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Automating Model Selection and Tuning for Multifidelity UQ (MFUQ)

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MS77: Advanced Multilevel and Multifidelity UQ Strategies: Applications, Generalized Model Hierarchies, and Data-Driven Approaches
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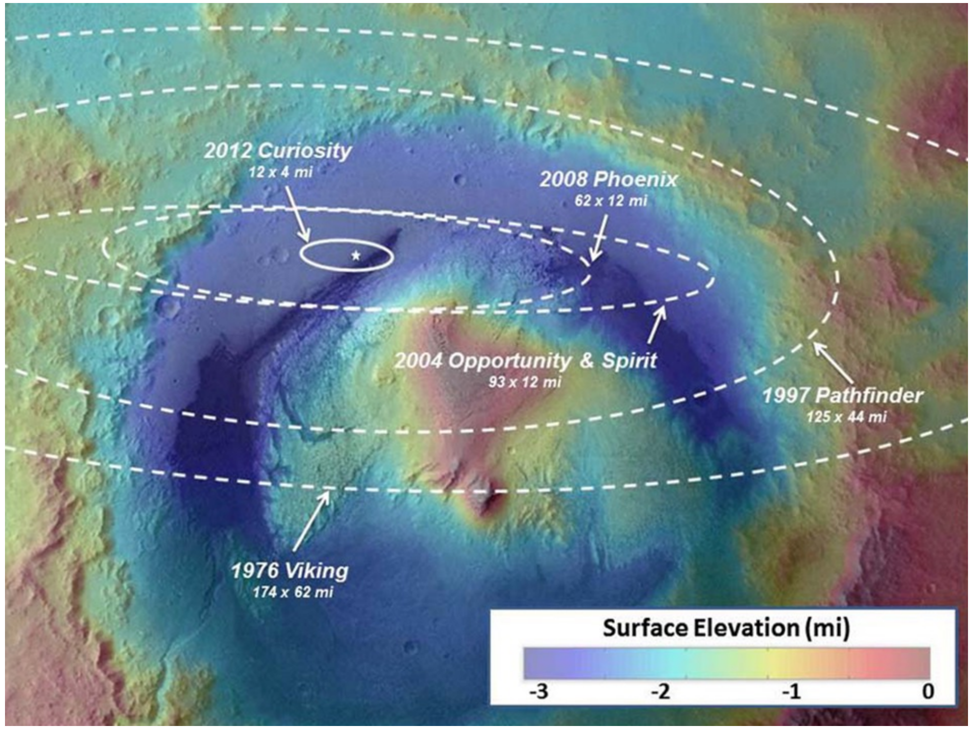
Motivation: Trajectory Guidance

- Orders of magnitude improvement in landing precision required to enable human Mars missions
  - **Long-term goal**: robust trajectory optimization under uncertainty

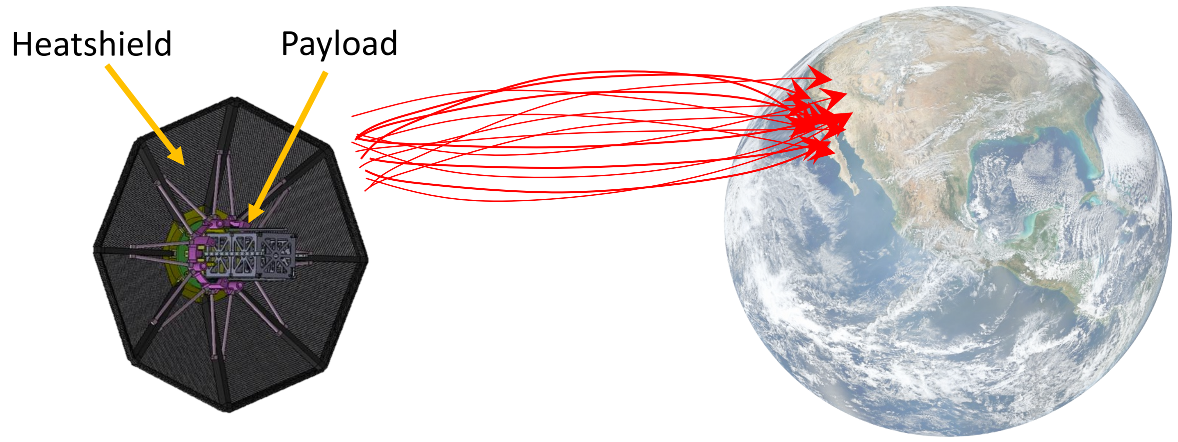


Mars landing precision over time

Motivation: Trajectory Guidance

- **Current focus:** uncertainty propagation for high-fidelity trajectory simulation
  - High dimensional inputs – e.g., atmosphere conditions, vehicle state
  - Multiple quantities of interest (QoIs) – e.g., landing location, flight time
  - Model: Program to Optimize Simulated Trajectories II (POST2)

Monte Carlo (MC) simulation



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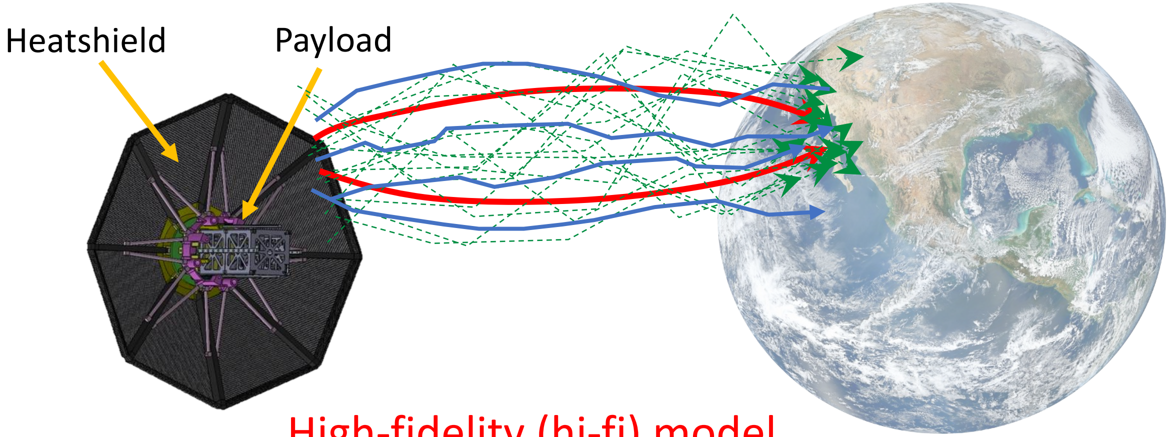
MFUQ



High-fidelity (hi-fi) model
Medium-fidelity (med-fi) model
Low-fidelity (lo-fi) model

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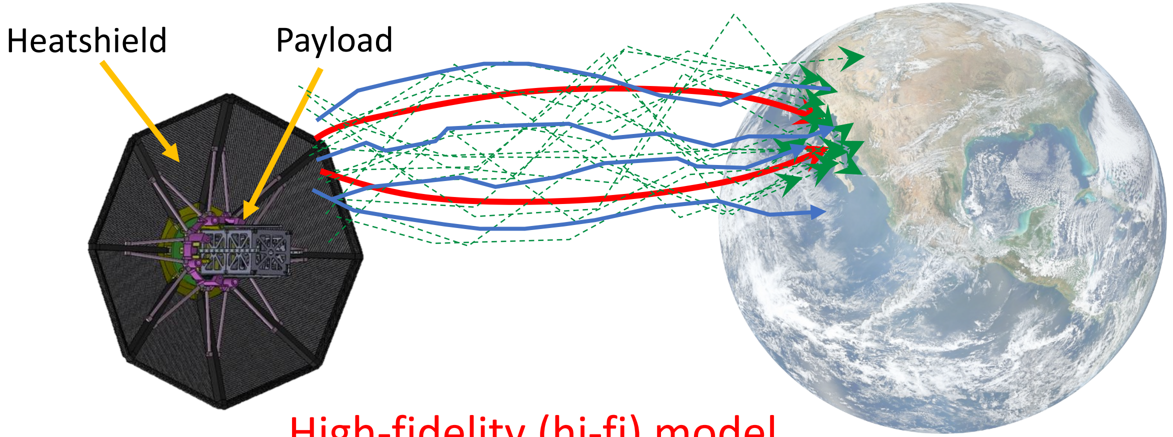
MFUQ

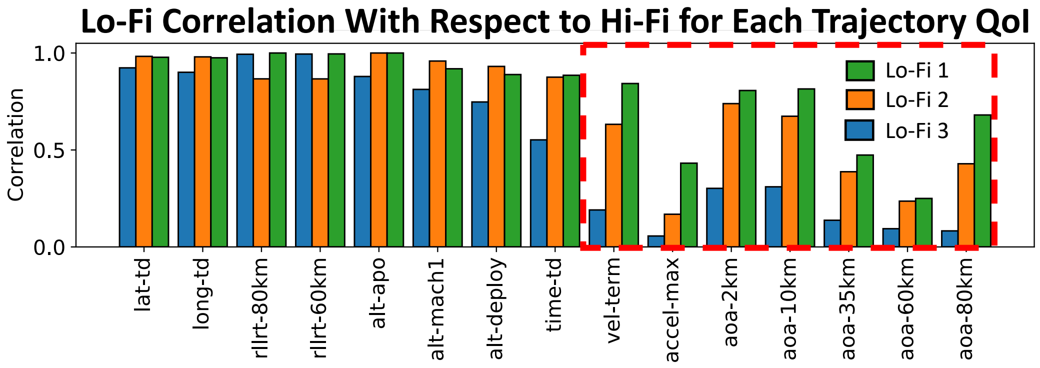


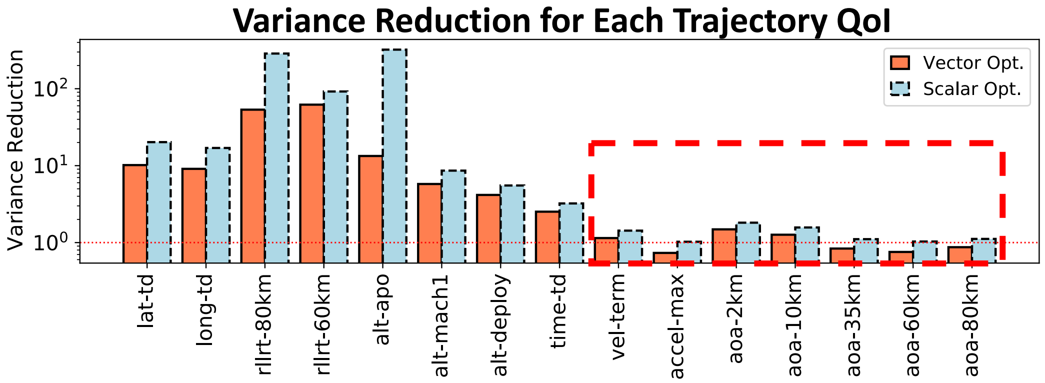
High-fidelity (hi-fi) model

Medium-fidelity (med-fi) model

Low-fidelity (lo-fi) model

AIAA SciTech 2021[1]:



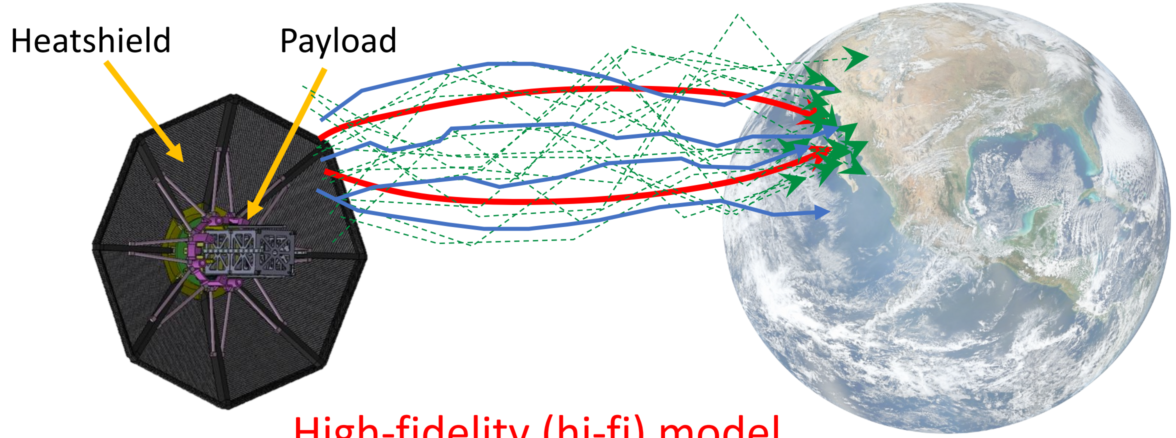


➢ **Sub-optimal lo-fi models = sub-optimal MFUQ**

[1] J. E. Warner et al. AIAA SciTech 2021.

Outline: Model Tuning for MFUQ

- Model tuning is important
- How we can do it optimally (In Progress)
- Application to trajectory simulation
  - Optimal time step selection for lo-fi models



High-fidelity (hi-fi) model
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Approximate Control Variates (ACV)[1]

$$\tilde{Q} = \hat{Q}(z) + \sum_{i=1}^{M} \alpha_i \left(\hat{Q}_i(z_i^1) - \hat{Q}_i(z_i^2) \right)$$

$Q:$ hi-fi model
Q_i: lo-fi models
$\hat{Q}$: MC estimator
α_i: CV weights

- Multilevel Monte Carlo (**MLMC**)[2] and Multifidelity Monte Carlo (**MFMC**)[3] are instances of this estimator
- New ACV estimators[1] based on independent sampling (**ACV-IS**), multifidelity sampling (**ACV-MF**) and their corresponding generalizations[4] (**GIS**, **GMF**)
- Estimator is unbiased (wrt $E[Q]$)
- ACV estimator variance: $Var[\tilde{Q}] = Var[\hat{Q}](1 - R_{ACV}^2)$

[1] Gorodetsky, A A., et al. Journal of Computational Physics (2020)
[2] Giles, M B. Operations Research (2008)
[3] Peherstorfer, B, et al. SIAM Journal on Scientific Computing (2016)
[4] Bomarito, G. F., et al. Journal of Computational Physics (2022)

ACV-MF Estimator Variance

$$Var[\tilde{Q}] = Var[\hat{Q}](1 - R^2_{ACV-MF})$$

cov of lo-fi models w.r.t. each other

cov of lo-fi models w.r.t. hi-fi

sampling ratios

$$R^2_{ACV-MF}(\vec{r}) = \frac{1}{Var[Q]}[diag[\boldsymbol{F}(\vec{r})] \circ \boldsymbol{c}]^T [\boldsymbol{C} \circ \boldsymbol{F}(\vec{r})]^{-1} [diag[\boldsymbol{F}(\vec{r})] \circ \boldsymbol{c}]$$

Matrix representing ACV-MF sampling strategy

Variance minimization for sample allocation:

$$\underset{N,\vec{r}}{\text{argmin}}\ Var[\tilde{Q}](N,\vec{r}) \quad \text{s.t.} \quad W^{total}(N,\vec{r}) \leq W^{target}$$

Estimator cost

Computational budget

ACV-MF Estimator Variance

Introduce model tuning parameters $\vec{\beta}$

cov of lofi models w.r.t. each other

cov of lofi models w.r.t. hifi

$$R^2_{ACVMF}(\vec{r},\vec{\beta}) = \frac{1}{Var[Q]}\left[diag[\boldsymbol{F}(\vec{r})] \circ \boldsymbol{c}(\vec{\beta})\right]^T \left[\boldsymbol{C}(\vec{\beta}) \circ \boldsymbol{F}(\vec{r})\right]^{-1}\left[diag[\boldsymbol{F}(\vec{r})] \circ \boldsymbol{c}(\vec{\beta})\right]$$

In general, these are not known a priori and must be estimated

- Can reformulate generally in terms of only model correlations
- Model costs are also a function of $\vec{\beta}$ (potentially known)

Optimization Approach*

$$\underset{N,\vec{r},\vec{\beta}}{\text{argmin}} \; Var[\tilde{Q}](N,\vec{r},\vec{\beta}) \quad \text{s.t.} \quad W^{total}(N,\vec{r},\vec{\beta}) \leq W^{target}$$

- Build global surrogate for $\boldsymbol{c}(\vec{\beta})$ from pilot samples
  - N_{tun}: number of values of tuning parameters to investigate
  - N_{pilot}: number of pilot samples at each set of tuning parameters
  - Local quadratic interpolant
- Assume known relationship of model costs
- Gradient based-optimization (SLSQP)

*work in progress

- Currently based on single iteration from pilot samples for all N_{tun}, N_{pilot}

Analytical Example[1]

- **Goal**: study the effect of hyperparameter, θ_1, for lo-fi model, Q_1, on estimator variance

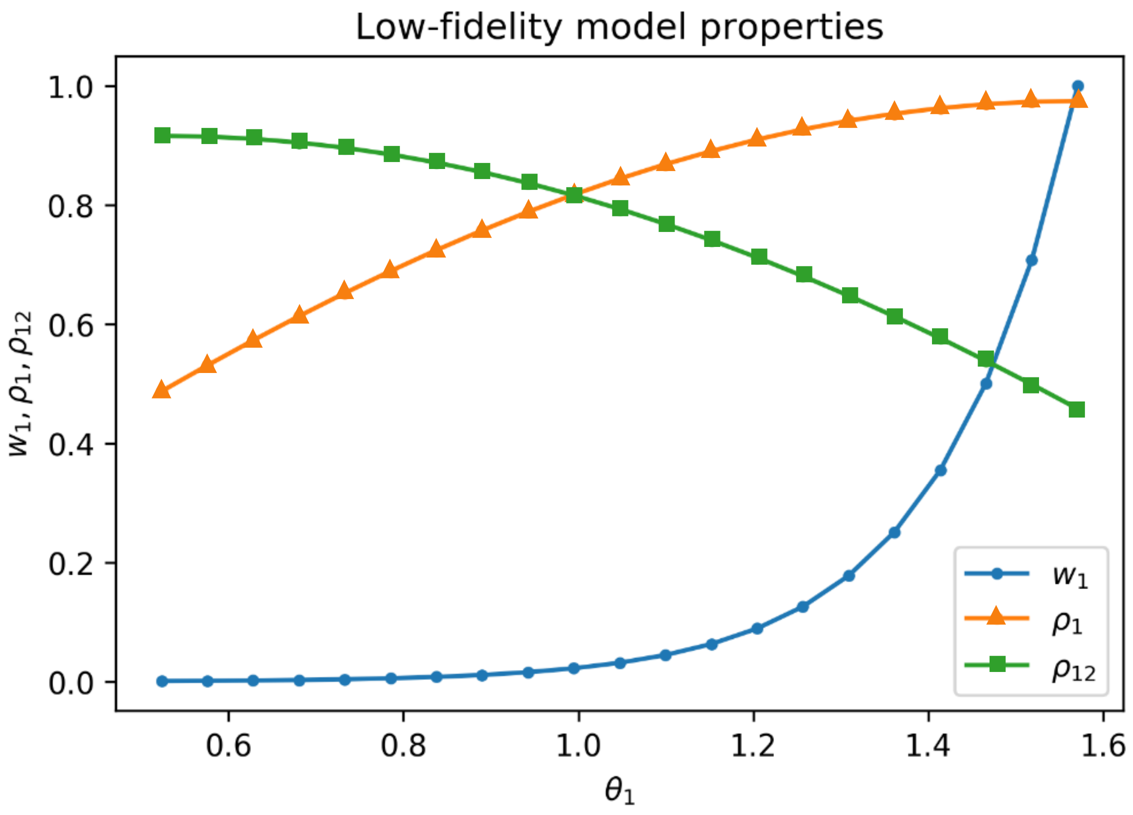
Hi-fi and lo-fi models

$$Q = A(\cos\theta x^5 + sin\theta y^5)$$
$$Q_1 = A_1(\cos\theta_1 x^3 + sin\theta_1 y^3)$$
$$Q_2 = A_2(\cos\theta_2 x + sin\theta_2 y)$$

Model costs:

$$w = 1$$
$$w_2 = 10^{-3}$$
$$\log w_1 = \log w_2 + \frac{\log w_2 - \log w}{\theta_2 - \theta}(\theta_1 - \theta_2)$$

A,A_1, A_2, θ, θ_2 are constants



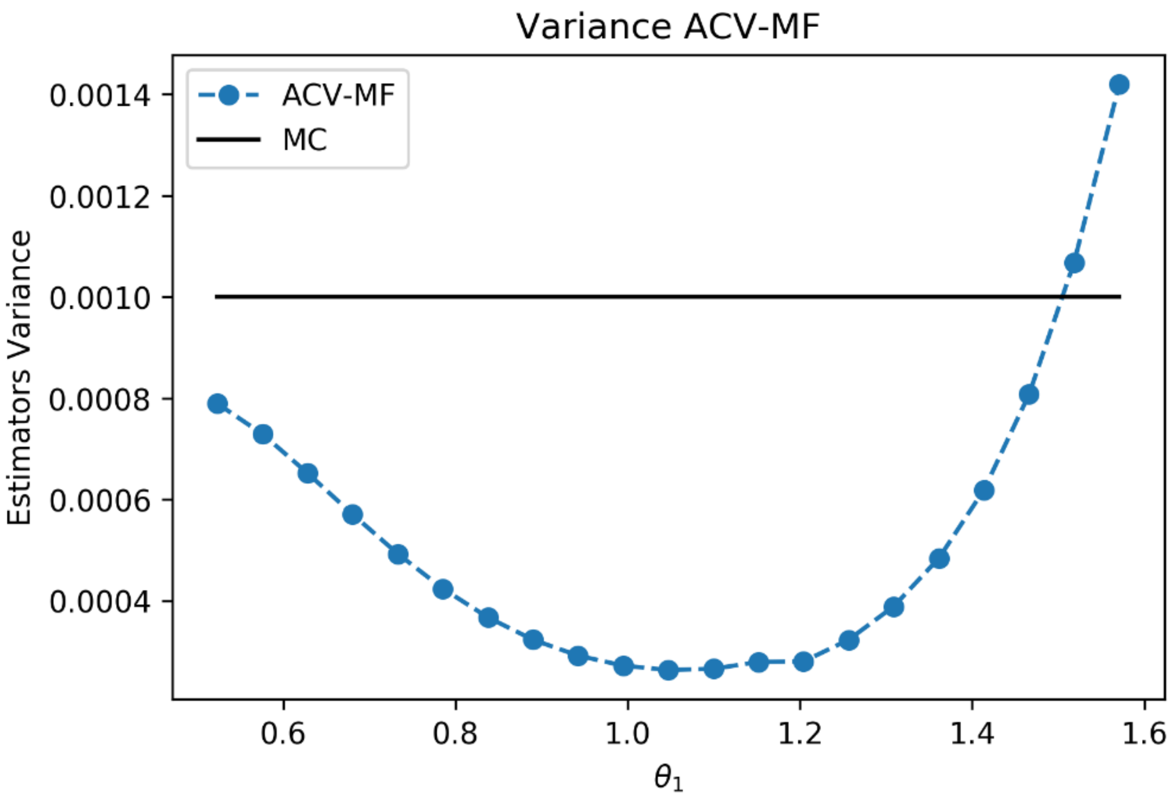
w_1: model cost

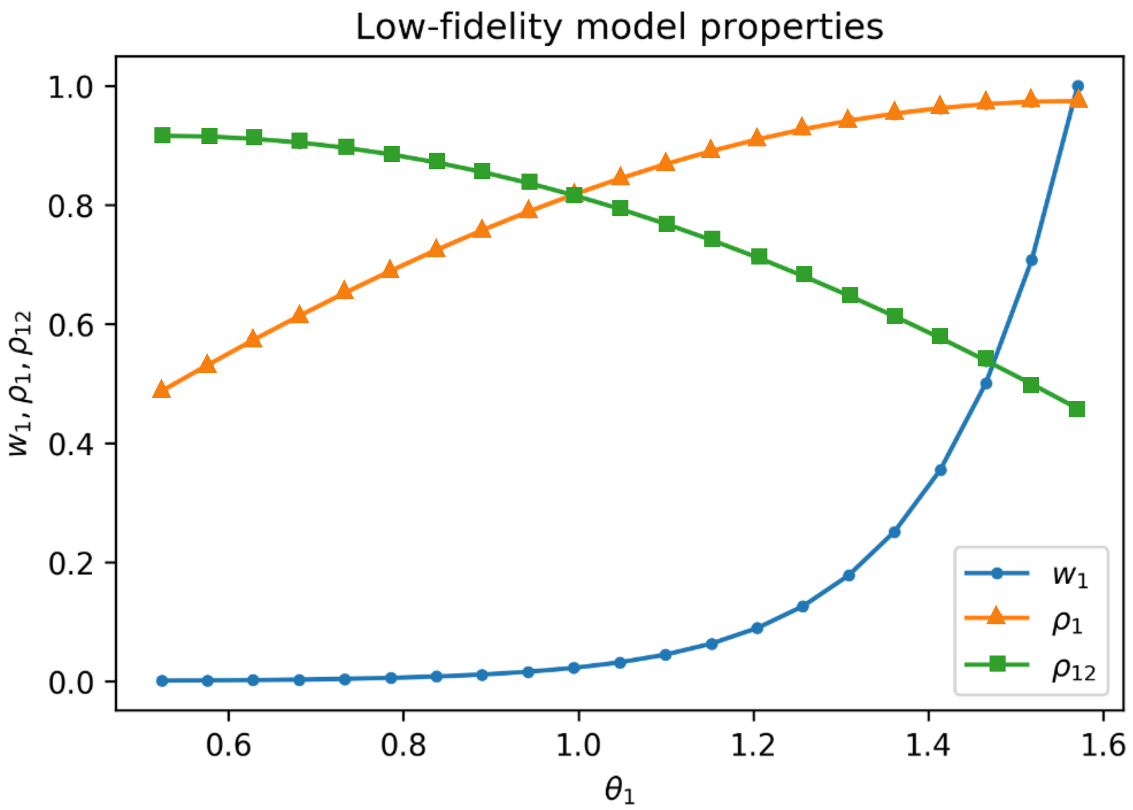
ρ_1 : correlation between Q_1 and Q

ρ_{12} : correlation between Q_1 and Q_2

[1] Gorodetsky, A A., et al. Journal of Computational Physics (2020)

Analytical Example[1]





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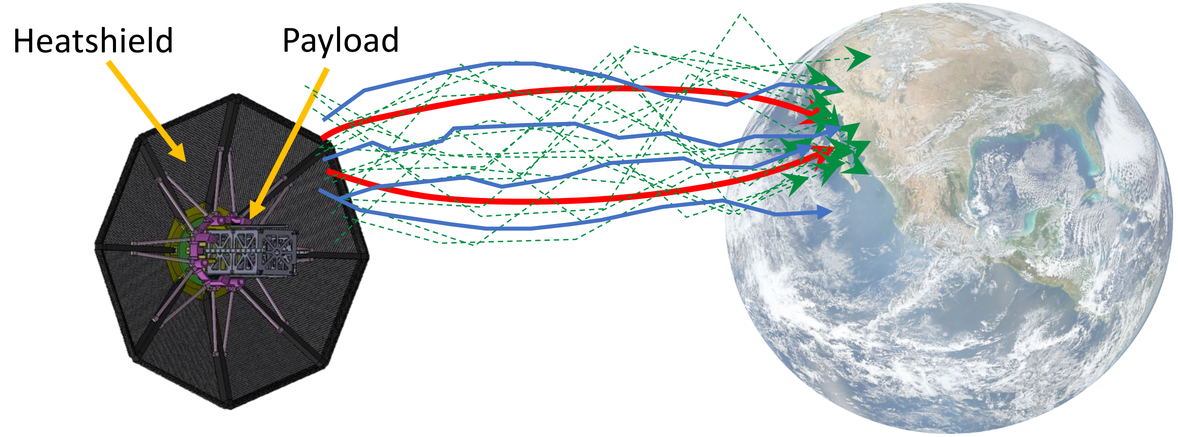
Model tuning can greatly affect estimator variance

[1] Gorodetsky, A. A., et al. Journal of Computational Physics (2020)

Trajectory Simulation Example

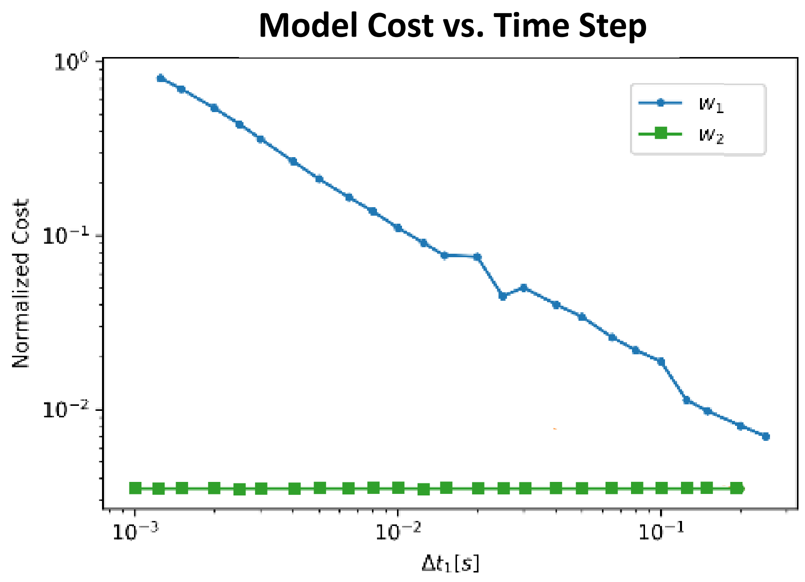
Goal: Predict the flight time of an umbrella heatshield reentering the Earth's atmosphere within computational budget

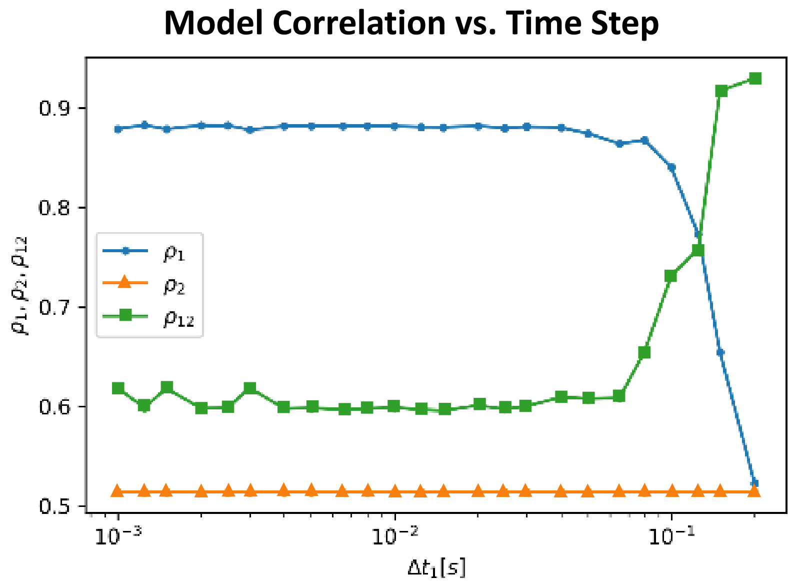


High-fidelity (Q): timestep = 0.001

Mid-fidelity (Q_1): timestep = $0.001 \leq \Delta t_1 \leq 0.25$

Low-fidelity (Q_2): timestep = 0.25





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Trajectory Simulation Example

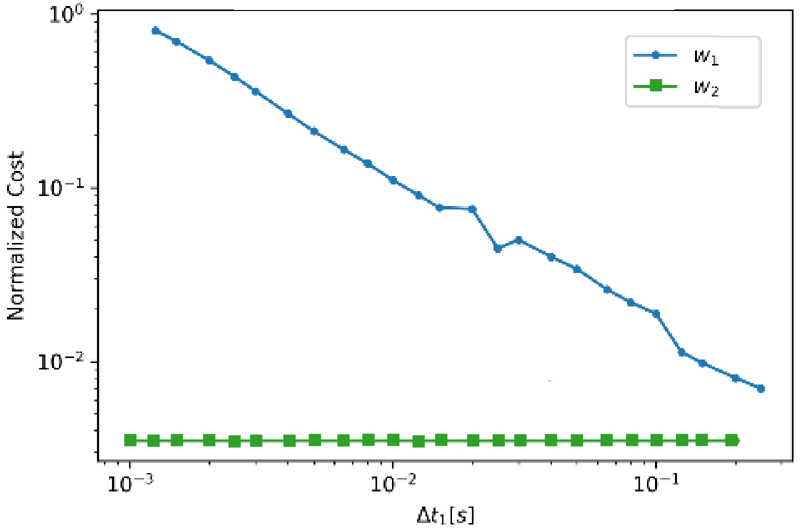
Goal: Predict the flight time of an umbrella heatshield reentering the Earth's atmosphere within computational budget

- Determine mid-fidelity time step through joint optimization:

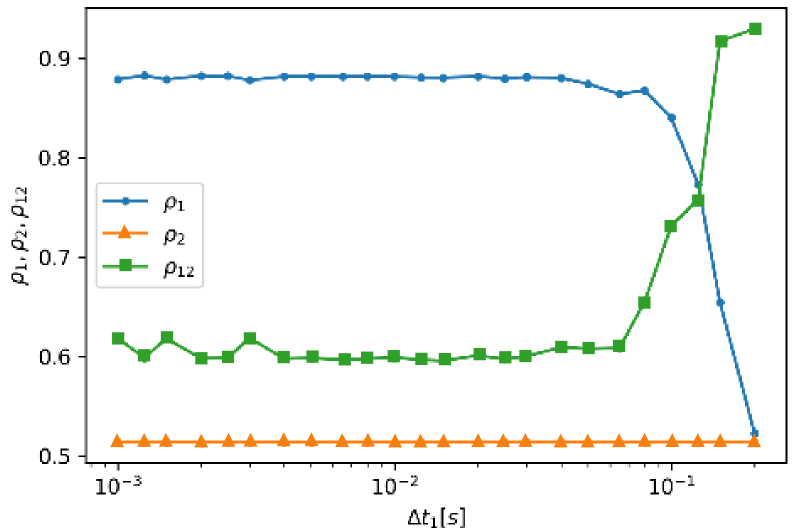
$$\underset{N, r_1, r_2, \Delta t_1}{\text{argmin}} \; Var[\tilde{Q}](N, r_1, r_2, \Delta t_1) \;\text{ s.t. }\; W^{total}(N, r_1, r_2, \Delta t_1) \leq W^{target}$$

- Compare correlation surrogate models with varying amounts of data
  1. $\mathrm{N_{tun}}$=24, $\mathrm{N_{pilot}} = 200$
  2. $\mathrm{N_{tun}}$=24, $\mathrm{N_{pilot}} = 50$
  3. $\mathrm{N_{tun}}$=6, $\mathrm{N_{pilot}} = 200$
  - Reference case (*Ref Surr*) with all data: $\mathrm{N_{tun}}$=24, $\mathrm{N_{pilot}} = 500$

Model Cost vs. Time Step



Model Correlation vs. Time Step

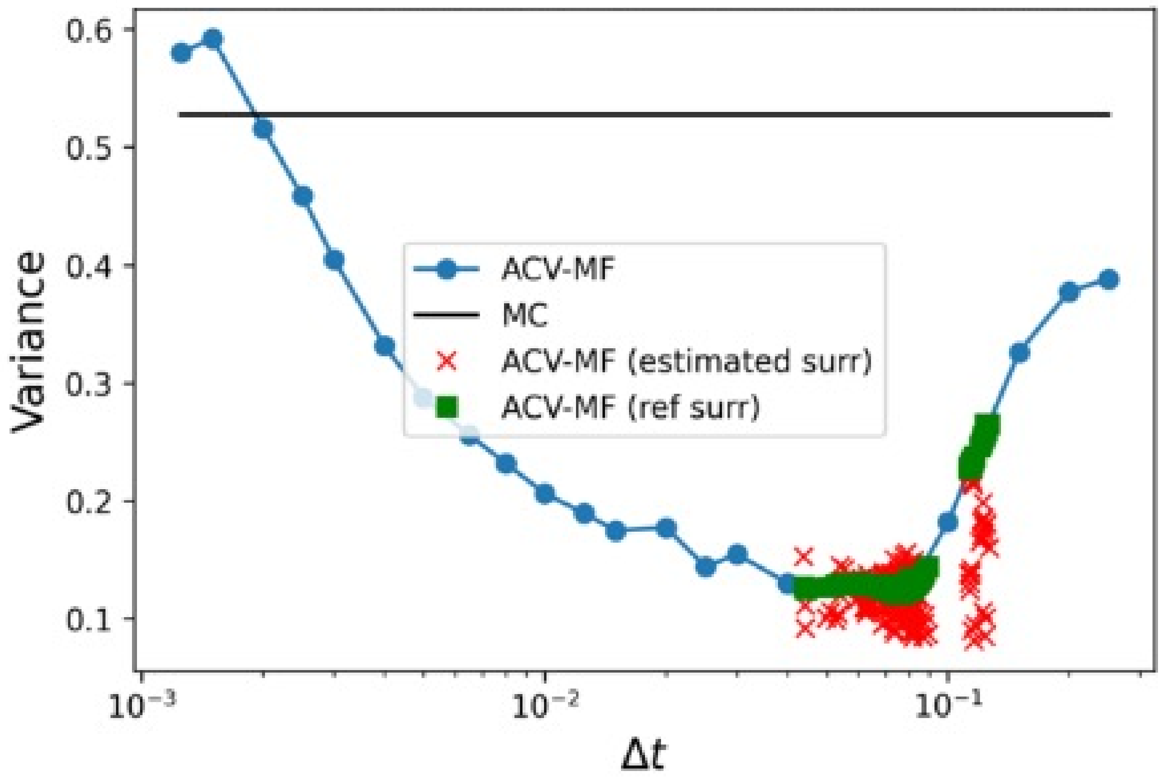


w_1: Q_1 model cost
ρ_1 : correlation between Q_1 and Q
ρ_{12} : correlation between Q_1 and Q_2

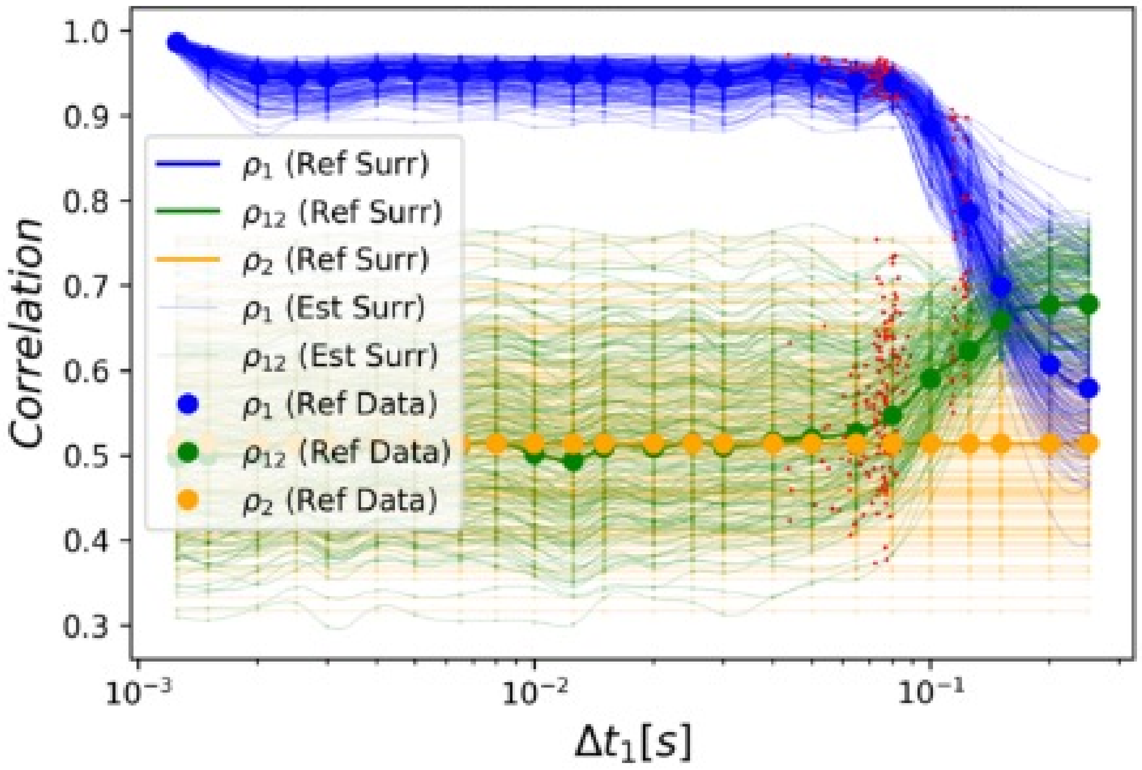
Results: Most Accurate Surrogate

- Optimization using $\mathrm{N_{tun}} = 24$, $\mathrm{N_{pilot}} = 200$ to build correlation surrogate models; 200 random trials

Estimator Variance vs. Time Step



Estimated Model Correlation vs. Time Step

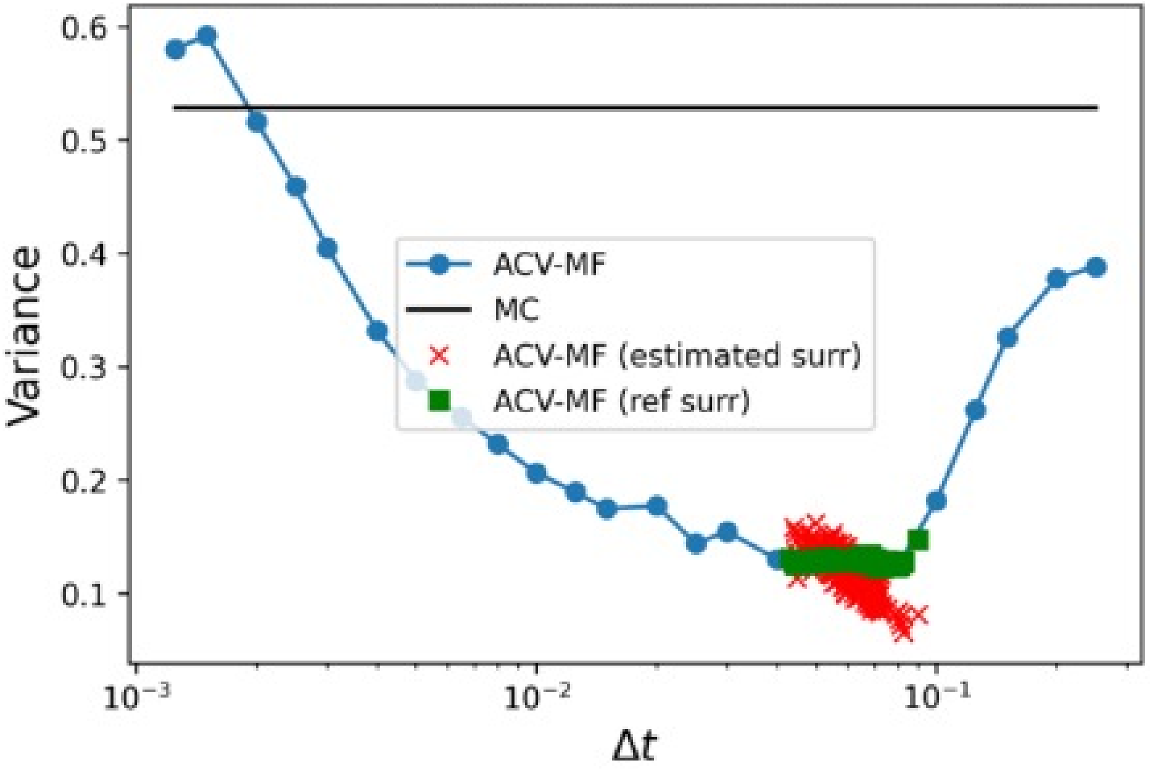


Optimal model tuning is achievable using surrogates for correlation

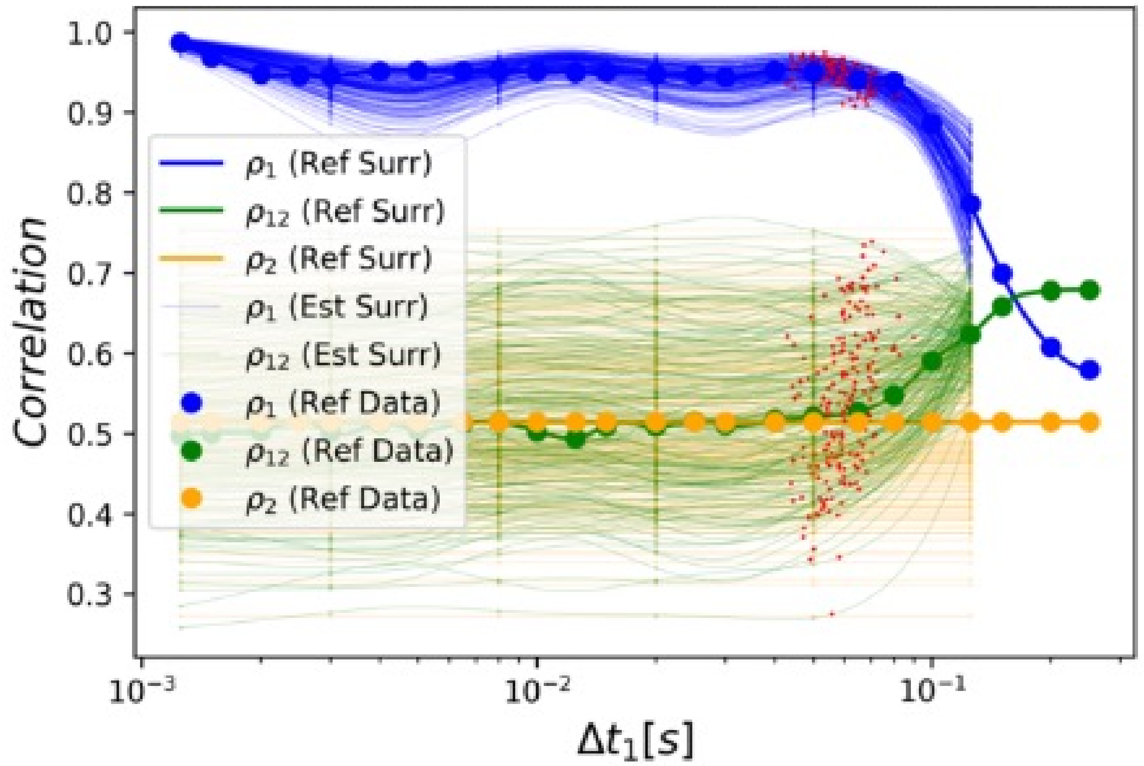
Results: Sparser Grid

- Optimization using $\mathbf{N_{tun} = 6}$, $\mathrm{N_{pilot}} = 200$ to build correlation surrogate models; 200 random trials

Estimator Variance vs. Time Step



Estimated Model Correlation vs. Time Step

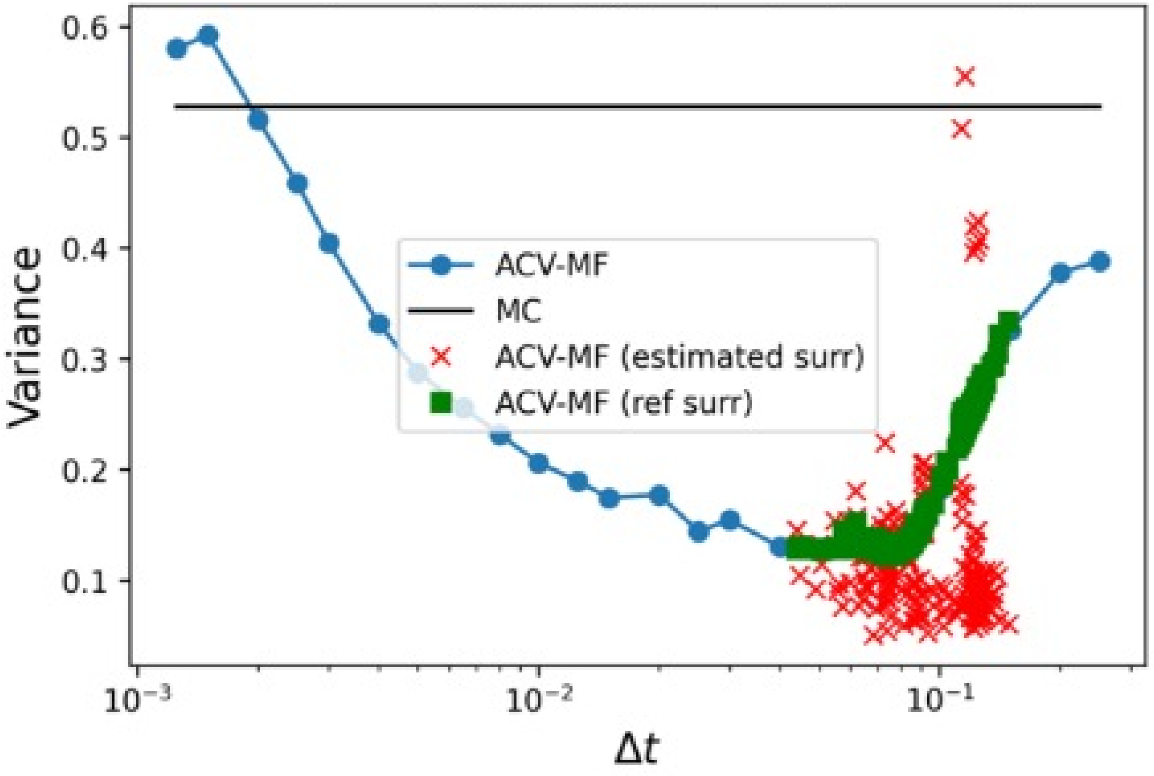


Smoothness is important for gradient-based optimization

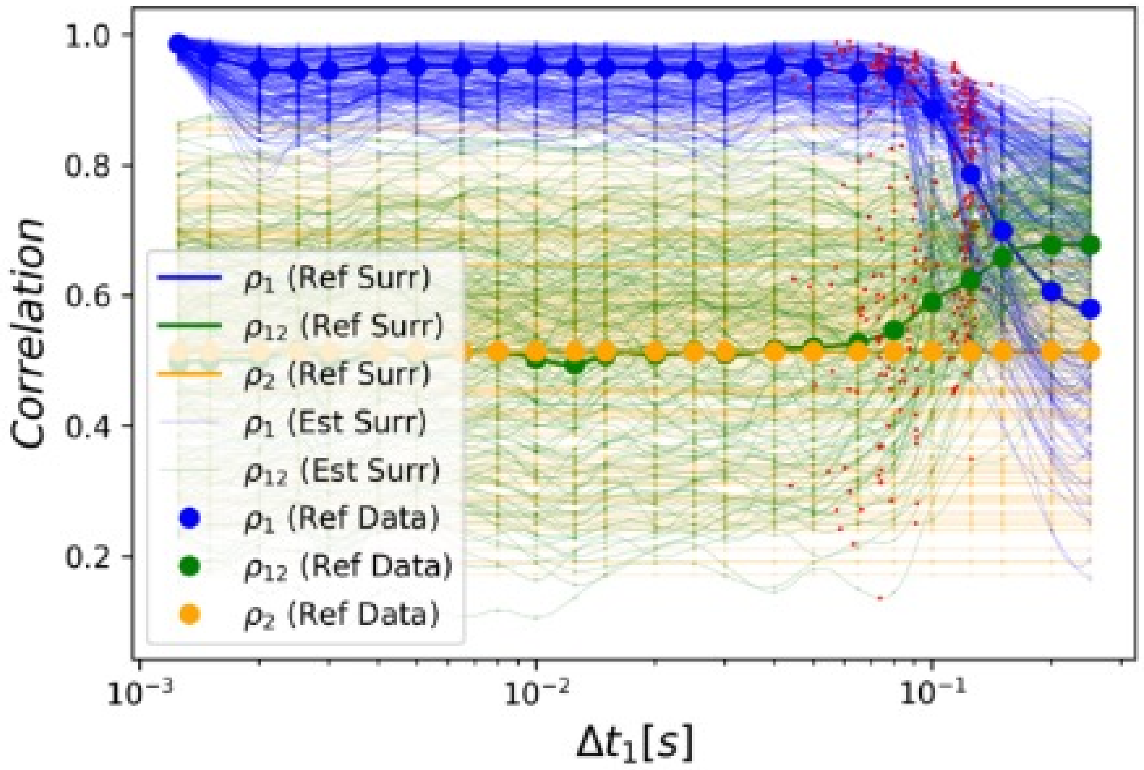
Results: Fewer Pilot Samples

- Optimization using $\mathrm{N_{tun}} = 24$, $\mathbf{N_{pilot} = 50}$ to build correlation surrogate models; 200 random trials

Estimator Variance vs. Time Step



Estimated Model Correlation vs. Time Step

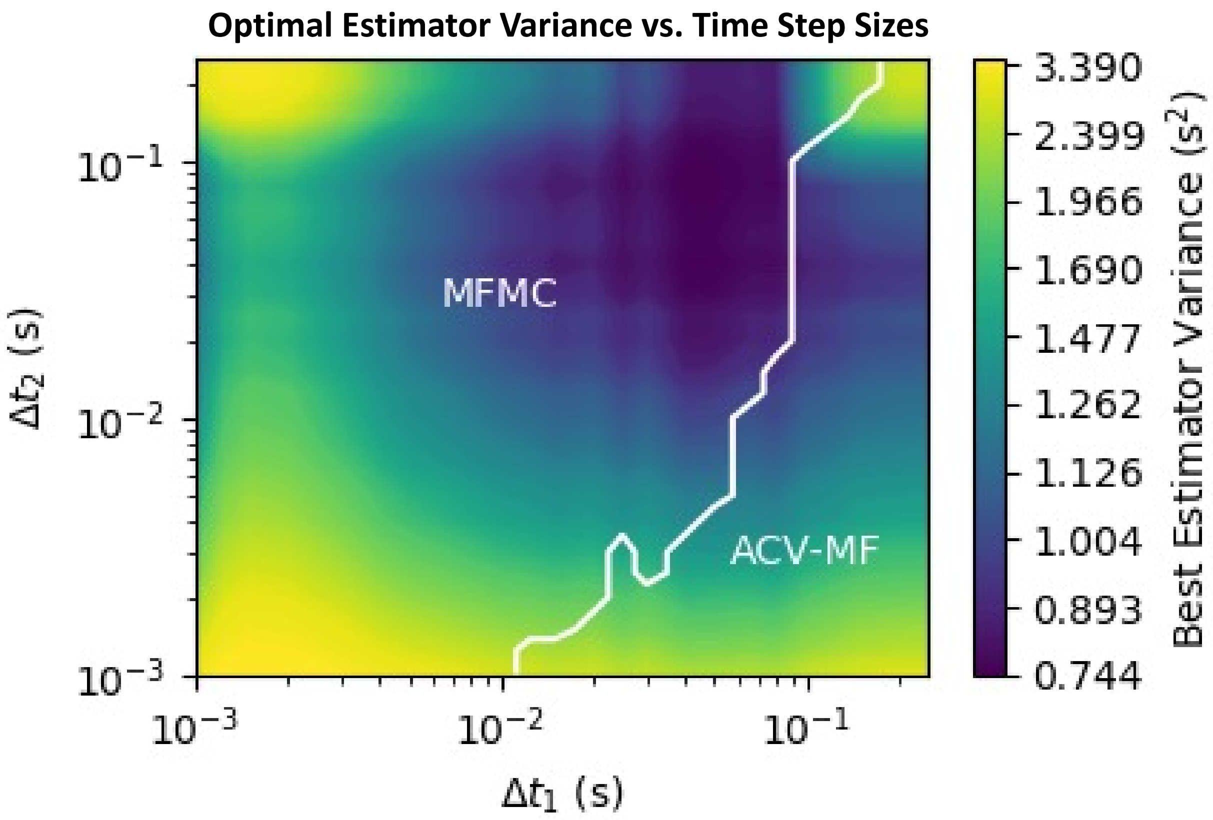


Statistical variability impacts optimization

Results: Two Tunable Lo-Fi Models

High-fidelity (Q): timestep = 0.001
Mid-fidelity (Q_1): timestep = $0.001 \leq \Delta t_1 \leq 0.25$
Low-fidelity (Q_2): timestep = 0.001 <= $\Delta t_2 \leq 0.25$

- Estimator variance was calculated directly for each $(\Delta t_1, \Delta t_2)$ pair using MFMC and ACV-MF and the optimal (minimum) value was plotted



Optimal ACV method (model graph) can be function of hyperparameters

Conclusions

- Model tuning can greatly affect estimator variance
- Optimization requires estimation (or knowledge) of correlations/costs as a function of tuning parameters
- Quality of the correlation surrogate is an important factor in tuning parameter optimization
- **Future Work:**
  - Automating sample allocation + model tuning optimization – implementation in Dakota
  - Global optimization with adaptive surrogate refinement
  - All-at-once optimization with model hierarchy

Questions?

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

- Reference:

    - G. F. Bomarito, G. Geraci, J. E. Warner, P. E. Leser, W. P. Leser, M. S. Eldred, J. D. Jakeman, A. A. Gorodetsky. *Improving Multi-Model Trajectory Simulation Estimators using Model Selection and Tuning*. 2022 AIAA Scitech Proceedings. January 2022. https://doi.org/10.2514/6.2022-1099.

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