

Agentic Systems for Calibrating Cosmological Simulations

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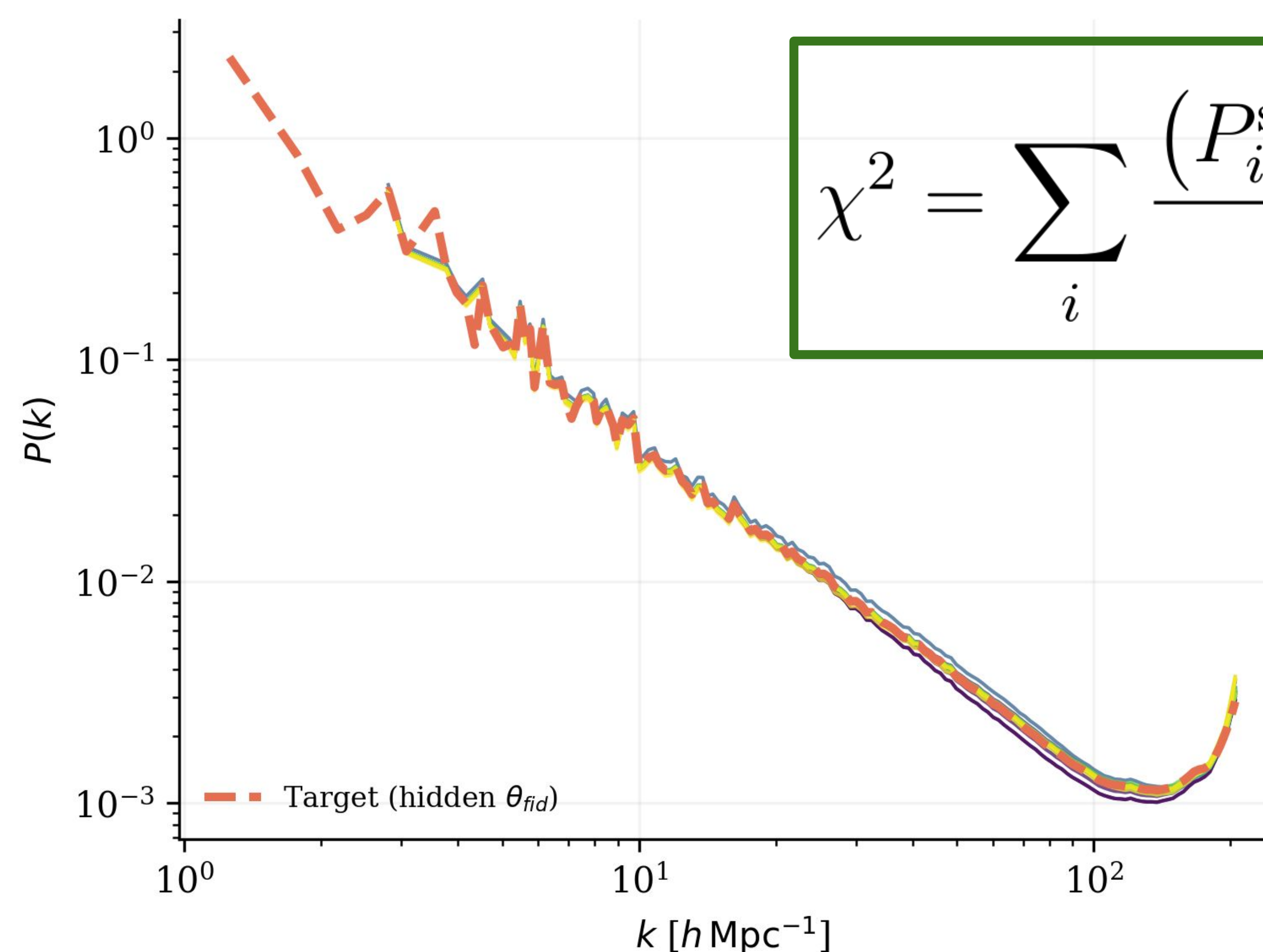
Setup: Calibration as Optimization

Sim $P^{\text{target}}(k) = P(k; \theta_{\text{true}})$

Goal: want to find θ that best **minimizes** the **discrepancy** between the **simulated spectra** and the **target spectra** under a **budget**

$$\hat{\theta} = \arg \min_{\theta \in \Theta} d(P(k; \theta), P(k; \theta_{\text{true}}))$$

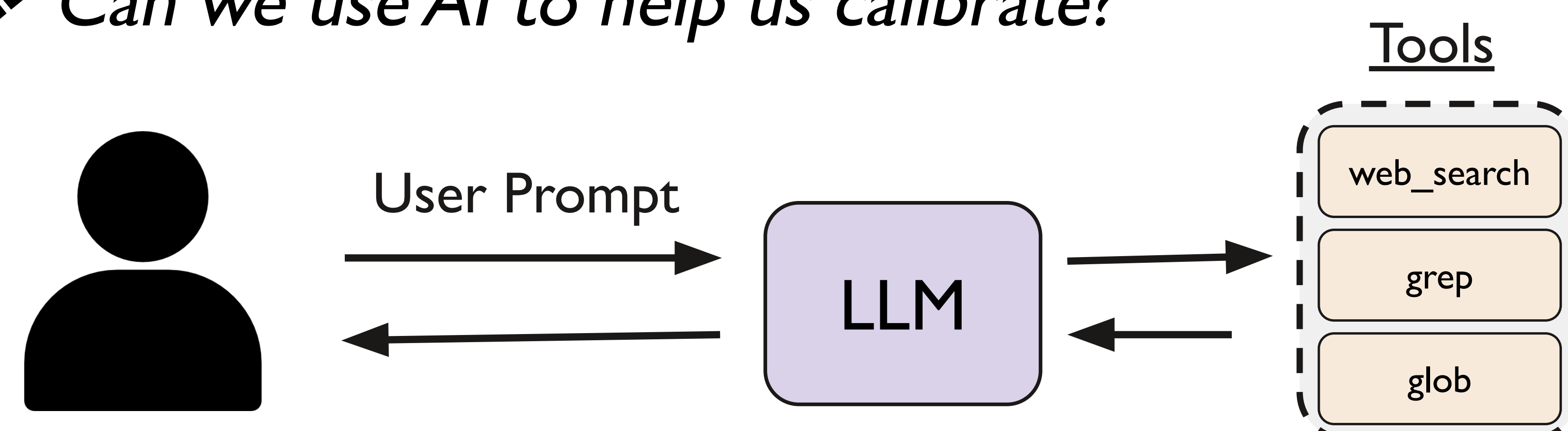
Simulated data Target data



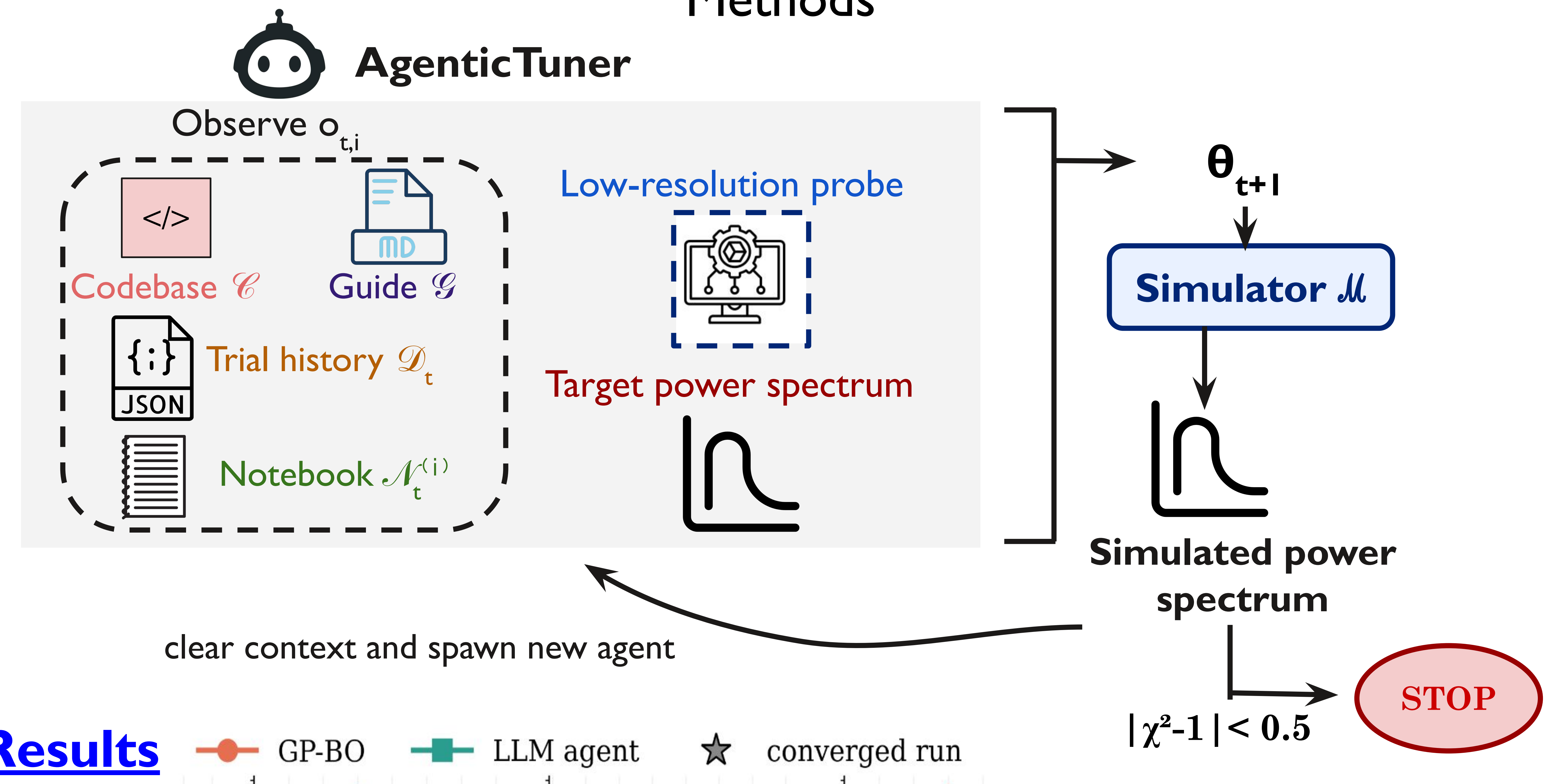
$$\chi^2 = \sum_i \frac{(P_i^{\text{sim}} - P_i^{\text{target}})^2}{\sigma_i^2}$$

Problem: Standard calibration pipelines use **Bayesian optimization (BO)**, but they scale poorly with dimensions!!

❖ Can we use AI to help us calibrate?



Methods



Results

— GP-BO — LLM agent ★ converged run

Giving LLM agents informal priors (such as codebase, documentation, and other contextual information that an expert human scientist may possess) can result in competitive calibration performance with less CPU time.

