Multi-Model Monte Carlo Estimators for Trajectory Simulation

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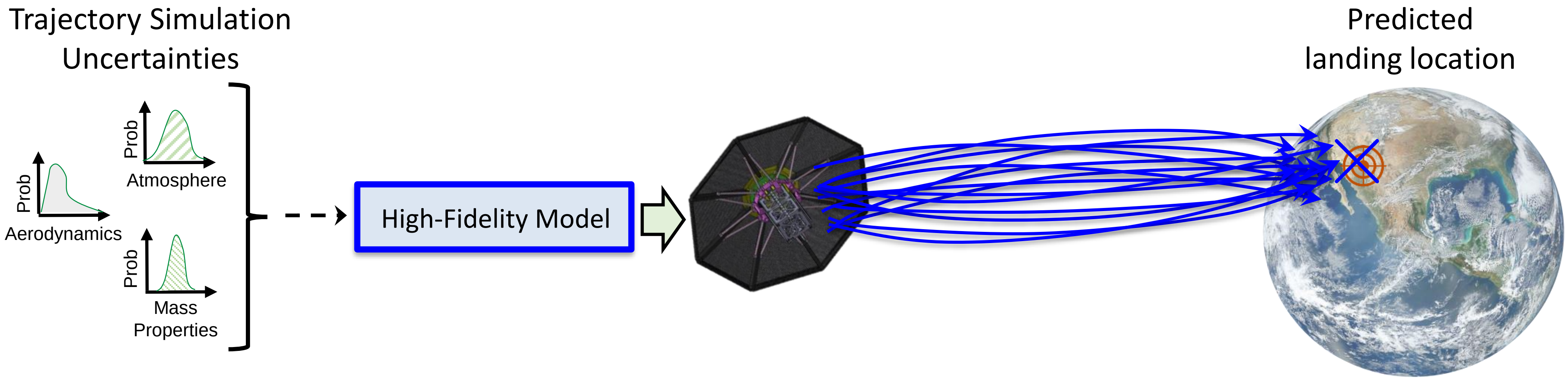
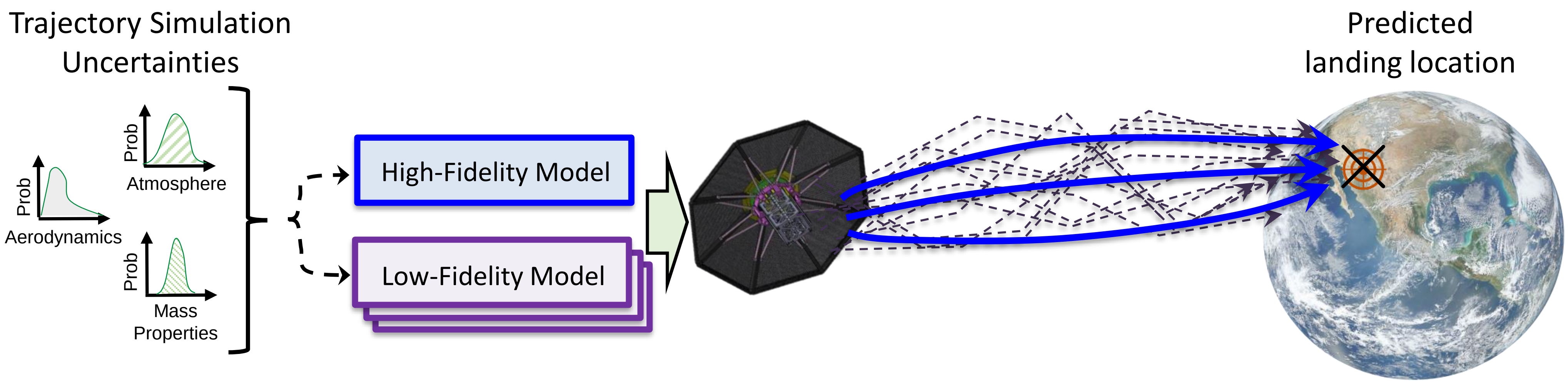
Motivation

- Significant advances in EDL capabilities are required to support NASA's aspirations for human class Mars Missions
  - Orders-of-magnitude improvement in trajectory simulation precision needed
- Current state-of-the-art uses Monte Carlo (MC) to simulate thousands or even millions of potential trajectories to account for uncertainty



Motivation

- Significant advances in EDL capabilities are required to support NASA's aspirations for human class Mars Missions
  - Orders-of-magnitude improvement in trajectory simulation precision needed
- Current state-of-the-art uses Monte Carlo (MC) to simulate thousands or even millions of potential trajectories to account for uncertainty
- This work explores emerging *multi-model MC* approaches for more efficient & accurate uncertainty quantification for trajectory simulation

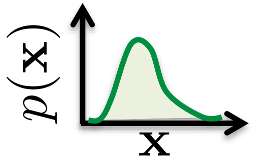


High-Fidelity Monte Carlo Simulation

Problem: estimate the expected value $\mathbb{E}[Y_0]$

Input Parameters

$\mathbf{X} \in \mathbb{R}^d$



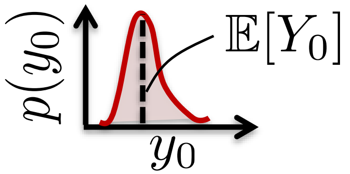
High-Fidelity Model

$\boxed{\mathcal{M}_0 : \mathbf{X} \rightarrow Y_0}$

Cost: C_0

Quantity of Interest (QoI)

$Y_0 \in \mathbb{R}$



Expected Value Estimator: $\mathbb{E}[Y_0] \approx \hat{Y}_0 = \frac{1}{N_0} \sum_{i=1}^{N_0} Y_0(\mathbf{x}^{(i)})$ where $\mathbf{x}^{(i)} \sim p(\mathbf{x})$, N_0 : # samples

Total Estimator Cost: $\boxed{\hat{C} = N_0 C_0}$

Mean Squared Error (MSE): $e(\hat{Y}_0) \equiv \mathbb{E}[(\hat{Y}_0 - \mathbb{E}[Y_0])^2] = (\mathrm{Bias}[\hat{Y}_0])^2 + \mathrm{Var}[\hat{Y}_0]$

$\boxed{\circ \ \mathrm{Bias}[\hat{Y}_0] = 0}$ $\boxed{\circ \ \mathrm{Var}[\hat{Y}_0] = \frac{\mathrm{Var}[Y_0]}{N_0}}$

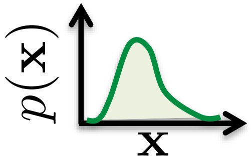
- **Unbiased estimator** provides convergence guarantee ($\mathbb{E}[\hat{Y}_0] = \mathbb{E}[Y_0]$)
- The convergence rate $O(N_0^{-1})$ is **slow**; prohibitive for expensive, high-fidelity models

Low-Fidelity Monte Carlo Simulation

Problem: estimate the expected value $\mathbb{E}[Y_0]$

Input Parameters

$\mathbf{X} \in \mathbb{R}^d$



Low-Fidelity Model

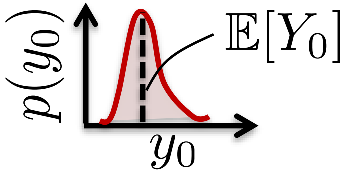
$\boxed{\mathcal{M}_1 : \mathbf{X} \rightarrow Y_1}$

Cost: $C_1 << C_0$

$Y_1 \approx Y_0$

Quantity of Interest (QoI)

$Y_0 \in \mathbb{R}$



Expected Value Estimator: $\mathbb{E}[Y_0] \approx \hat{Y}_1 = \frac{1}{N_1} \sum_{i=1}^{N_1} Y_1(\mathbf{x}^{(i)})$ where $\mathbf{x}^{(i)} \sim p(\mathbf{x})$, N_1 : # samples

Total Estimator Cost: $\boxed{\hat{C} = N_1 C_1}$

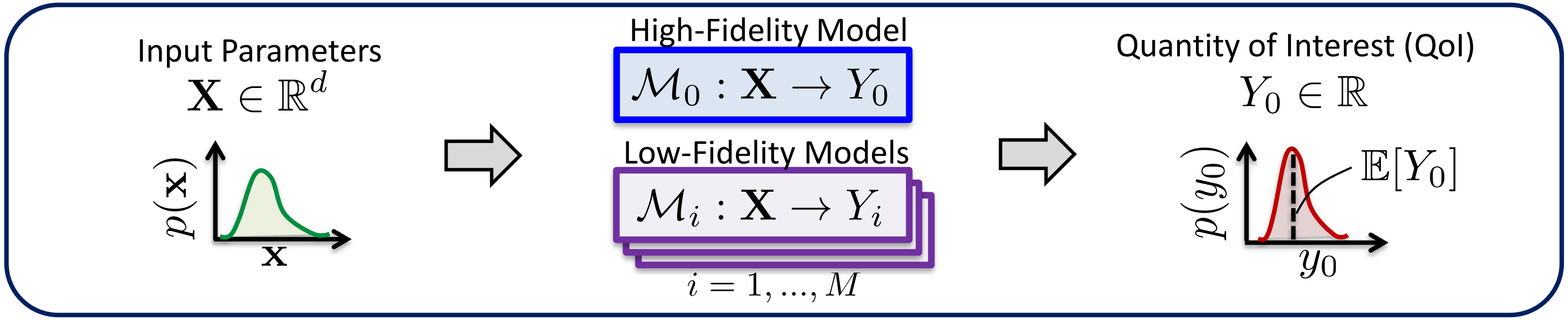
Mean Squared Error (MSE): $e(\hat{Y}_1) \equiv \mathbb{E}[(\hat{Y}_1 - \mathbb{E}[Y_0])^2] = (\mathrm{Bias}[\hat{Y}_1])^2 + \mathrm{Var}[\hat{Y}_1]$

$\boxed{\circ \ \mathrm{Bias}[\hat{Y}_1] \neq 0}$ $\boxed{\circ \ \mathrm{Var}[\hat{Y}_1] = \frac{\mathrm{Var}[Y_1]}{N_1}}$

- **Computationally efficient** variance reduction ($N_1 >> N_0$)
- **Irreducible error** from estimator bias ($\mathbb{E}[\hat{Y}_1] \neq \mathbb{E}[Y_0]$)

Multi-Model Monte Carlo Simulation

Problem: estimate the expected value $\mathbb{E}[Y_0]$



Expected Value Estimator: $\mathbb{E}[Y_0] \approx \tilde{Y}_0(\boldsymbol{\alpha}, \{\mathbf{x}\}) = \hat{Y}_0(\mathbf{x}_0) + \sum_{i=1}^{M} \alpha_i(\hat{Y}_i(\mathbf{x}_{i+}) - \hat{Y}_i(\mathbf{x}_{i-}))$ (Linear combination of MC estimators)

Total Estimator Cost: $\boxed{\tilde{C} = N_0 C_0 + \sum_{i=1}^{M} N_i C_i}$

Mean Squared Error (MSE): $e(\tilde{Y}_0) \equiv \mathbb{E}[(\tilde{Y}_0 - \mathbb{E}[Y_0])^2] = (\mathrm{Bias}[\tilde{Y}_0])^2 + \mathrm{Var}[\tilde{Y}_0]$

$\boxed{\circ\ \mathrm{Bias}[\tilde{Y}_0] = 0}$ $\boxed{\circ\ \mathrm{Var}[\tilde{Y}_0] << \mathrm{Var}[\hat{Y}_0]}$

- **Unbiased** estimator provides convergence guarantee
- More **efficient** variance reduction versus standard MC

Multi-model MC combines strengths of high- & low-fidelity MC

Optimal Sample Allocation

Expected Value Estimator: $\tilde{Y}_0(\boldsymbol{\alpha}, \{\mathbf{x}\}) = \hat{Y}_0(\mathbf{x}_0) + \sum_{i=1}^{M} \alpha_i (\hat{Y}_i(\mathbf{x}_{i+}) - \hat{Y}_i(\mathbf{x}_{i-}))$

Goal: Select $\boldsymbol{\alpha}$ and $\{\mathbf{x}\} \equiv \{\mathbf{x}_0, \mathbf{x}_{1+}, \mathbf{x}_{1-}, ..., \mathbf{x}_{M+}, \mathbf{x}_{M-}\}$ to yield the most accurate estimator for total cost C^*

$$\boxed{\begin{gathered}\boldsymbol{\alpha}^{opt}, \{\mathbf{x}\}^{opt} = \min_{\boldsymbol{\alpha}, \{\mathbf{x}\}} \mathrm{Var}[\tilde{Y}_0(\boldsymbol{\alpha}, \{\mathbf{x}\})] \\ \text{s.t. } \tilde{C} \leq C^*\end{gathered}}$$

- The optimization solution depends on the cost of each model and the covariance between their predictions
  - ***Fast low-fidelity models that are highly correlated with high fidelity model are more beneficial***
- The approach can handle vector-valued QoIs by minimizing the total sum of QoI variances
- Several multi-model MC methods have been developed that differ on the strategy used for solving the optimization problem [1-4]

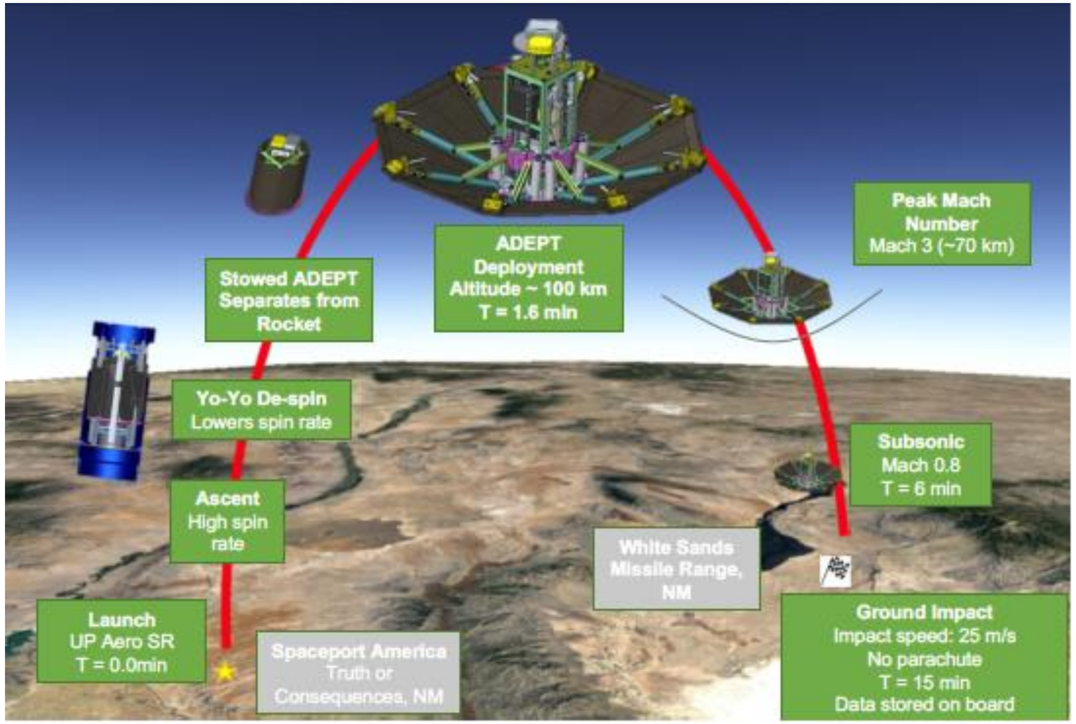
[1] Multilevel Monte Carlo (MLMC). Giles, 2008.
[2] Multifidelity Monte Carlo (MFMC). Peherstorfer, 2016.
[3] Approximate Control Variates (ACV). Gorodetsky, 2020.
[4] Parametrically-defined ACV. Bomarito, 2020.

Multi-Model Monte Carlo with Python (MXMCPy)
https://github.com/nasa/mxmcpy

Application

Analysis of the Adaptable Deployable Entry & Placement Technology (ADEPT) Sounding Rocket 1 (SR-1) test flight

ADEPT SR-1 Test Flight Schematic [5]



Trajectory QoIs Considered

Abbreviation	Description
lat-td	Geodetic latitude at touchdown
long-td	Longitude at touchdown
rllrt-80km	Roll rate at 80km geodetic altitude
rllrt-60km	Roll rate at 60km geodetic altitude
alt-apo	Apoapsis altitude
alt-mach1	Altitude at Mach 1
alt-deploy	ADEPT deploy altitude
time-td	Touchdown time
vel-term	Terminal velocity
accel-max	Max acceleration (Earth g's)
aoa-2km	Total angle of attack at 2km geodetic altitude
aoa-10km	Total angle of attack at 10km geodetic altitude
aoa-35km	Total angle of attack at 35km geodetic altitude
aoa-60km	Total angle of attack at 60km geodetic altitude
aoa-80km	Total angle of attack at 80km geodetic altitude

- Program to Optimize Simulated Trajectories II (POST2) was used to model the flight trajectory
- The accuracy of multi-model MC QoI estimates was quantified versus both high- and low-fidelity MC

[5] Dutta et al. AIAA Aviation 2019 Forum

Trajectory Simulation Models

High-fidelity model:

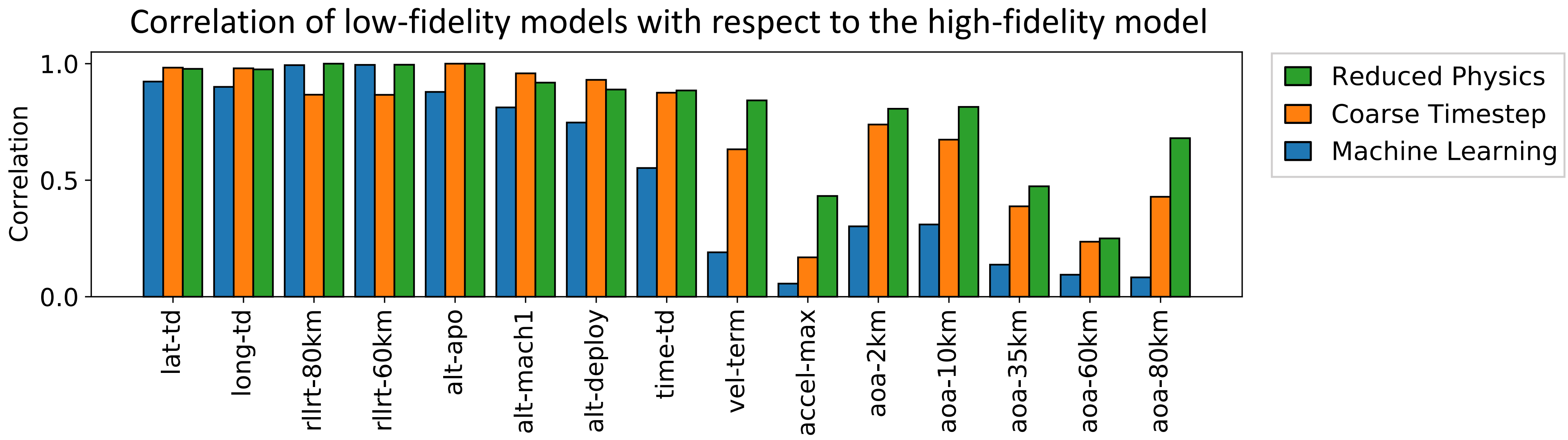
- POST2 with time step $\Delta t = 10^{-3}$ sec

Low-fidelity models:

1. Reduced physics: POST2 with simplified atmosphere model
2. Coarse time step: POST2 with $\Delta t = 10^{-1}$ sec
3. Machine learning: Support vector machine (SVM) regression trained with input/output data from 250 POST2 simulations

Trajectory Simulation Model Run Times

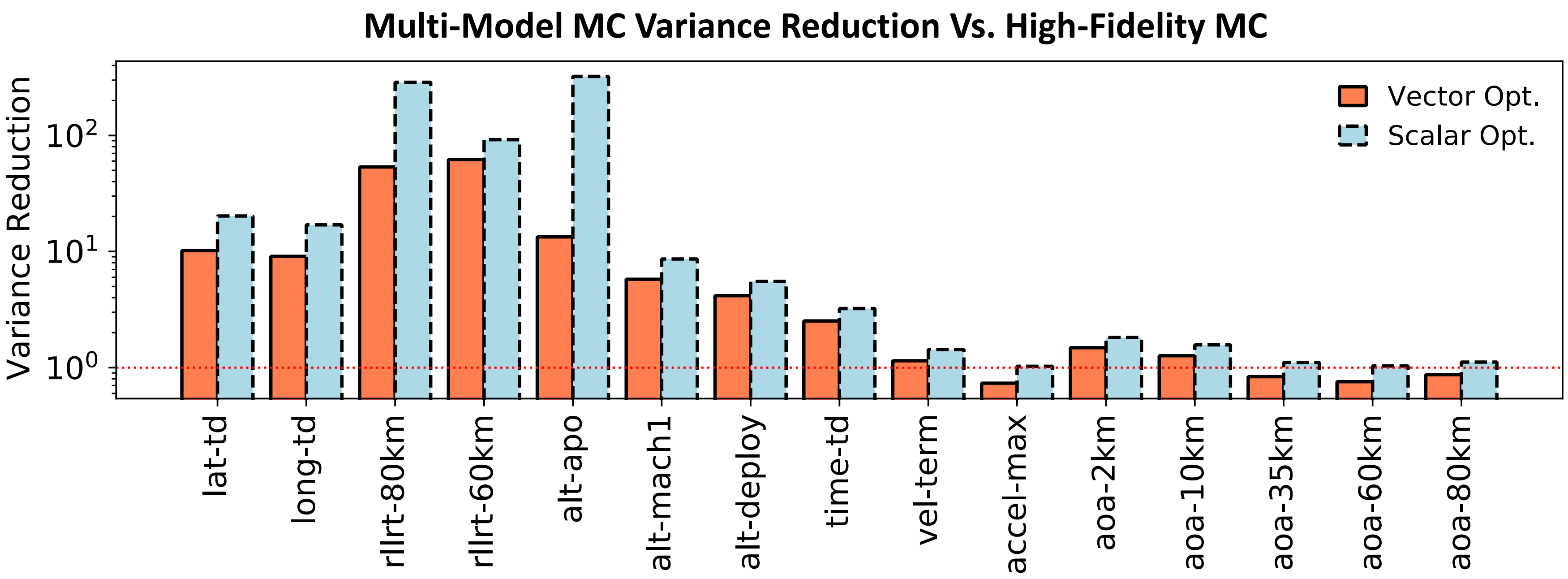
Model	Run Time (sec)	Speedup (X)
High Fidelity	2.2×10^{2}	1.0×10^{0}
Reduced Physics	4.7×10^{1}	4.6×10^{0}
Coarse Time Step	2.8×10^{0}	7.8×10^{1}
Machine Learning	7.0×10^{-4}	3.1×10^{5}



Estimator Variance Comparison

For a computational budget of 10^4 seconds, the sample allocation optimization was solved for two cases

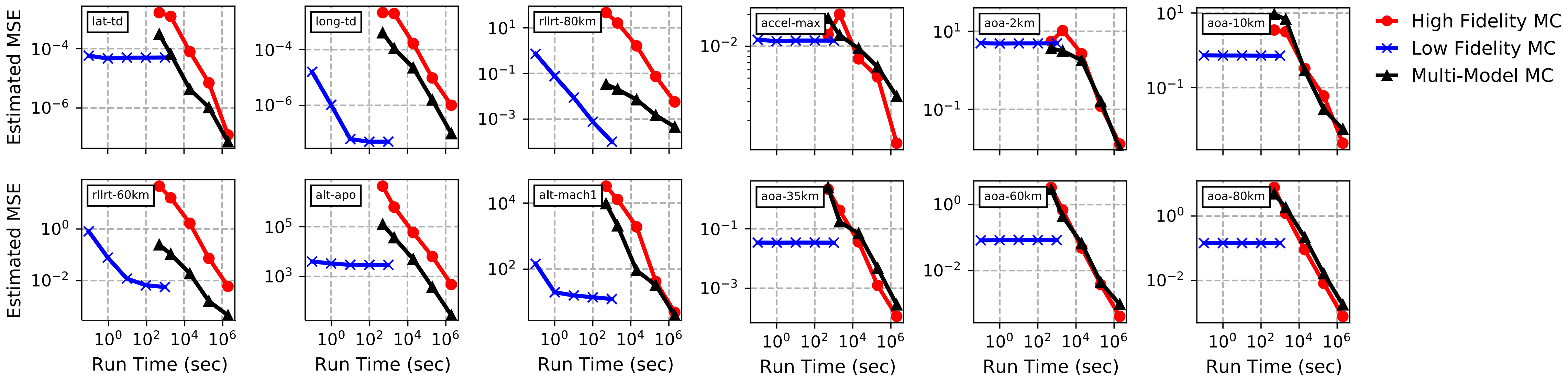
- **Vector Opt.:** minimizes variance for all QoIs simultaneously
- **Scalar Opt.:** minimizes variance for each QoI individually



Estimator Accuracy Vs. Run Time

- The MSE was calculated for high-, low-, and multi-model MC estimators versus a reference solution using high-fidelity MC with 100,000 samples

MSE versus Run Time for Several Trajectory QoIs



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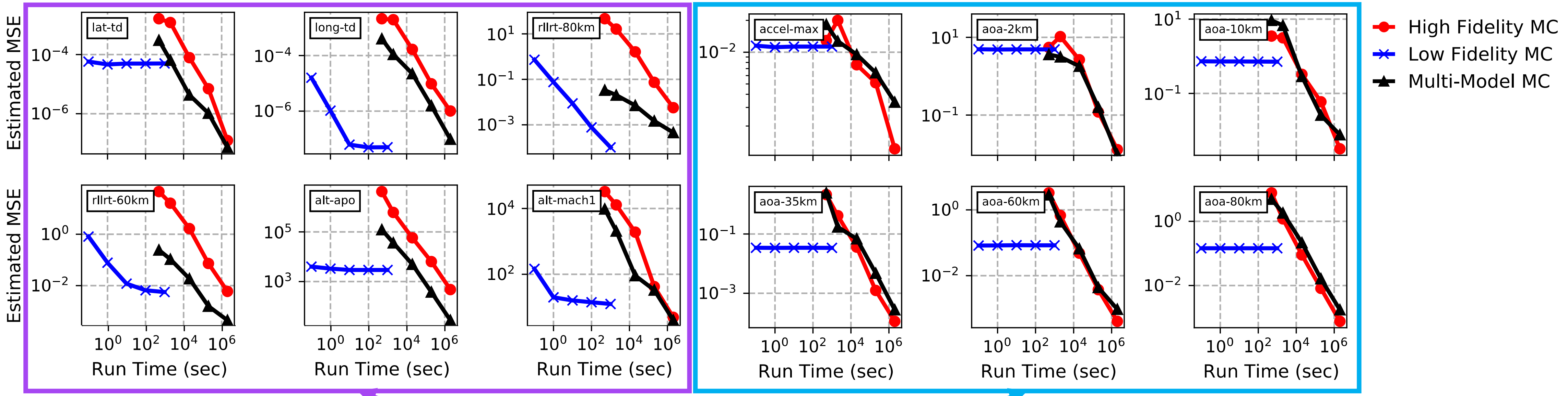
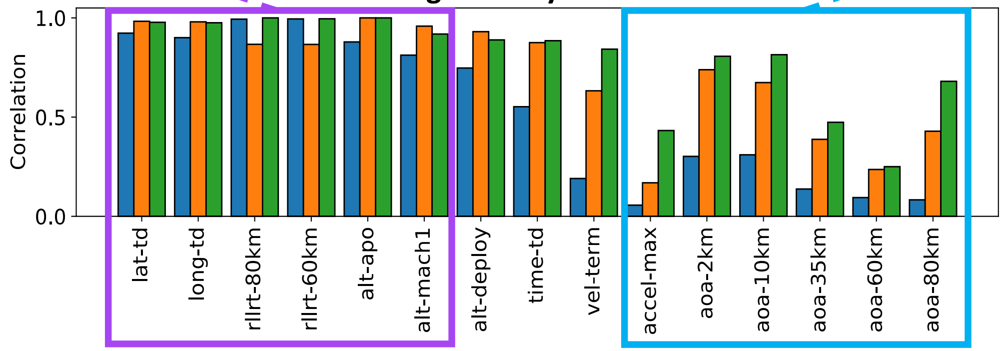
MSE versus Run Time for Several Trajectory QoIs



Low-to-high fidelity model correlation



Higher correlations yield large accuracy improvement relative to high-fidelity MC

Lower correlations yield accuracy comparable to high-fidelity MC

Conclusions & Future Work

- Established a proof of concept for performing trajectory simulation using a multi-model MC approach as an alternative to standard MC that relies exclusively on a high- *or* low- fidelity model
- Demonstrated the potential to deliver up to two orders of magnitude accuracy improvement, while in the worst case the accuracy is only comparable to high-fidelity MC
- **Future Work:**
  - Develop low-fidelity models that have higher correlation with respect to the high-fidelity model for dynamic trajectory QoIs
  - Extend the multi-model MC approach to predict more advanced statistical quantities (probability distributions, rare event probabilities, landing ellipses, etc.)

References

[1] Giles, M. B., “Multilevel Monte Carlo path simulation,” *Operations Research*, Vol. 56, No. 3, 2008

[2] Peherstorfer, B., Willcox, K. , and Gunzburger, M., “Optimal model management for multifidelity Monte Carlo estimation,” SIAM Journal on Scientific Computing, Vol. 38, 2016.

[3] Gorodetsky, A., Geraci, G. , Eldred, M., and Jakeman, J. D., “A generalized approximate control variate framework for multifidelity uncertainty quantification,” Journal of Computational Physics, Vol. 408, 2020.

[4] Bomarito, G. F., Leser, P. E., Warner, J. E., and Leser, W. P., “On the optimization of approximate control variates with parametrically defined estimators,” In Preparation, 2020.

[5] Dutta, S., and Green, J. S., “Flight mechanics modeling and post-flight analysis of ADEPT SR-1,” AIAA Aviation 2019 Forum, AIAA, Dallas, TX, 2019.

Software:

- POST2: https://post2.larc.nasa.gov/
- MXMCPy: https://github.com/nasa/mxmcpy