SAND2021-15264C

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

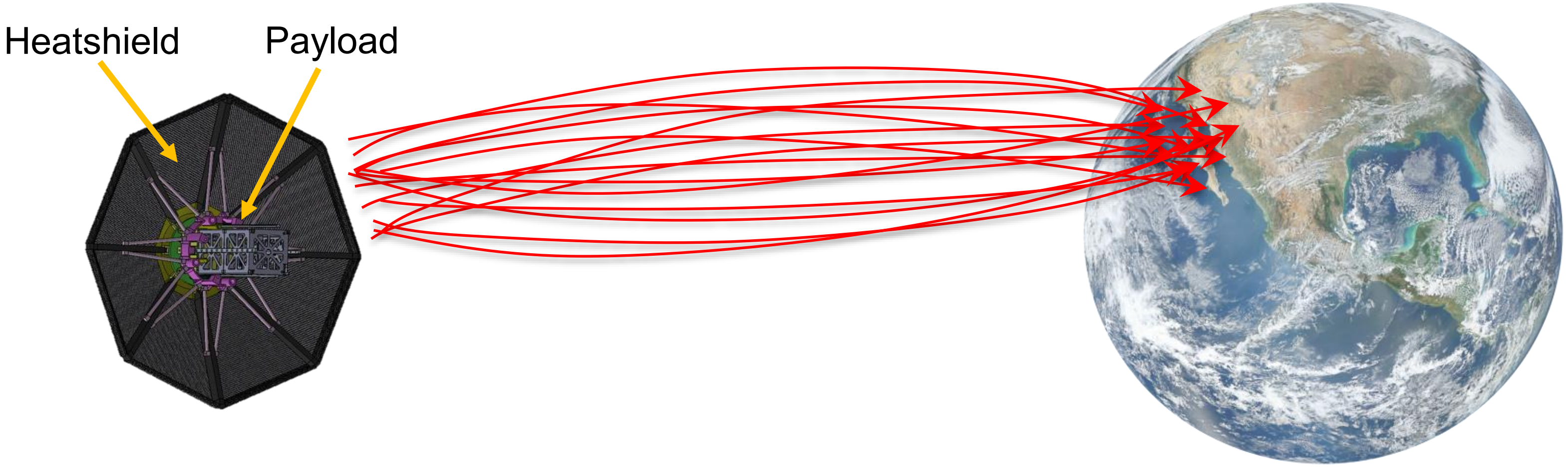
Geoffrey Bomarito†, Gianluca Geraci‡, James Warner†, Patrick Leser†, Paul Leser†, Michael Eldred‡, John Jakeman‡, Alex Gorodetsky₺

† NASA Langley Research Center, Hampton, VA
‡ Sandia National Laboratories, Albuquerque, NM
₺ University of Michigan, Ann Arbor, MI

Motivation: Trajectory Simulation

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

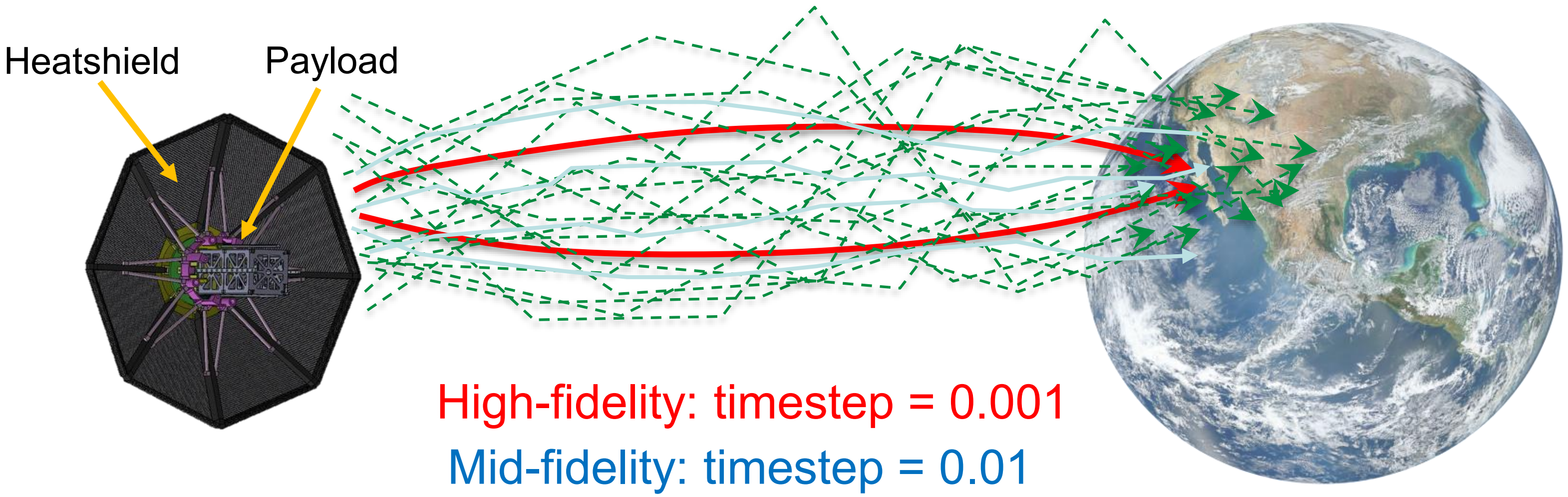
- Uncertain inputs: initial velocity, wind speeds, etc.
- Quantity of interest: flight time
- Model : Program to Optimize Simulated Trajectories (POST2)



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)

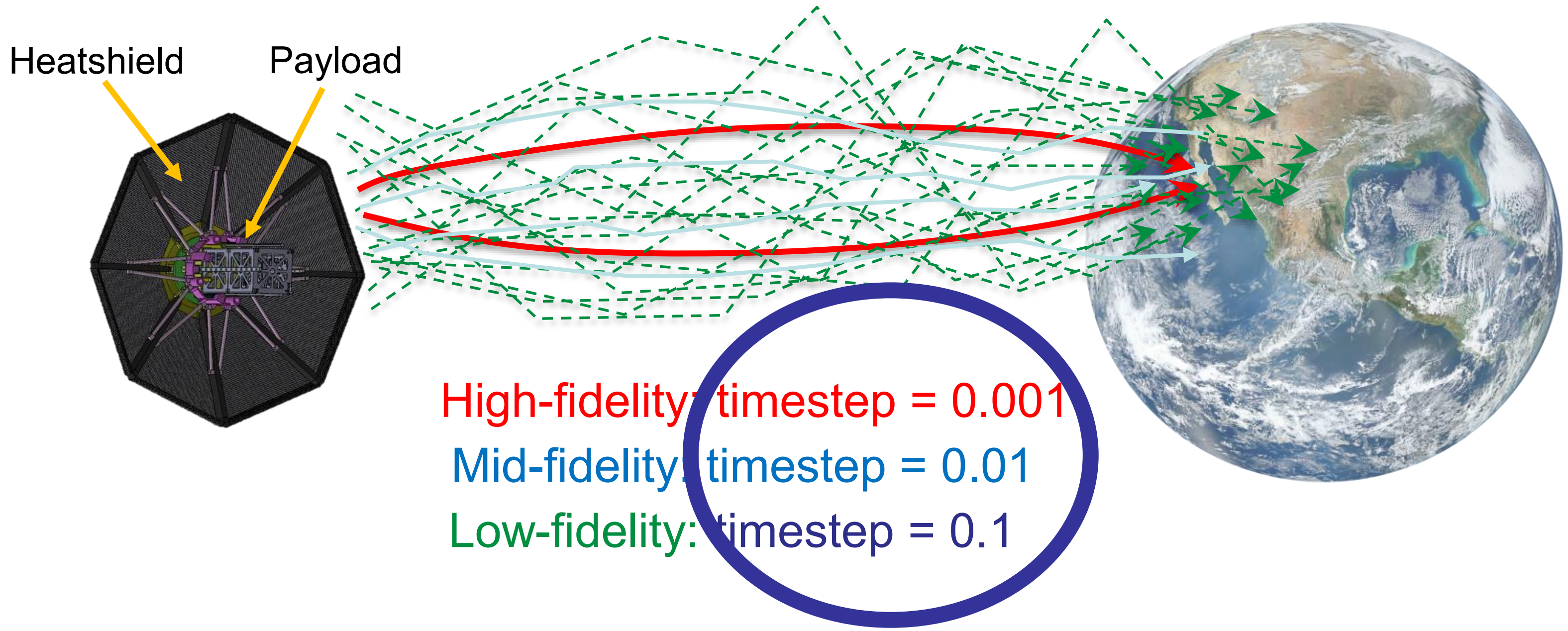


High-fidelity: timestep = 0.001
Mid-fidelity: timestep = 0.01
Low-fidelity: timestep = 0.1

- 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

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

sampling ratios

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

cov of lofi models w.r.t. hifi

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

Matrix representing ACVMF sampling strategy

ACV-MF Variance

Model tuning parameters β

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

cov of lofi models w.r.t. hifi

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

In general, these are not known and must be estimated

Model cost may also be a function of β

Analytical example

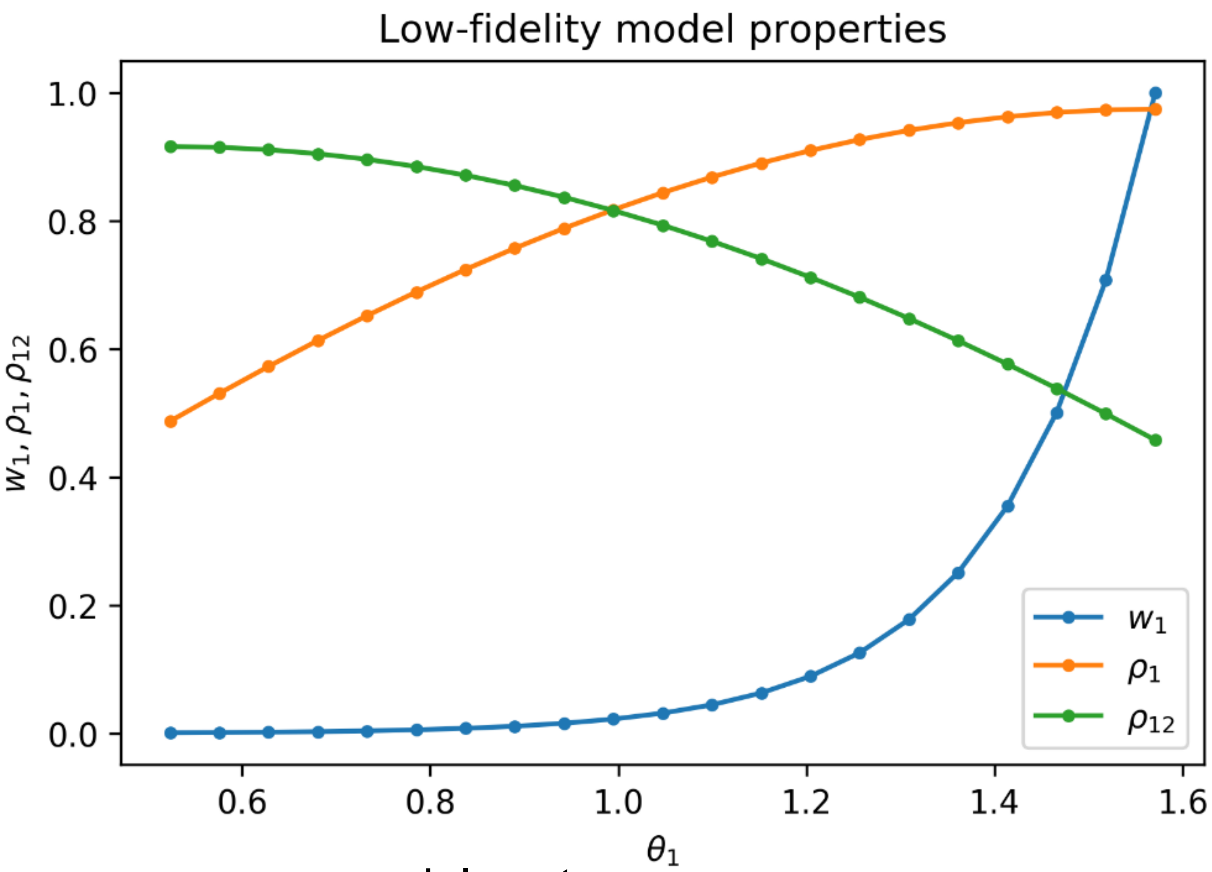
$$Q = \sqrt{11} y^5$$

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

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

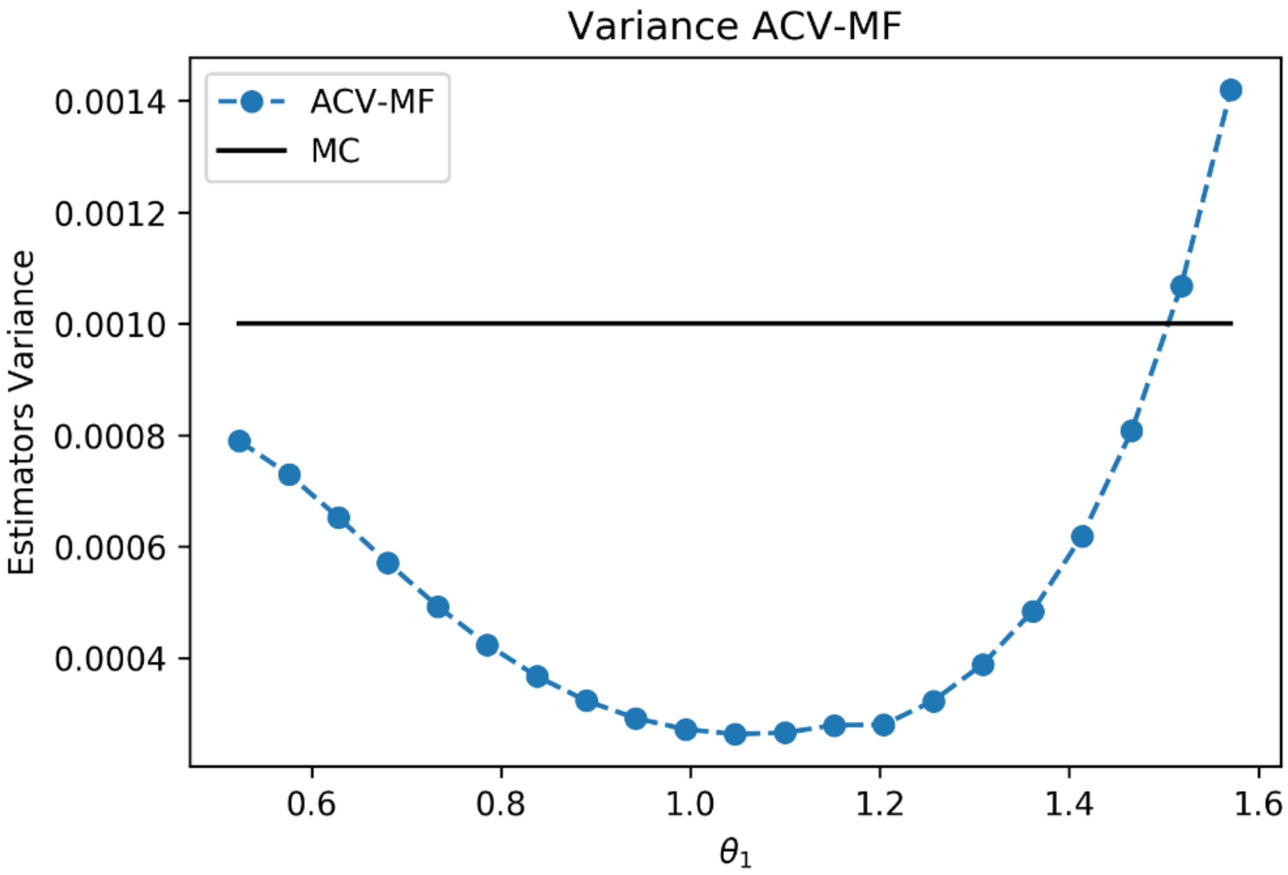
$$w = 1 \text{ and } w_2 = 10^{-3}$$

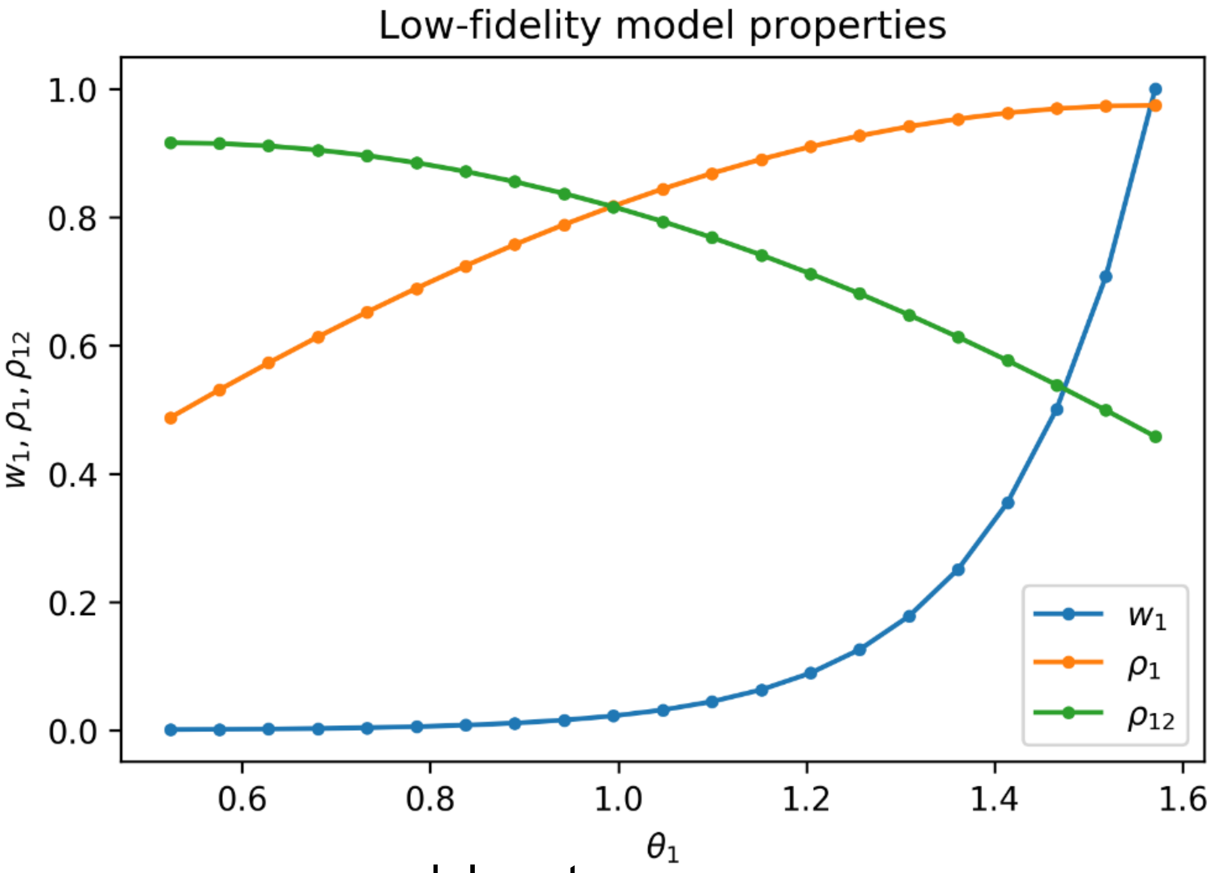
$$\log w_1 = \log w_2 + \frac{\log w_2 - \log w}{\theta_2 - \theta}(\theta_1 - \theta_2)$$



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

Analytical example





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

Model tuning can greatly affect estimator variance

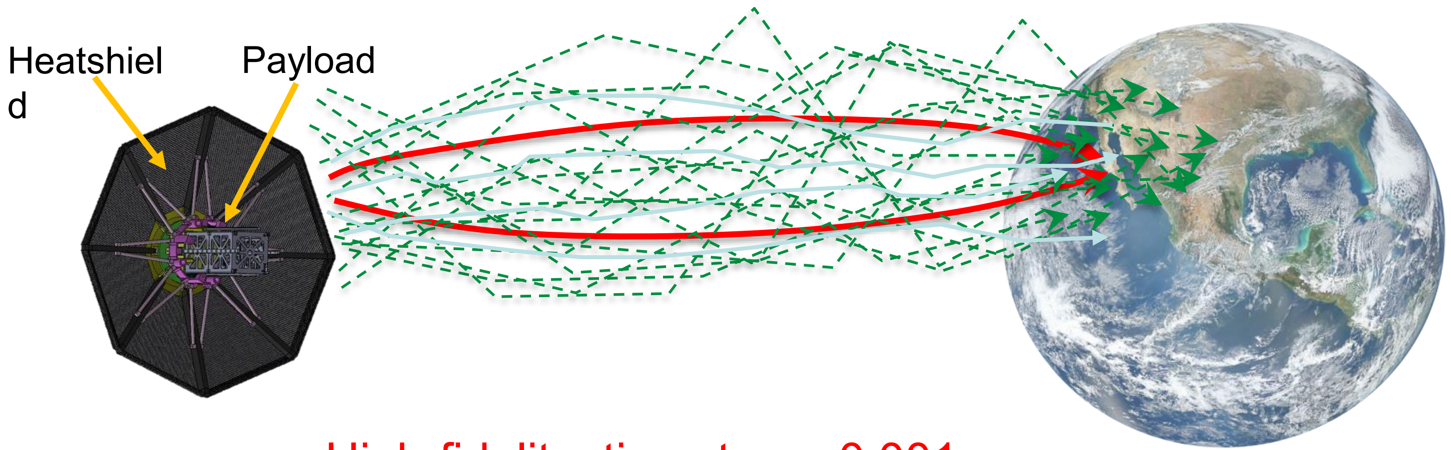
Optimization approach*

- Minimize $Var[\tilde{Q}](N, r, \beta)$ st. cost < budget constraint
- Build global surrogate for $\boldsymbol{c}(\beta)$ 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
  - Local 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

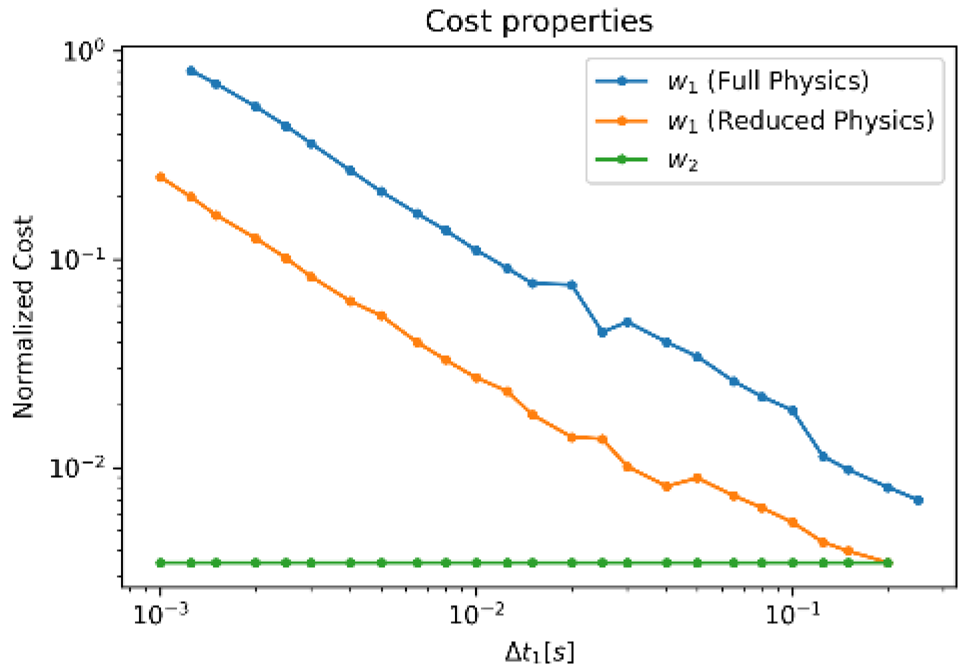


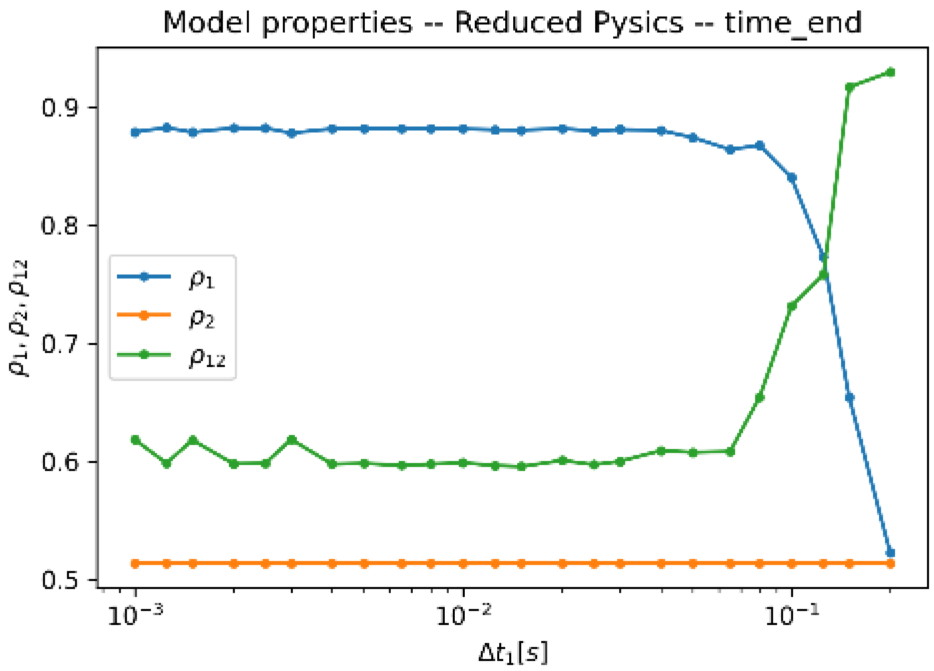
High-fidelity: timestep = 0.001

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

Low-fidelity: timestep = 0.25

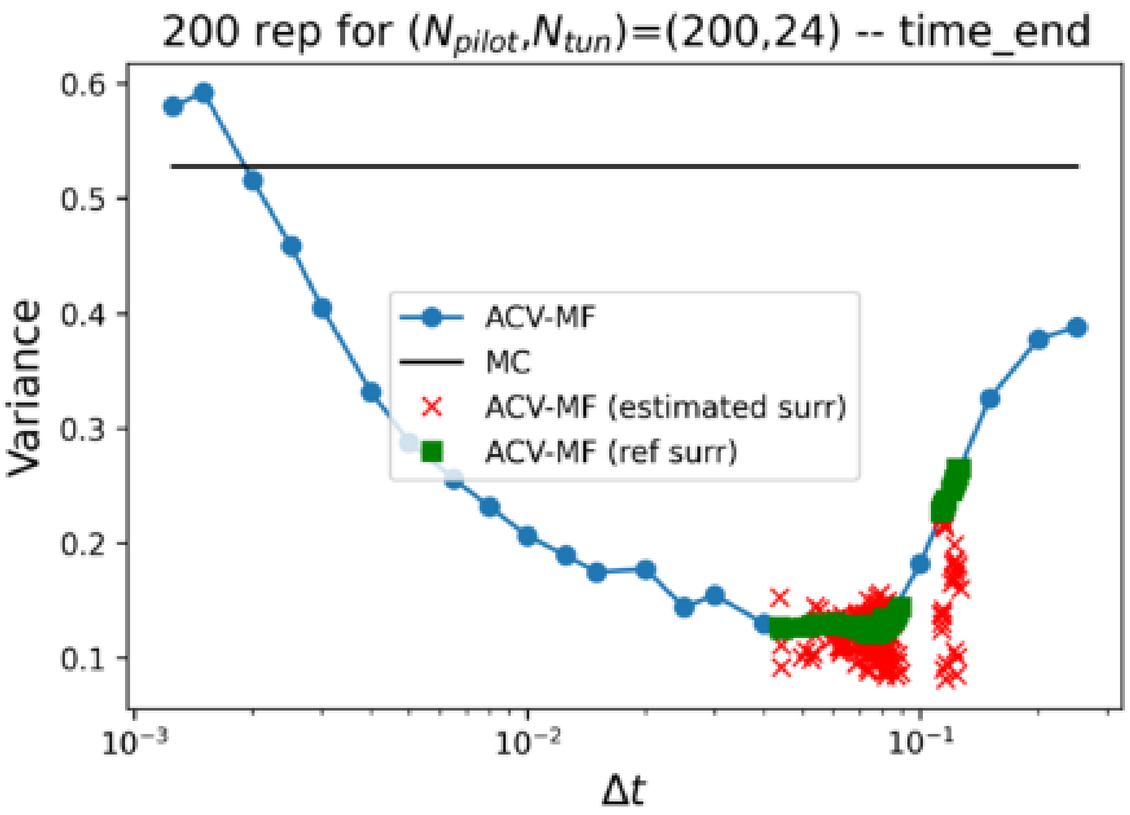
w_1: model cost
ρ_1 : correlation between Q_1 and Q
ρ_{12} : correlation between Q_1 and Q_2

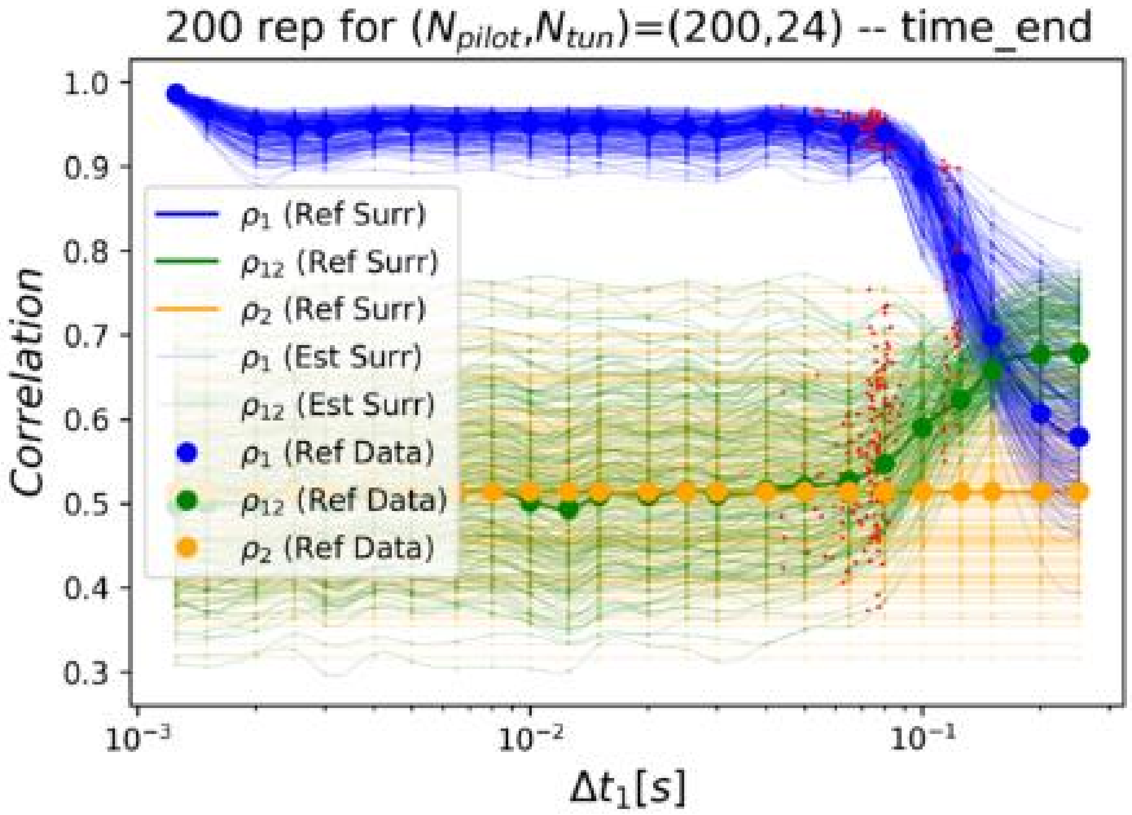




Results: most accurate surrogate

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



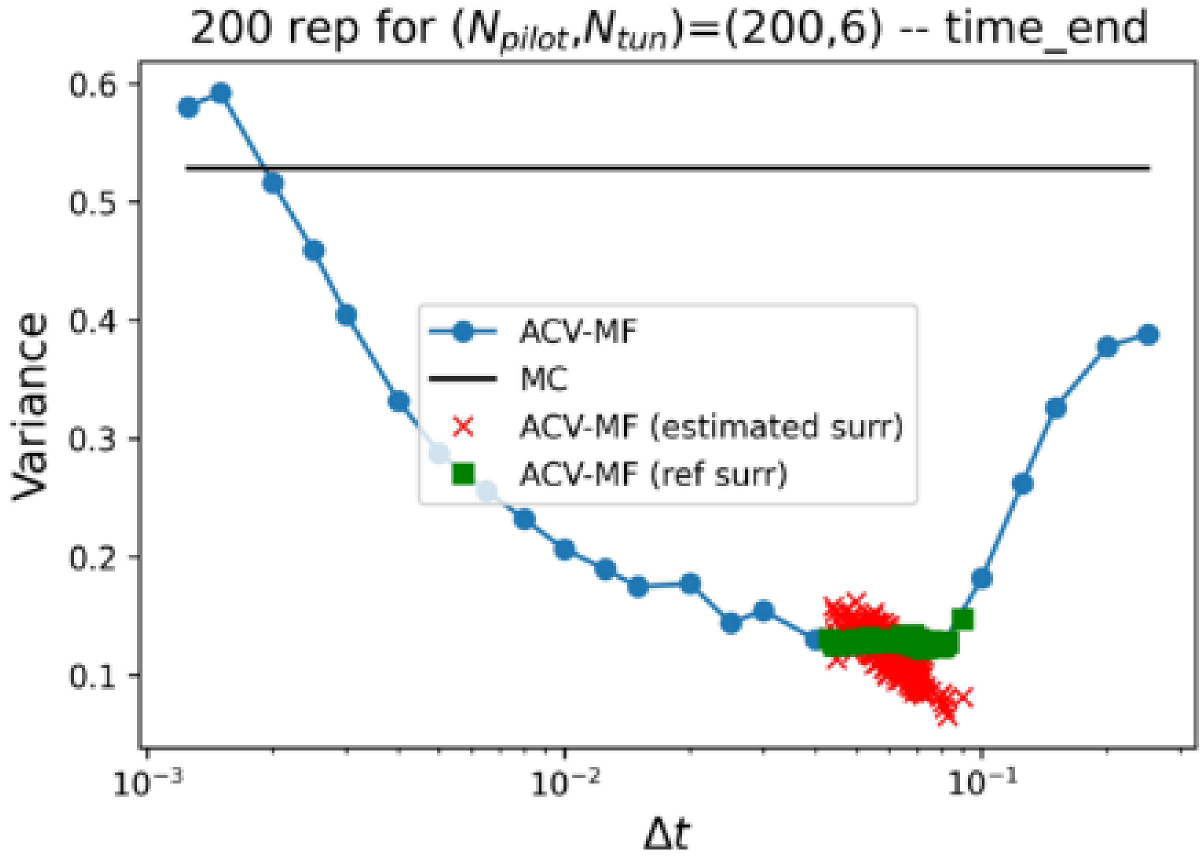


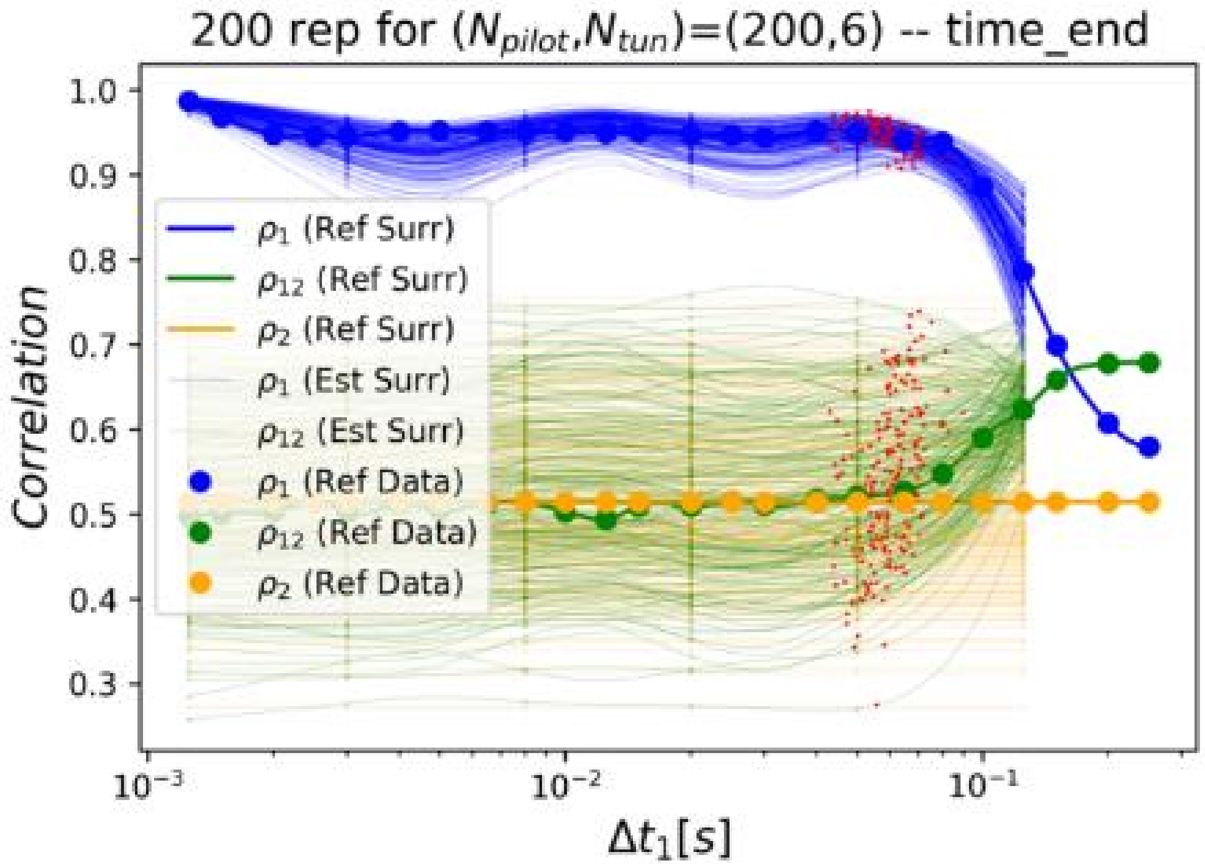
Optimal model tuning is achievable using surrogates for correlation

SHAPING THE FUTURE OF AEROSPACE

Results: more sparse measurements

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

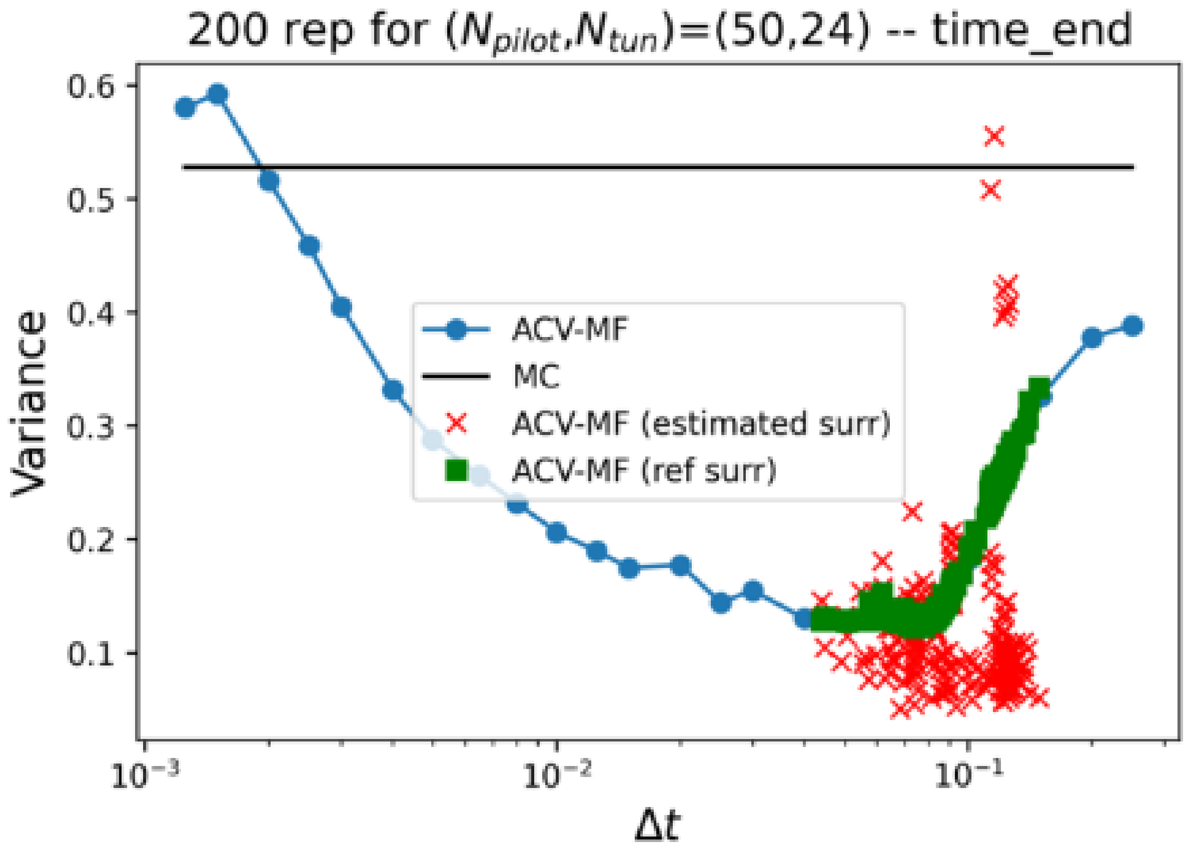


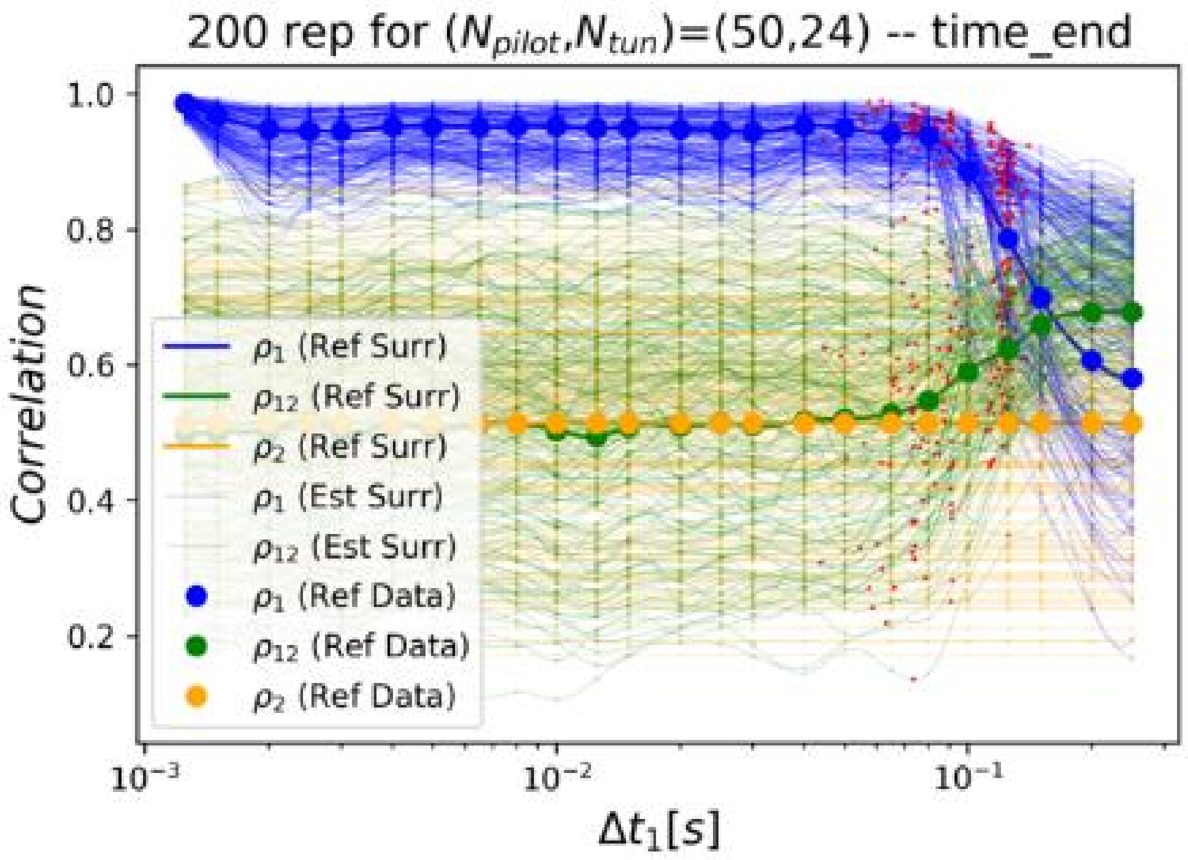


Smoothness is important for gradient-based optimization

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!

geoffrey.f.bomarito@nasa.gov