

An Uncertainty-Based Active Sampling Method for Coupled Multidisciplinary Systems

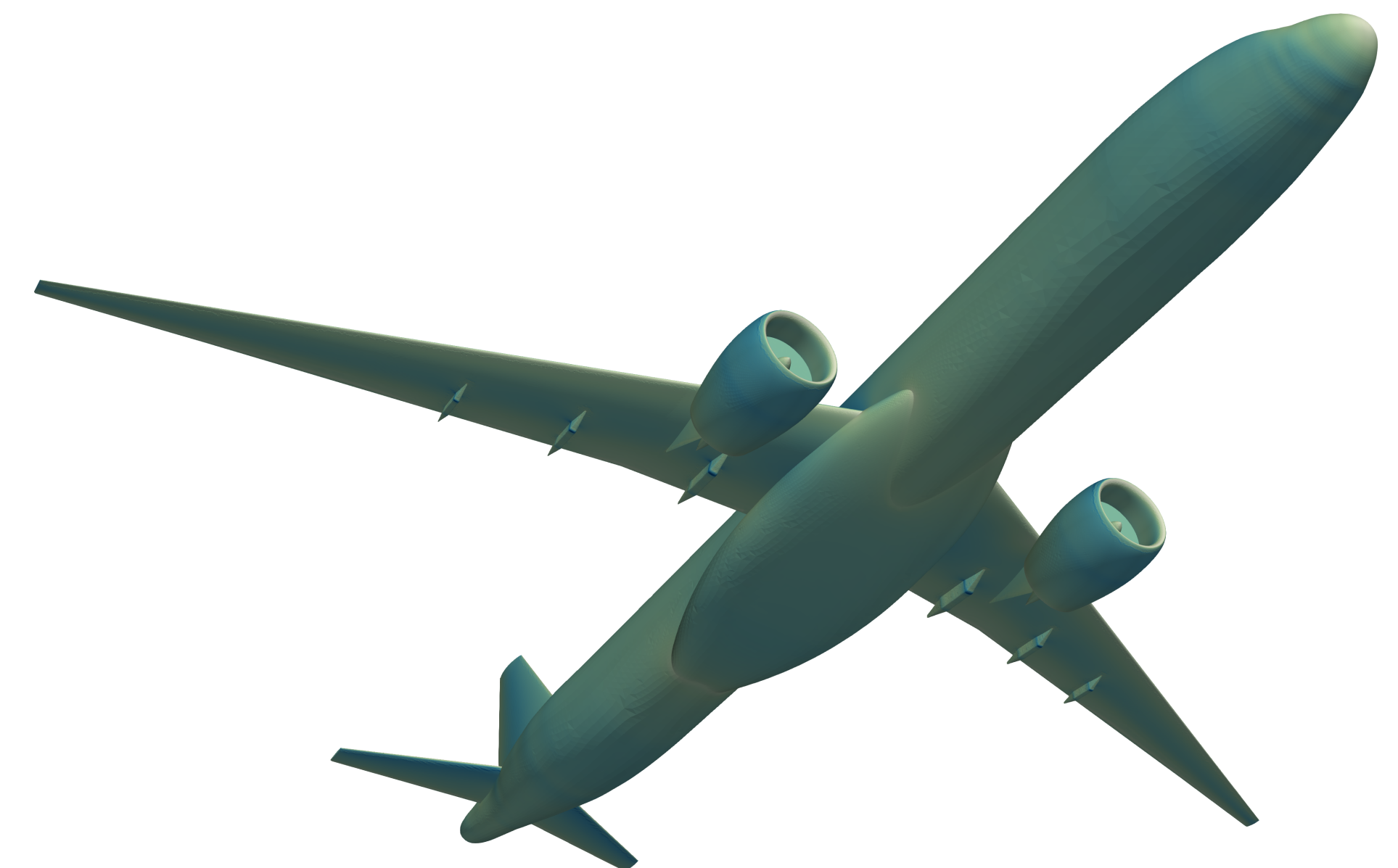
Pablo Norczyk Simon

Joaquim R.R.A. Martins (Advisor), Rodrigo Castellanos (Tutor), Rauno Cavallaro (Advisor)

Motivation and state of the art

MDO plays a vital role in complex system design, enabling the capture of coupled discipline interactions and system-level trade-offs. However, it faces an inherent **tension between mission fidelity and disciplinary fidelity**: tools simulating a complete mission across all subsystems must rely on simplified disciplinary models [1], while high-fidelity shape optimizations are limited to single or few operating points.

Surrogate models alleviate this by learning system responses from sparse data, but introduce epistemic uncertainty that propagates through the coupled system and impacts reliability. Reducing this uncertainty with uniform sampling is inefficient, often wasting resources on uninformative regions [2]. **Uncertainty-based active sampling** overcomes this by adaptively selecting new samples based on uncertainty, concentrating effort where it most impacts the objective, showing promising results on co-design problems [3-4].



Objectives

The objective of this thesis is to develop a **unified uncertainty-based active sampling method** for coupled multidisciplinary systems, enabling adaptive refinement of surrogate models across the full mission envelope to support high-fidelity aerodynamic shape optimization of complete aircraft configurations.

Methodology

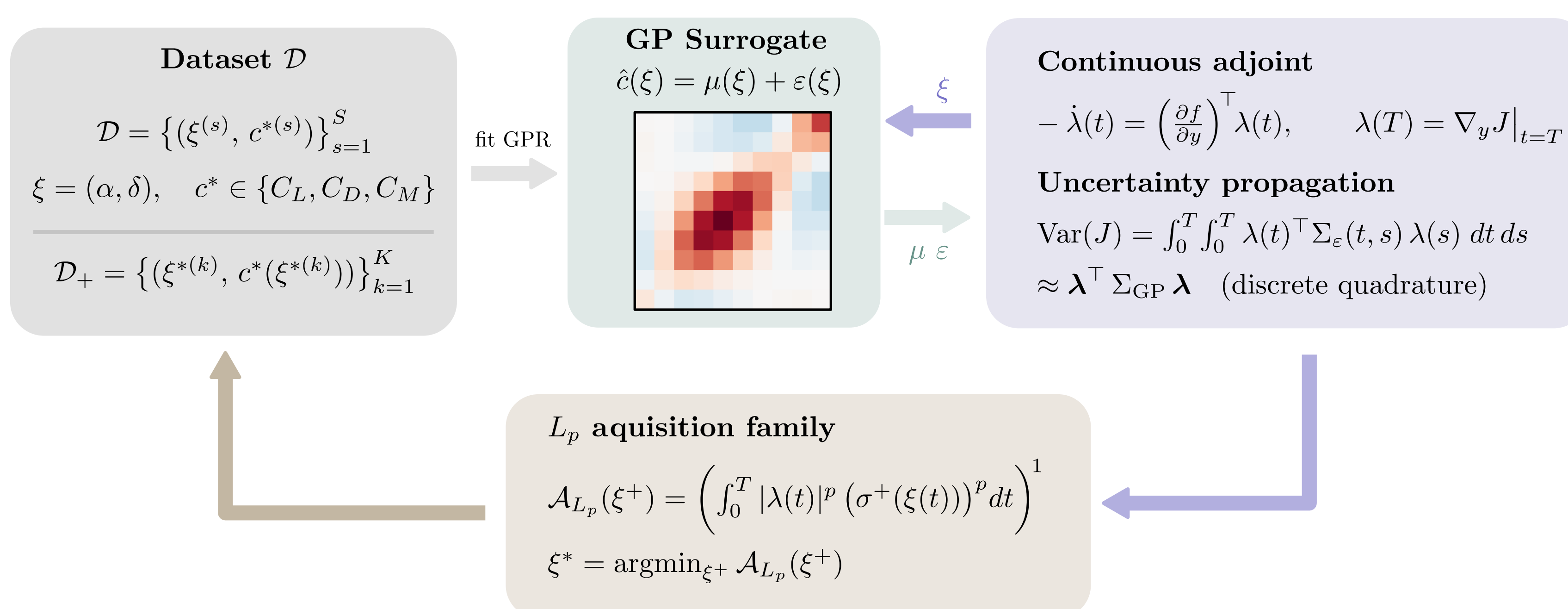


Figure 1. Active sampling framework: GP surrogates are fitted to a growing dataset, adjoint-based uncertainty propagation scores each candidate point, and the L_p acquisition criterion selects the optimal next sample.

To perform these optimizations we develop an uncertainty-based active sampling framework that refines surrogate models where it most impacts mission-level performance:

- **Gaussian Process surrogates** replace expensive disciplinary models embedded in a full mission simulation that evaluates the QoI.
- **Direct/adjoint sensitivities** propagate across the full coupled system, capturing how local surrogate perturbations affect the QoI.
- **GP posterior uncertainty** quantifies the probable magnitude of those potential errors.
- Combining the two, every candidate is scored, within and across surrogates, by its expected impact on QoI uncertainty.

Results

Results on an analytical ODE trajectory test case compare three uncertainty-propagated strategies (L_1 , L_2 , Σ), a non-propagated baseline (σ), and passive Halton sampling.

$$\mathcal{A}_{\text{exact}} = \sum_i \int_0^T \int_0^T \psi_i(t) \Sigma_i^+(t, s) \psi_i(s) dt ds$$

$$\mathcal{A}_{L_p} = \left(\sum_i \left(\int_0^T |\psi_i|^p (\sigma_i^+)^p dt \right)^{1/p} \right)^p$$

$$\mathcal{A}_\sigma = \sum_i \sigma_{\text{GP},i}(\xi^+)$$

At $N=15$ samples, **L_1 achieves the lowest RMSE (2.51) — 4.6× lower than the non-propagated baseline (σ , 11.63) and 300× lower than Halton (762).** The success rate (trajectory error $< \pm 1$ m) reaches 100% for L_1 versus 80.7% for σ and just 2.3% for Halton, confirming that the coupled adjoint-based uncertainty propagation is the key performance driver when concentrating effort where it most impacts the objective.

Proof of concept for coupled systems — extension to full aircraft configurations is ongoing.

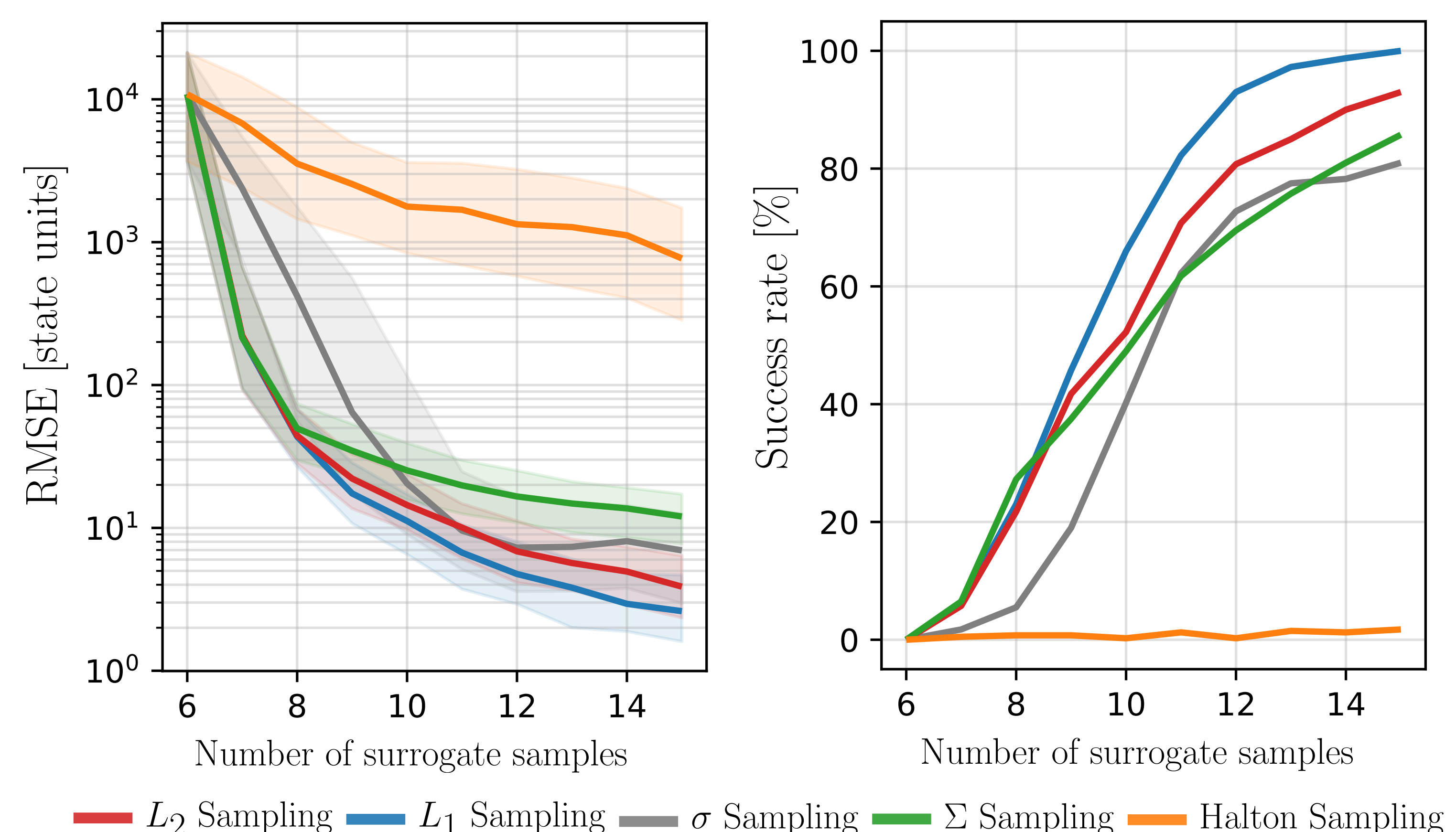


Figure 2. RMSE (left) and success rate, defined as trajectory error $< \pm 1$ m, (right) vs. number of surrogate samples across five sampling strategies

- [1] P. Norczyk Simon, R. Quiben Figueroa, A. Cini, and R. Cavallaro, "Multidisciplinary Design and Optimization of H2-Powered Regional Aircraft Architectures," AIAA 2025-0360, AIAA SciTech 2025 Forum, January 2025.
- [2] J. T. Hwang, J. P. Jasa, and J. R. R. A. Martins, "High-Fidelity Design-Allocation Optimization of a Commercial Aircraft Maximizing Airline Profit," Journal of Aircraft, vol. 56, no. 3, pp. 1164–1178, 2019.
- [3] J. R. Cangelosi and M. Heinkenschloss, "Sensitivity-Driven Adaptive Surrogate Modeling for Simulation and Optimization of Dynamical Systems," arXiv:2509.04651, September 2025.
- [4] J. T. Needels, Efficient Multidisciplinary Analysis and Optimization of Hypersonic Vehicles Using Multi-Fidelity Surrogate Models, Ph.D. dissertation, Stanford University, August 2024.



PhD Student:

Pablo Norczyk - pnorczyk@bsc.es

Advisors:

Rauno Cavallaro - rcavalla@bsc.es

Joaquim R.R.A. Martins - jram@umich.edu

Rodrigo Castellanos - rcastell@ing.uc3m.es