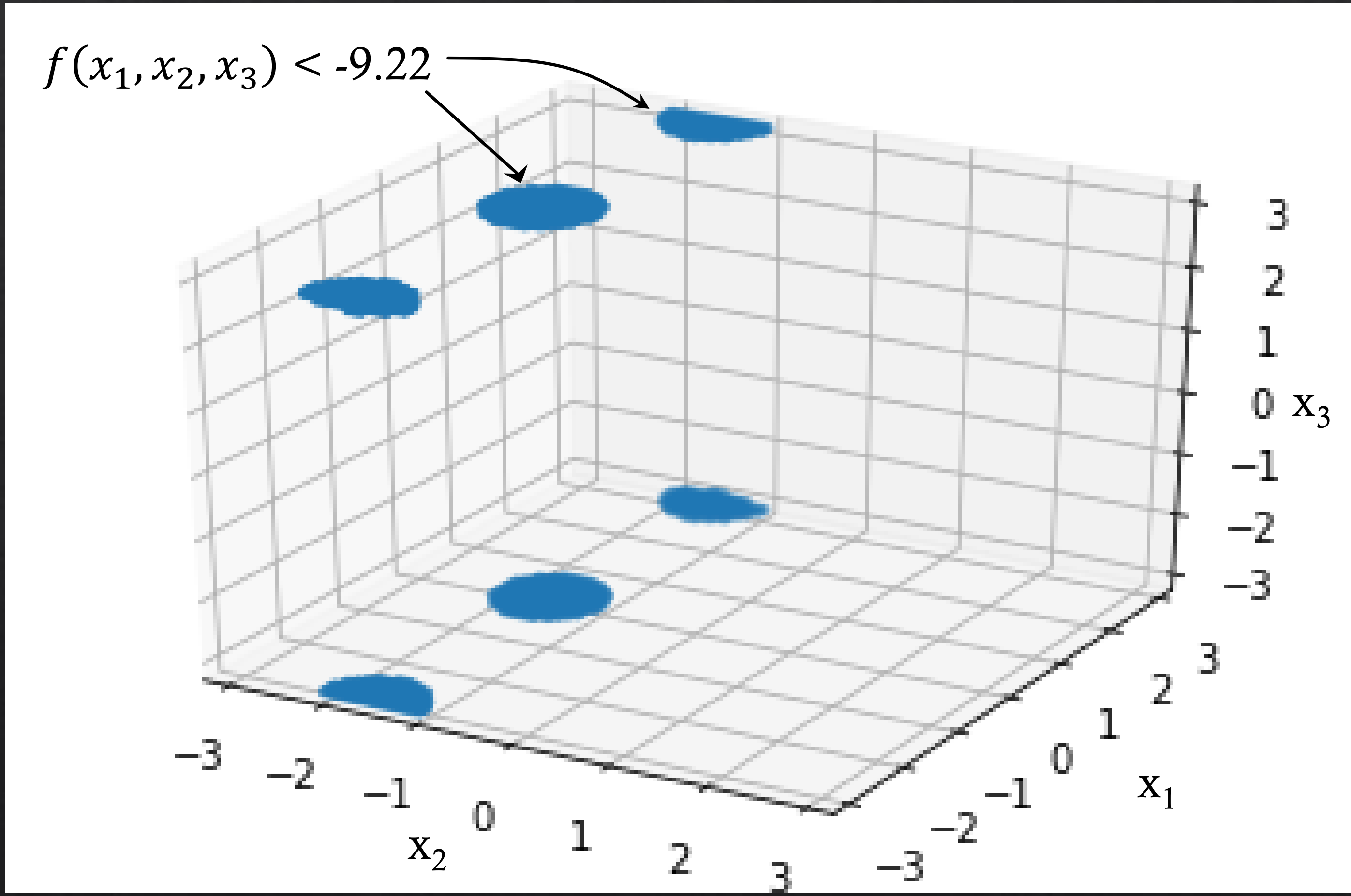
$$f(x_1, x_2, x_3) = \sin(x_1) + 5\sin^2(x_2) + 0.1x_2^4 \sin(x_1)$$

- Low-fidelity equation:

$$\bar{f}(x_1, x_2, x_3) = \sin(x_1) + 3\sin^2(x_2) + 0.9x_2^2 \sin(x_1)$$

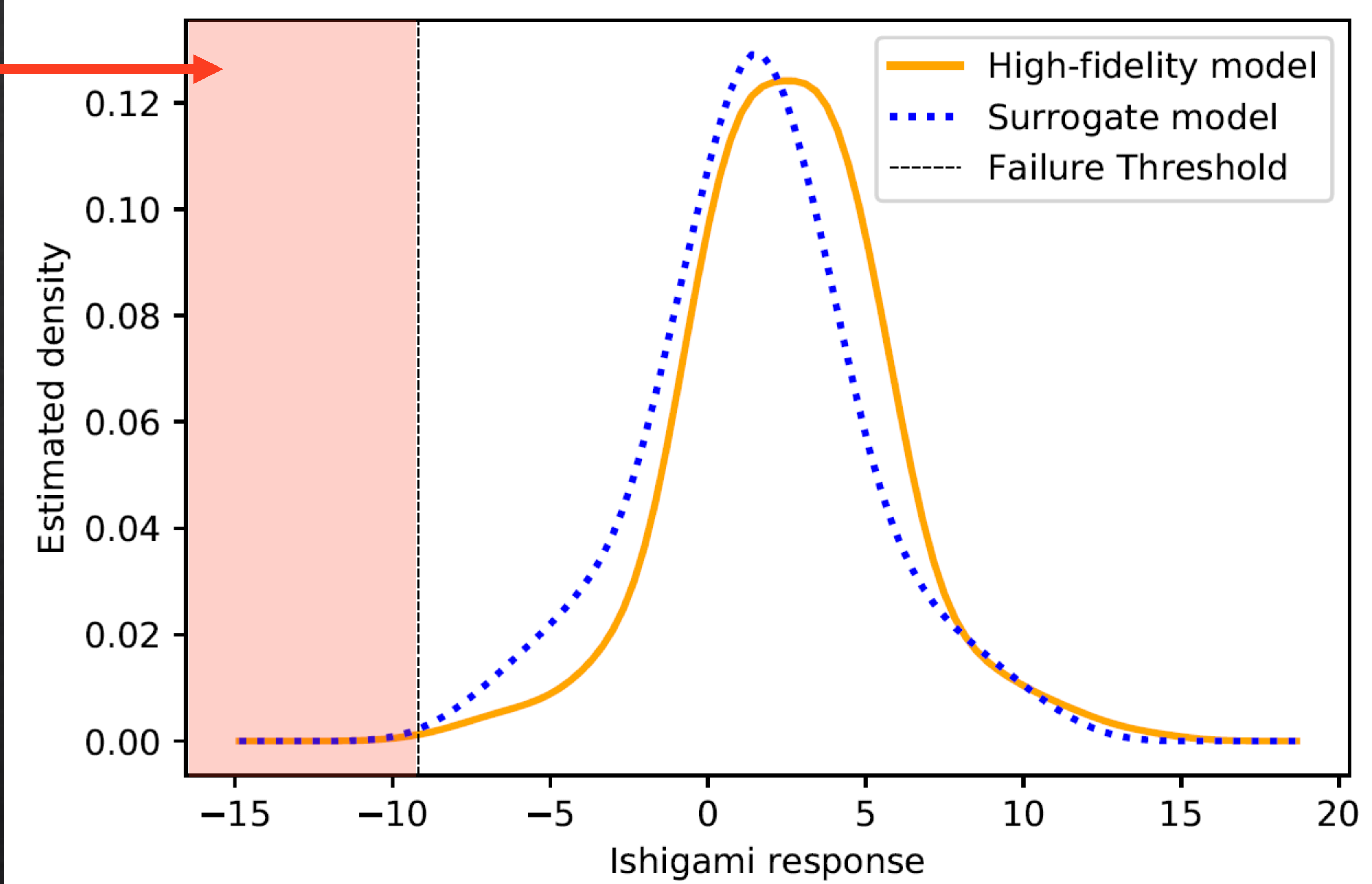
- Failure threshold set at **-9.22**, producing a failure probability of **1e-3**

# Failure Regions in the Input Space



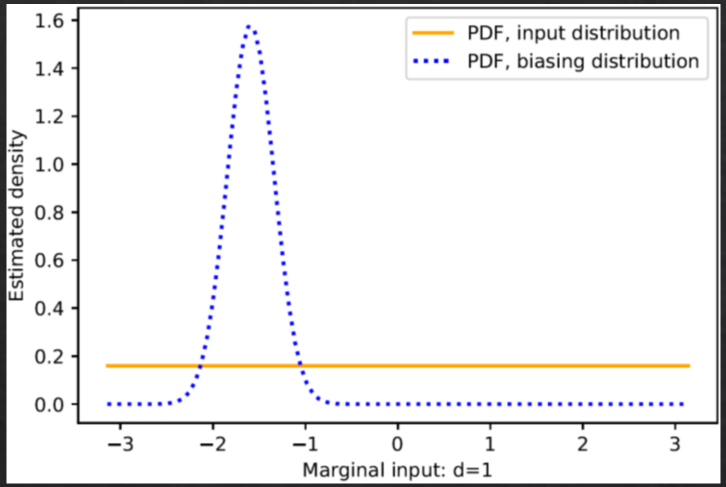
# Failure Region in the Output Space

Failure region

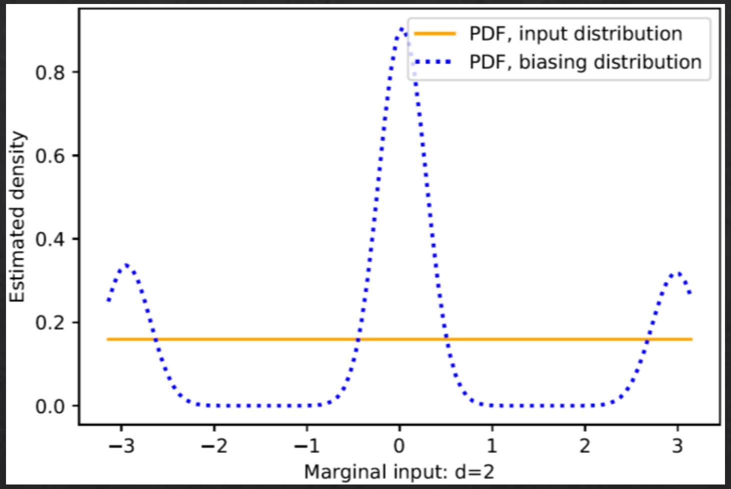


# Bias Distributions

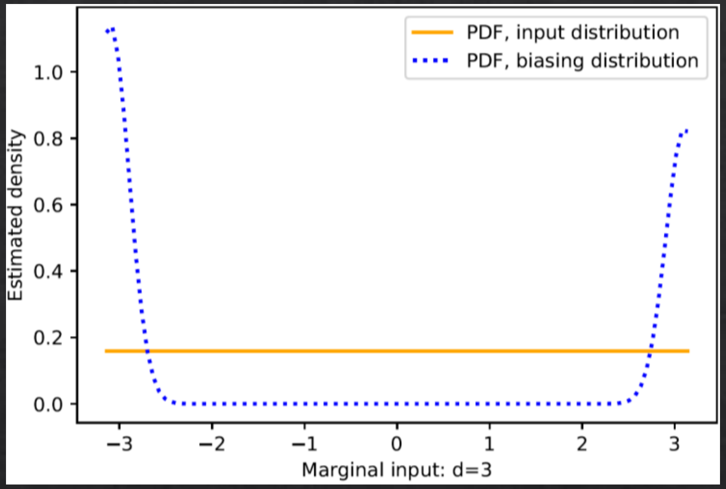
Input Parameter 1




Input Parameter 2

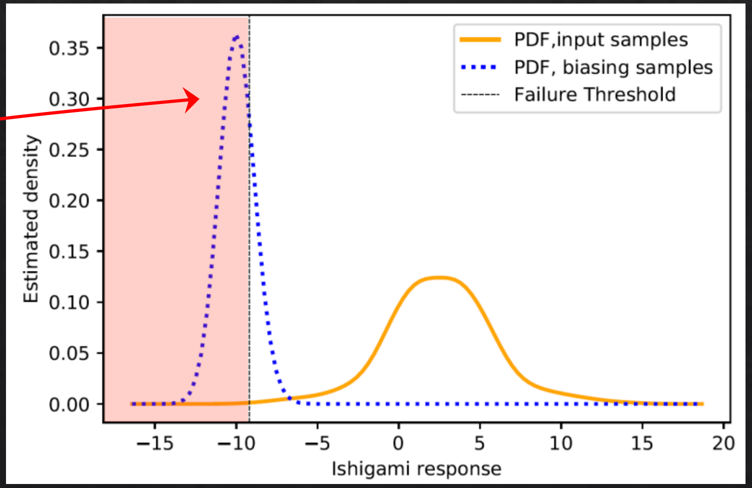



Input Parameter 3



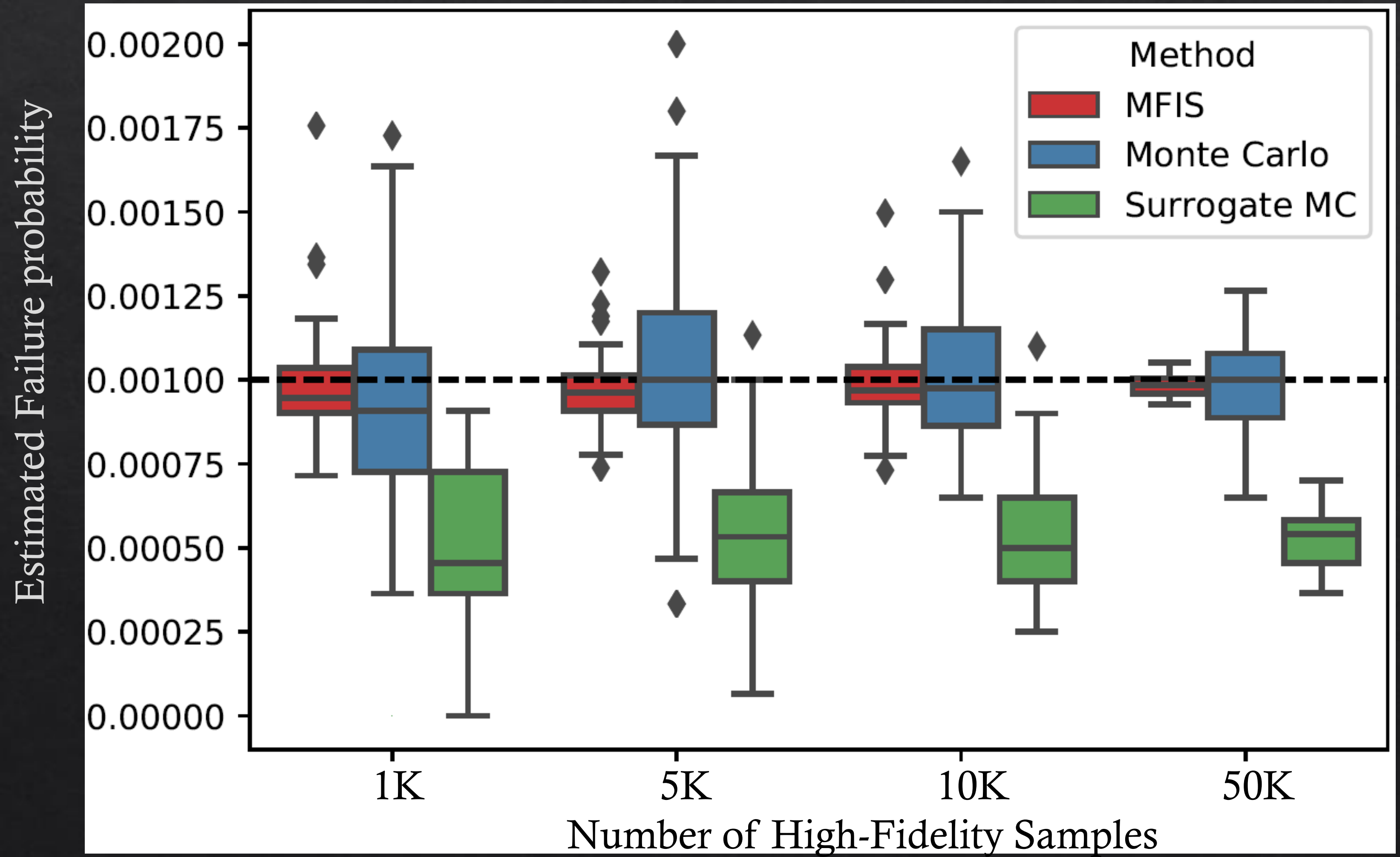

Output Distributions

Bias distribution leads to significantly higher rate of failures



# Estimation of Failure Probability Results

over 50 repetitions




If each simulation run took 2.5 minutes…

| # of High Fidelity Samples | Total Runtime |
|---|---|
| 1,000 | ≈42 hours |
| 5,000 | ≈8.7 days |
| 10,000 | ≈2.5 weeks |
| 50,000 | ≈3 months |

# Conclusion

- Multifidelity Monte Carlo methods combine predictions from high-fidelity models with low-fidelity models to yield fast, unbiased estimators for UQ
- NASA is actively researching new multifidelity UQ methods and their application to a range of pertinent problems including trajectory simulation for EDL and estimating reliability of space systems like the xEMU spacesuit and frangible joints
- We are actively recruiting/hiring student interns!
  - Email us: Geoffrey.f.bomarito@nasa.gov, james.e.warner@nasa.gov
  - View NASA-wide project listings at: https://intern.nasa.gov/
- Relevant software:
  - Multi-model Monte Carlo with Python: https://github.com/nasa/mxmcpy