

Improving Multi-Model Trajectory Simulation Estimators using Model Selection and Tuning

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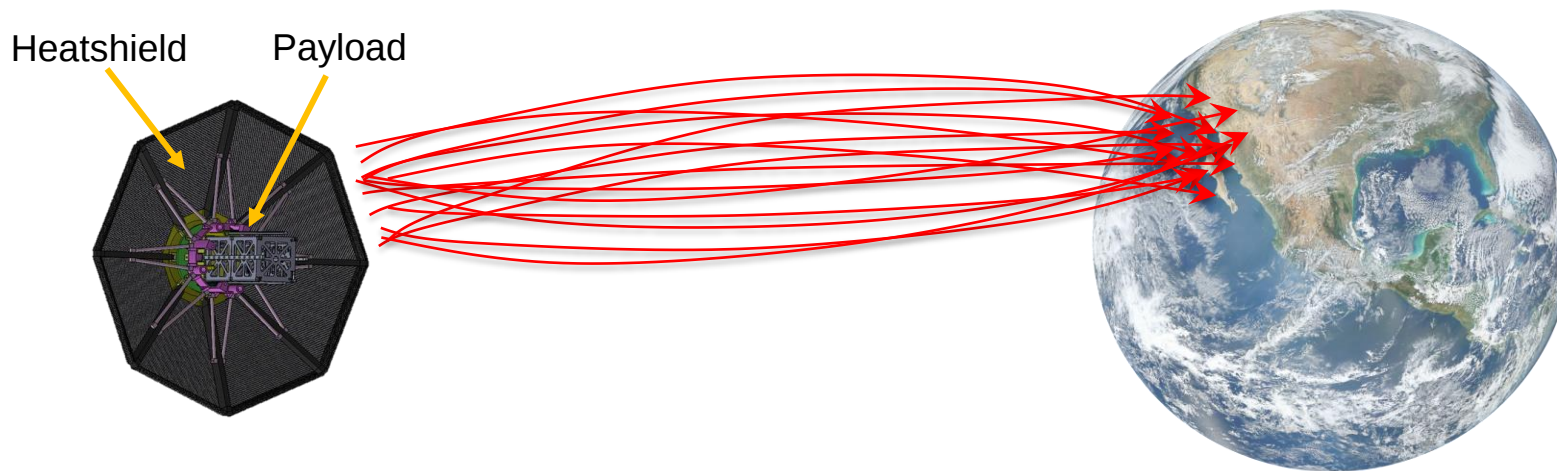
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Motivation: Trajectory Simulation

Goal: Predict the flight time of an umbrella heatshield reentering the Earth's atmosphere with target precision

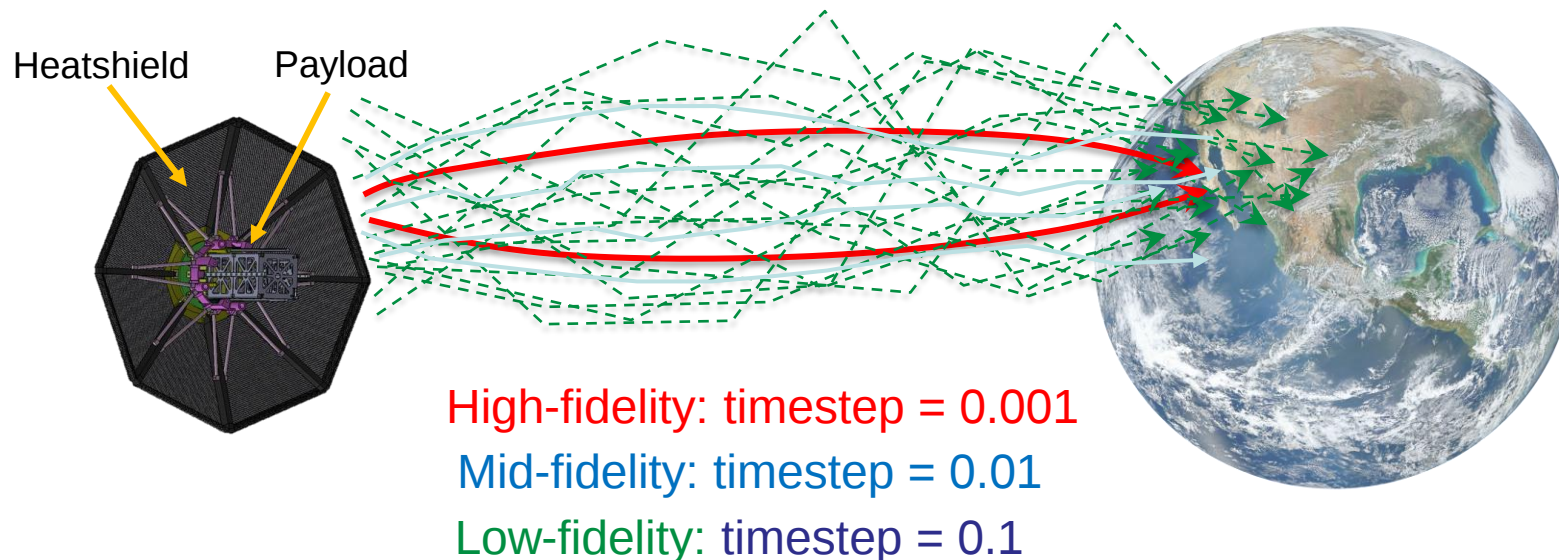
- Uncertain inputs: initial velocity, wind speeds, etc.
- Quantity of interest: flight time
- Model : Program to Optimize Simulated Trajectories (POST2)



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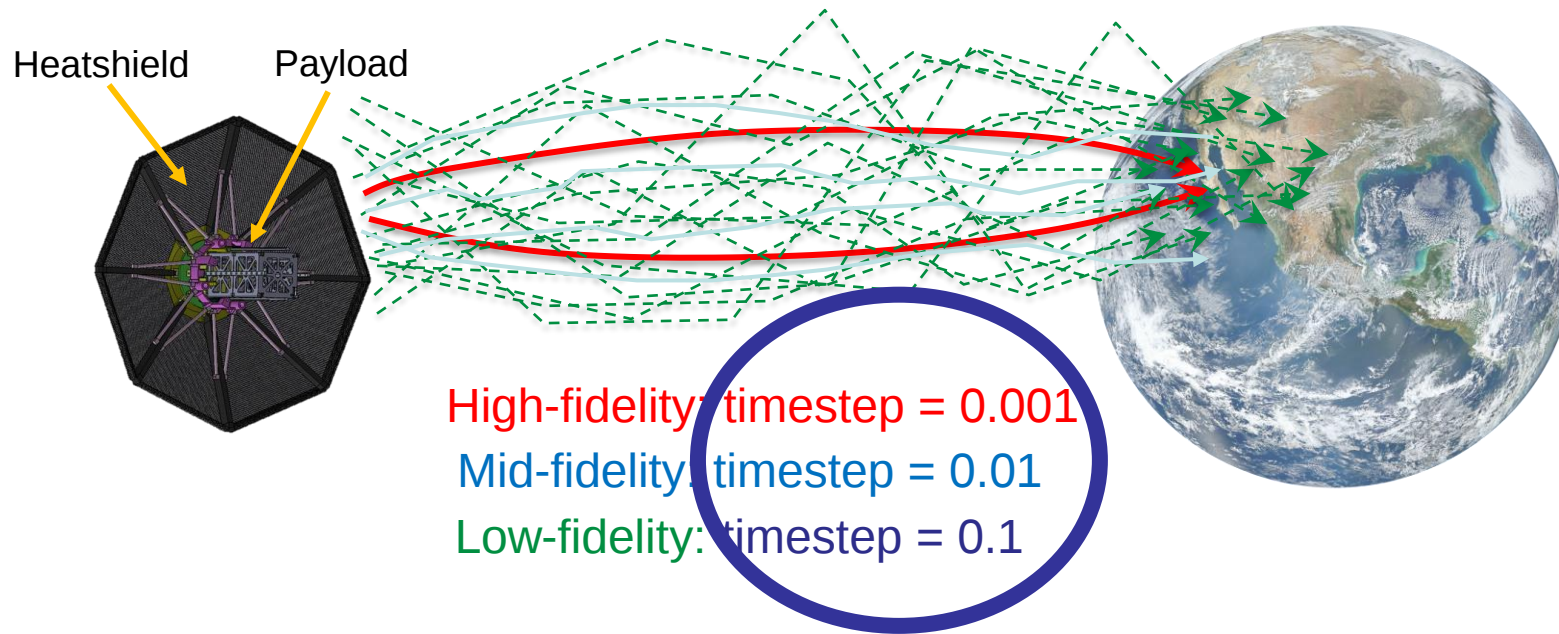
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- Model : Program to Optimize Simulated Trajectories (POST2)



- Use multi-model Monte Carlo to precisely predict vehicle flight time in less time by leveraging low-fidelity models and relatively few expensive, high-fidelity model evaluations

Outline

- Model tuning is important
- How we can do it optimally
- Application to trajectory simulation



Approximate Control Variates^[1] (ACV)

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

- Multilevel Monte Carlo (**MLMC**)^[2] and Multifidelity Monte Carlo (**MFMC**)^[3] are instances of this estimator
- New ACV estimators^[1] based on independent sampling (**ACVIS**), multifidelity sampling (**ACVMF**)
- Estimator is unbiased (wrt $E[Q]$)
- $Var[\tilde{Q}] = Var[\hat{Q}](1 - R_{ACV}^2)$

[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)

ACV-MF Variance

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

$$R_{ACV-MF}^2(r) = \frac{1}{\text{Var}[Q]} [\text{diag}[\mathbf{F}(r)] \circ \mathbf{c}]^T [\mathbf{C} \circ \mathbf{F}(r)]^{-1} [\text{diag}[\mathbf{F}(r)] \circ \mathbf{c}]$$

Diagram illustrating the components of the ACV-MF Variance formula:

- sampling ratios** (blue arrow) points to $\mathbf{c}$.
- cov of lofi models w.r.t. each other** (red arrow) points to $\mathbf{C}$.
- cov of lofi models w.r.t. hifi** (purple arrow) points to $\mathbf{F}(r)$.
- Matrix representing ACVMF sampling strategy** (green arrow) points to $[\mathbf{C} \circ \mathbf{F}(r)]^{-1}$.

ACV-MF Variance

Model tuning parameters β

$$R_{ACVMF}^2(r, \beta) = \frac{1}{Var[Q]} [diag[F(r)] \circ \mathbf{c}(\beta)]^T [\mathbf{C}(\beta) \circ F(r)]^{-1} [diag[F(r)] \circ \mathbf{c}(\beta)]$$

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

cov of lofi models w.r.t. hifi

In general, these are not known and must be estimated

Model cost may also be a function of β

Analytical example

$$Q = \sqrt{11}y^5$$

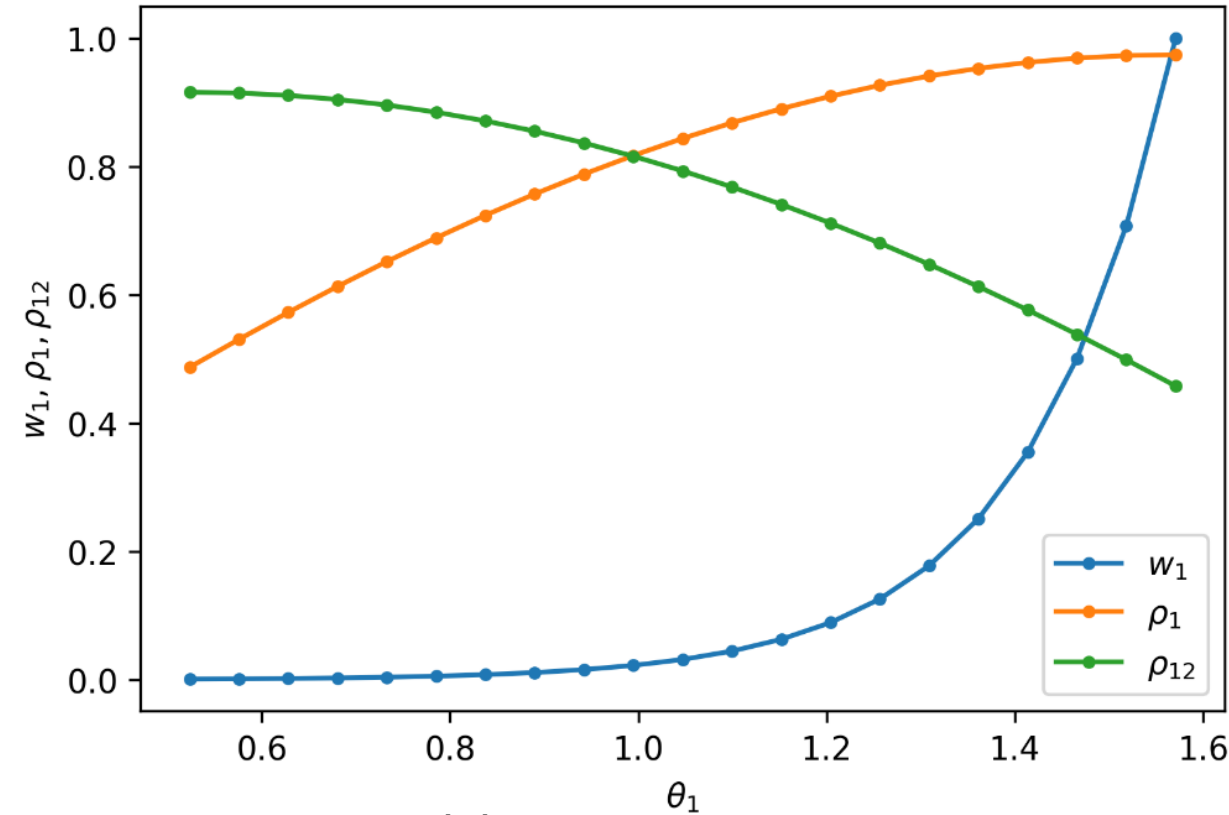
$$Q_1 = \sqrt{7} \left(\cos \theta_1 x^3 + \sin \theta_1 y^3 \right)$$

$$Q_2 = \sqrt{3} \left(\frac{\sqrt{3}}{2}x + \frac{1}{2}y \right),$$

$$w = 1 \text{ and } w_2 = 10^{-3}$$

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

Low-fidelity model properties



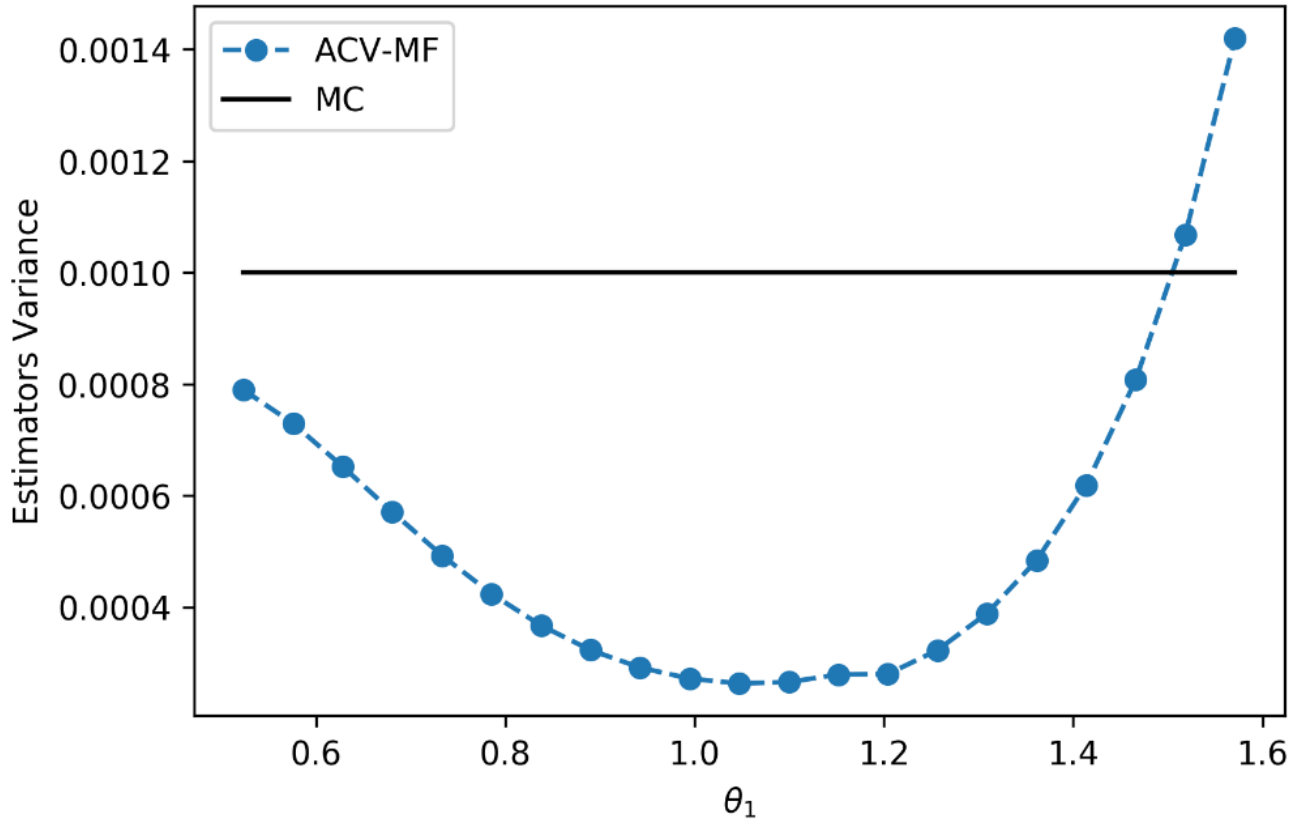
w_1 : model cost

ρ_1 : correlation between Q_1 and Q

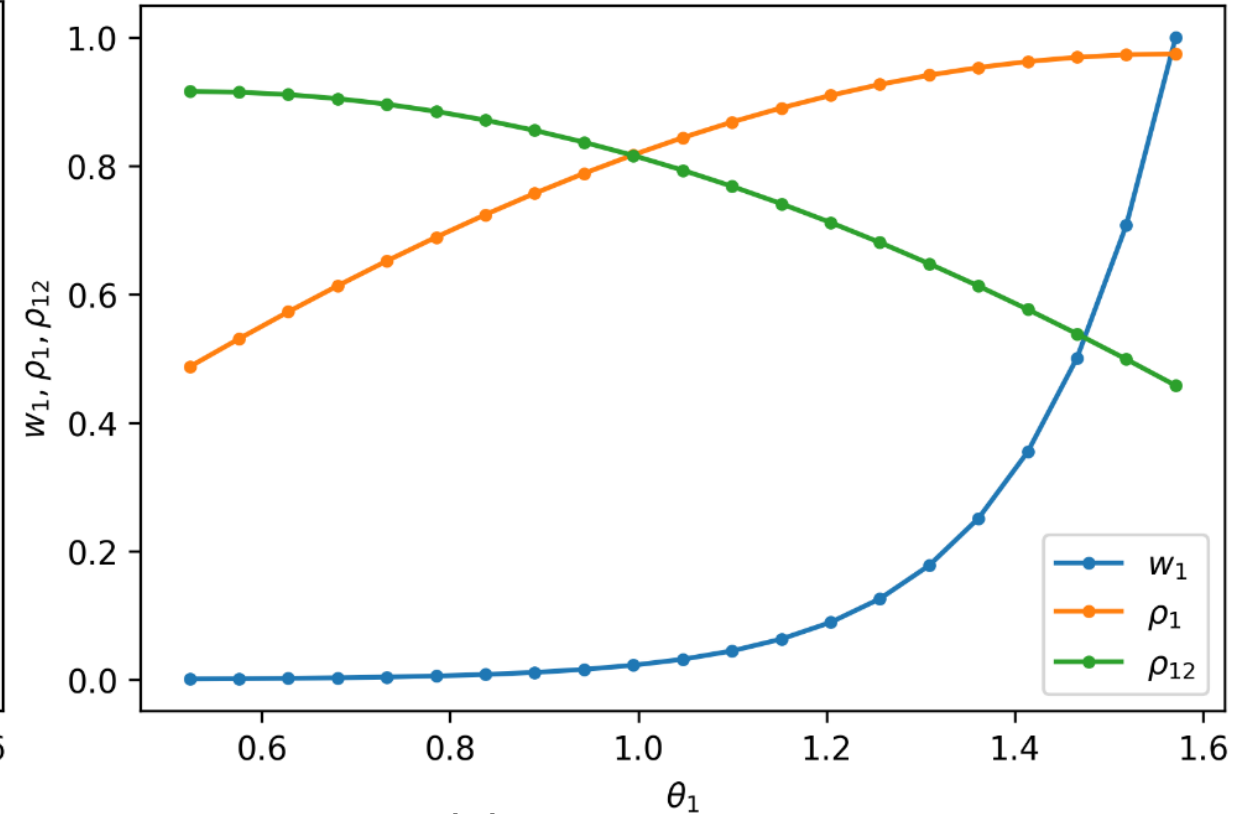
ρ_{12} : correlation between Q_1 and Q_2

Analytical example

Variance ACV-MF



Low-fidelity model properties



Model tuning can greatly affect estimator variance

w_1 : model cost

ρ_1 : correlation between Q_1 and Q

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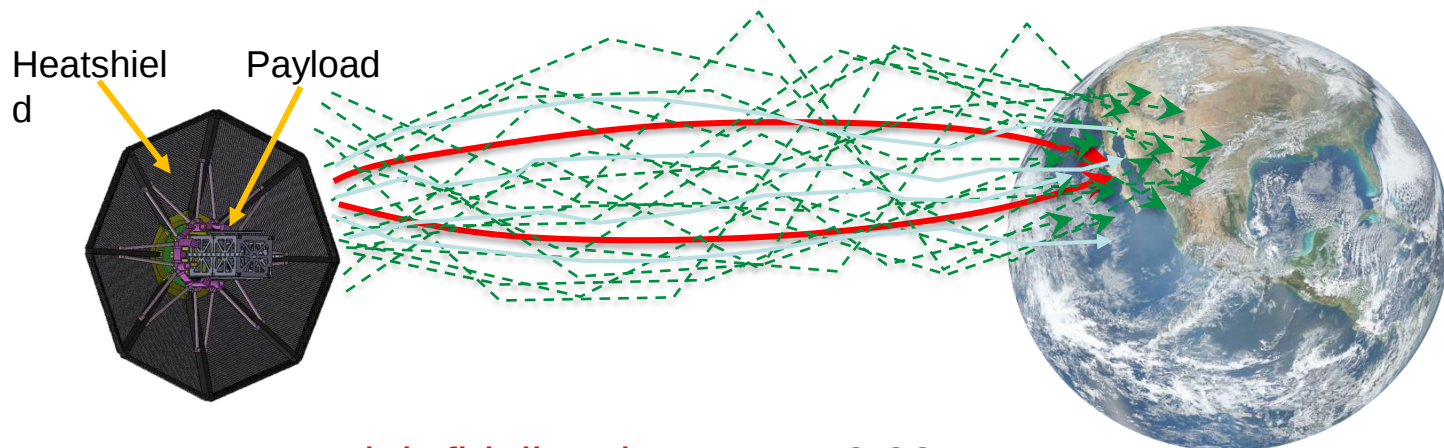
Optimization approach*

- Minimize $Var[\tilde{Q}](N, r, \beta)$ st. cost < budget constraint
- Build global surrogate for $c(\beta)$ and $\mathbf{C}(\beta)$ from pilot samples
 - N_{tun} : number values of tuning parameters to investigate
 - N_{pilot} : number of pilot samples at each set of tuning parameters
 - Quadratic interpolant
- Assume known relationship of model costs
- Gradient based-optimization (SLSQP)

* work in progress

Trajectory Simulation

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



High-fidelity: timestep = 0.001

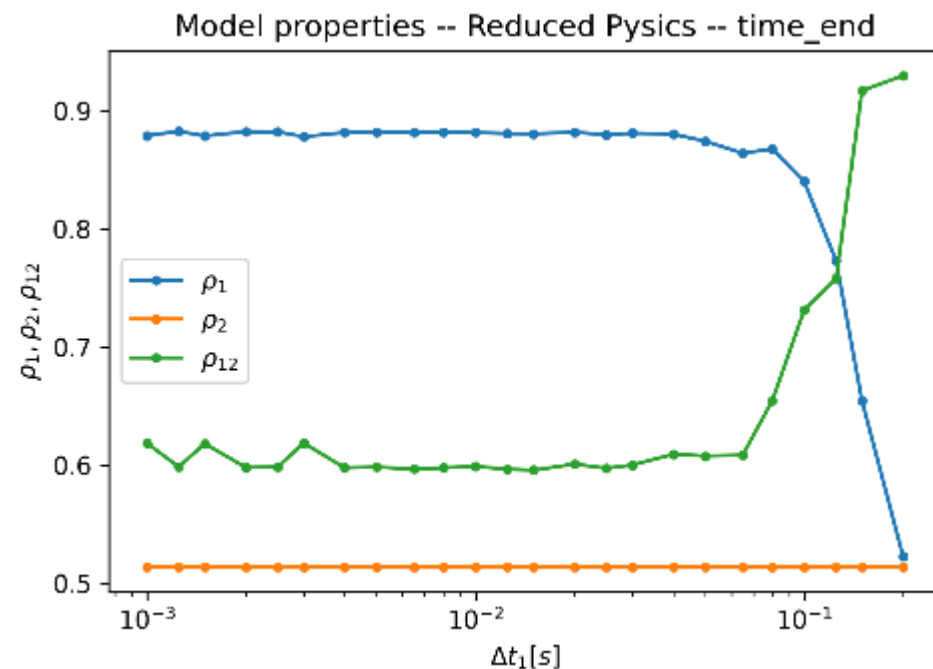
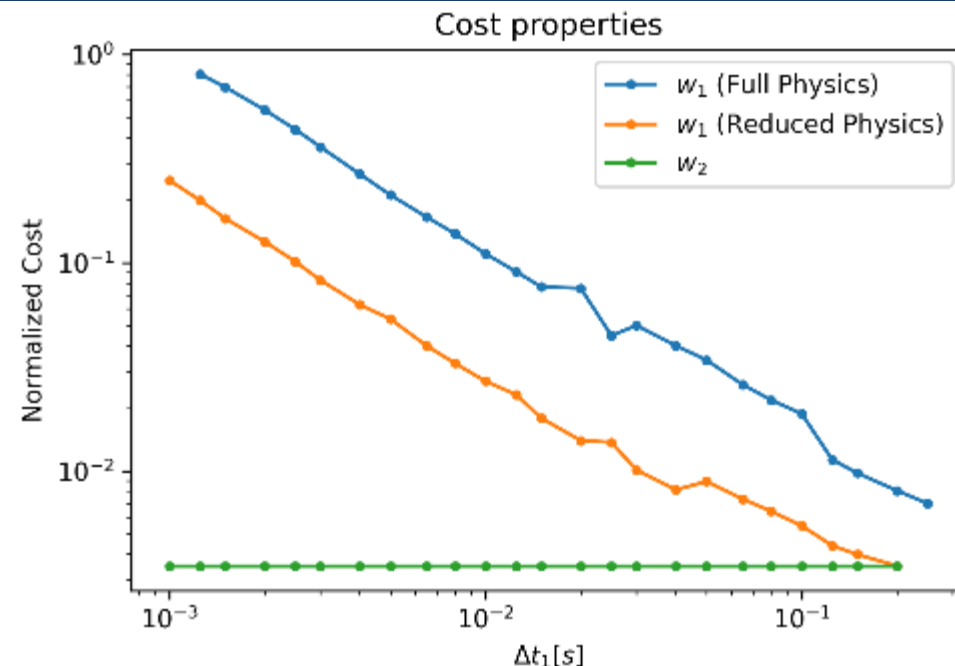
Mid-fidelity: timestep = $0.001 \leq \Delta t_1 \leq 0.25$

Low-fidelity: timestep = 0.25

w_1 : model cost

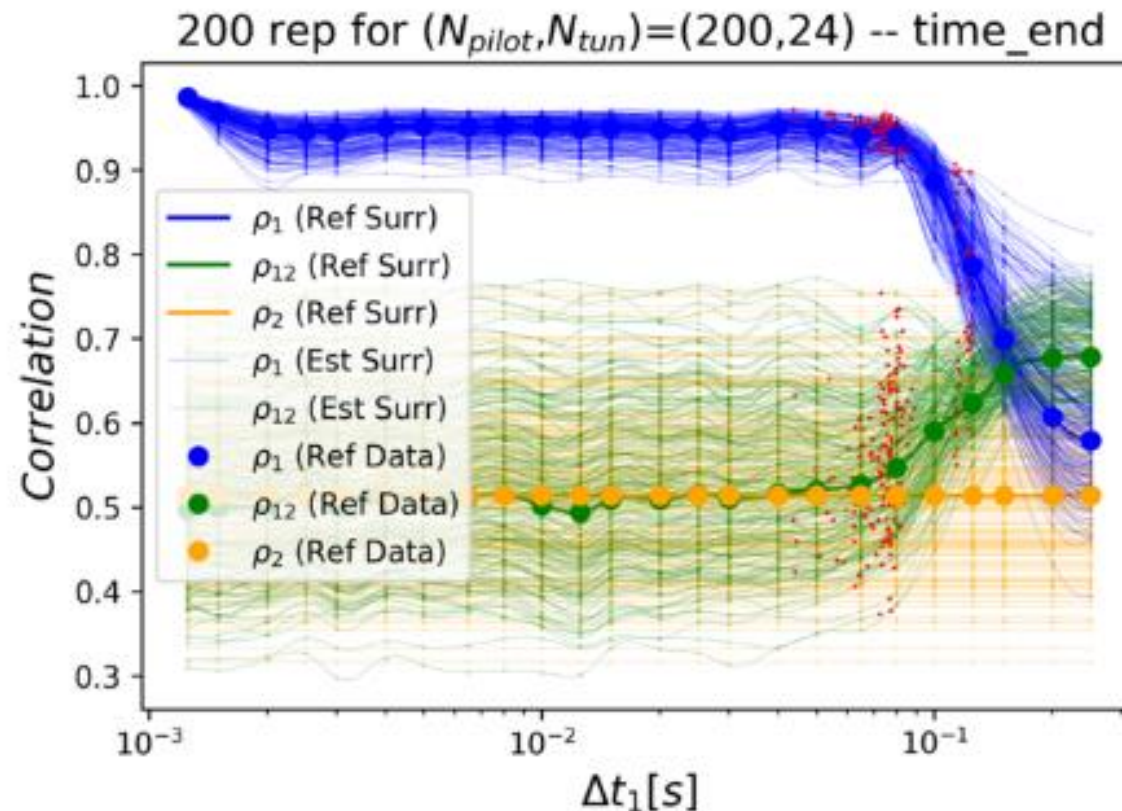
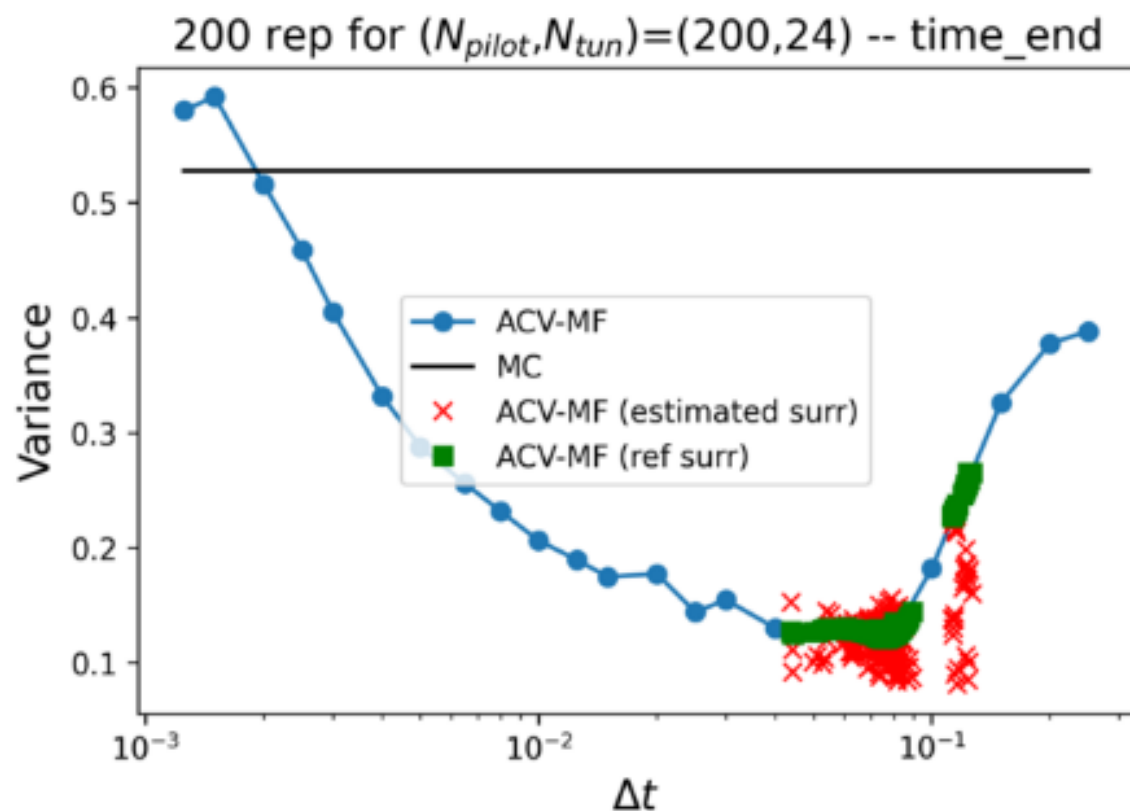
ρ_1 : correlation between Q_1 and Q

ρ_{12} : correlation between Q_1 and Q_2



Results: most accurate surrogate

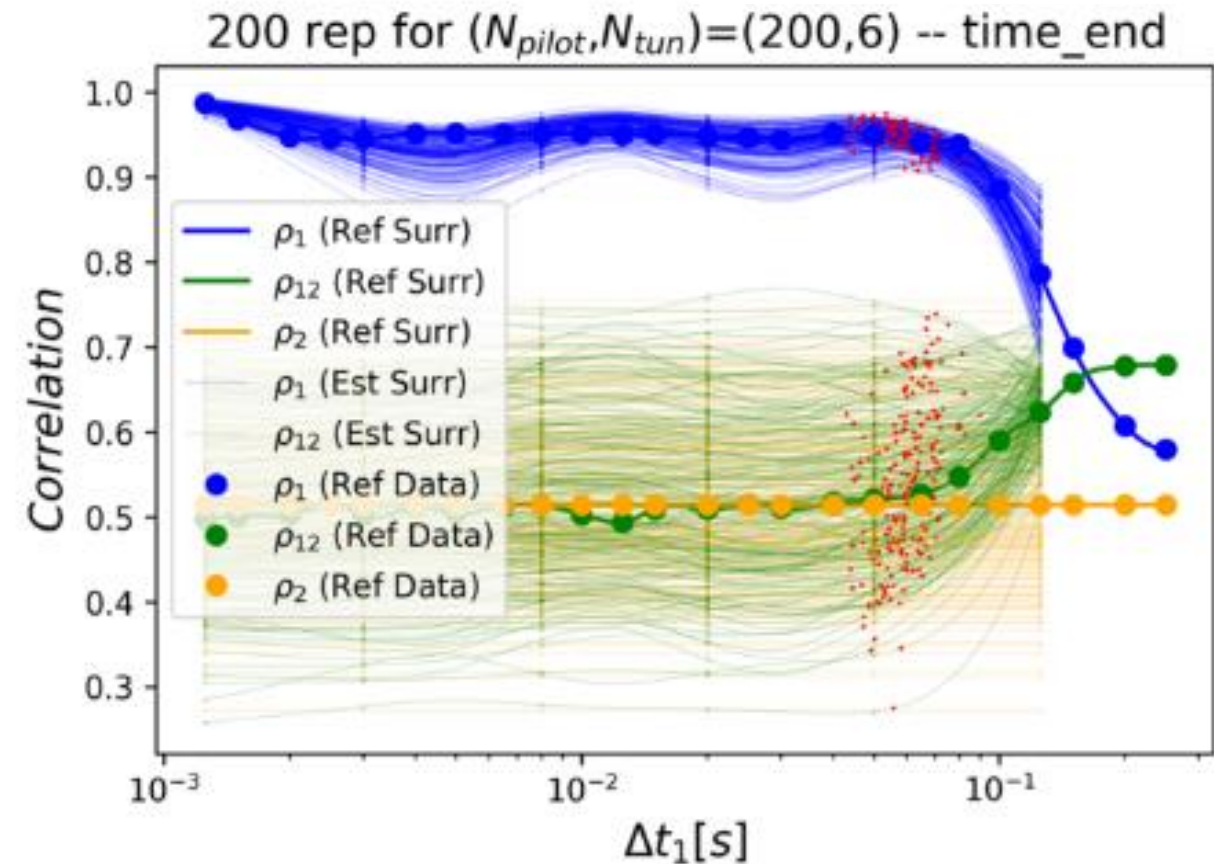
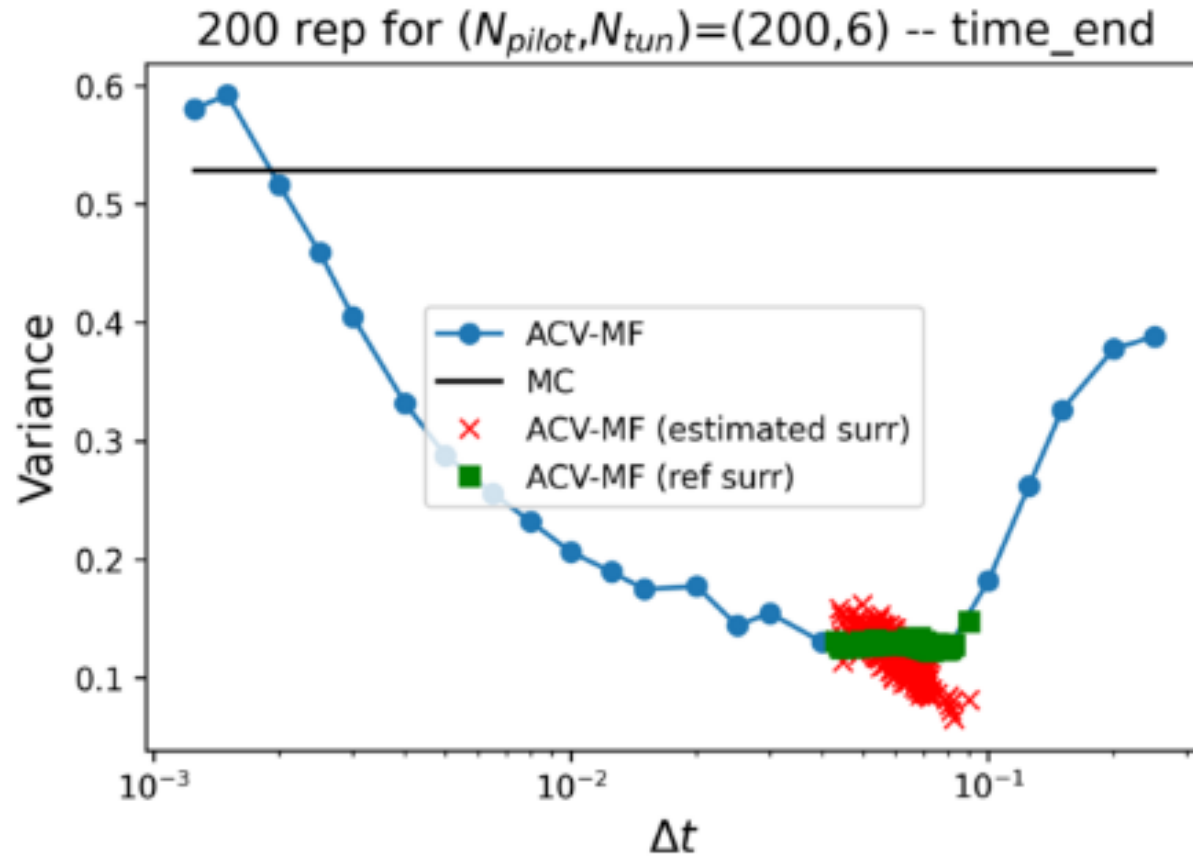
w_1 : model cost
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Optimal model tuning is achievable using surrogates for correlation

Results: more sparse measurements

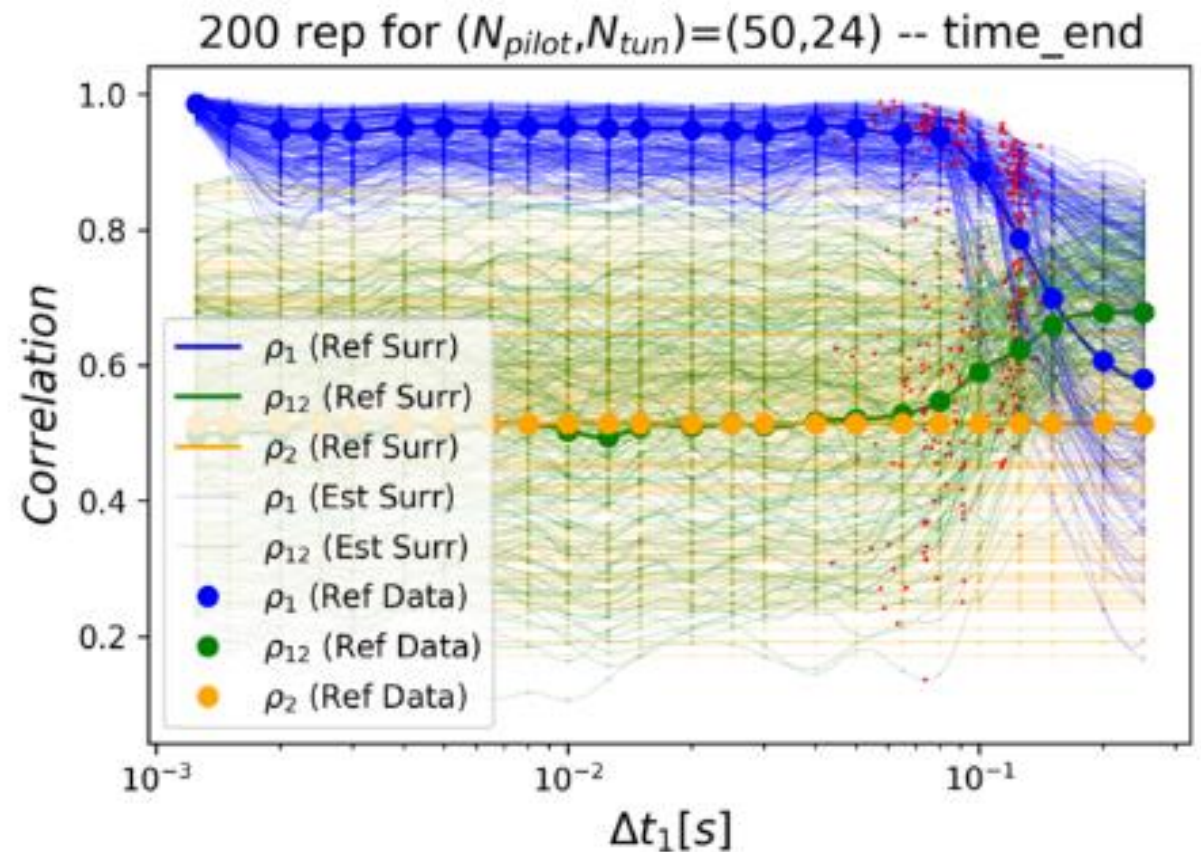
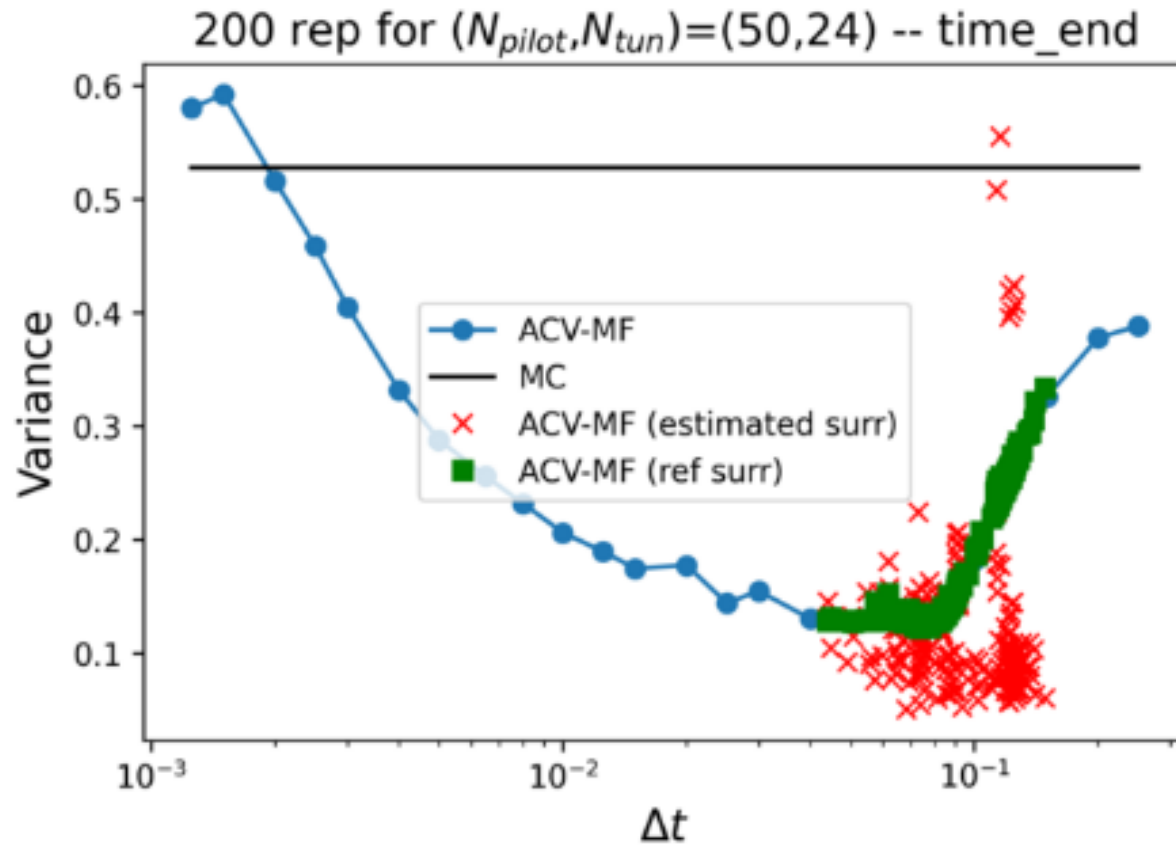
w_1 : model cost
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Smoothness is important for gradient-based optimization

Results: fewer pilot samples

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



More accuracy of surrogates impacts optimization

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

- Improved surrogates, with adaptive refinement
- Use global optimization rather than local optimization to reduce effect of noisy correlation estimates
- All-at-once optimization with model hierarchy

Thank You For Watching!

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