

Safe Bayesian Optimization with Physics Residuals

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Motivation

Optimizing chemical reactors requires finding the "sweet spot" (max profit) without violating safety constraints [1][2]

- **Data Scarcity:** Real plant experiments are expensive and time-consuming
- **The Risk:** Standard "Black-Box" Machine Learning (Bayesian Optimization) is blind to physics. It often explores dangerous regions just to learn where the boundaries are

We embed **known physical laws** (mass/energy balances) into optimization logic to prevent **unsafe exploration**

Methodology

We modified the standard Acquisition Function to include a **Physics Penalty**. This turns "Black Box" into "Gray Box"

$$\alpha_{PI}(\mathbf{x}) = \underbrace{J(\mathbf{x})}_{\text{Cost}} + \underbrace{E(\mathbf{x})}_{\text{Exploration}} + \underbrace{\lambda \cdot P_{\text{safe}}(\mathbf{x})}_{\text{Safety (UCB)}} + \underbrace{\gamma \cdot P_{\text{phys}}(\mathbf{x})}_{\text{Physics Penalty}}$$

We substitute the GP mean predictions (μ) directly into the system's governing equations. If the GP's predictions are physically consistent, the residual is zero. We penalize deviations from this consistency:

$$P_{\text{phys}}(\mathbf{x}) = ||\mathcal{F}(\mu_s(\mathbf{x}), \mathbf{x})||$$

- If the model predicts a state that violates physics, P_{phys} spikes, discouraging the optimizer from sampling that region

Case Study: Non-isothermal CSTR with two parallel reactions

It is described by a set of 5 coupled Ordinary Differential Equations (ODEs) representing the dynamic behavior, e.g. the energy balance:

$$\frac{dT}{dt} = \frac{F}{V}(T_{in} - T) + \frac{1}{\rho c_p} \sum_{j=1}^2 (-\Delta H_j) r_j + \frac{UA}{V\rho c_p} (T_c - T)$$

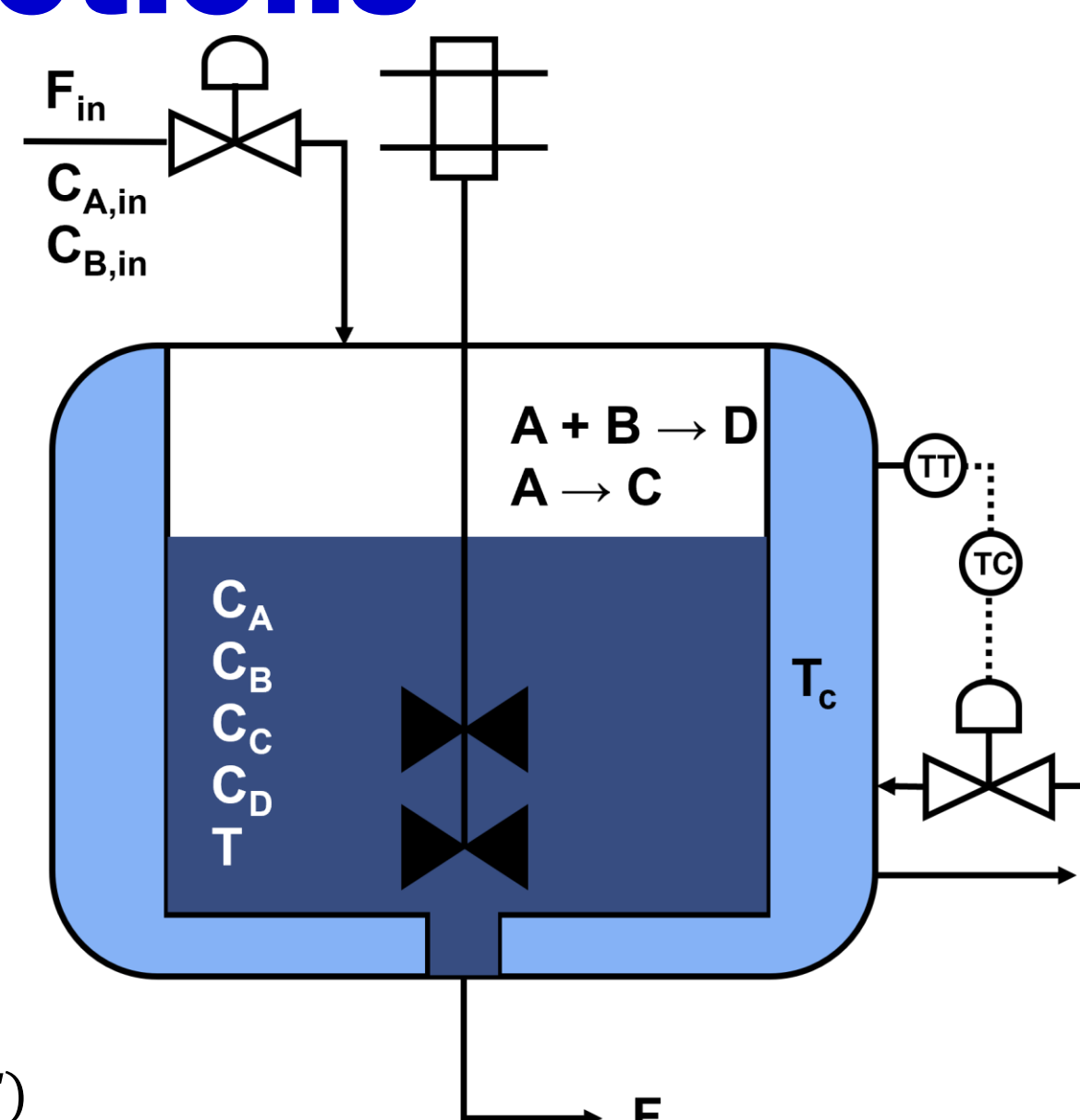


Fig 1: CSTR Schematic showing inputs (A, B) and outputs (C, D, Heat)

Target: Maximize the profit

Constraint: Temperature must stay below **650K**

Results & Discussion

Trajectory Analysis

- We compared a **Baseline BO** vs. **Our Algorithm**

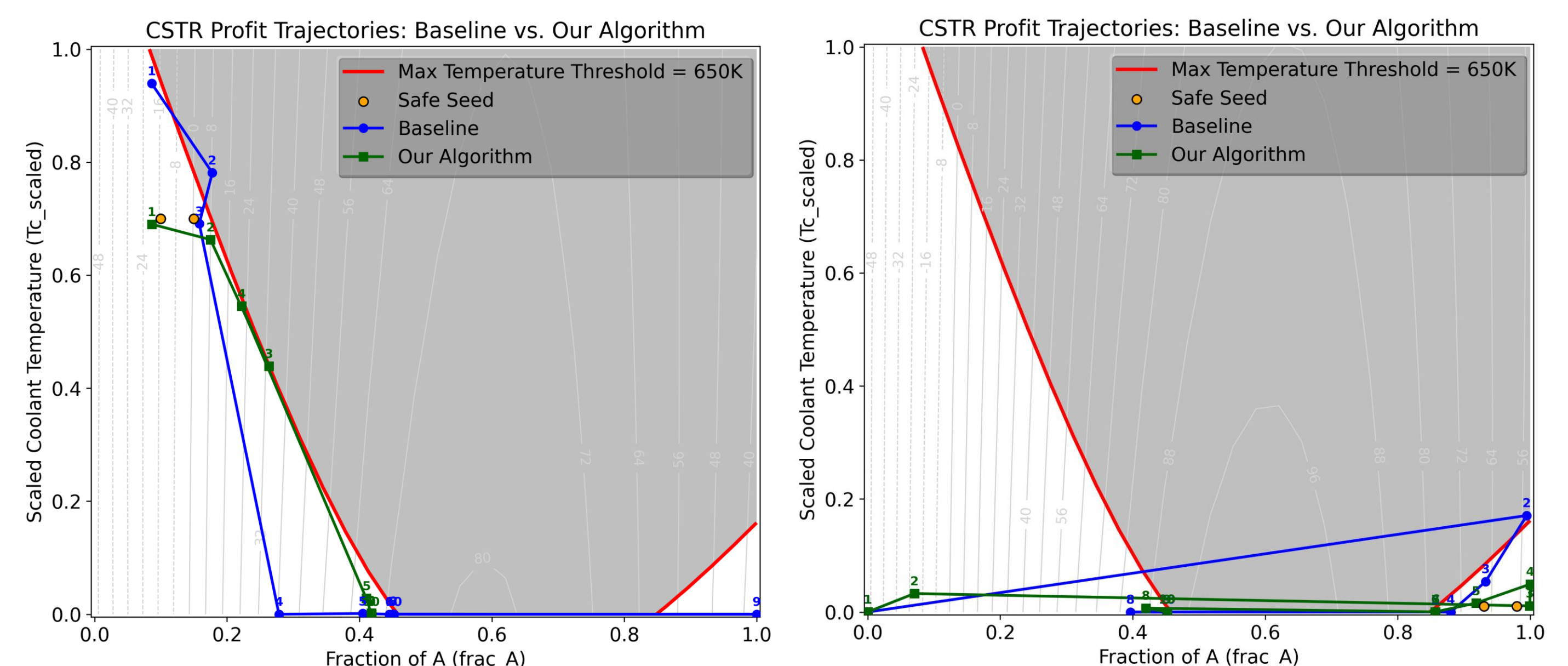


Fig 2: Optimization trajectories overlaid on ground-truth economic profit landscape

Robustness & Convergence

- Tested on 15 independent runs with random seed pairs

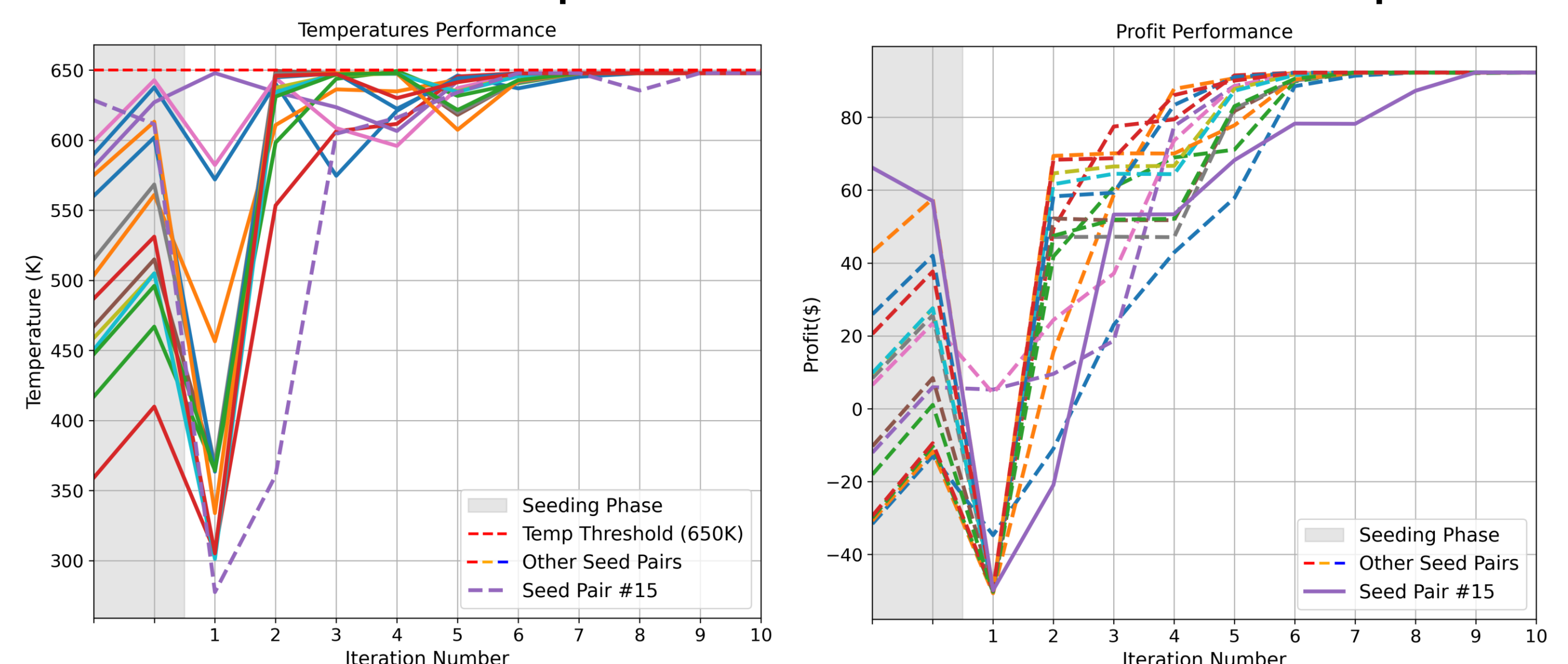


Fig 3: Temperature and Profit performance profiles

Residual Evolution

- Shown for a case with four seed points

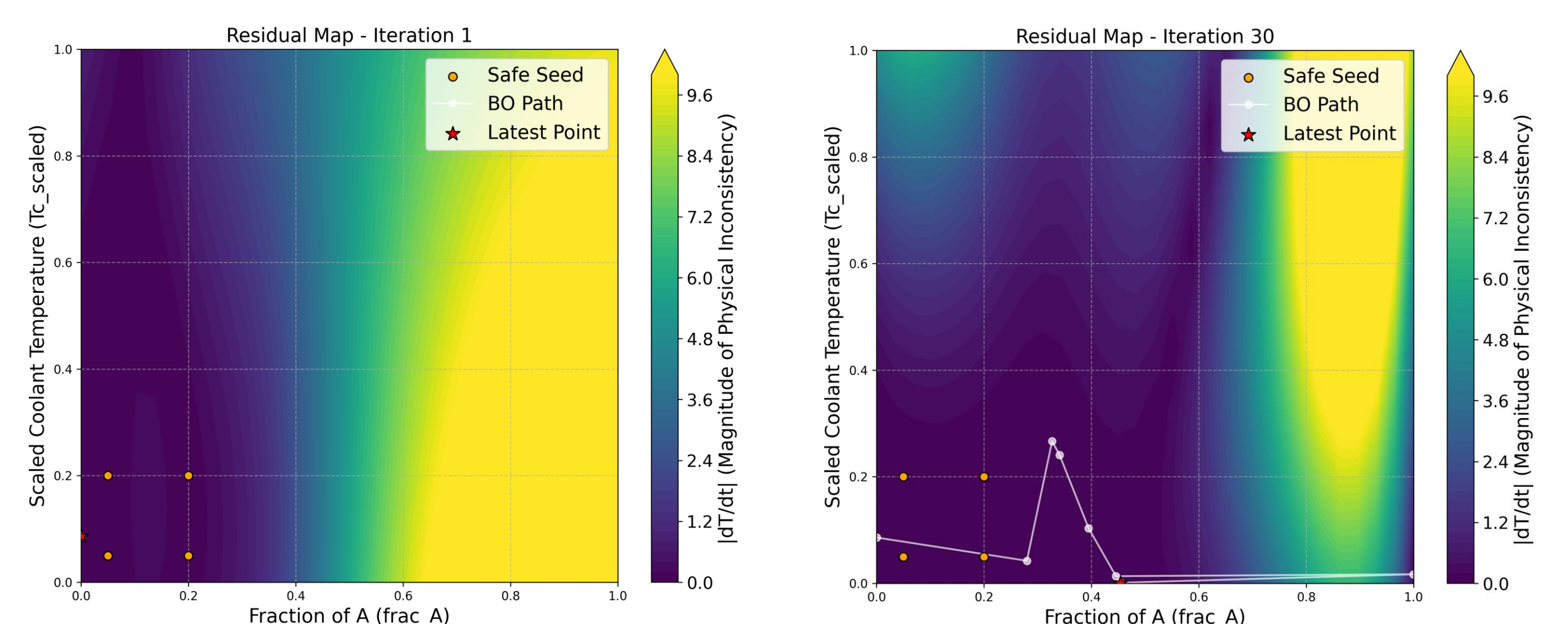


Fig 4: Global residual evolution over ground-truth landscape

Conclusion & Outlook

- This framework allows for **safe, real-time optimization** of chemical processes even with very limited initial data
- **Future Work:** Application to industrial systems with uncertain parameters or measurement noise.

References

- [1] Sui, Y., Gotovos, A., Burdick, J., and Krause, A. (2015). Safe Exploration for Optimization with Gaussian Processes. In Proceedings of the 32nd International Conference on Machine Learning, 997–1005. PMLR.
- [2] Dong, L., Zagórowska, M., Liu, T., Durkin, A., and Mercangöz, M. (2024). Pi-cof: A bilevel optimization framework for solving active learning problems using physics-information. In 2024 IEEE Conference on Control Technology and Applications (CCTA), pages 101–106. IEEE.