Agentic AI for Scientific Model Discovery

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with

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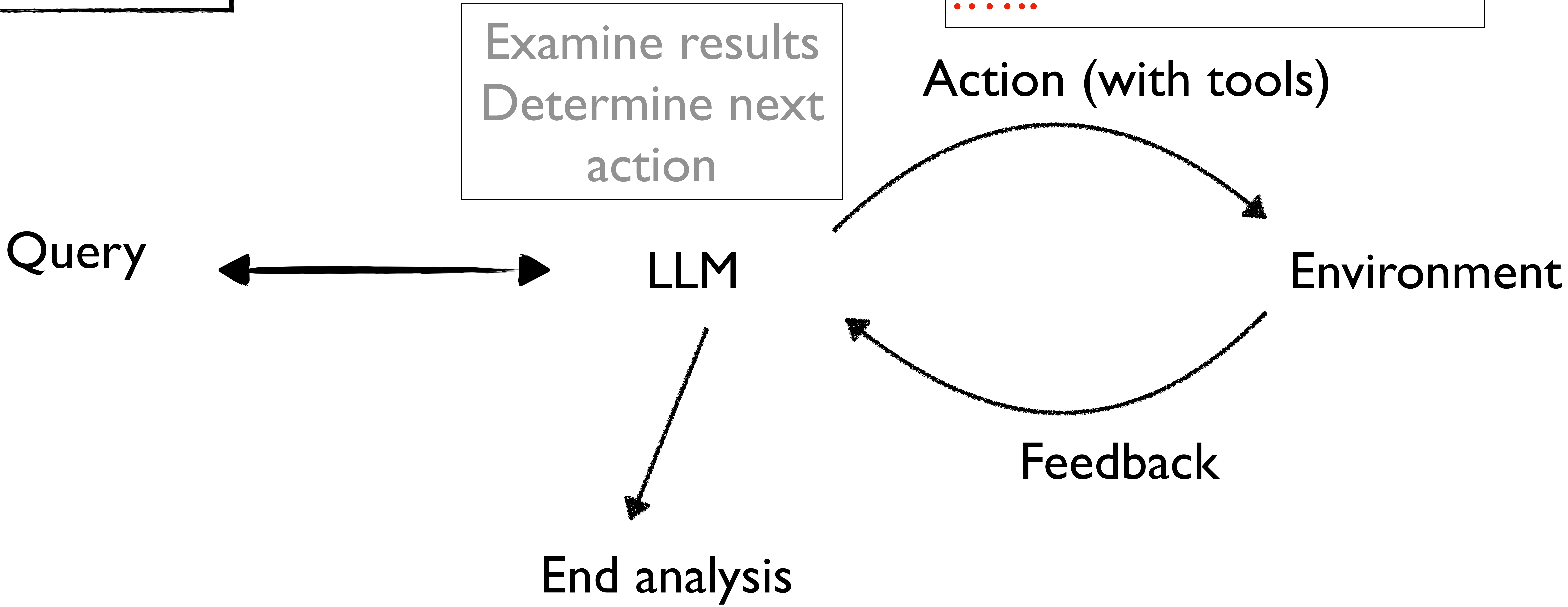
(Traditional) LLM workflow

Query $\longrightarrow$ LLM $\longrightarrow$ Output

Agentic framework

1. Read documents/code
2. Execute code
3. Web search
4. Make plots

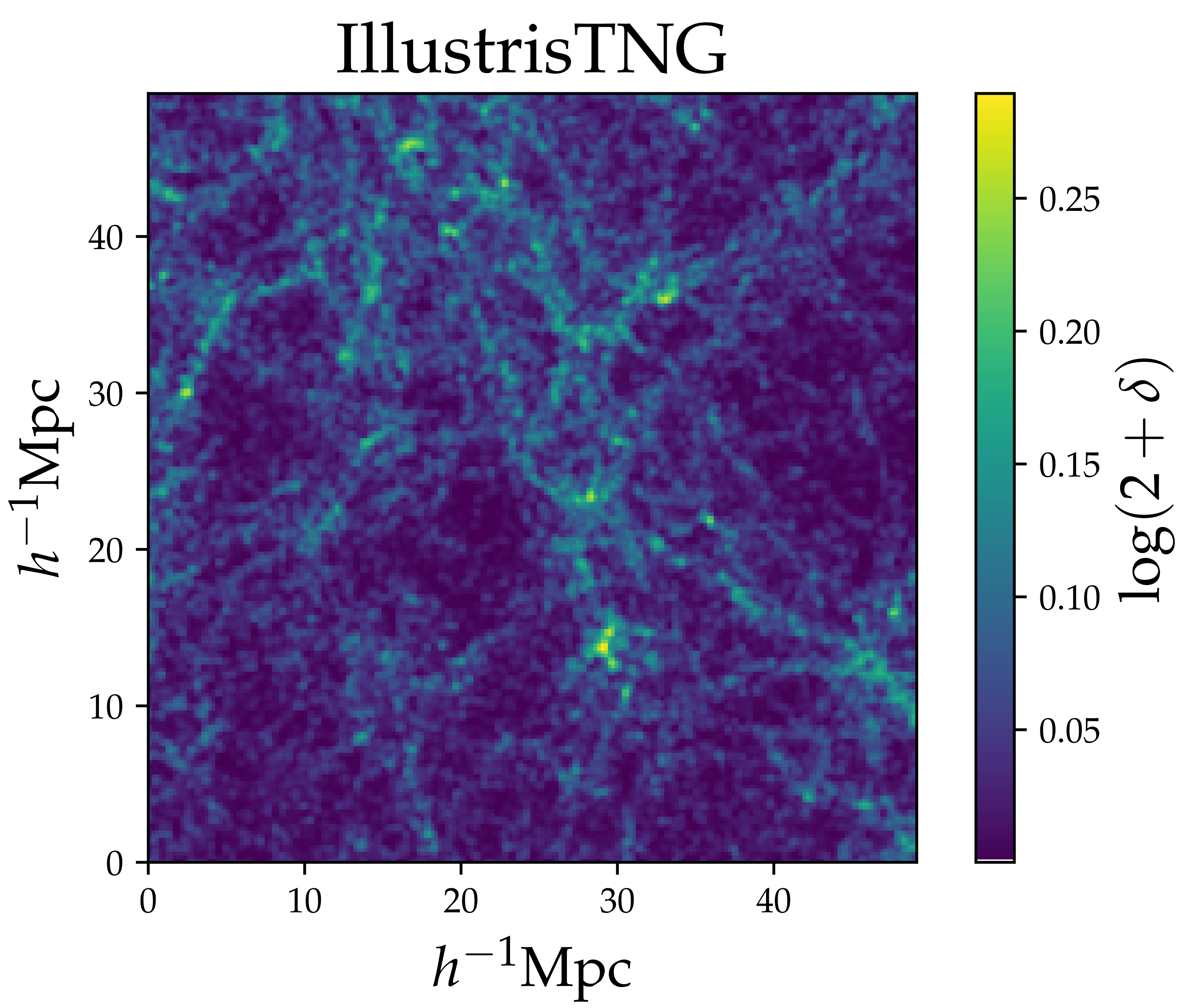
……..

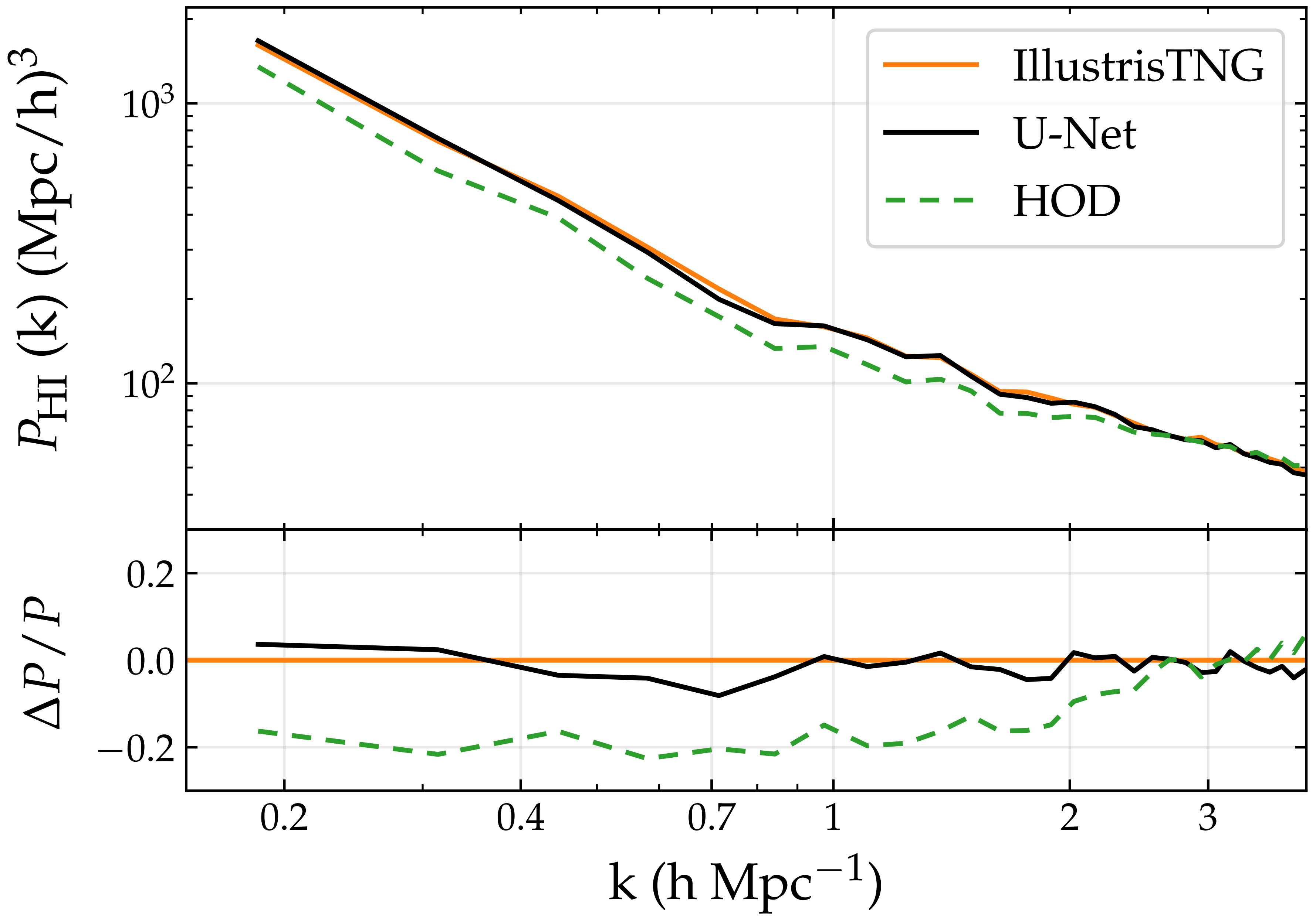


Agent = LLM + scaffold

1. Agents for (analytic) surrogate modeling
2. Agents for transient searches
3. Agents for cross-disciplinary workflows

Surrogate models are ubiquitous in sciences

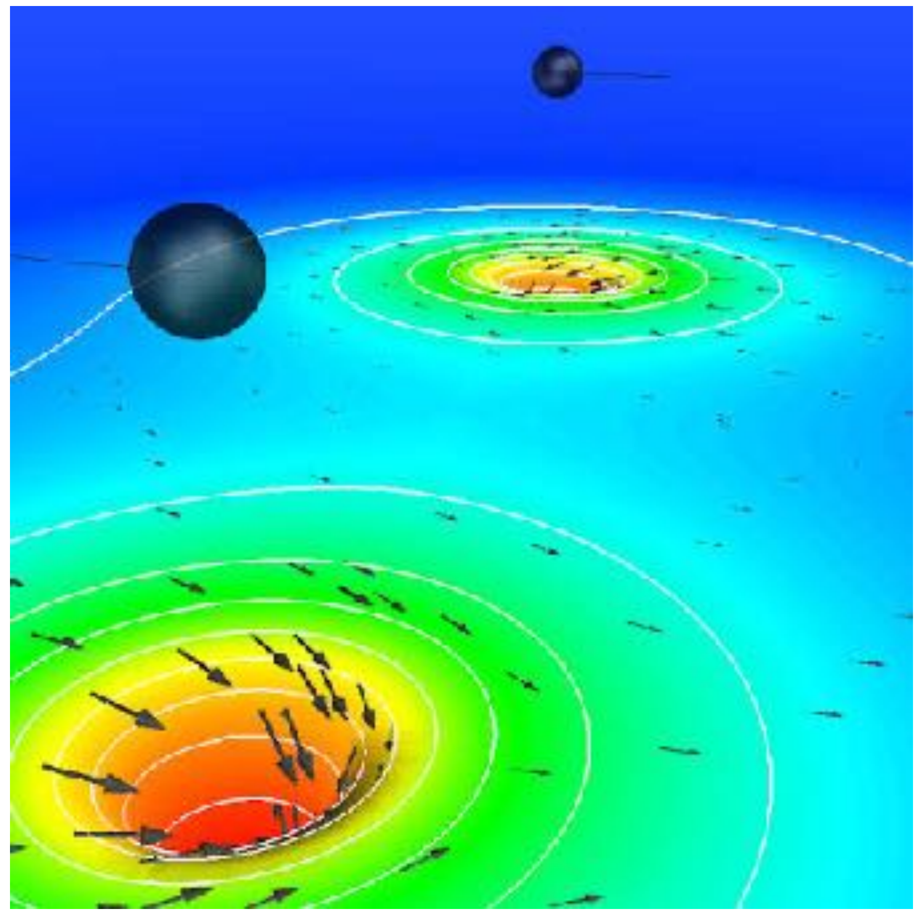


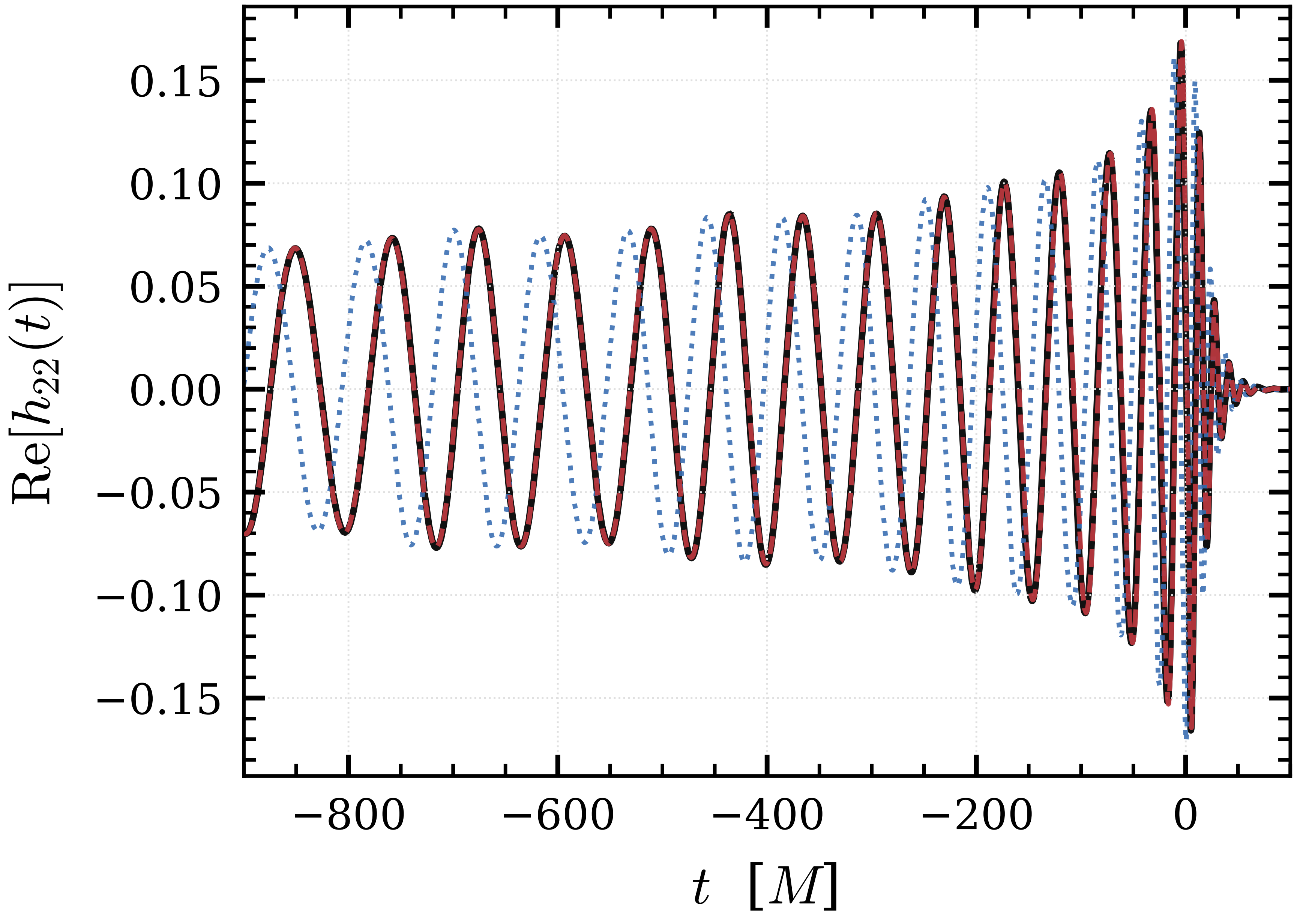


(Simulation ~10^{8-9} CPU hours)

(ML surrogate/emulator)

(Analytic surrogate)





(Simulation ~10^{5-6} CPU hours)

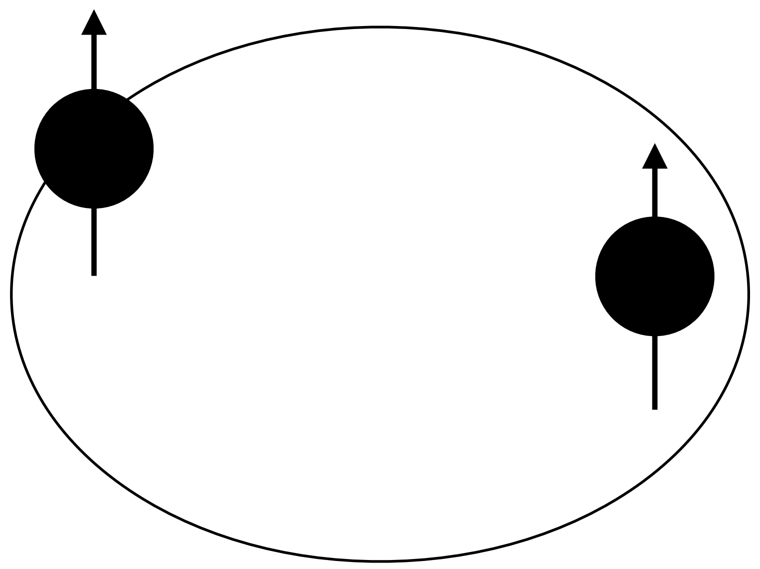
(ML surrogate)

(Analytic surrogate)

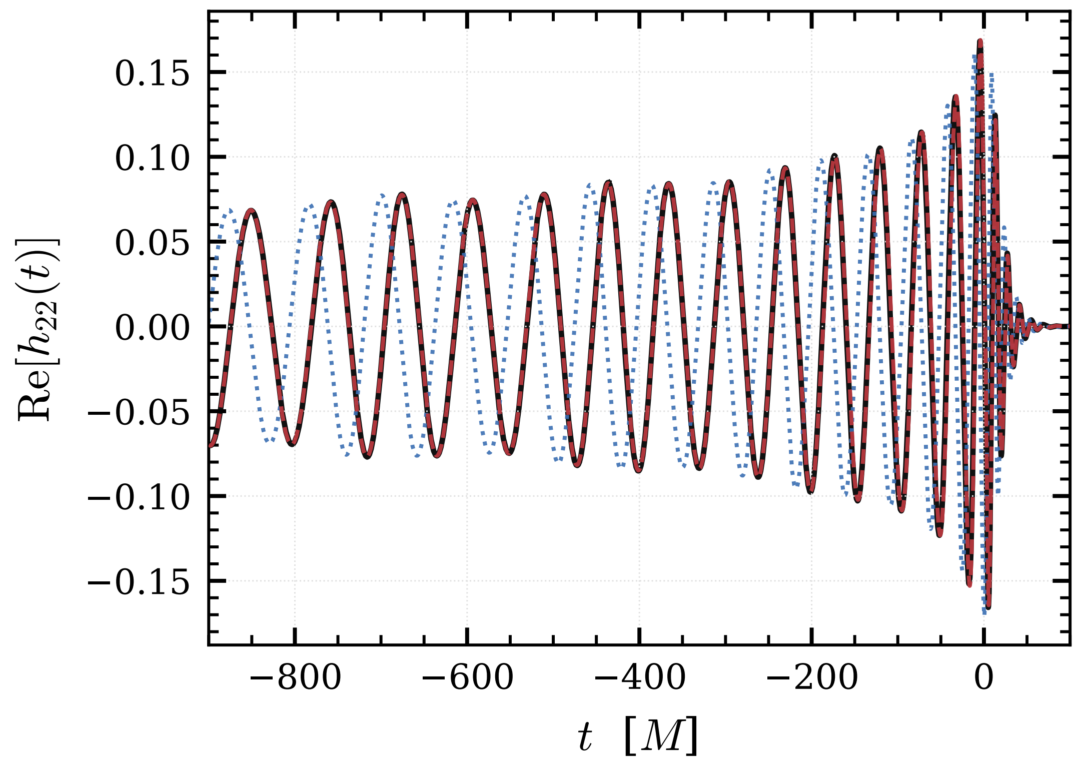
1. Agents for surrogate/emulator modeling

- Surrogates are computationally cheap models used to approximate expensive simulations

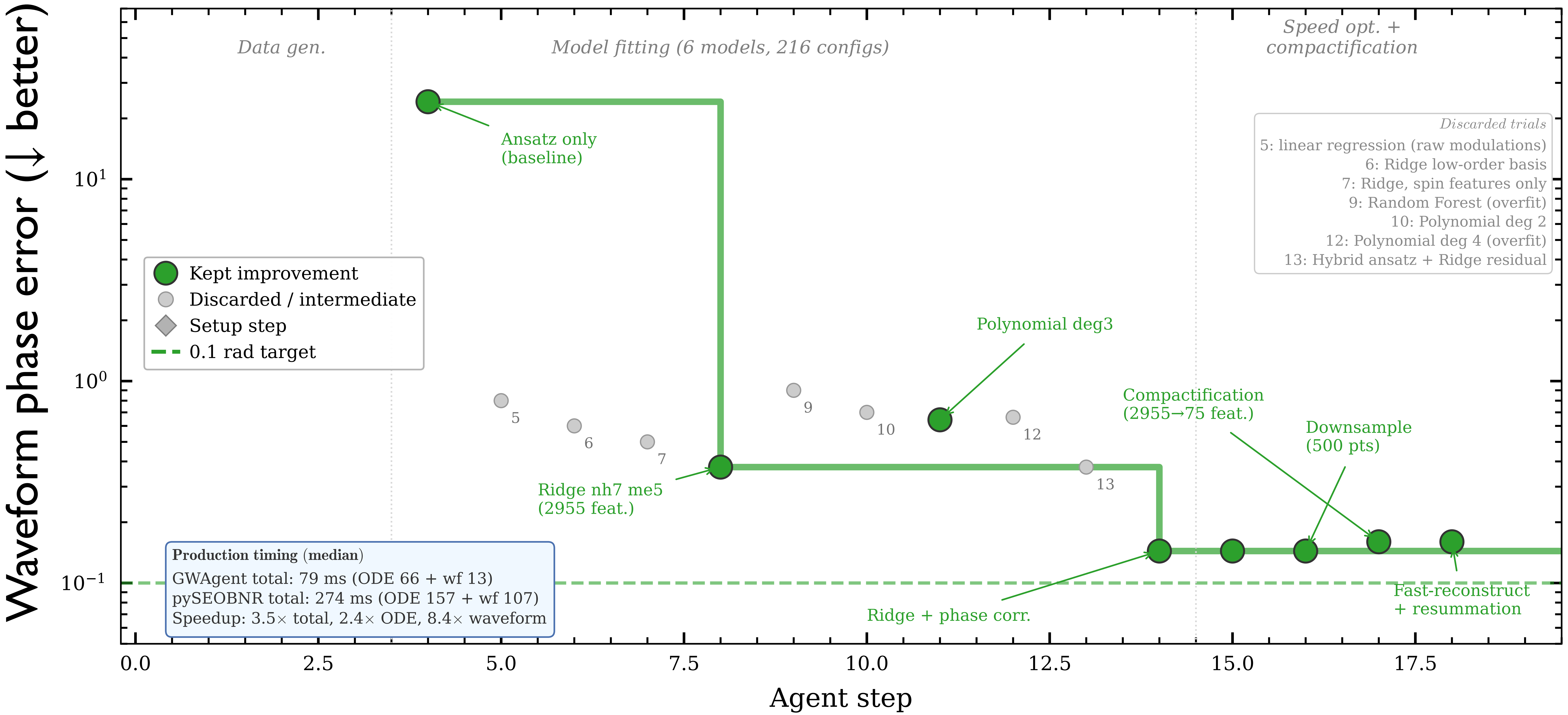
- Strong case for agents:
  1. Verifiable objective function (simulator ground truth is known)
  2. Rapid low-cost Iterations
  3. Rich/high-dimensional search space



$$[m_2/m_1, \chi_{1z}, \chi_{2z}, e, \zeta] \longrightarrow$$



Generate candidates → Fit sim.data → Validate and simplify



See also: AlphaEvolve (arXiv:2506.13131), Autoresearch (Andrej Karpathy)

Analytic/symbolic target model
+ Compactification/Interpretation

~3000 terms

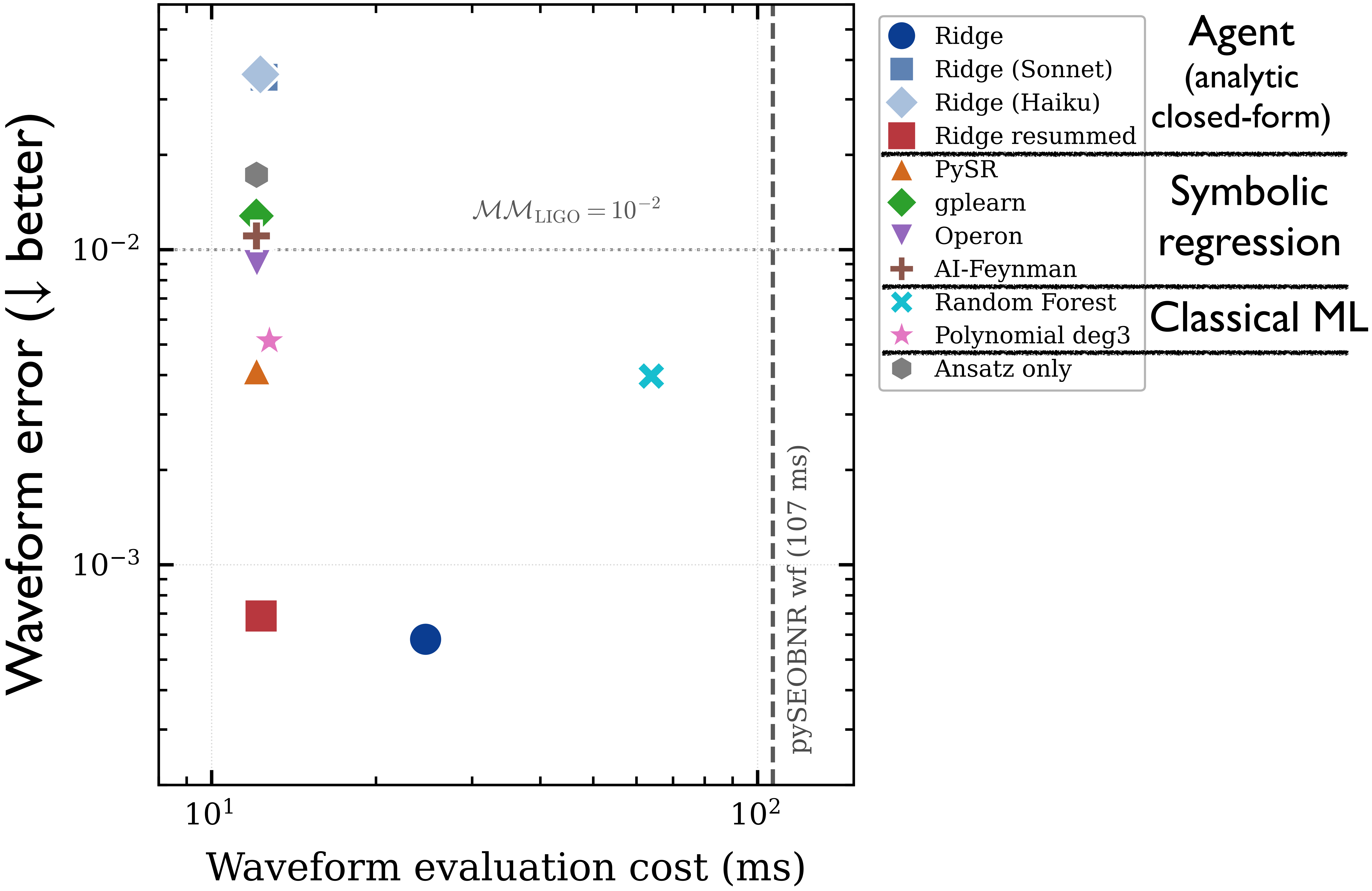
$$F_{\text{agent}}(x, e, \zeta) = \sum_{j=1}^{N\sim 2955} c_j \cdot e_i^{a_j} \cdot x_i^{b_j} \cdot \nu_i^{c_j} \cdot \mathrm{Trig}(k_j, \zeta)$$

$\downarrow$

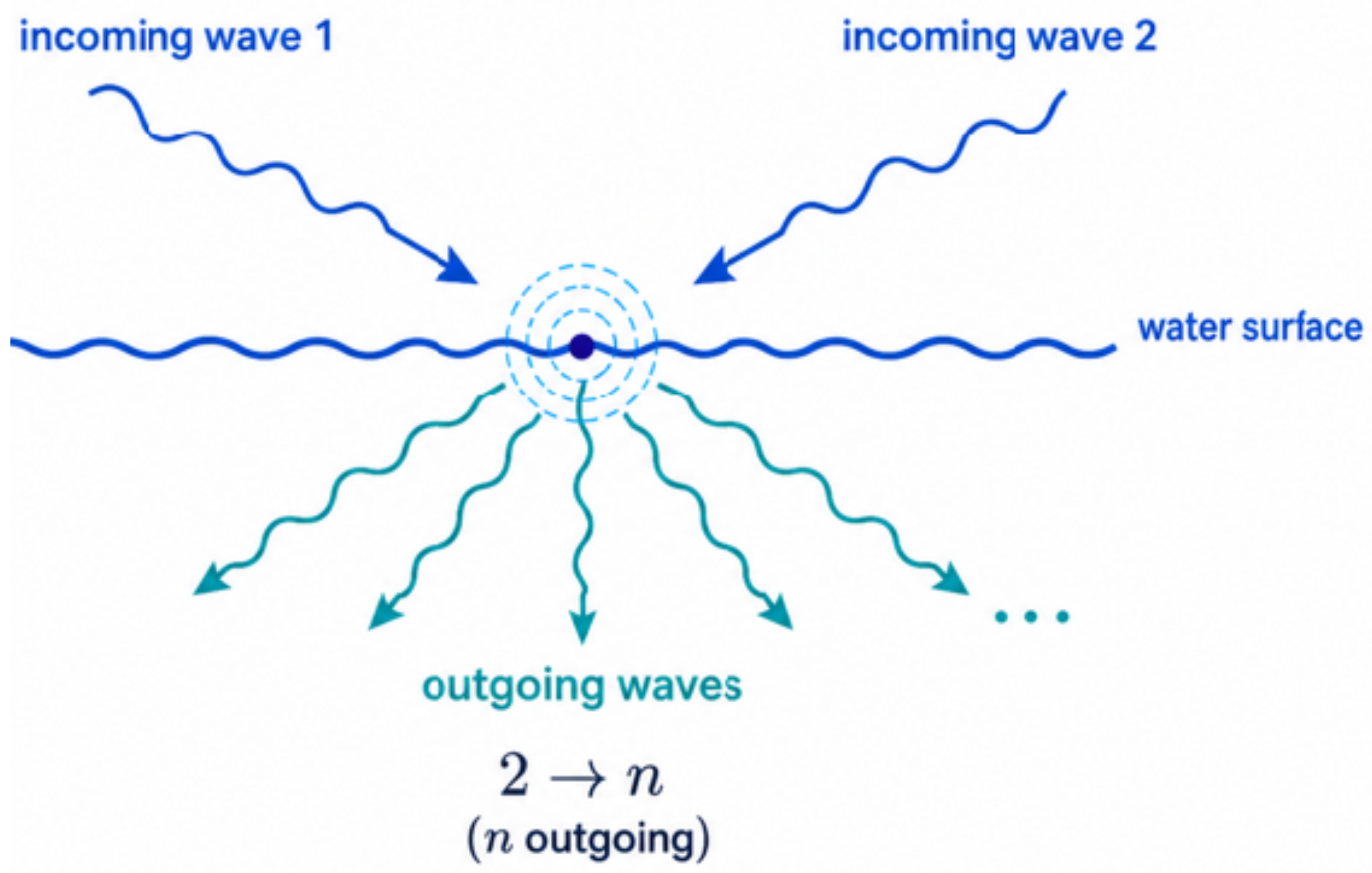
~10 terms

$$F_{\text{agent}}(x, e, \zeta) \approx \sum_{i=1}^{N\sim 10} \frac{e^{a_i}}{(1-e^2)^{1/2}} x^{b_i} \nu^{c_i} \chi_S^{d_i} \chi_A^{f_i} \left[c_0^{(i)} + \sum_{k=1}^{3} \left(\alpha_k^{(i)} \cos(k\zeta) + \beta_k^{(i)} \sin(k\zeta) \right) \right]$$

Agentic solution outperforms



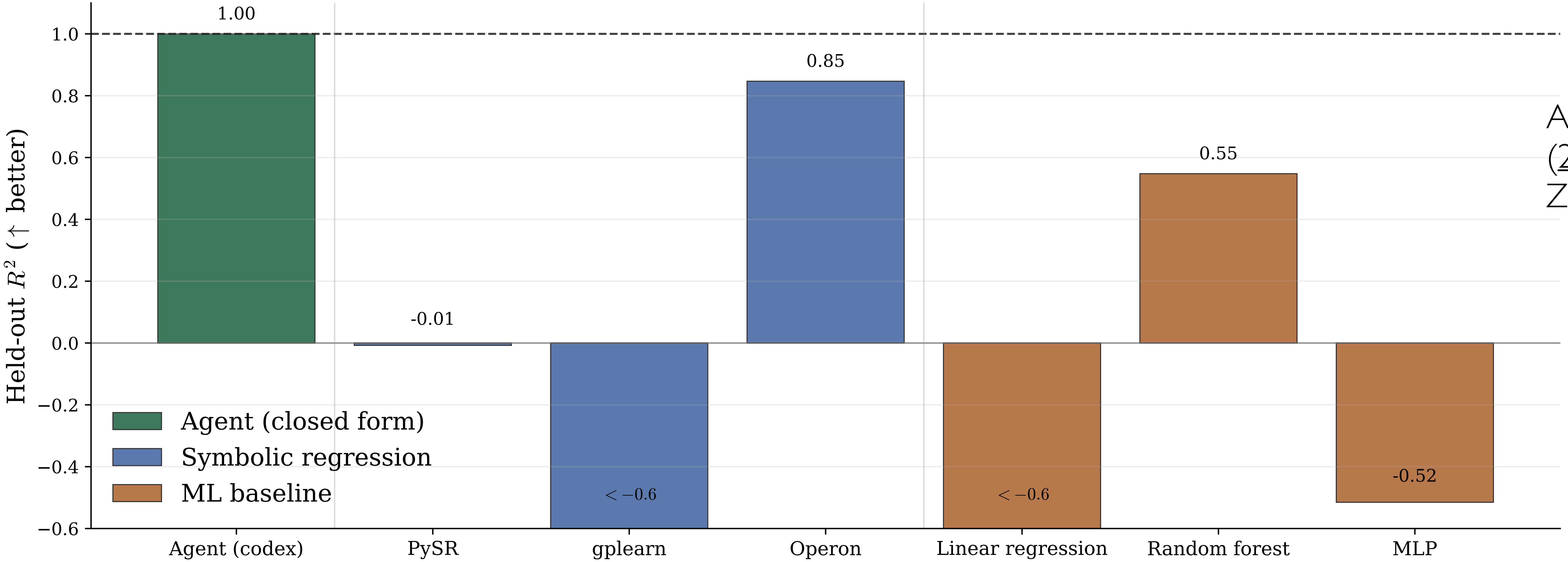
Islam, DW, et al (2605.11280)



Another example of agentic analytic modeling: Surface water wave scattering

$$A_n^{(--+\cdots+)} = \omega_1\omega_2\, 2^{\,n-1} \sum_{S\subseteq\{3,\ldots,n\}} (-1)^{|S|}\left[\beta^2 - \sum_{i\in S}\omega_i^2\right]_+^{n-3}$$

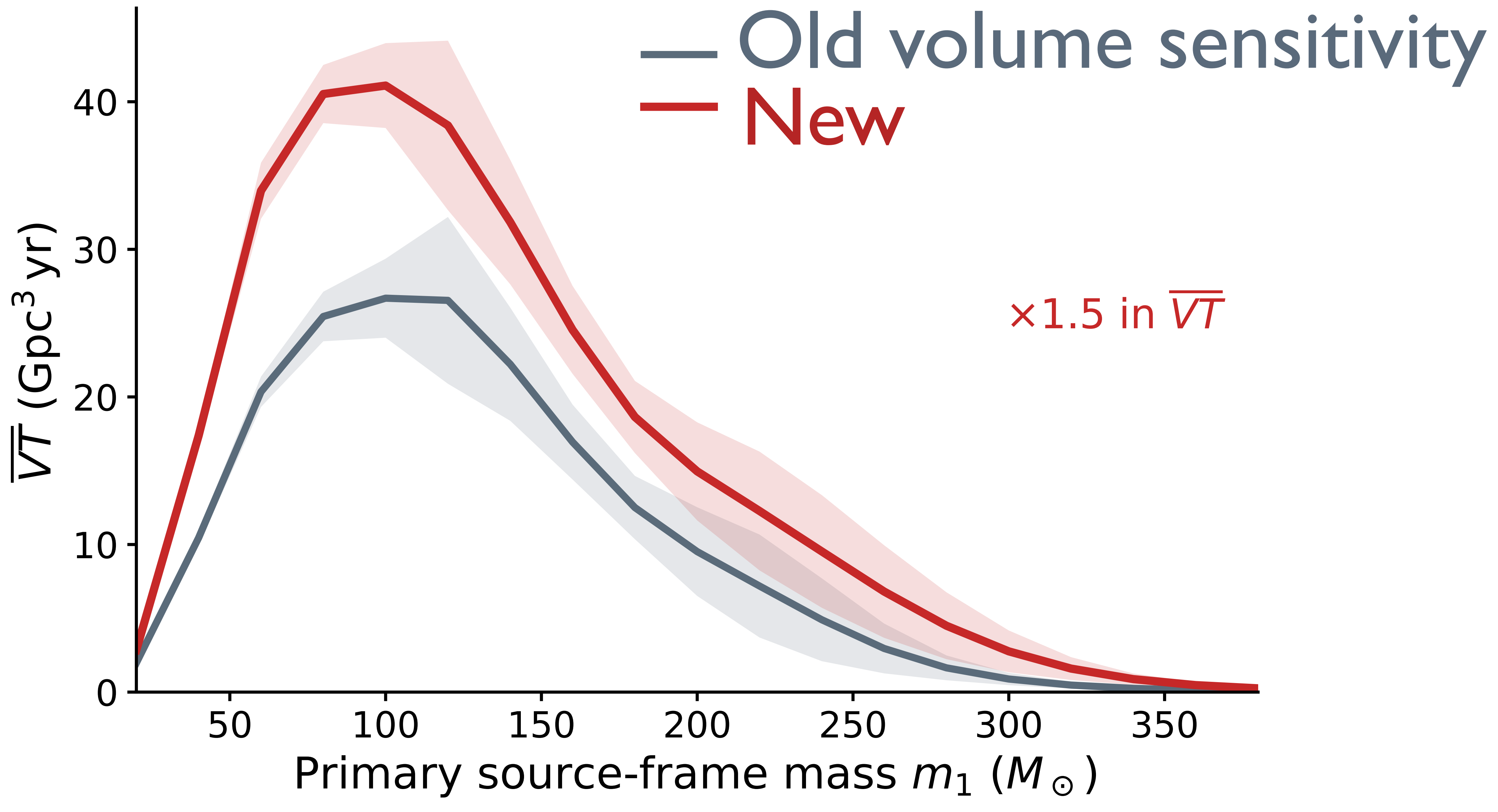
$$n=5: \quad A_5 = 16\omega_1\omega_2\Big[\beta^4 - [\beta^2-\omega_3^2]_+^2 - [\beta^2-\omega_4^2]_+^2 - [\beta^2-\omega_5^2]_+^2 + [\beta^2-\omega_3^2-\omega_4^2]_+^2 + [\beta^2-\omega_3^2-\omega_5^2]_+^2 + [\beta^2-\omega_4^2-\omega_5^2]_+^2 - [\beta^2-\omega_3^2-\omega_4^2-\omega_5^2]_+^2\Big]$$

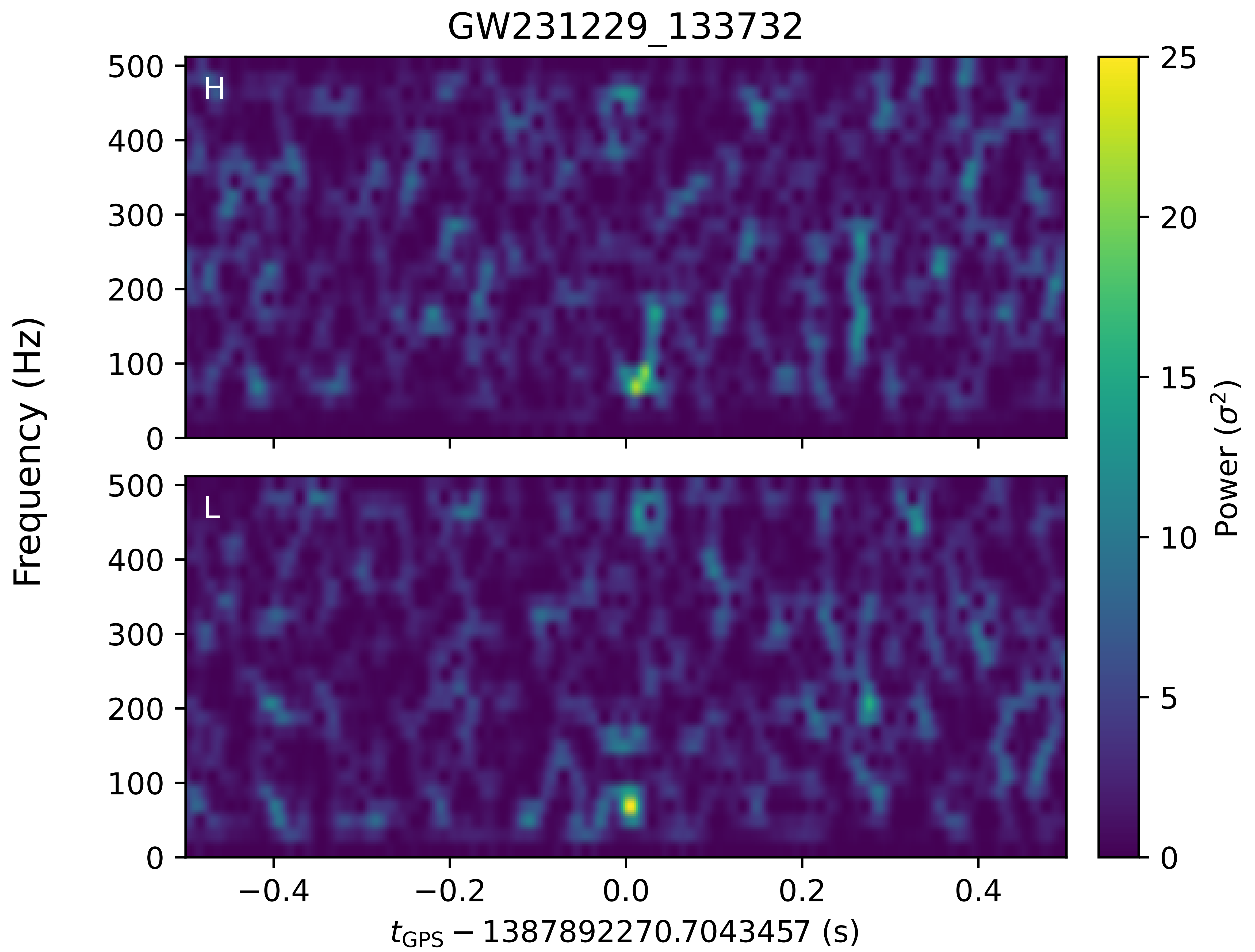


Arkani-Hamed, et al (2606.28280)
Zhou, DW et al (in prep)

2. Transient searches → new black hole mergers

1. Verifiable objective function (maximize synthetic signal detection)
2. Rapid low-cost Iterations
3. Rich/high-dimensional search space

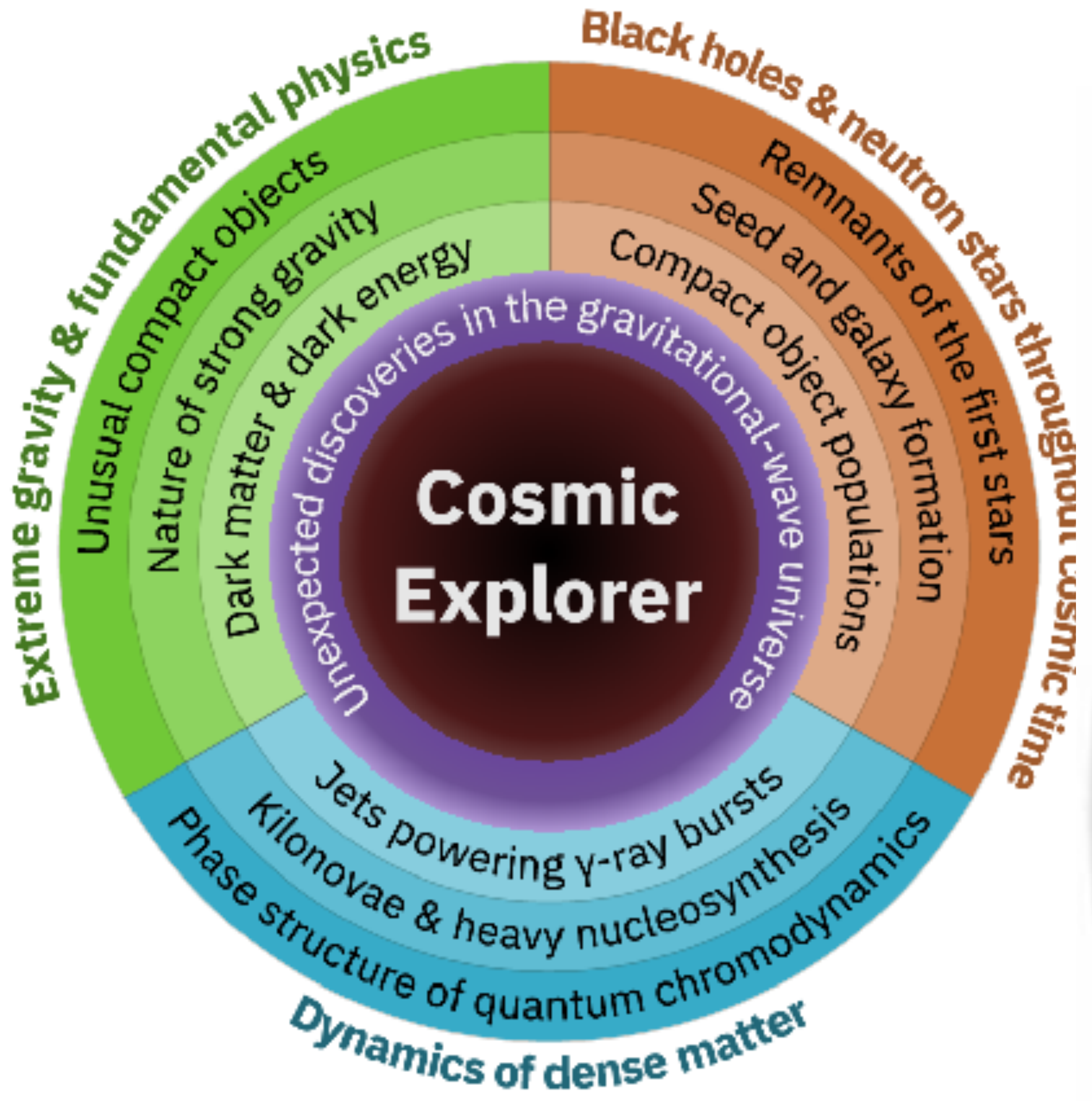


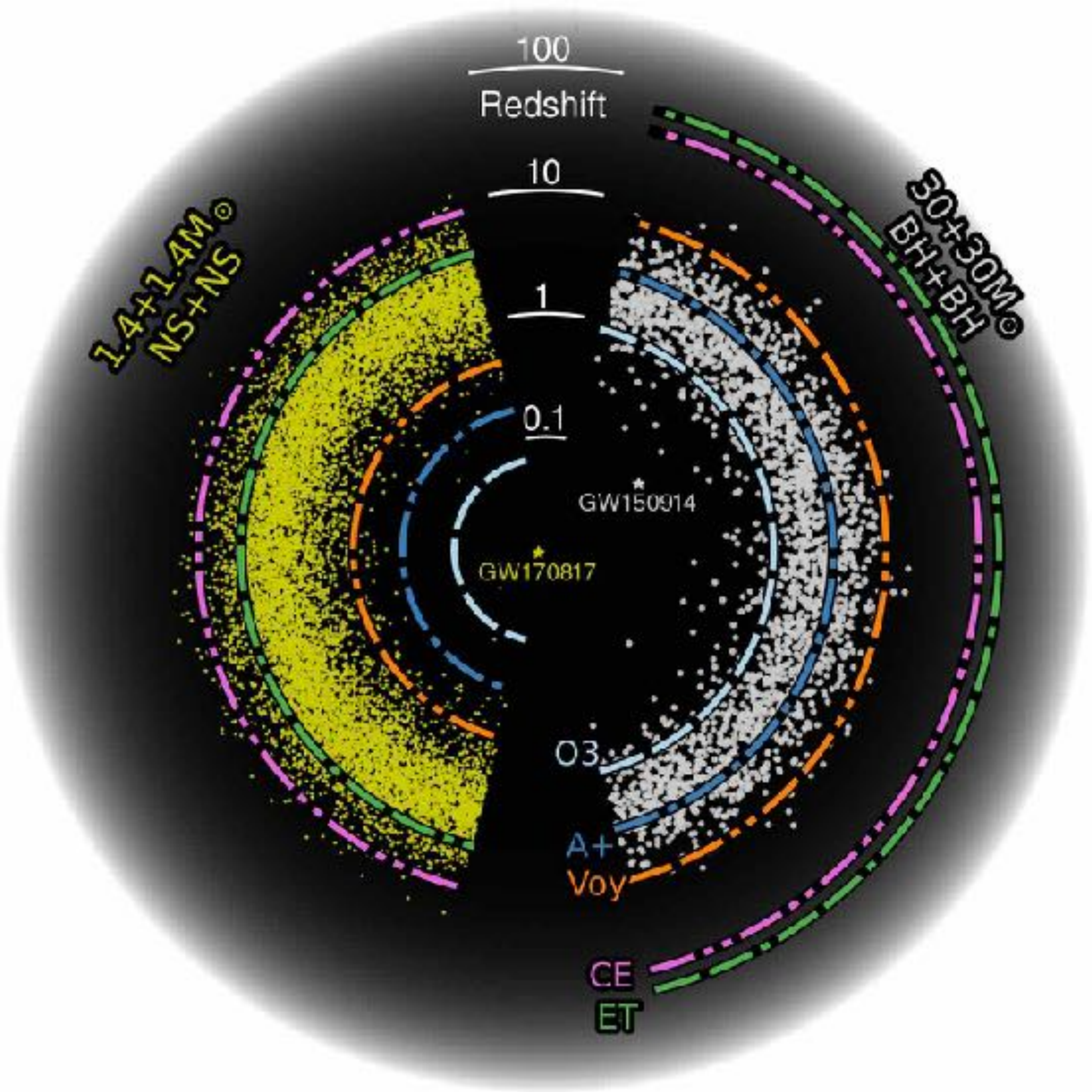


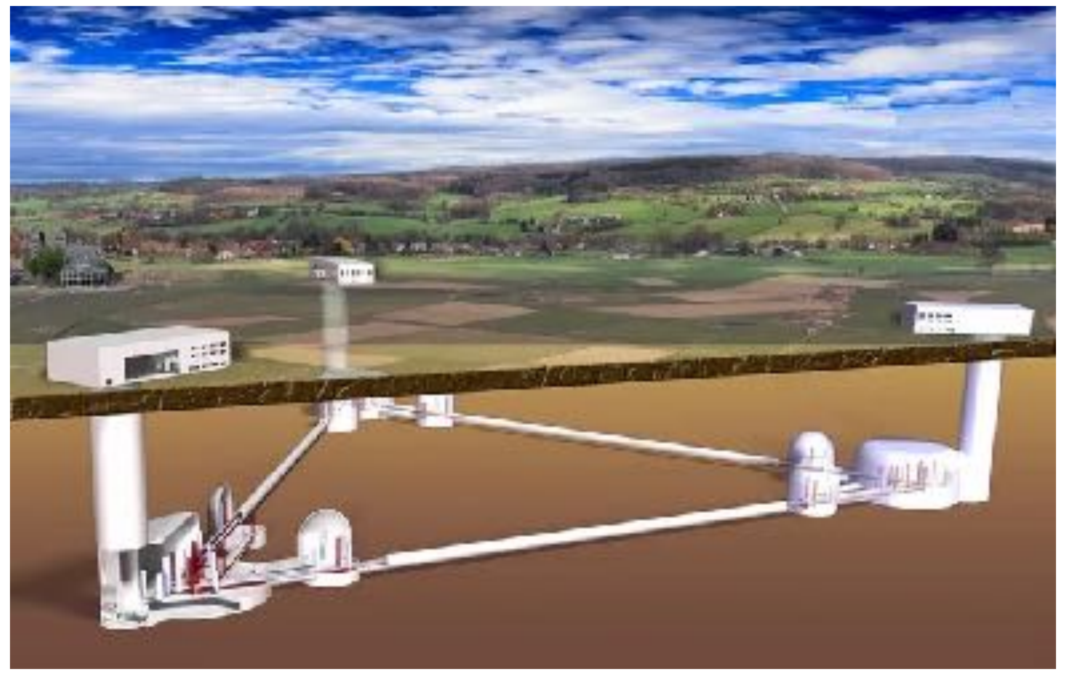
DW et al (in prep)

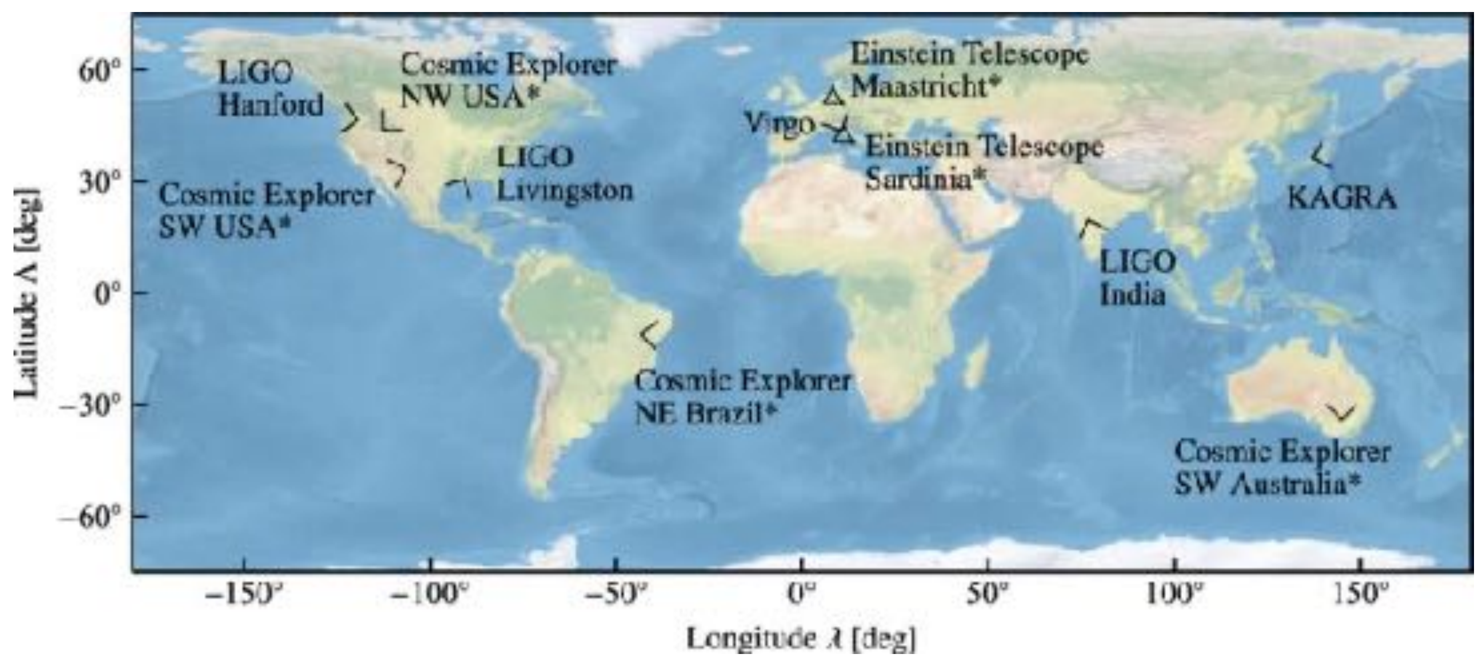
3. Agents for cross-disciplinary scientific forecasting

Science cases × Astrophysical distribution of compact objects × Detector configurations × Forecast models







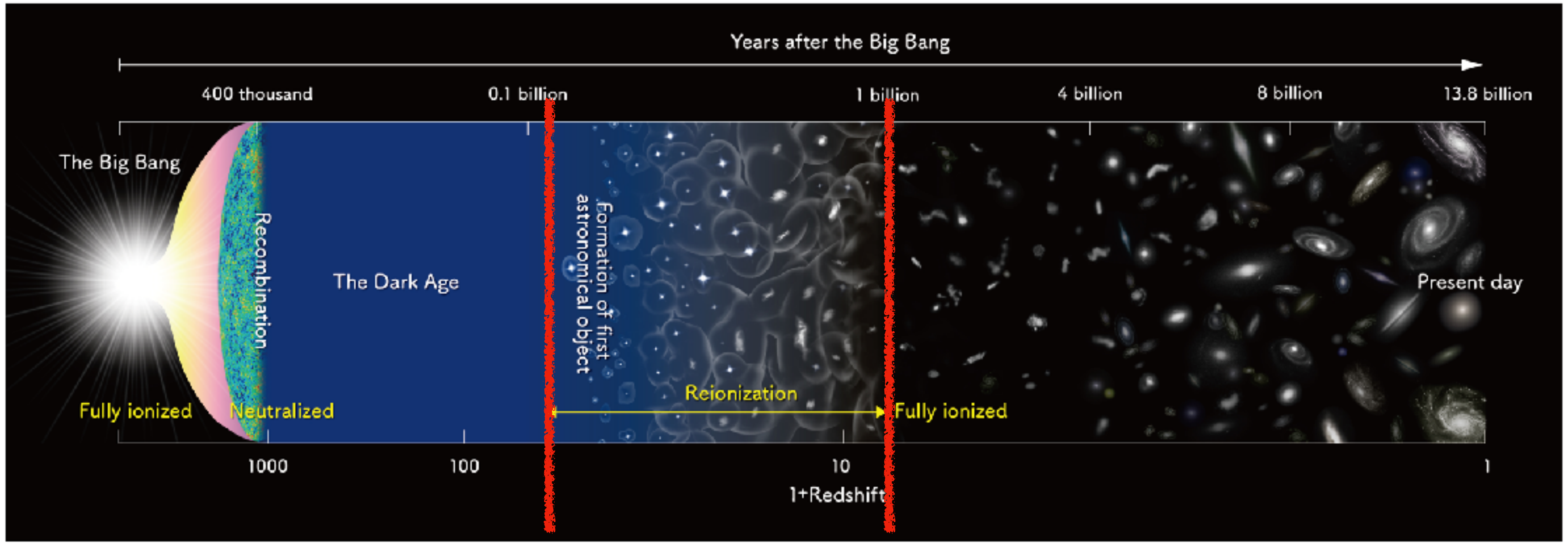


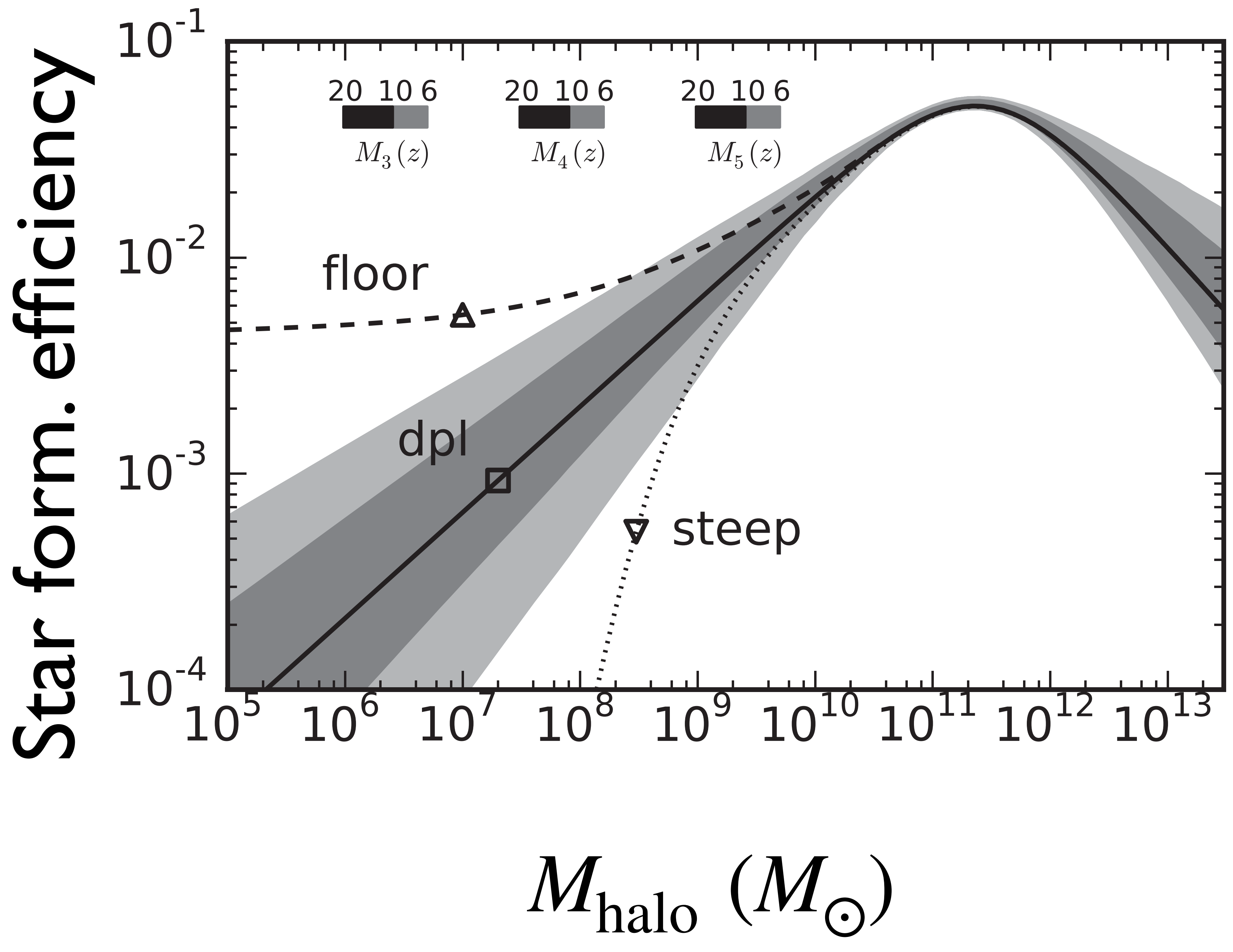
CosmoStatGW / gwfast

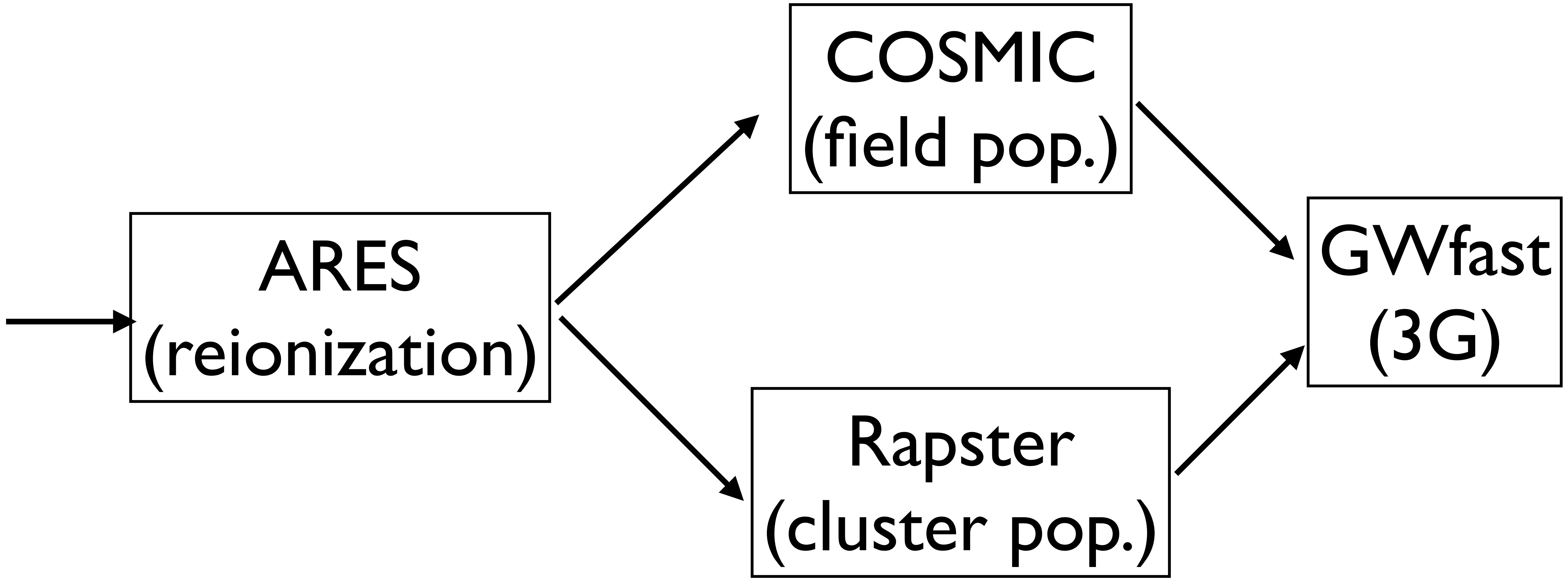
janosch314 / GWFish

sborhanian / gwbench

Probing cosmic reionization with gravitational detectors

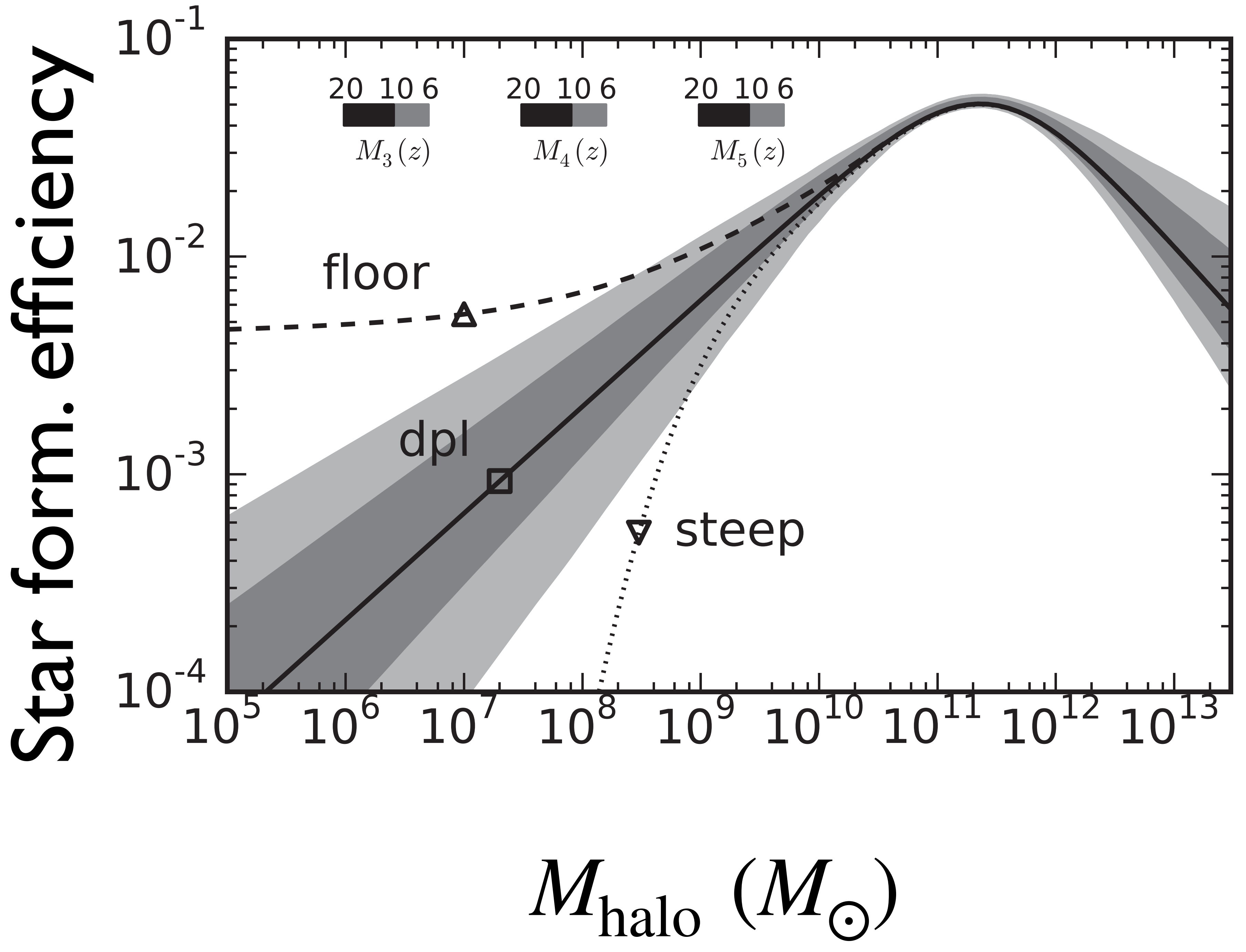




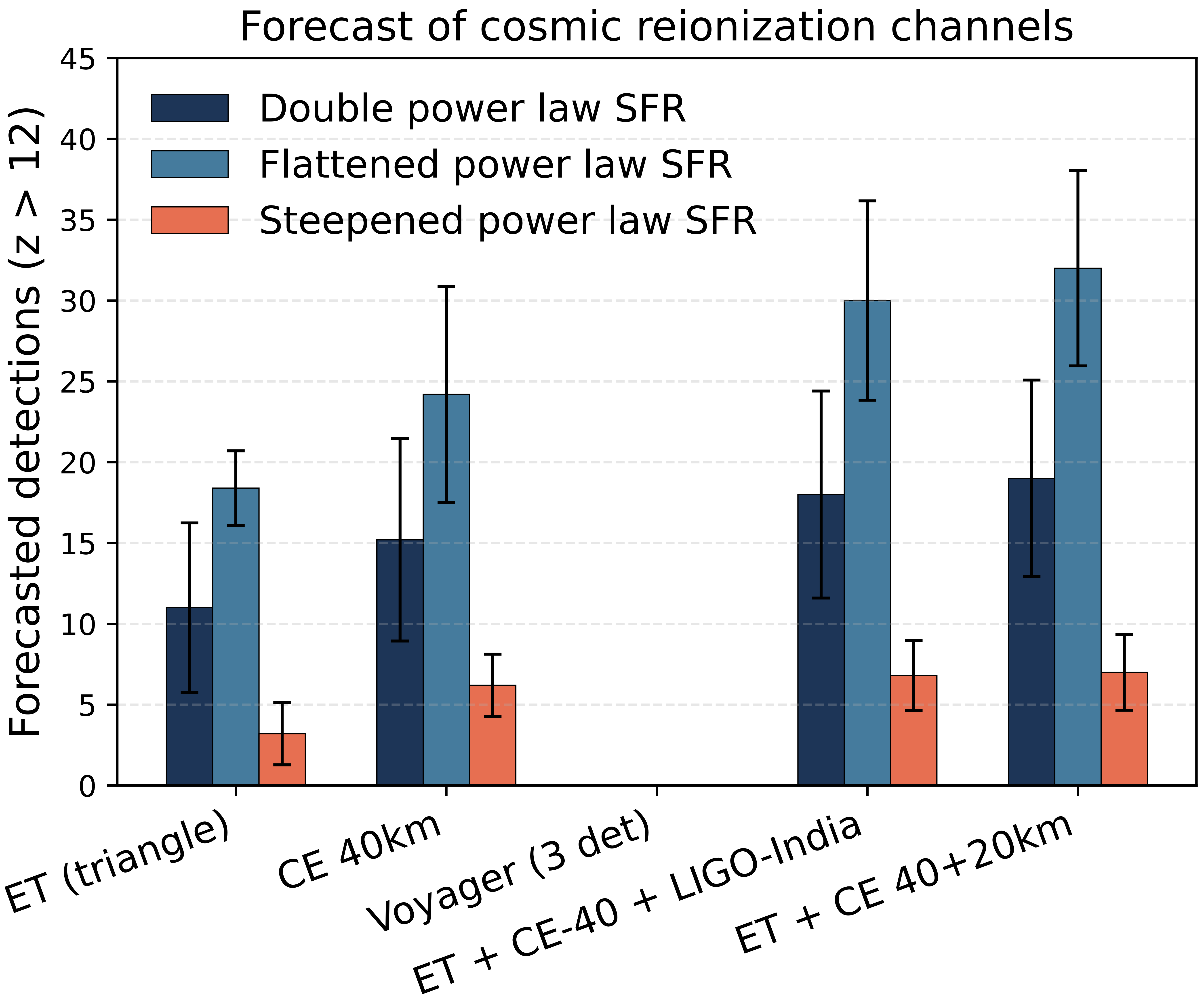


Enables using multiple codebases from different fields

Probing cosmic reionization with gravitational detectors



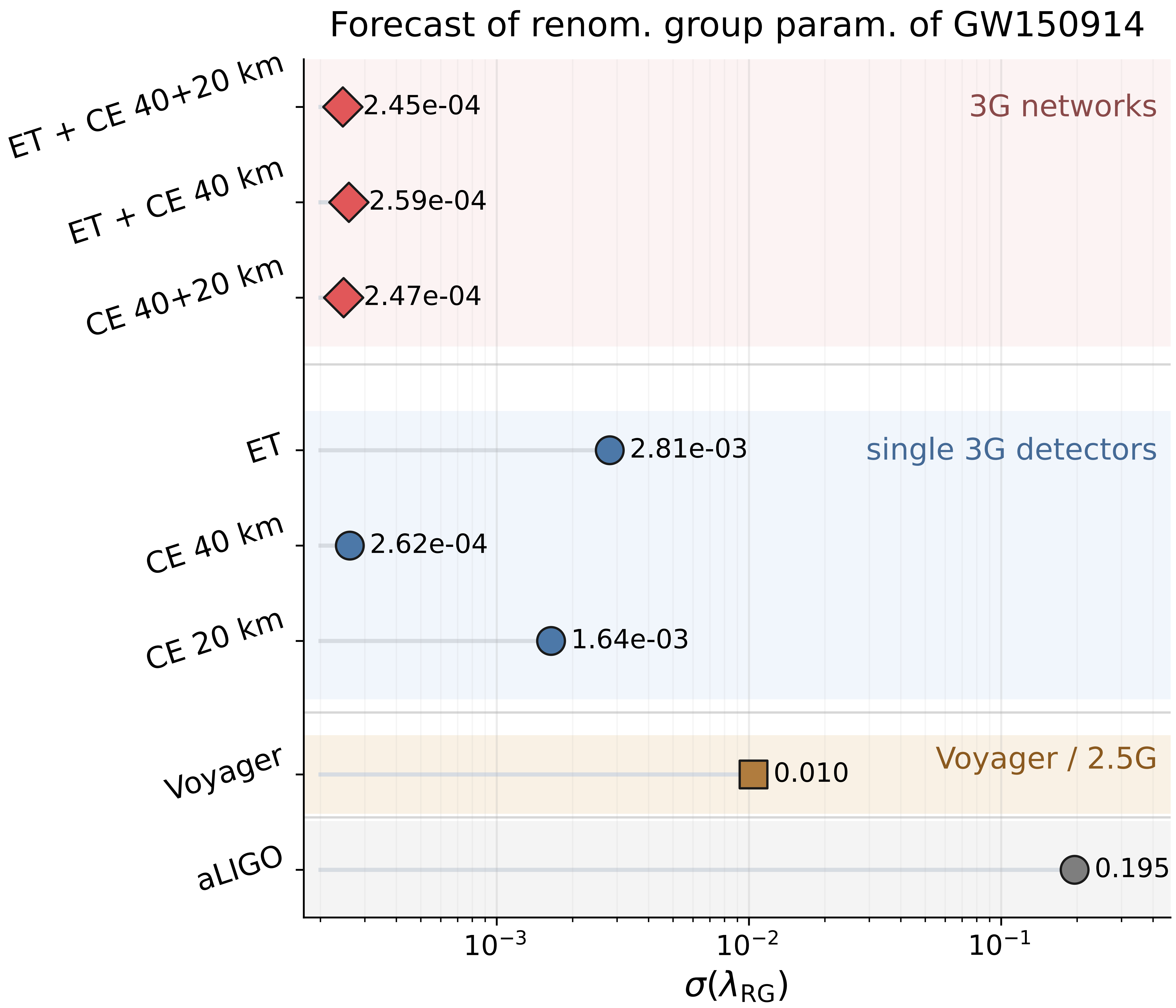
Mirocha et al. 17



Probing renormalization group running with 3G detectors

Renormalized angular momentum quantum number

$$\hat{\hat{\ell}} = \ell + \lambda_{\rm RG}\gamma_{\ell m}^{\rm univ}$$



NASA AI/ML STIG group

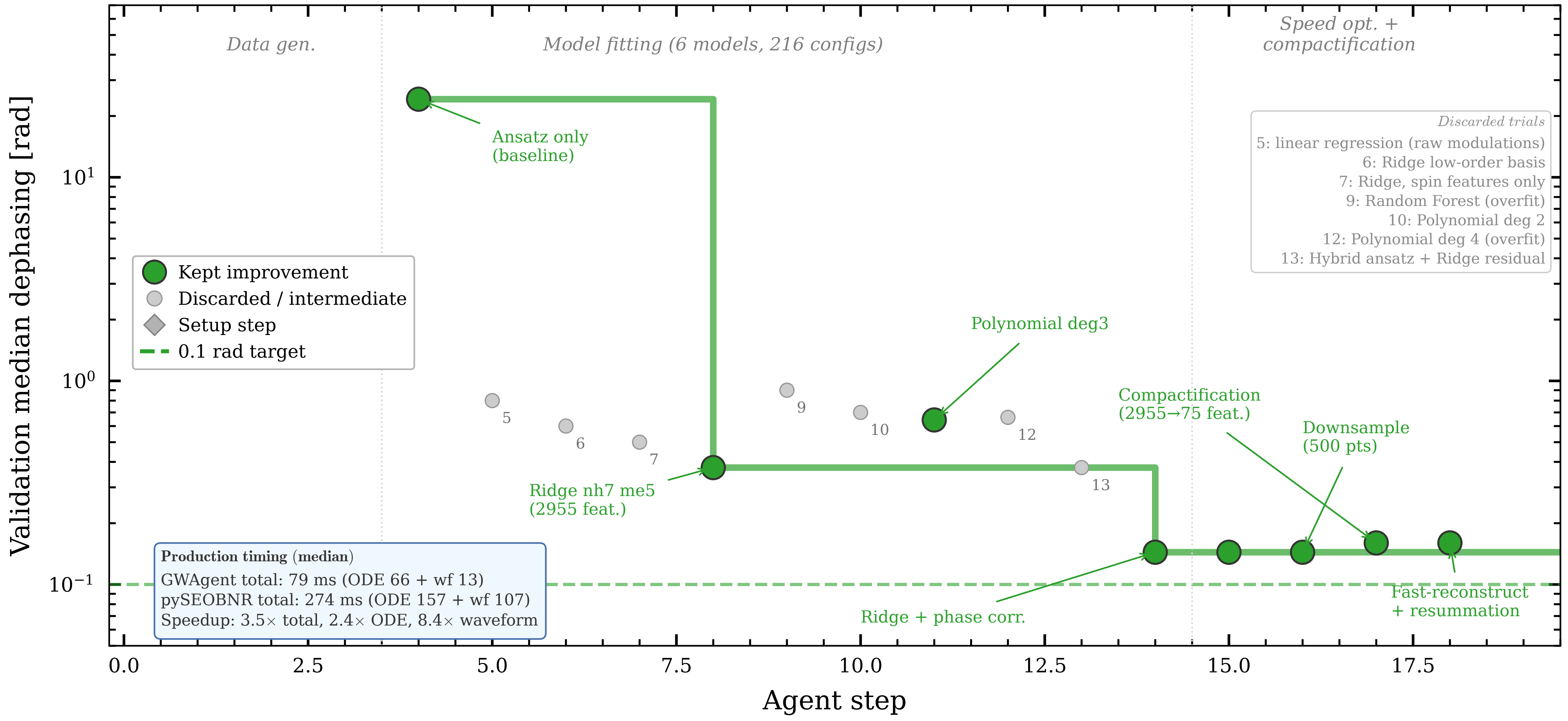
WEEK	DATE	TOPIC	SPEAKER
1	Nov 3	Overview · Video & Materials	Jesse Thaler, MIT
Module 1: Large Language Models as Autonomous Agents			
2	Nov 10	LLM API Basics · Video & Materials	Yuan-Sen Ting, OSU
3	Nov 17	RAG & Function Tools · Video & Materials	Yuan-Sen Ting, OSU
4	Nov 24	LLM as Agent · Video & Materials	Francisco Villaescusa-Navarro, Flatiron
5	Dec 8	Model Context Protocol (MCP) · Video & Materials	Yuan-Sen Ting, OSU
Module 2: Deep Learning Frameworks			
6	Dec 15	PyTorch and Autodifferentiation · Video & Materials	Phill Cargile, Harvard-Smithsonian
7	Dec 22	JAX · Video & Materials	Phill Cargile, Harvard-Smithsonian
Module 3: Neural Network Basics			
8	Jan 12	Inductive Biases · Video & Materials	John Wu, STScI
9	Jan 26	Convolutional Neural Networks (CNNs) · Video & Materials	John Wu, STScI

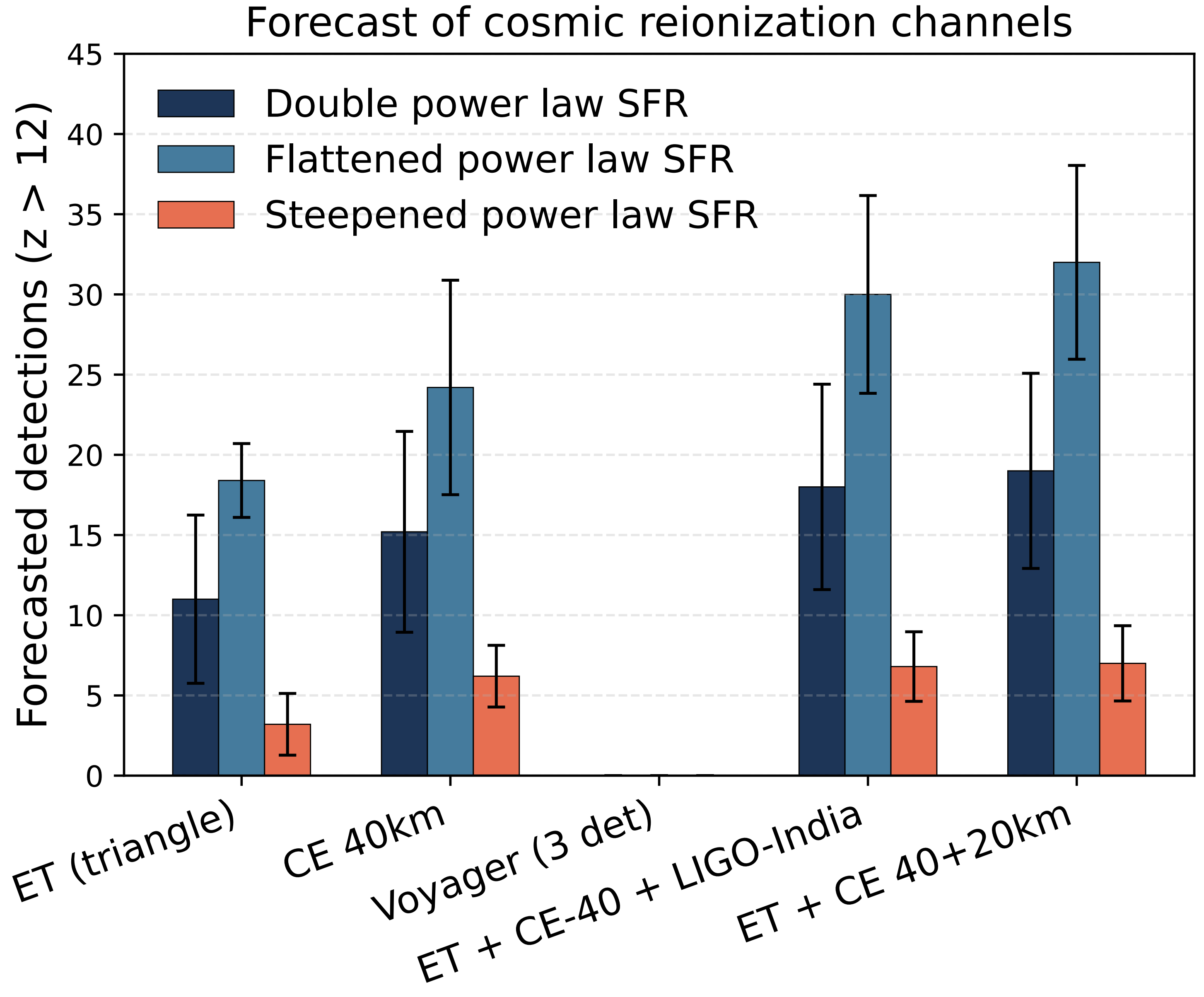
https://ai4astro.org/

Summary

- Agentic systems can be powerful in areas with:
  1. 1. Verifiable objective function
  2. Rapid low-cost Iterations
  3. Rich/high-dimensional search space

- Agents can help in multiple areas of astrophysical data analysis:
  1. Surrogate modeling
  2. Next gen. detector forecasts
  3. Transient searches





What open problems in your field are naturally suited for agentic applications?

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