

Expediting Astronomical Discovery with Large Language Models

Yuan-Sen Ting (丁源森)

Australian National University
The Ohio State University



NSF awarded over \$200 million for *AI Research Institutes*

Biological Sciences
~ 2 centers

Physical Sciences
~ 1 + (1+1) centers

Environmental Sciences
~ 2 centers

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6 centers x
15M ~ 100M

Hype, myth, or *real deal*?

[nature](#) > [articles](#) > [article](#)

Article | [Open access](#) | Published: 15 July 2021

Highly accurate protein structure prediction with **AlphaFold**

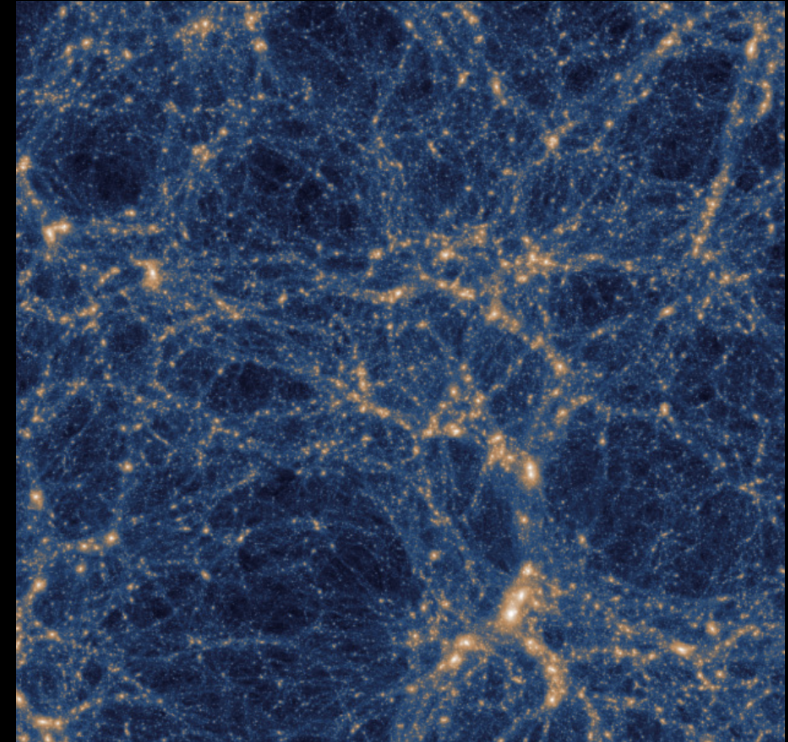
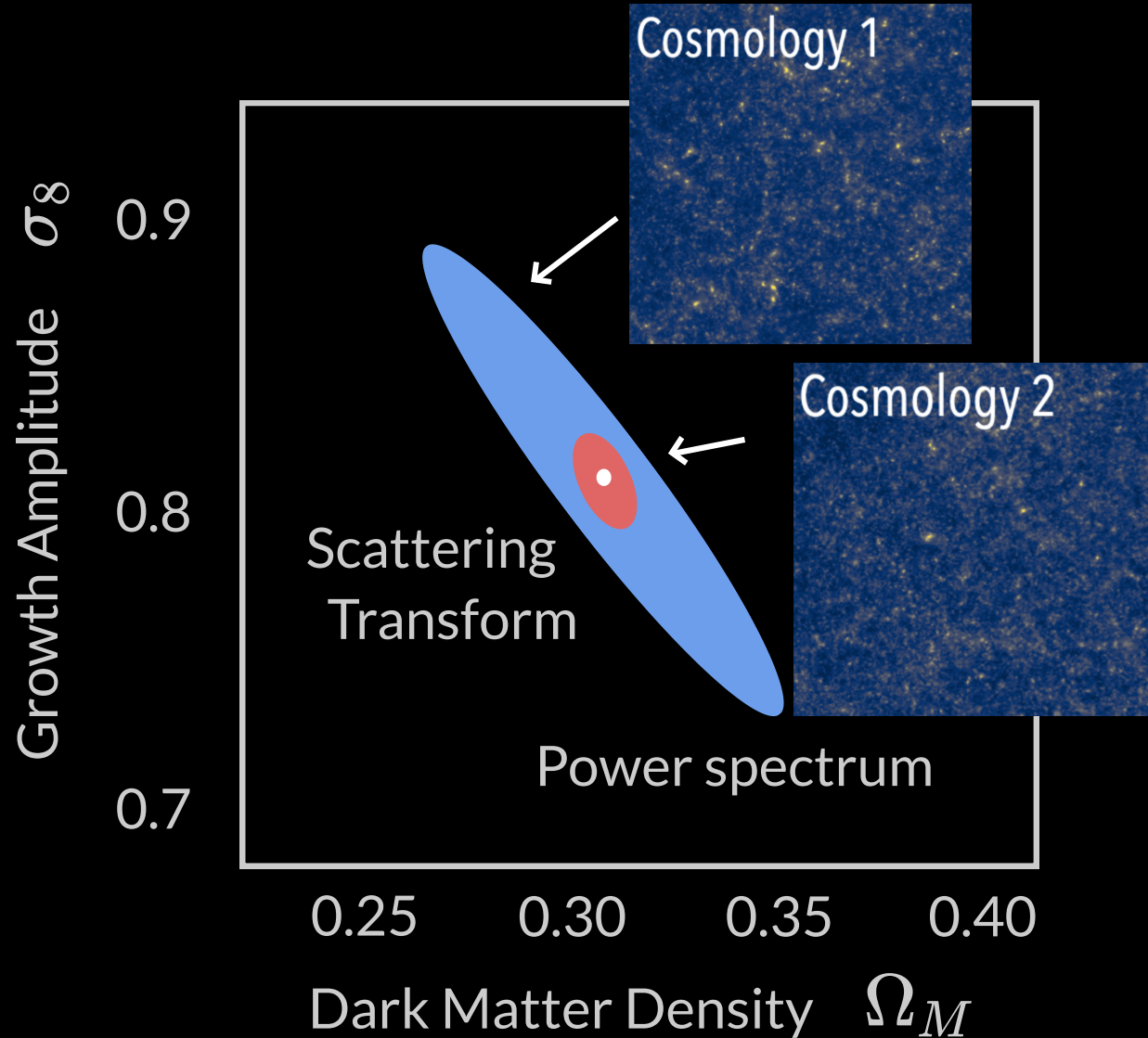
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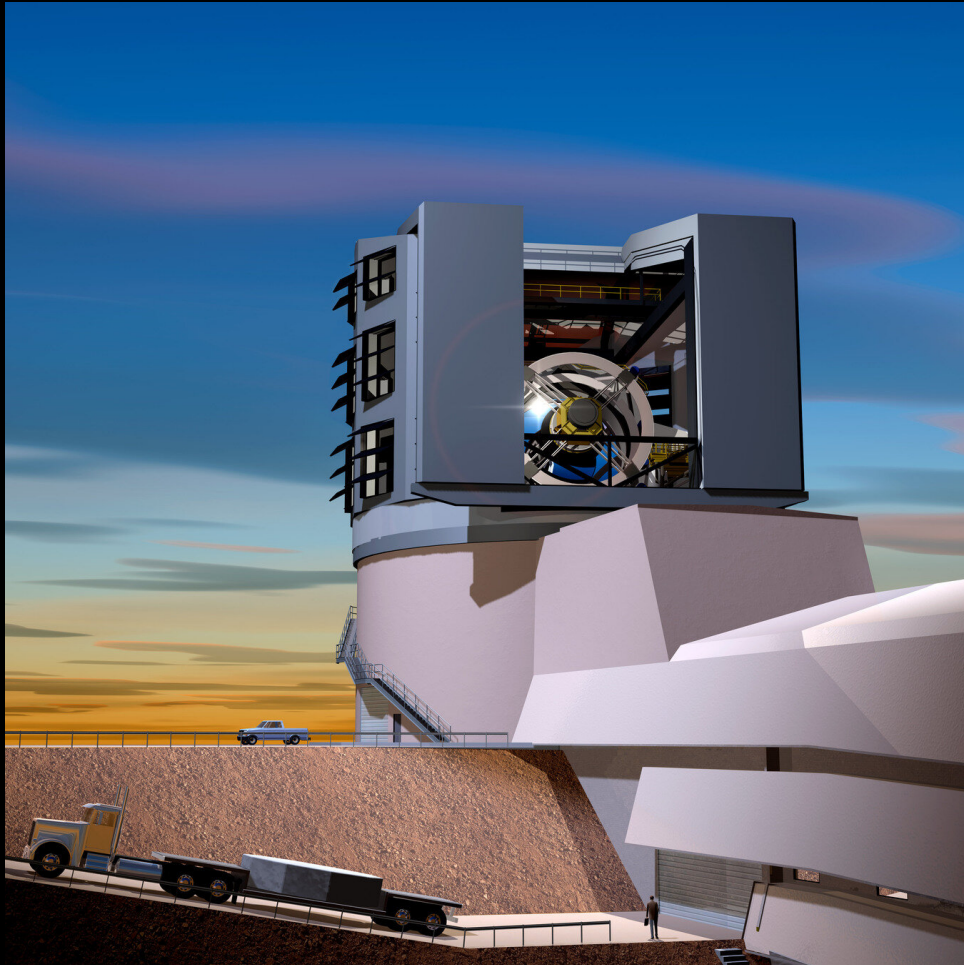
Why hasn't astronomy had its
"AlphaFold" moment yet?"

Most AI in Astronomy focuses on *extending* statistical methods



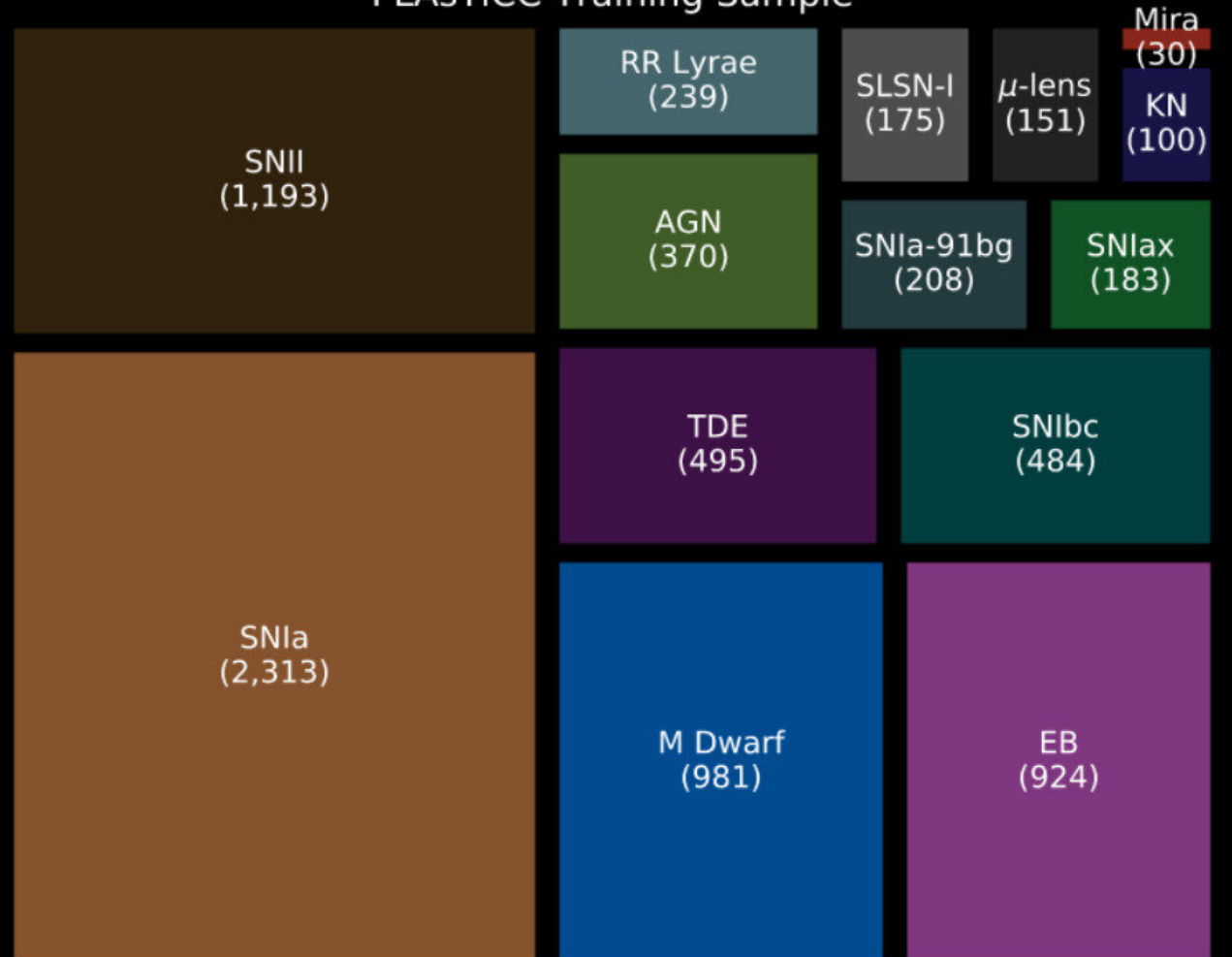
International Astrostatistics Association Award
Cheng, YST, Menard & Bruna + 20

or building effective brokers / *classifiers*



Rubin Observatory

PLAsTiCC Training Sample



Improving individual downstream tasks with
AI will *not* revolutionize astronomy

The Bitter Lesson - Rich Sutton, 2019

The Bitter Lesson - Rich Sutton, 2019

"We should build in only the *meta-methods* that can find and capture this arbitrary complexity.

Essential to these methods is that they can find good approximations, but the search for them should be *by our methods, not by us.*

We want AI agents that can *discover like we can*, not which contain what we have discovered."

- Where are we in AI for Astronomy - What's the problem?
- What could be the AlphaFold moment for astronomy?
- How do we get there in a cost-effective way?

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Knowledge Graph in Astronomical Research with Large Language Models: Quantifying Driving Forces in Interdisciplinary Scientific Discovery

Zechang Sun^{1*}, Yuan-Sen Ting^{2,3}, Yaobo Liang⁴, Nan Duan⁴, Song Huang¹, Zheng Cai¹

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³School of Computing, Australian National University, Canberra, Australia

⁴Microsoft Research Asia, Beijing, China

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nanduan.nlp@outlook.com, {shuang, zcai}@mail.tsing

Abstract

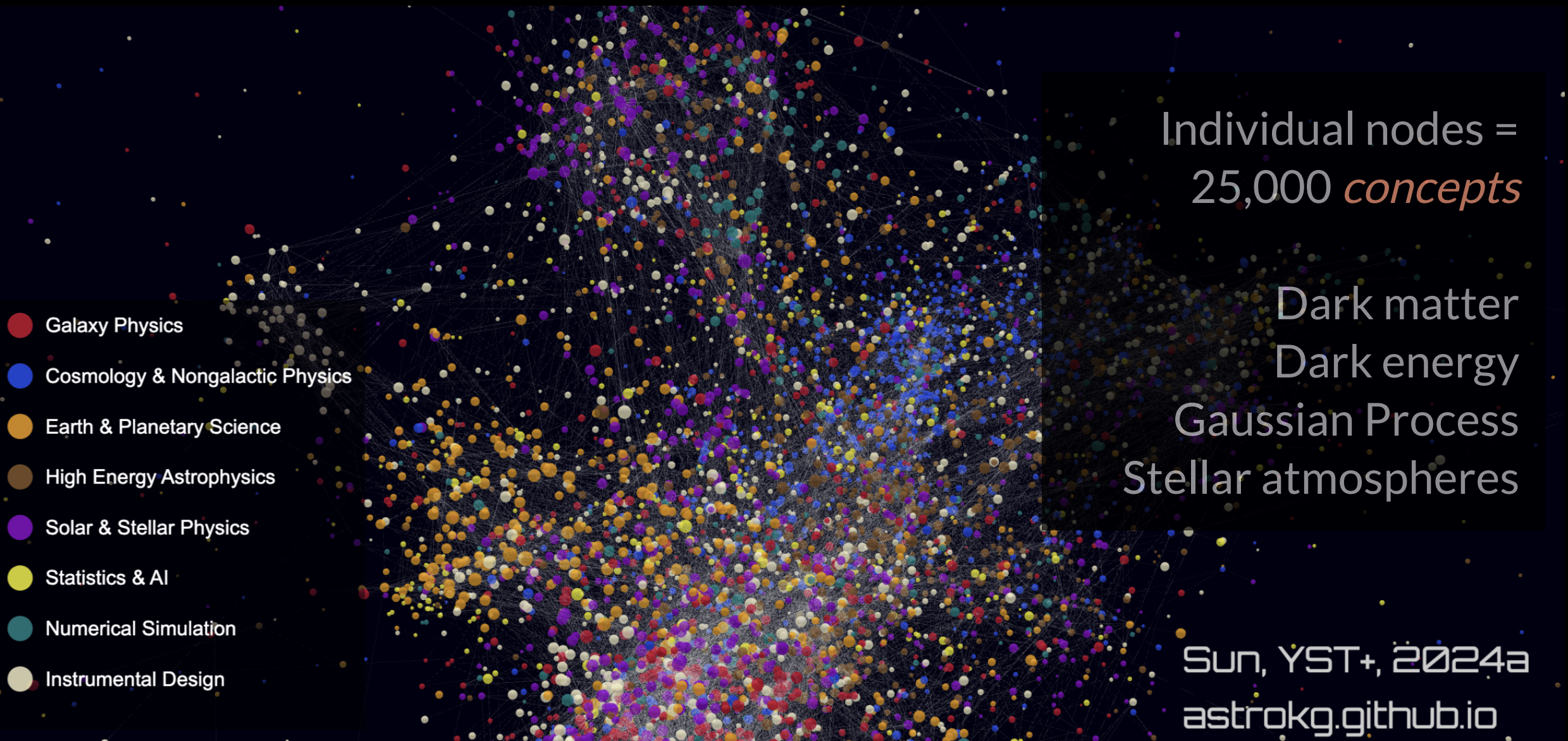
Identifying and predicting the factors that contribute to the success of interdisciplinary research is crucial for advancing scientific discovery. However, there is a lack of methods to quantify the integration of new ideas and technological advancements in astronomical research and how these new technologies drive further scientific breakthroughs.

Large language models, with their ability to ex-

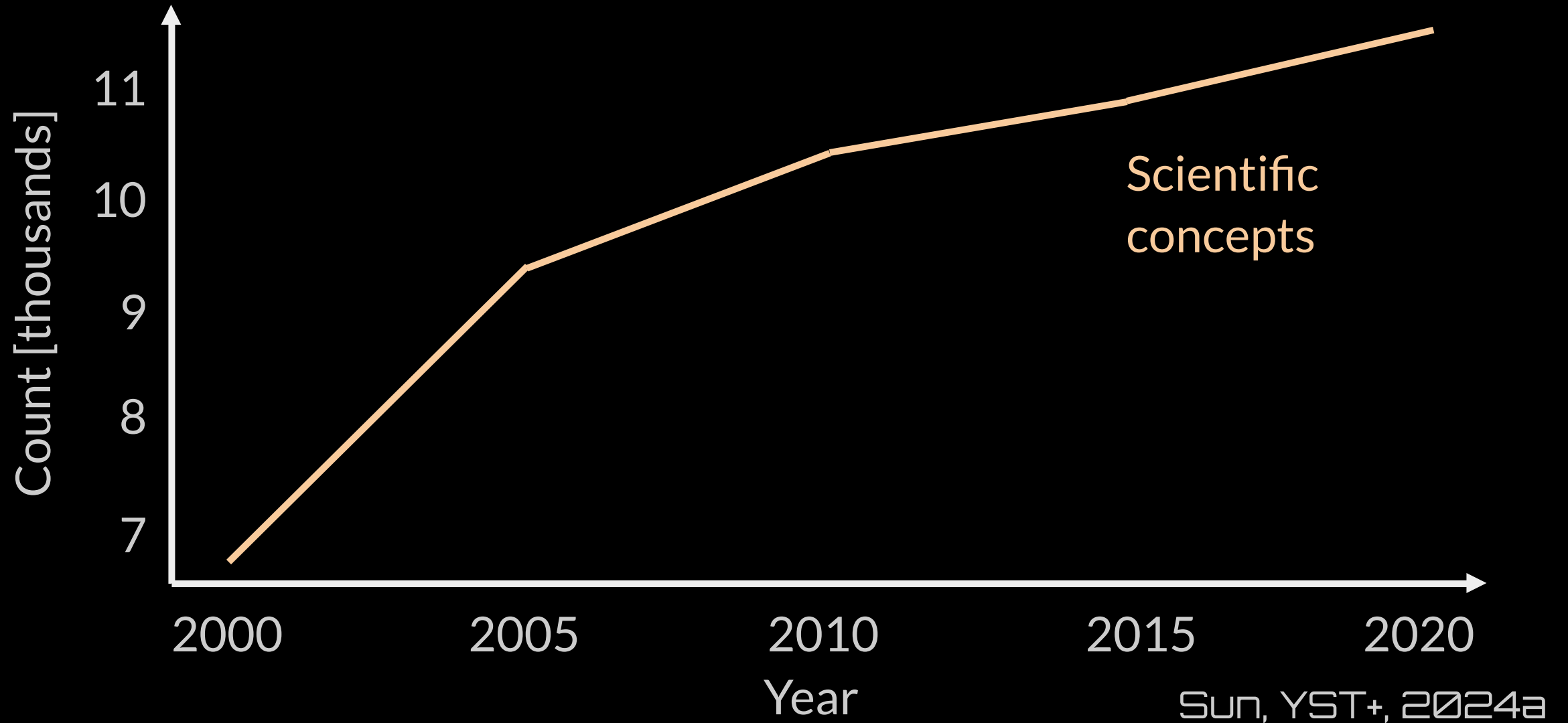
the theoretical understand-
eral relativity has driven
berg, 2008], and each s
leads to new windows
the detection of gravita
al., 2016], which was
cutting-edge technologi
high-performance comp
standing complex syste



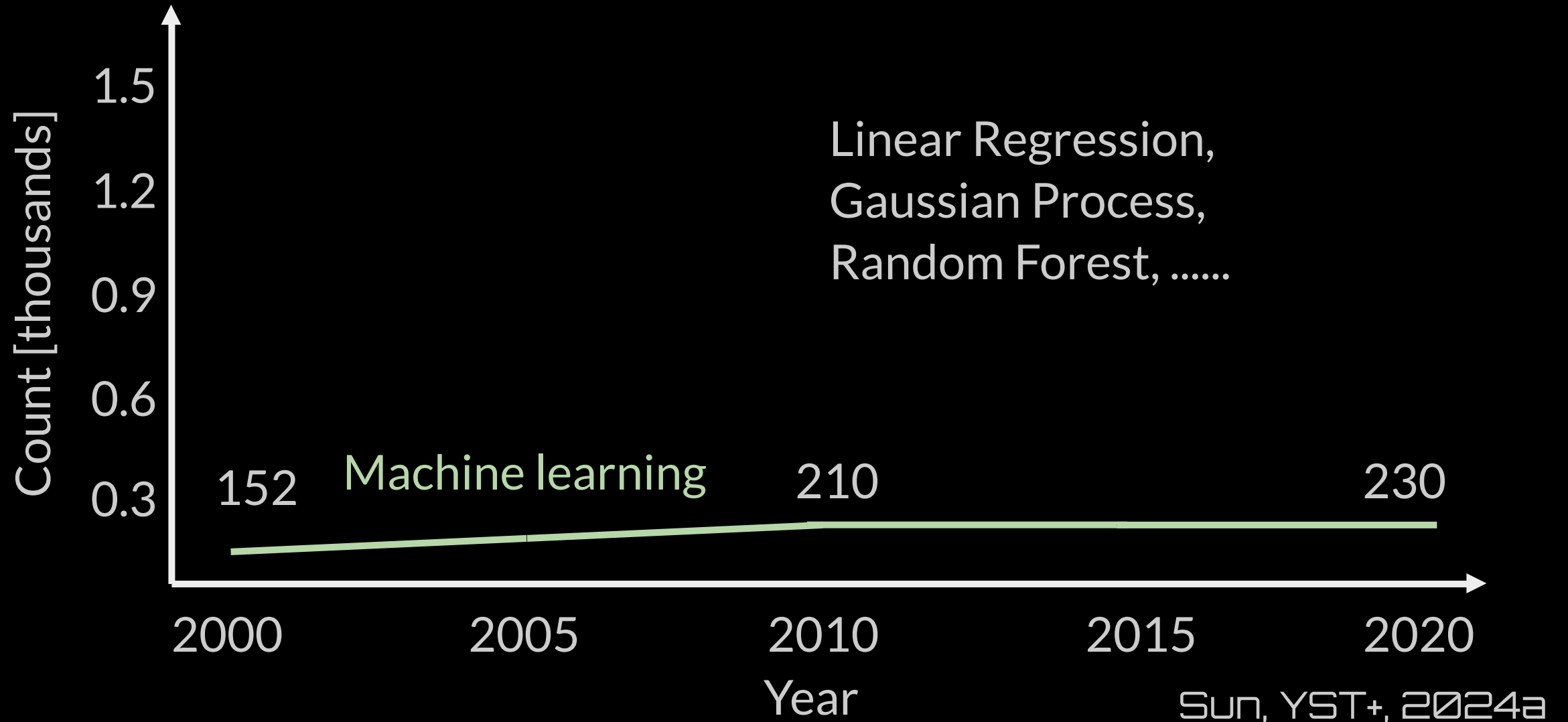
Visualizing the *knowledge graph* and evolution in astronomy



Quantifying the growth of the field -- by groups of concepts

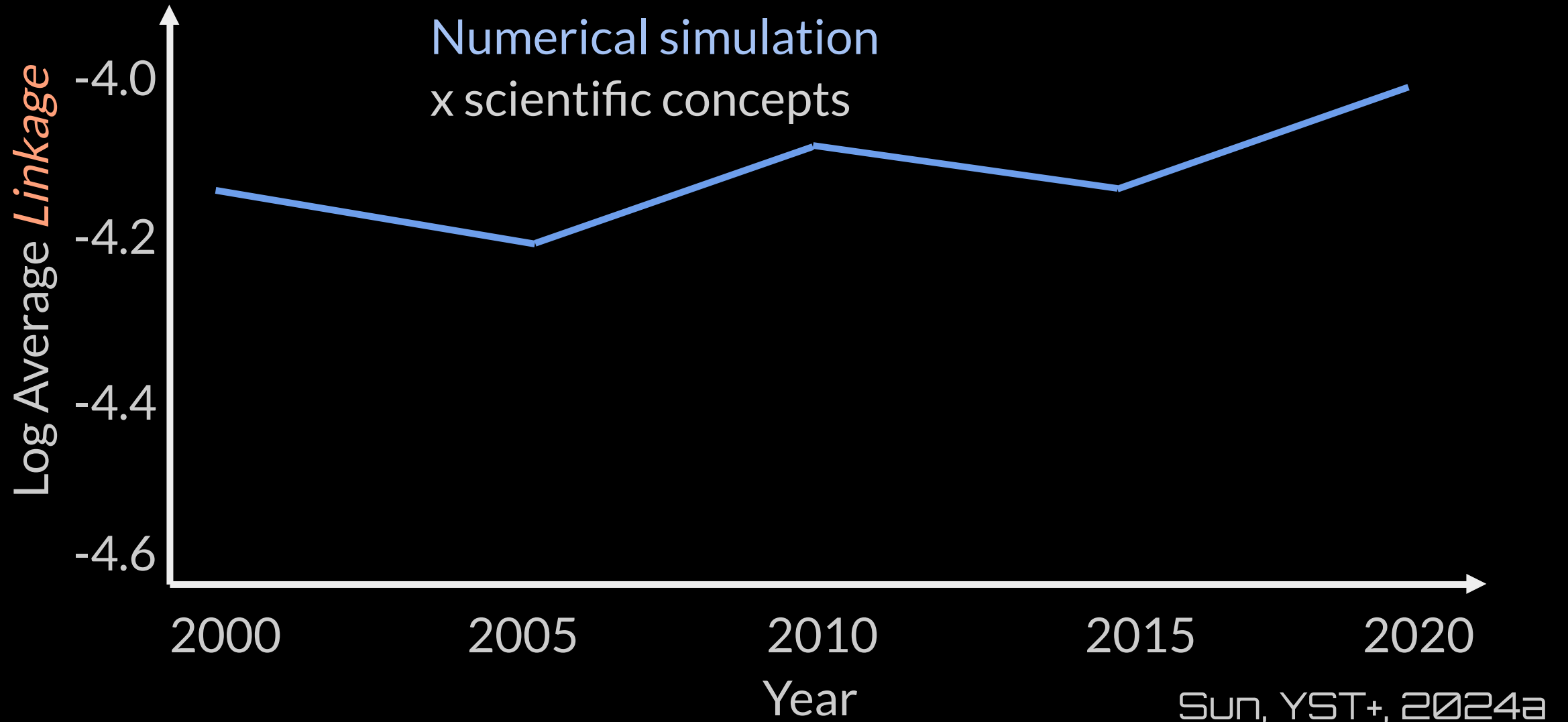


The number of ML concepts in astronomy has *not grown*

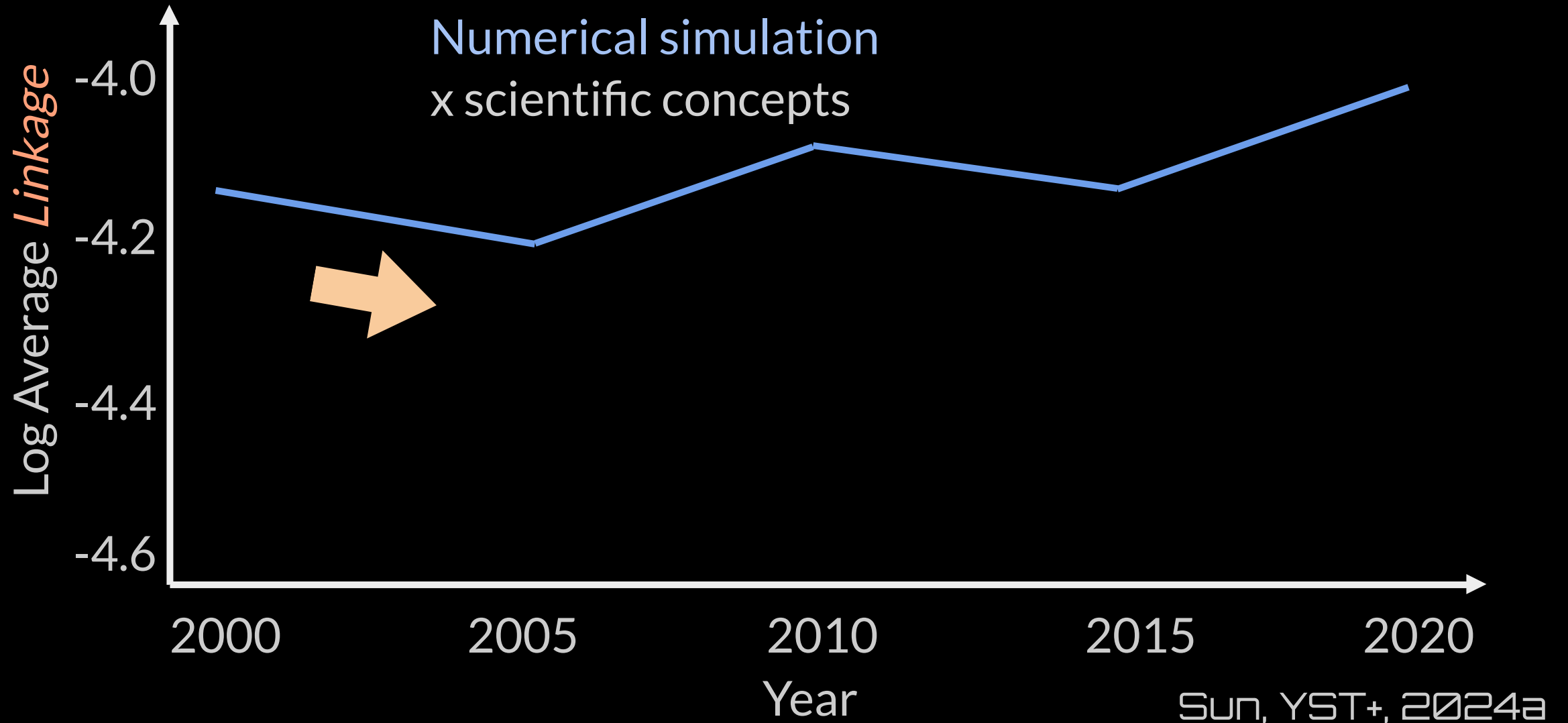


Quantifying the *cross-domain* interaction:
How technical concepts inspire scientific ones

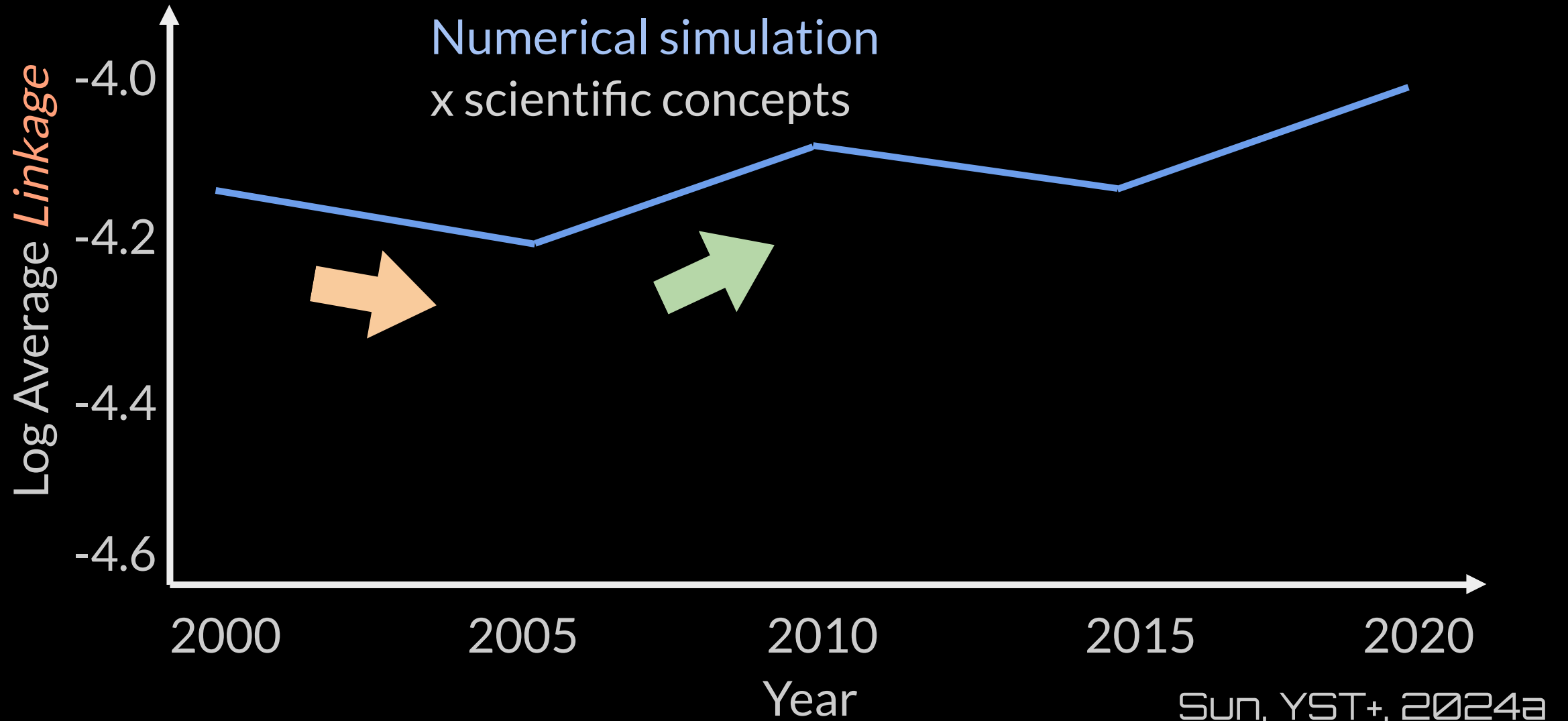
Cross-domain linkage shows a *two-phase* evolution



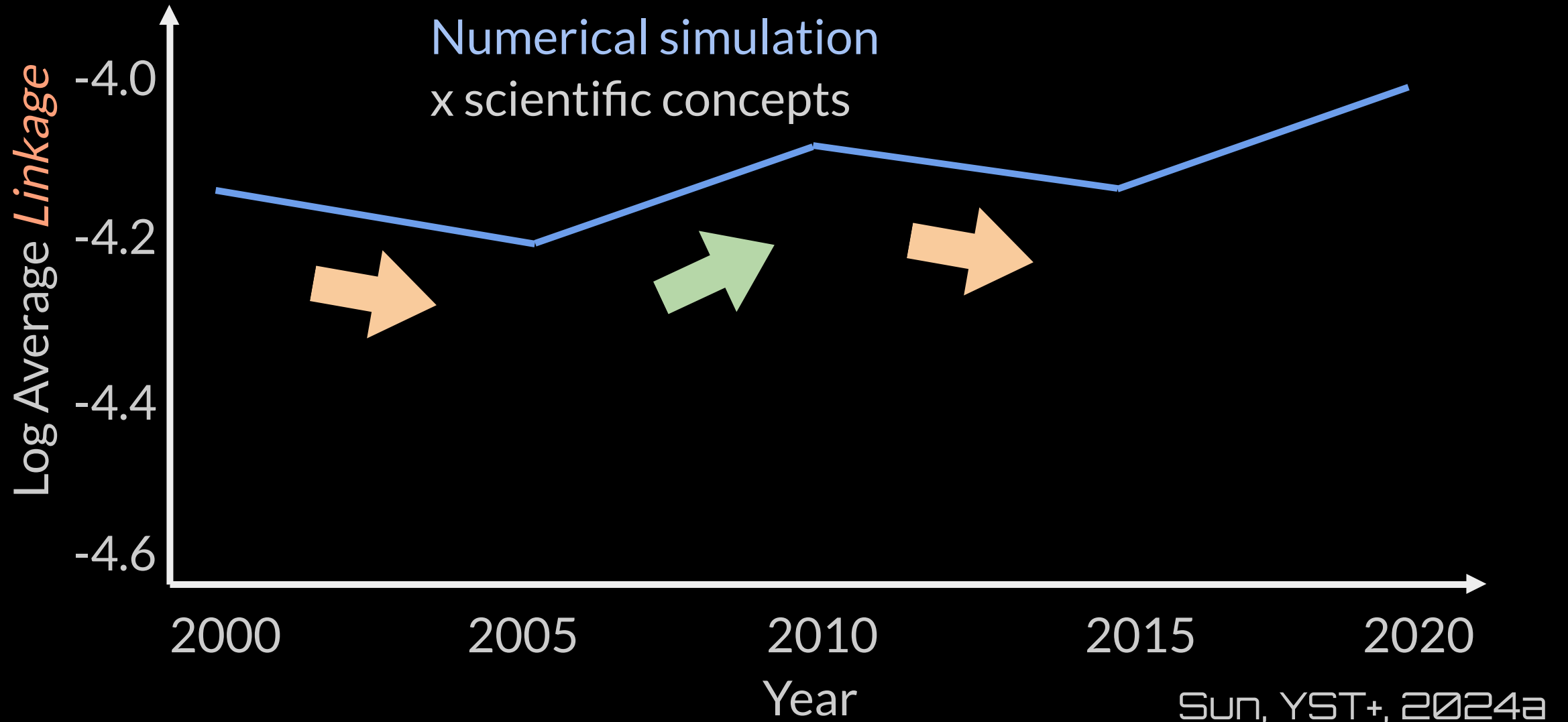
Cross-domain linkage shows a *two-phase* evolution



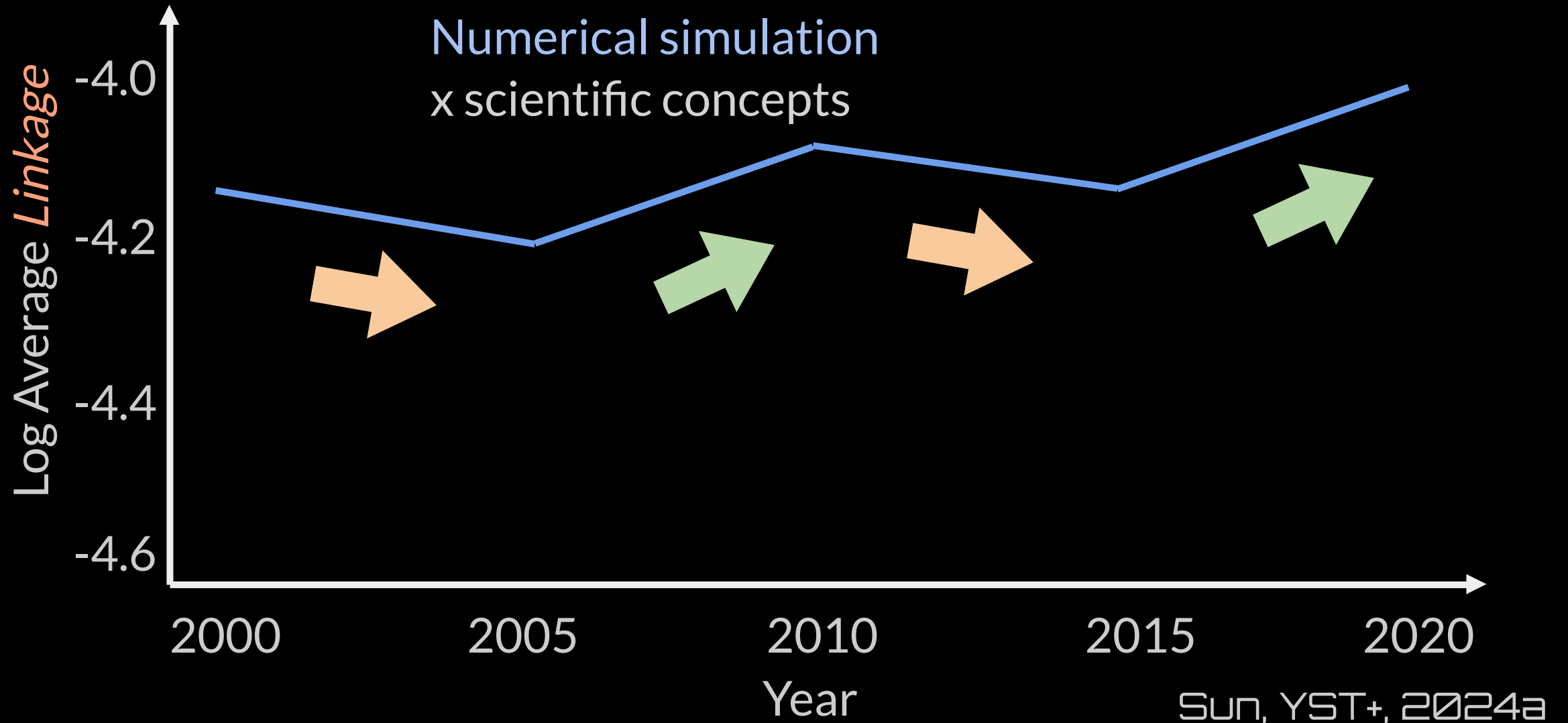
Cross-domain linkage shows a *two-phase* evolution



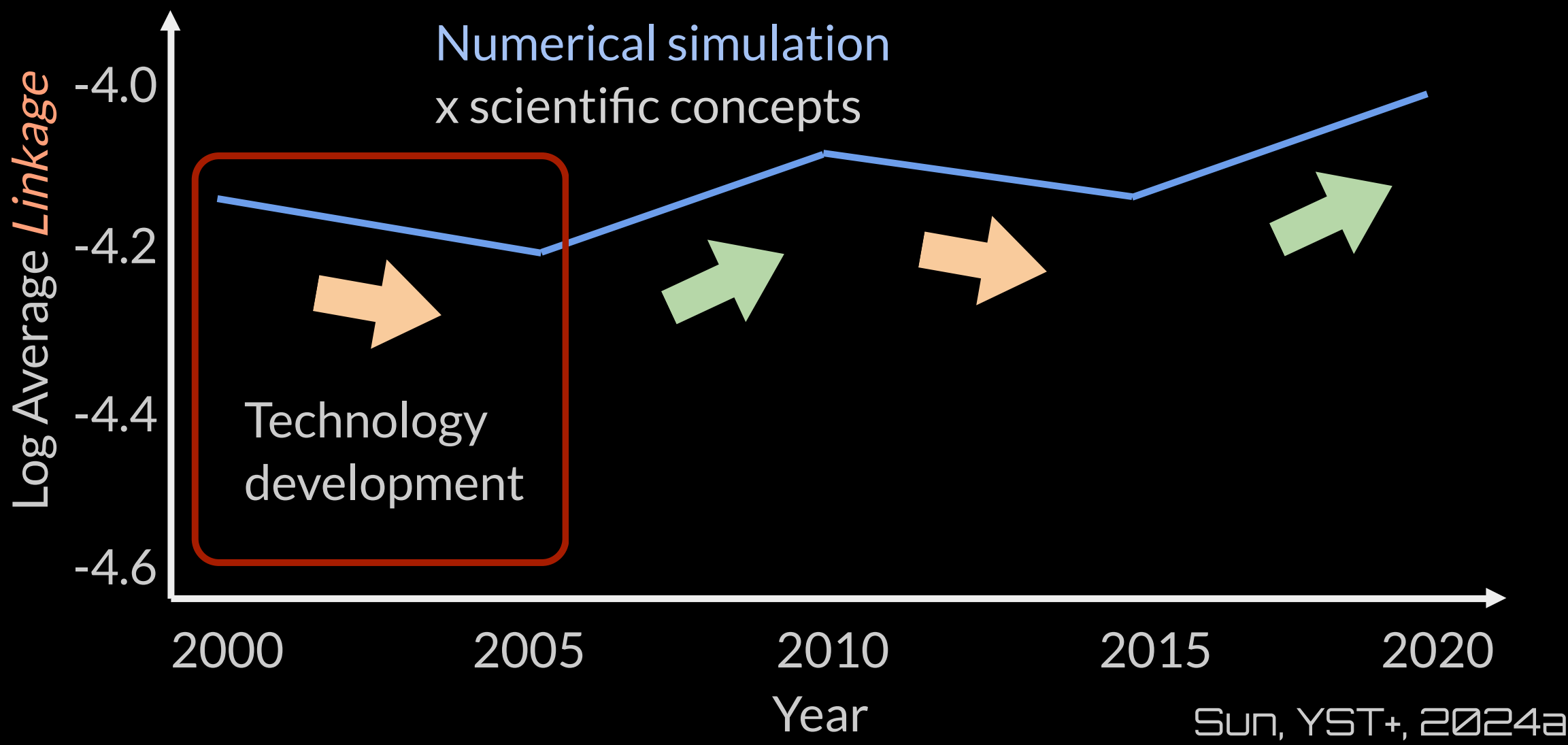
Cross-domain linkage shows a *two-phase* evolution

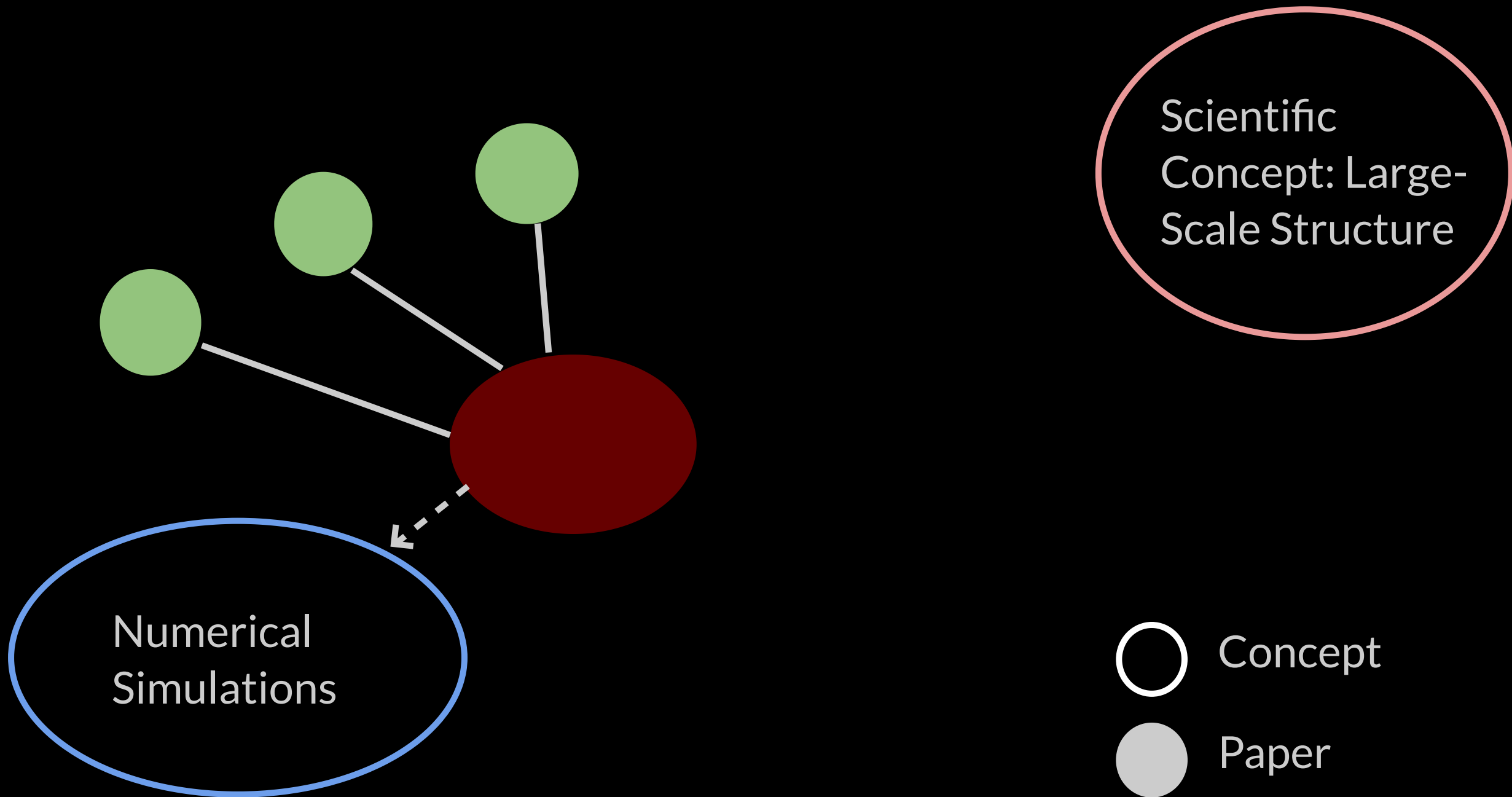


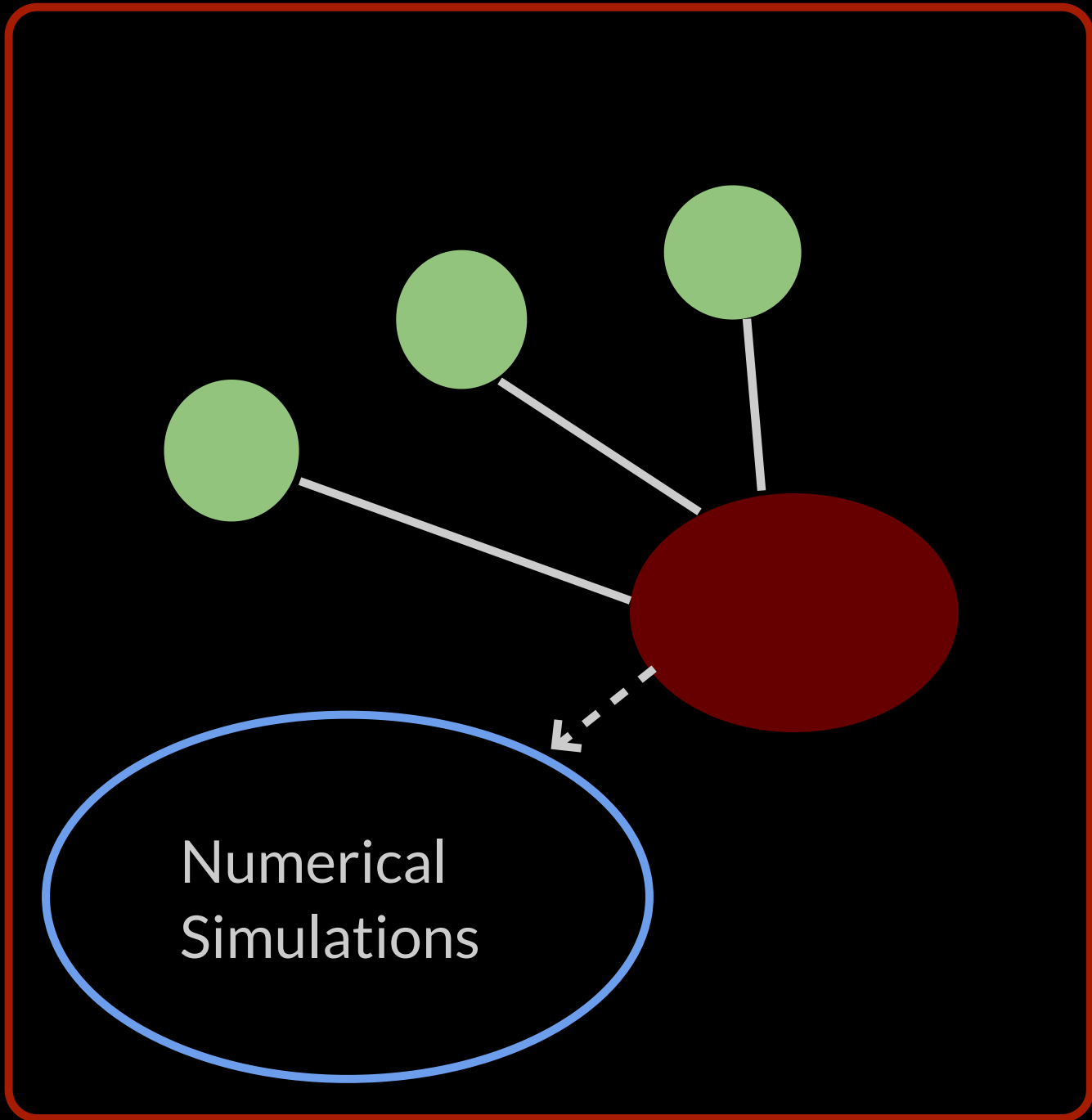
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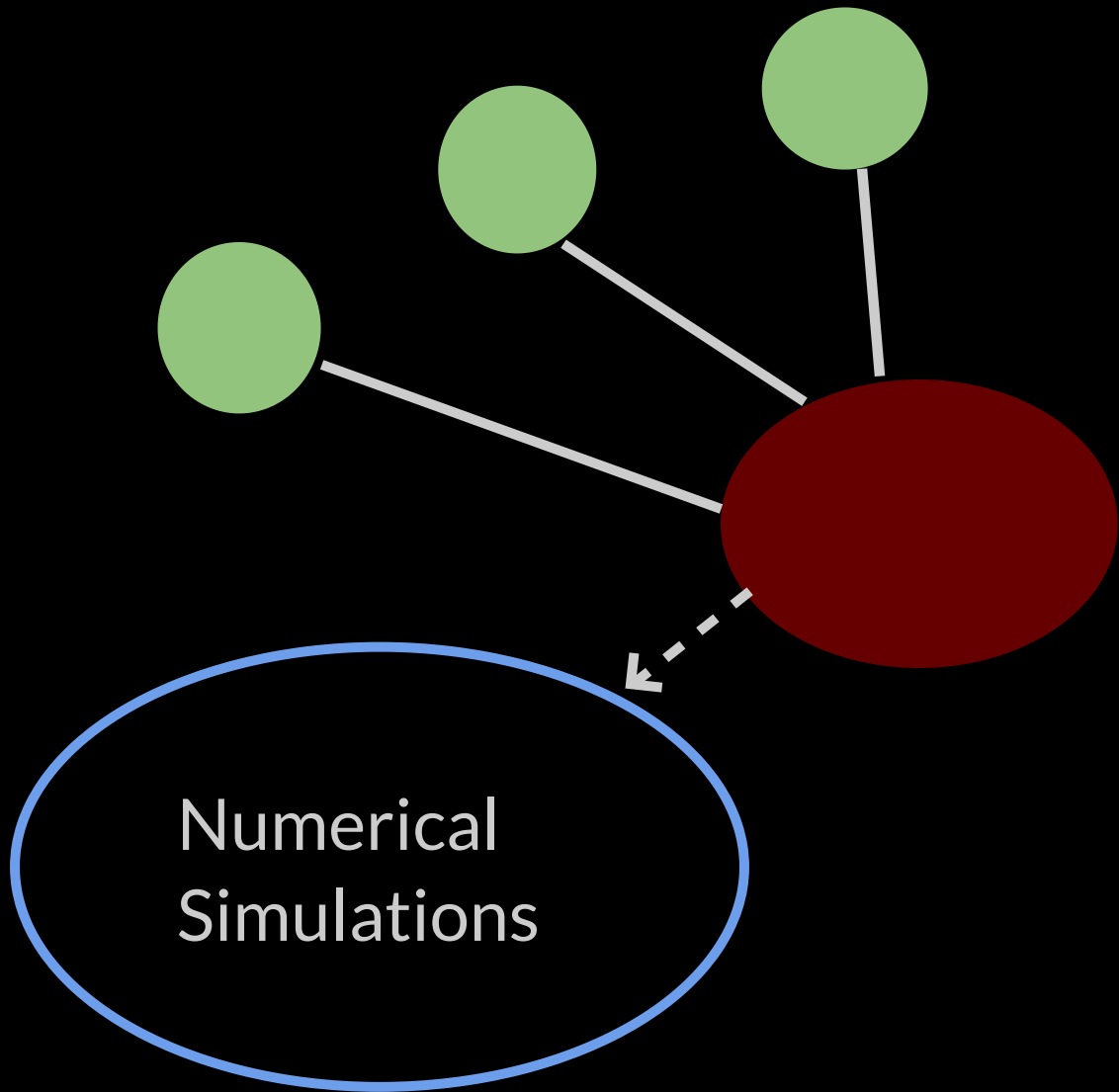




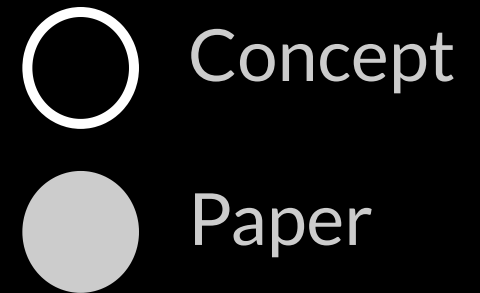
Scientific
Concept: Large-
Scale Structure

- Concept
- Paper

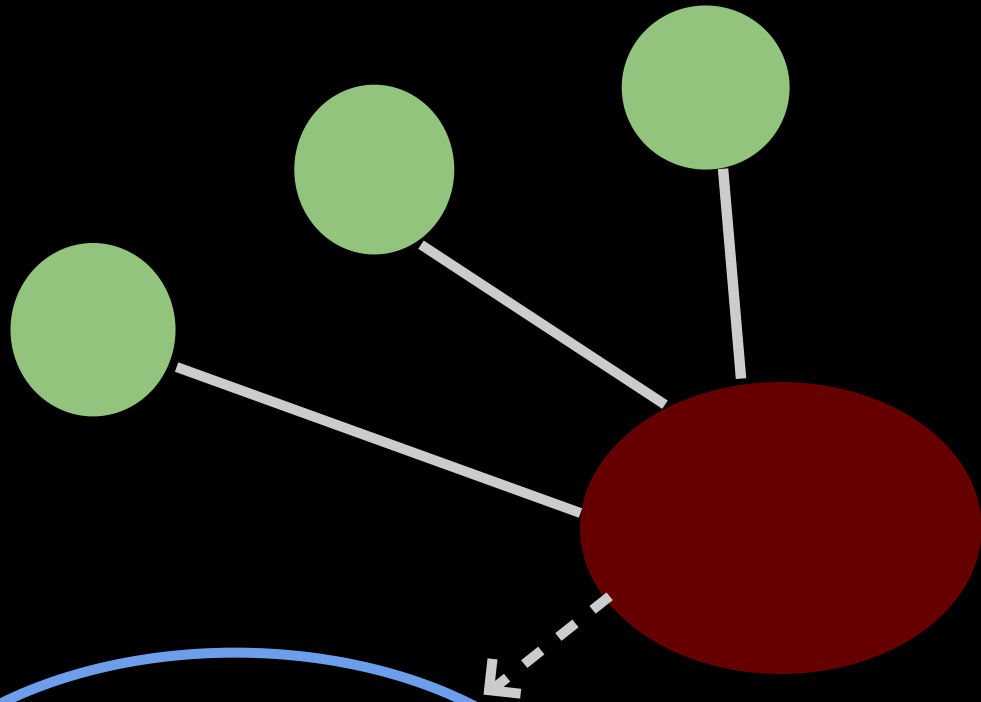
N-body solver being developed



Scientific
Concept: Large-
Scale Structure



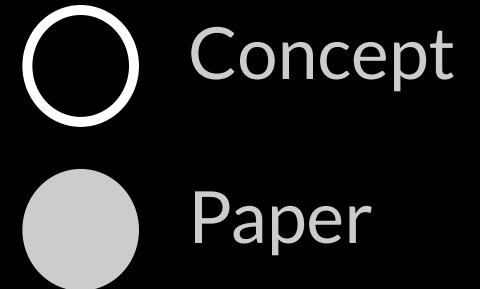
N-body solver being developed



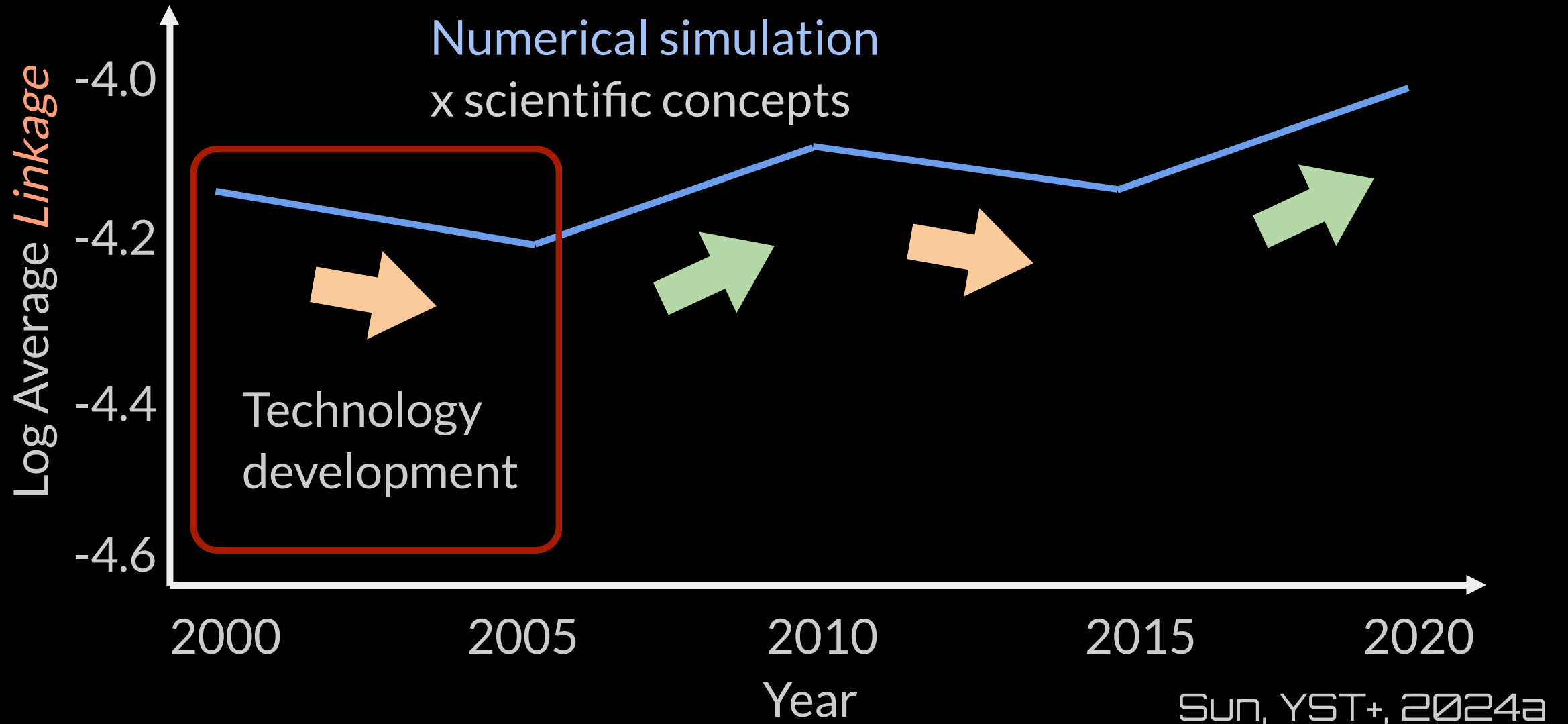
Numerical
Simulations

Linkage
decoupled

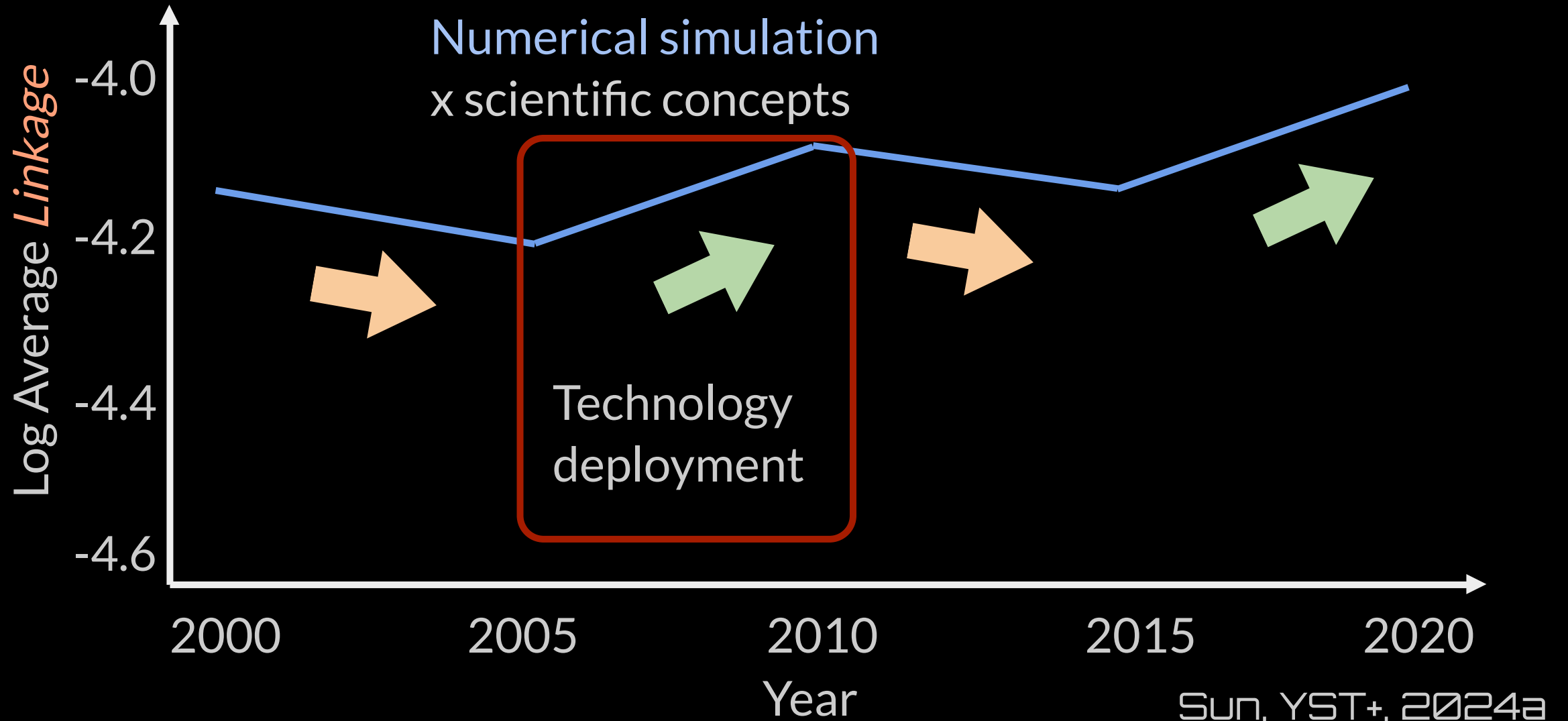
Scientific
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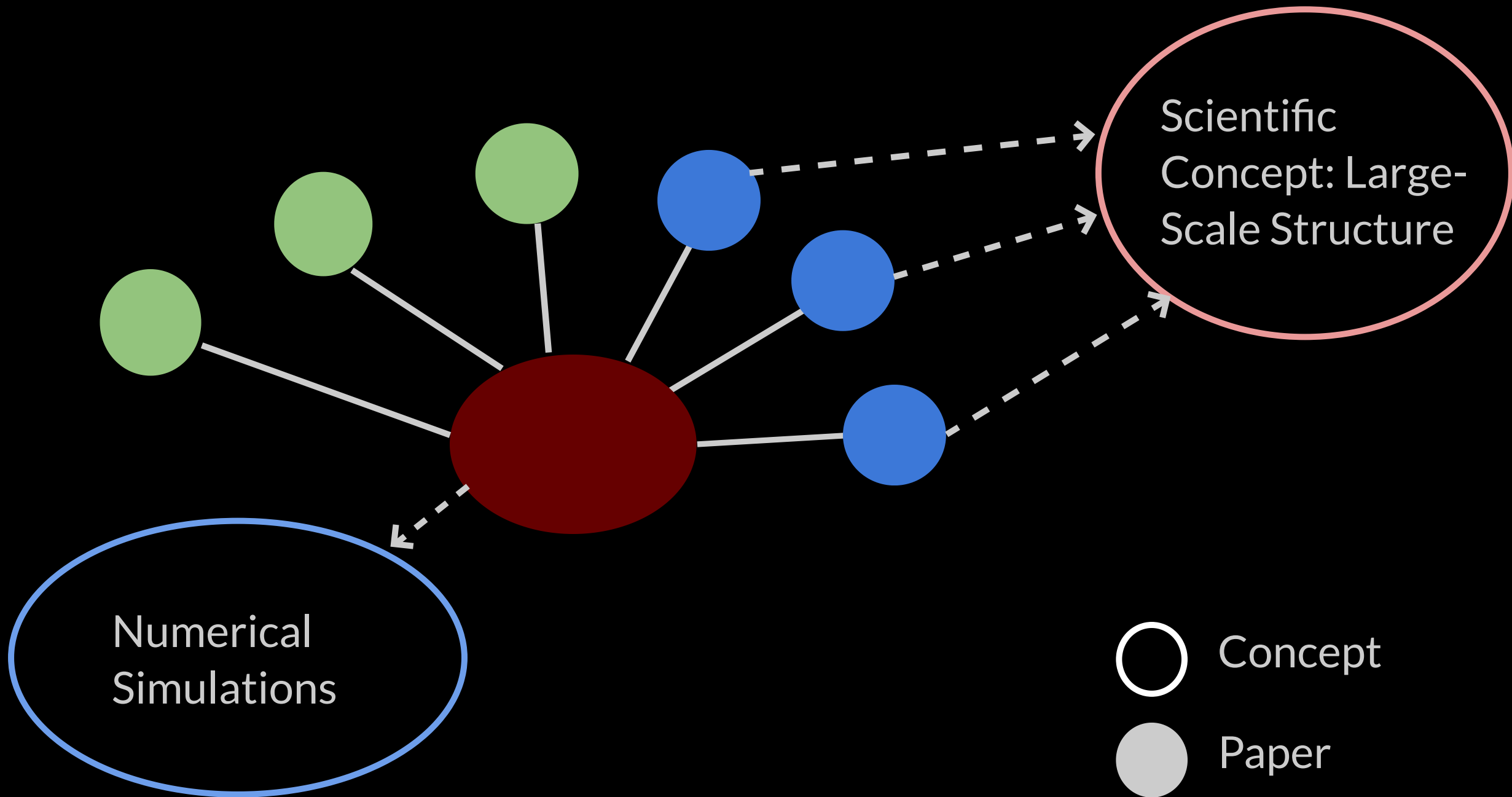


Cross-domain linkage shows a *two-phase* evolution

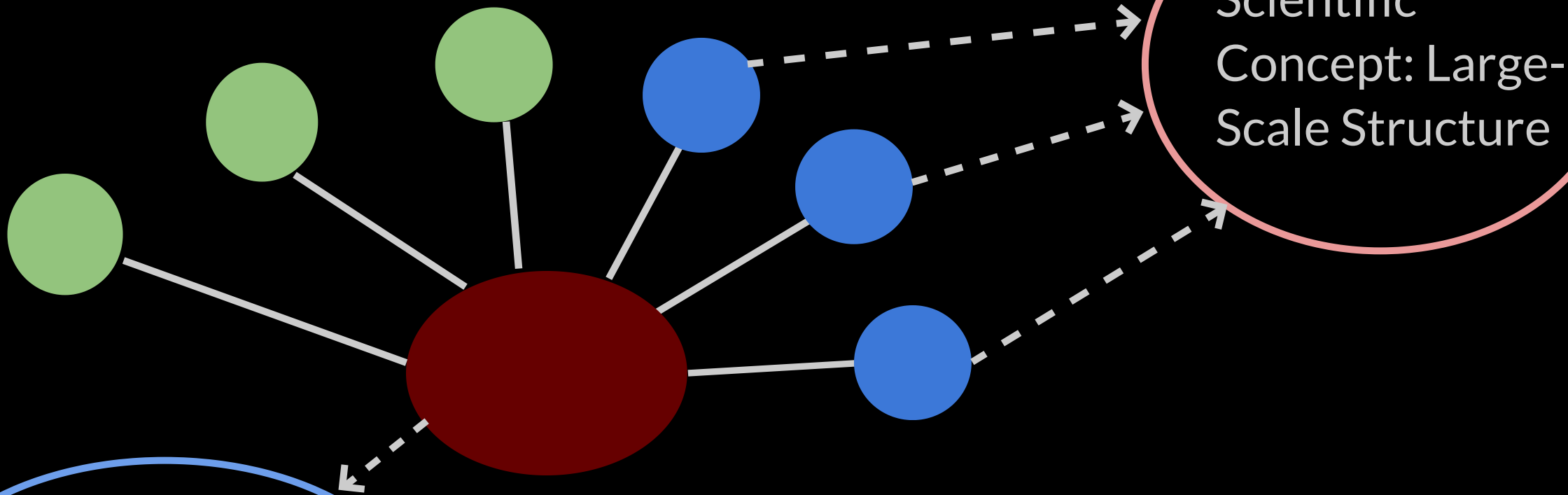


Cross-domain linkage shows a *two-phase* evolution



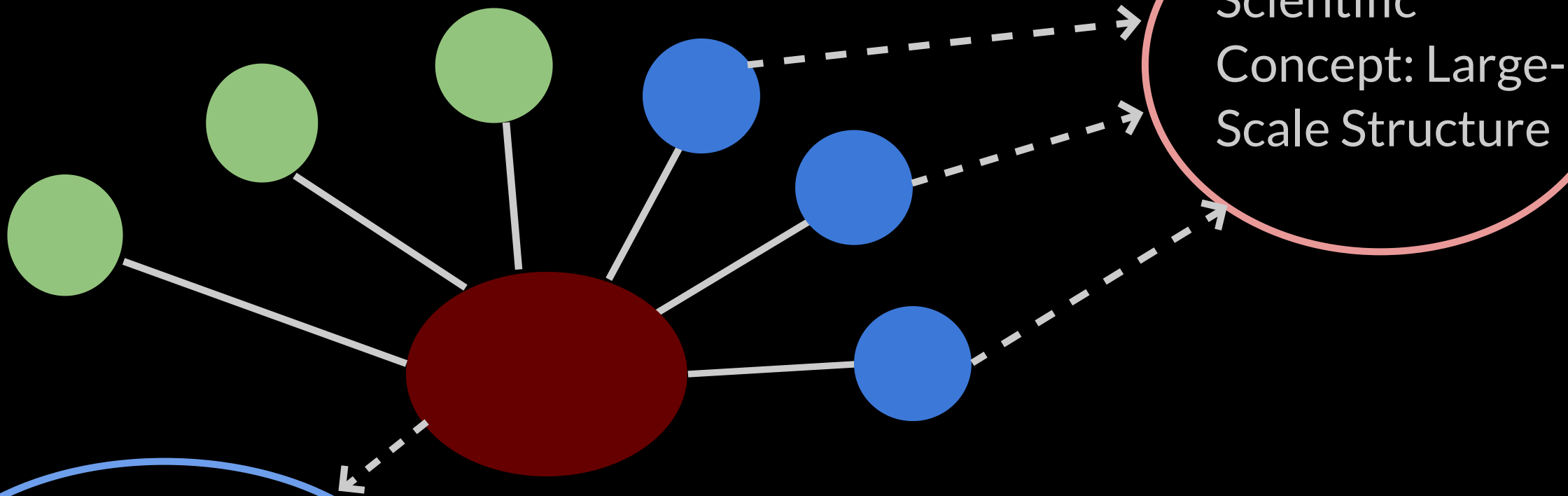


N-body solver being deployed to simulations



- Concept
- Paper

N-body solver being deployed to simulations



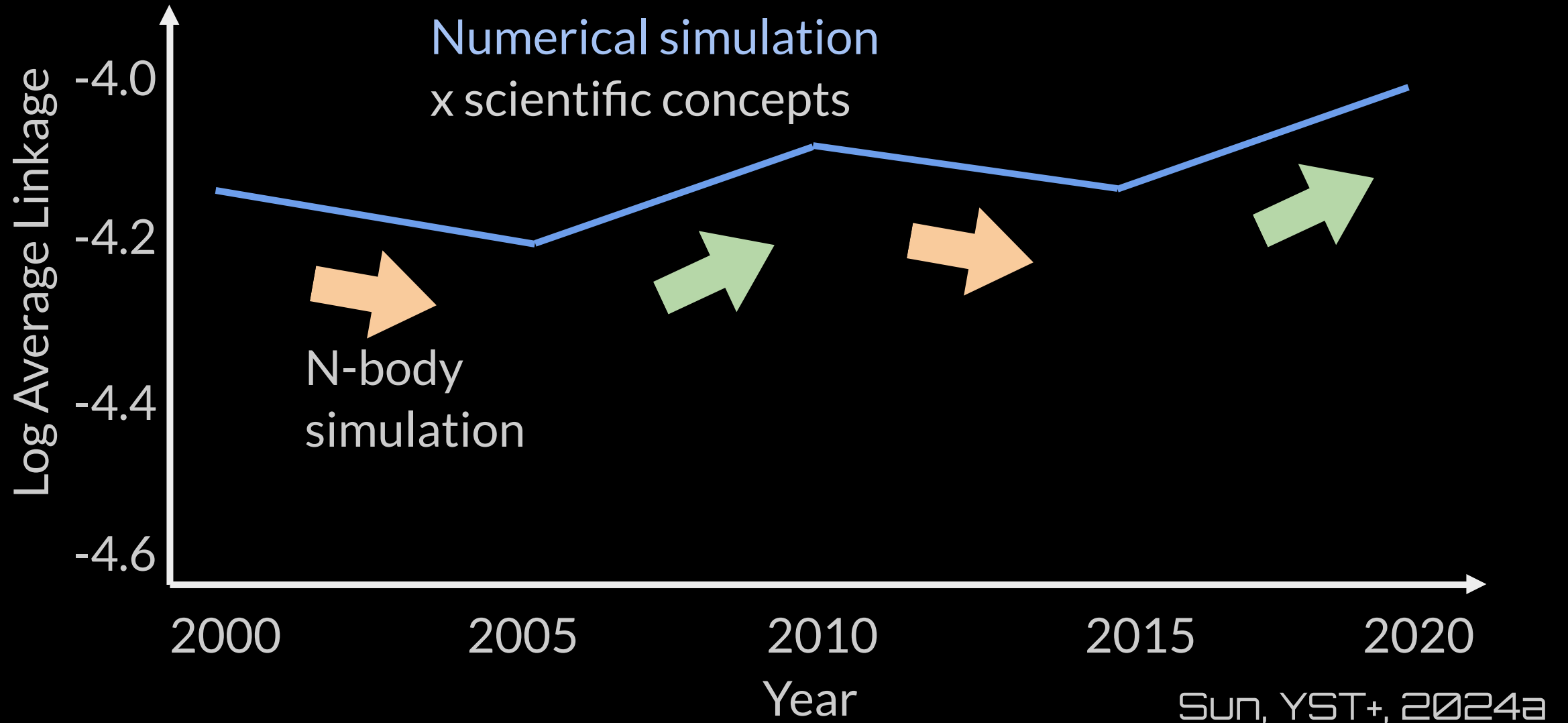
Numerical
Simulations

Linkage increases

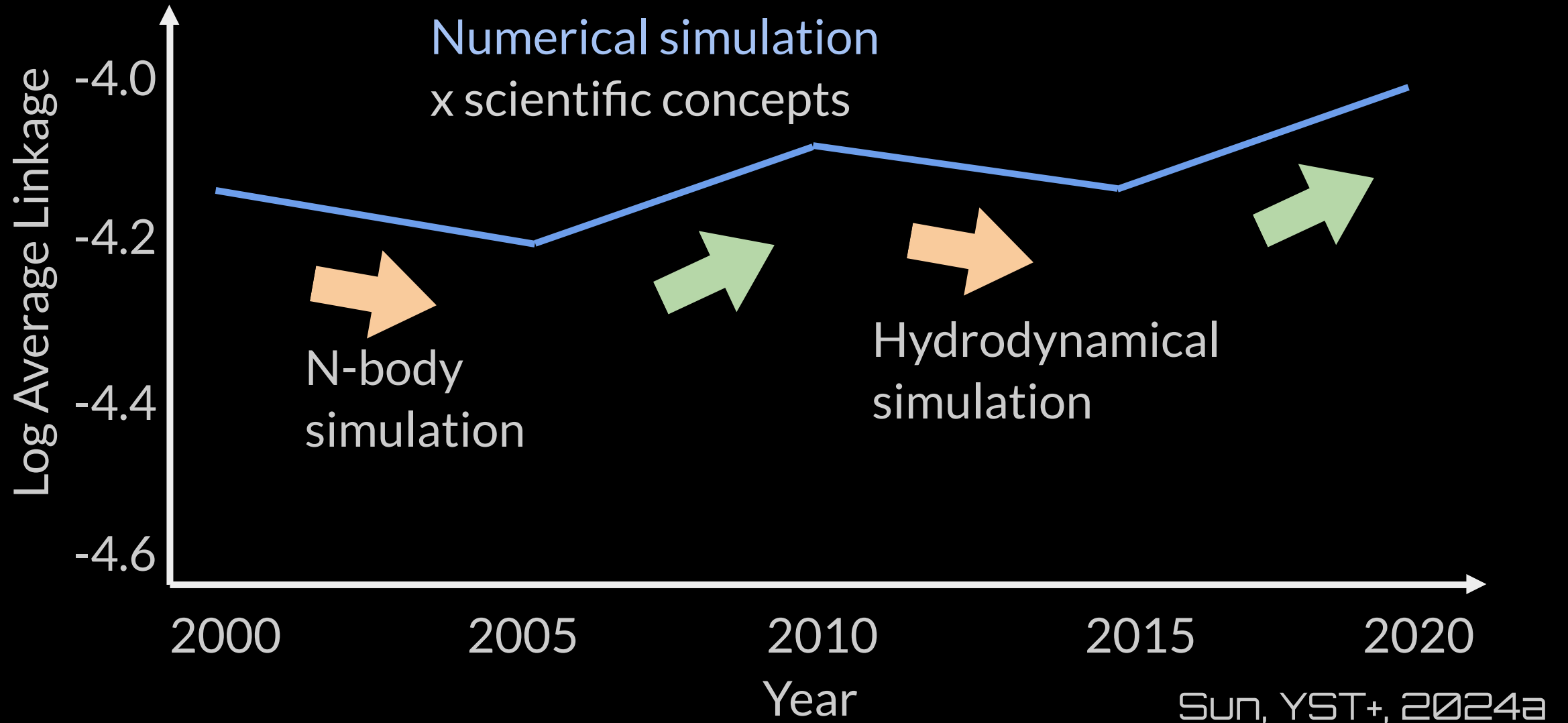
○ Concept

● Paper

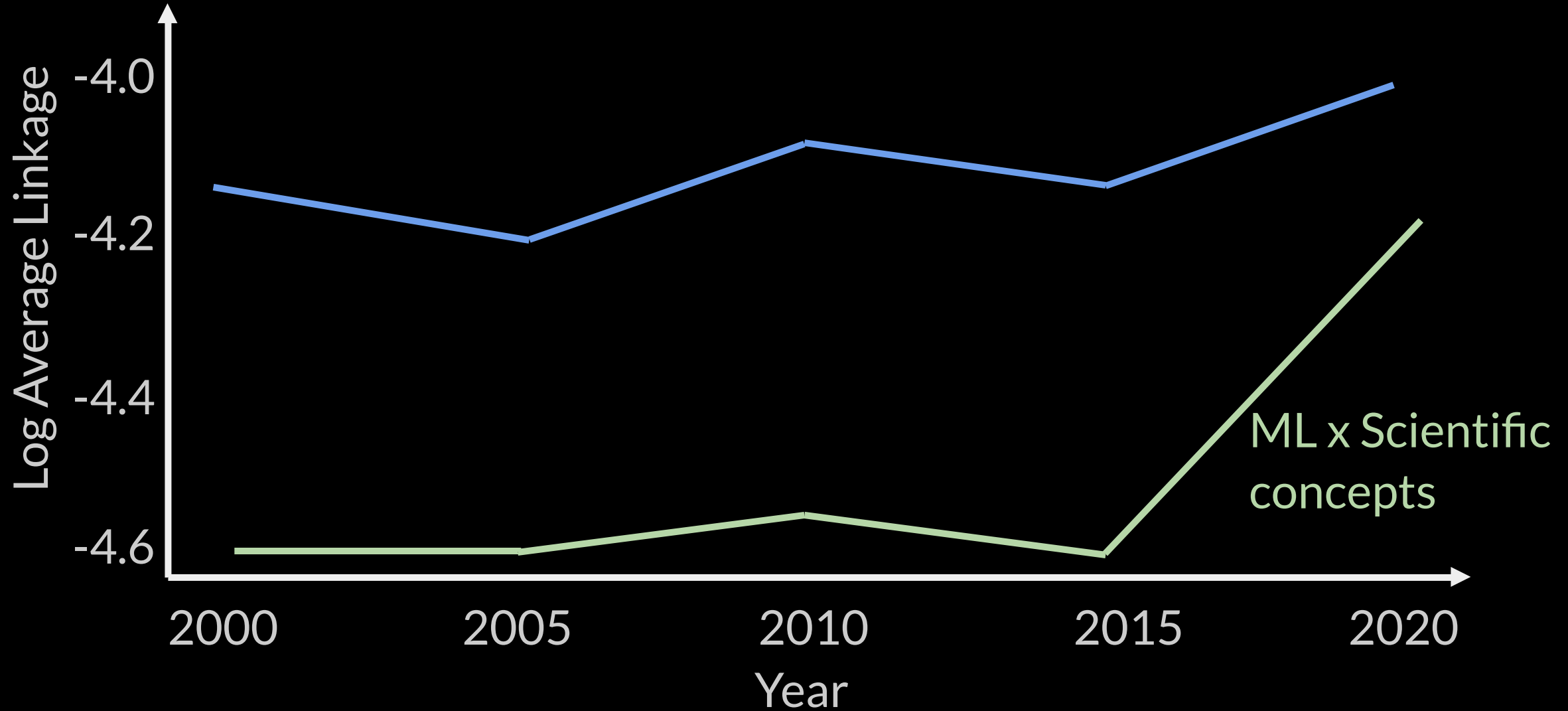
Cross-domain linkage shows a *two-phase* evolution



Cross-domain linkage shows a *two-phase* evolution



Interest in AI x Astronomy *outpaces* technological development



Machine learning is becoming *increasingly integrated* into astronomy,

However, the field has been *slow to incorporate new concepts* and techniques.

Astronomy is *not* biology

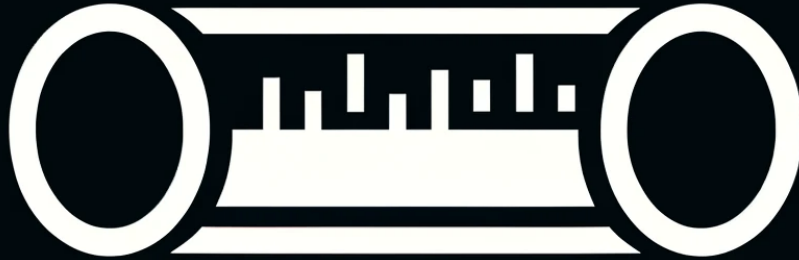
Data /
Observation

Theory /
Hypothesis

Astronomy is *not* biology

Data /
Observation

Theory /
Hypothesis

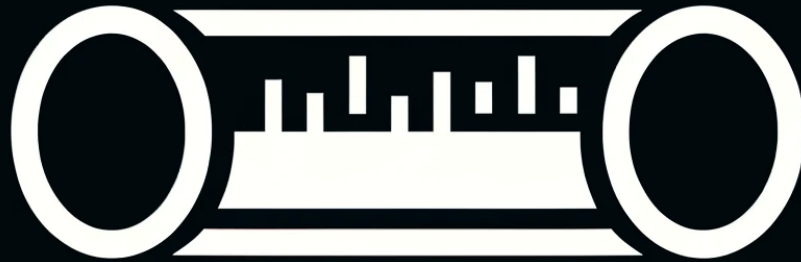


Analysis
Pipelines

Astronomy is *not* biology

Data /
Observation

Theory /
Hypothesis



Analysis
Pipelines



True

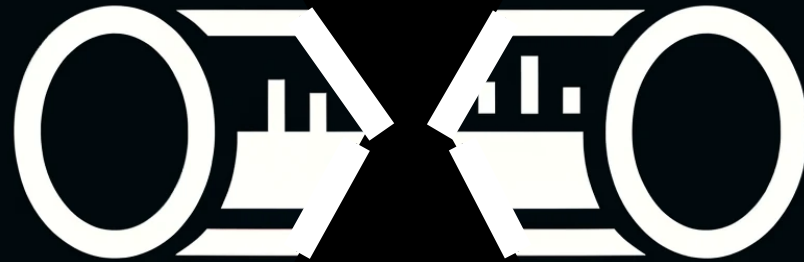


False

Biology faced a fundamental *bottleneck*

Data /
Observation

Theory /
Hypothesis



Analysis
Pipelines



True



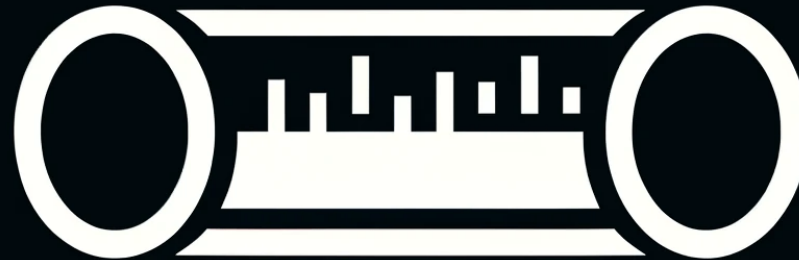
False

Biology faced a fundamental *bottleneck*

Data /
Observation

Theory /
Hypothesis

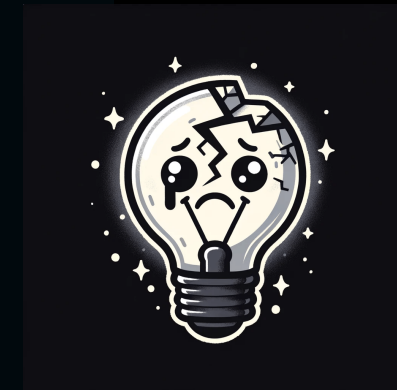
Alphafold



Analysis
Pipelines



True

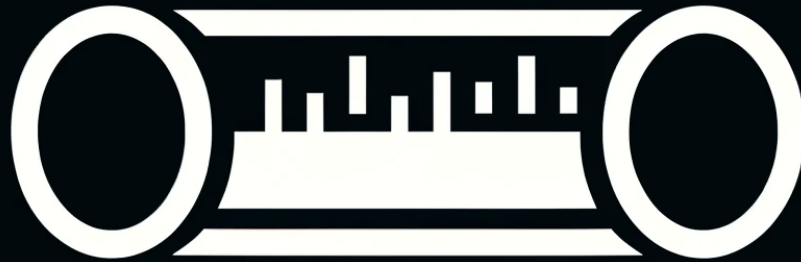


False

Astronomy already has a successful *standard model*

Data /
Observation

Theory /
Hypothesis



LambdaCDM



True



False



- Where are we in AI for Astronomy - What's the problem?
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- What could be the AlphaFold moment for astronomy?

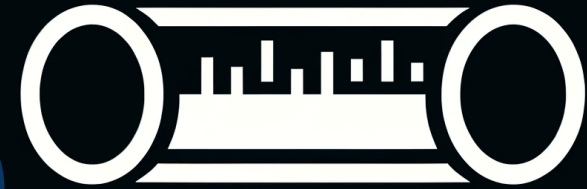
- How do we get there in a cost-effective way?

Toward an *AI Astronomer*

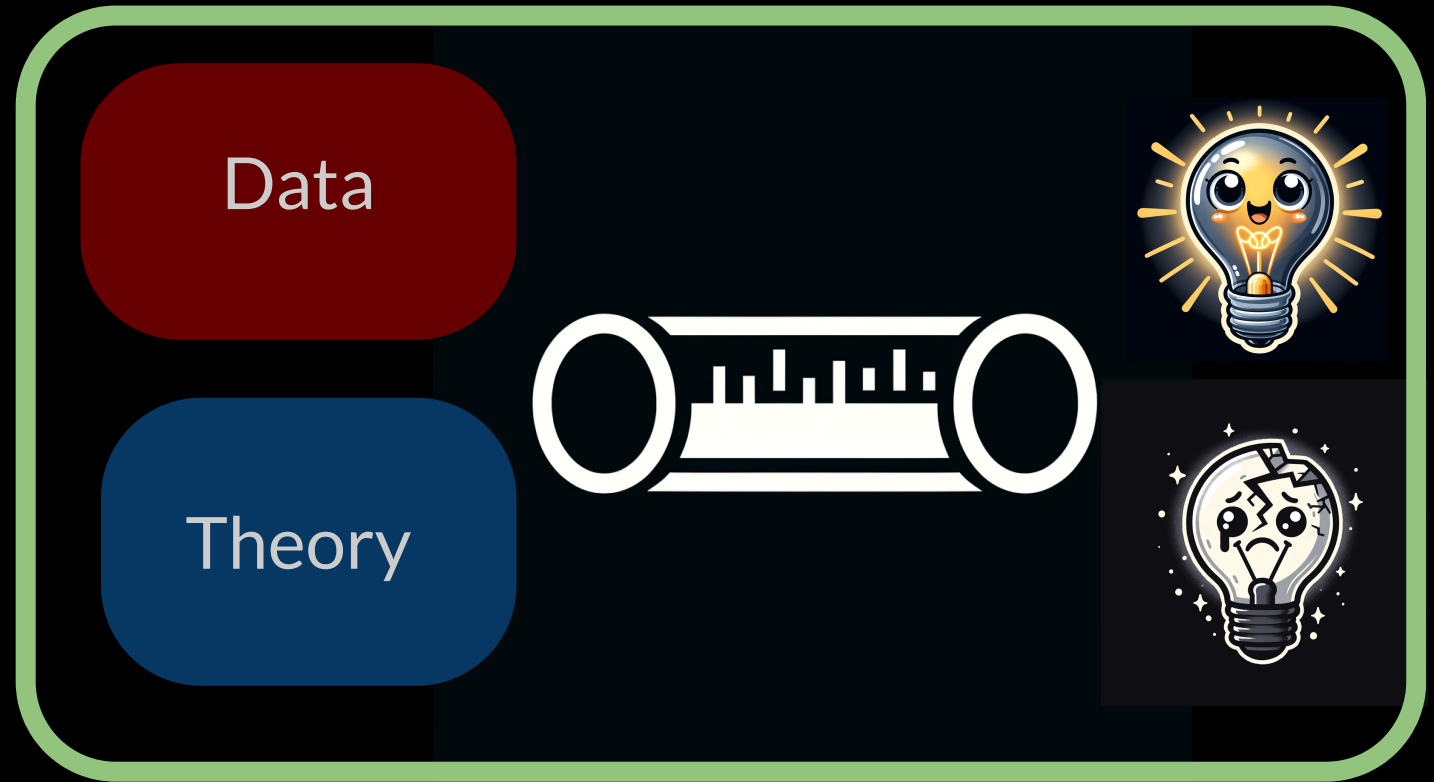
Research is essentially a *reinforcement learning* process

Data

Theory



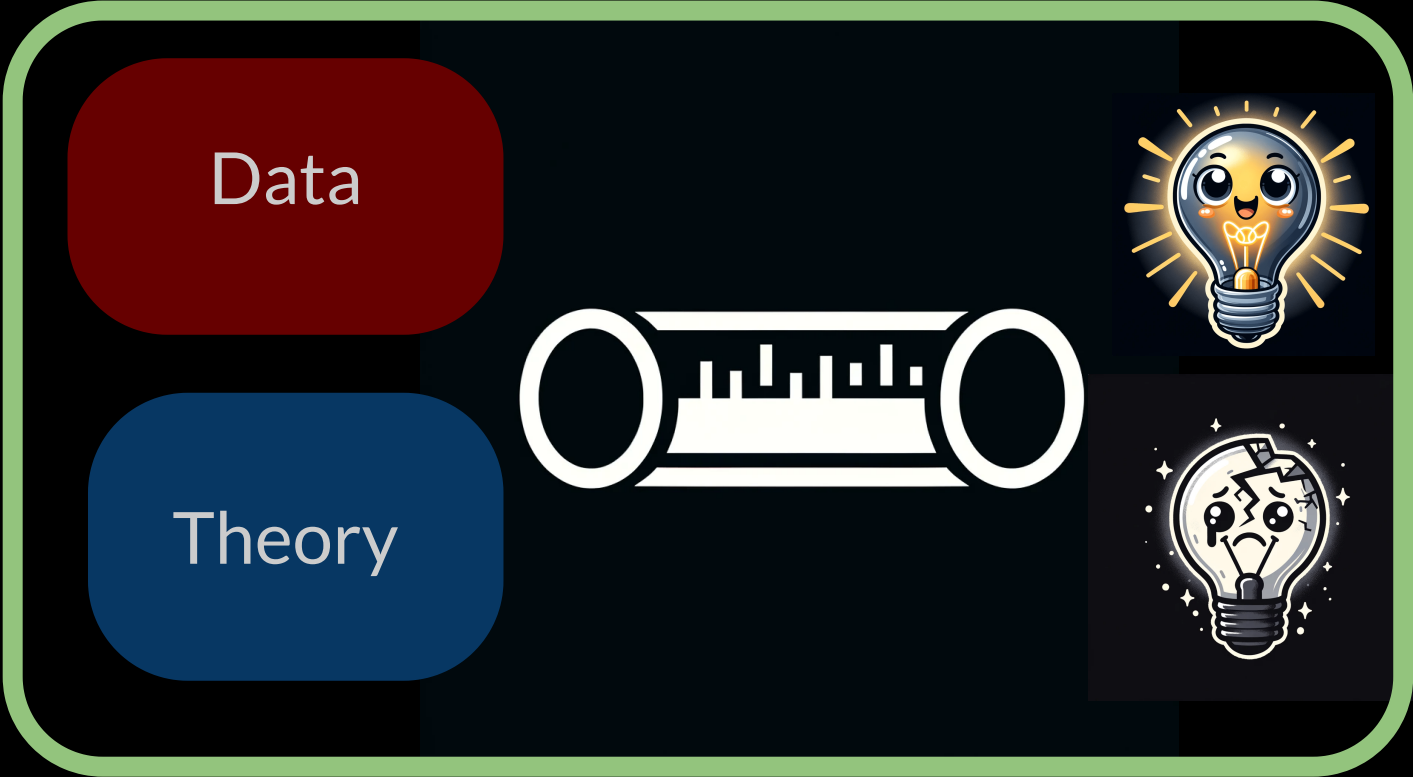
Research is essentially a *reinforcement learning* process



State of the research

Research is essentially a *reinforcement learning* process

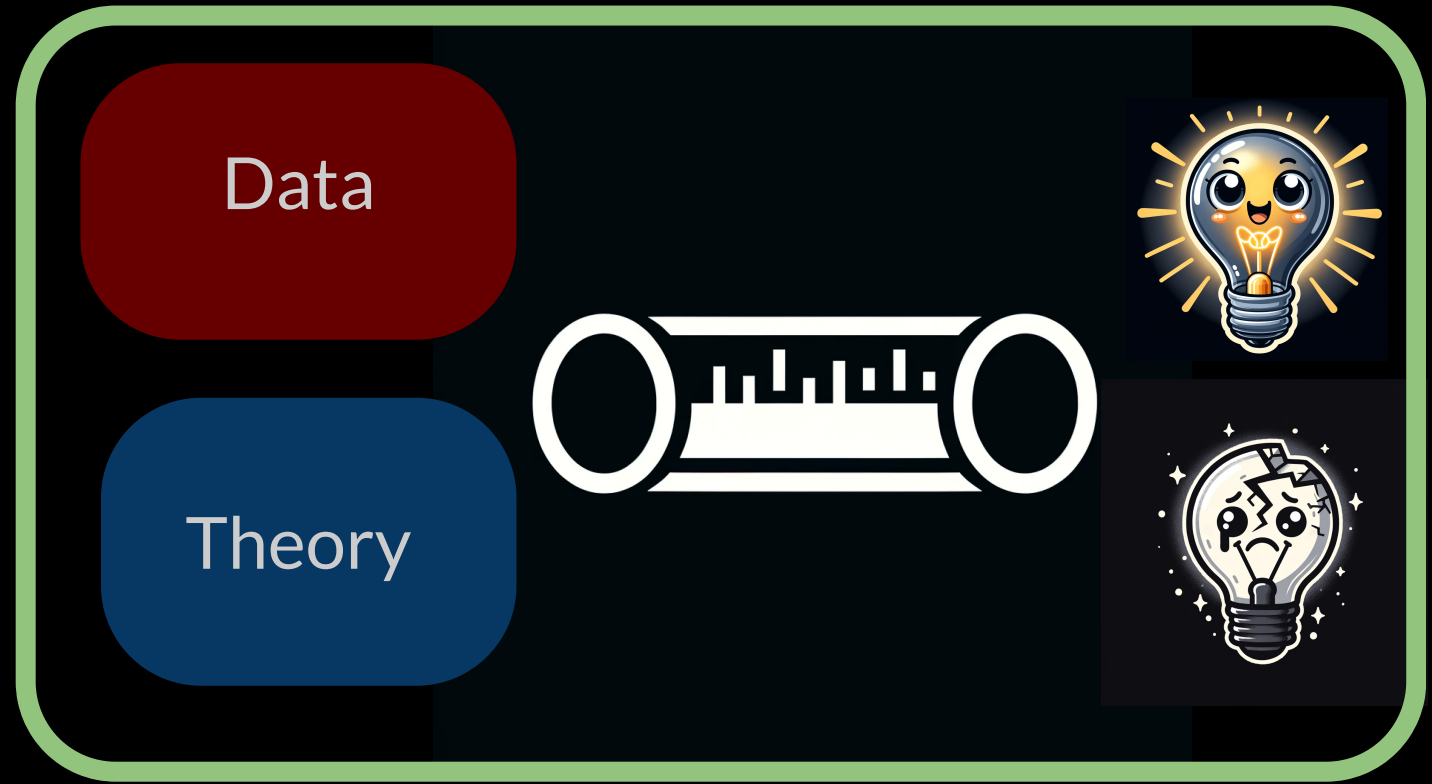
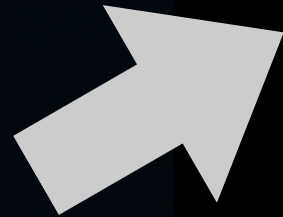
Evaluate the state



State of the research

Research is essentially a *reinforcement learning* process

Evaluate the state
propose new theory or data

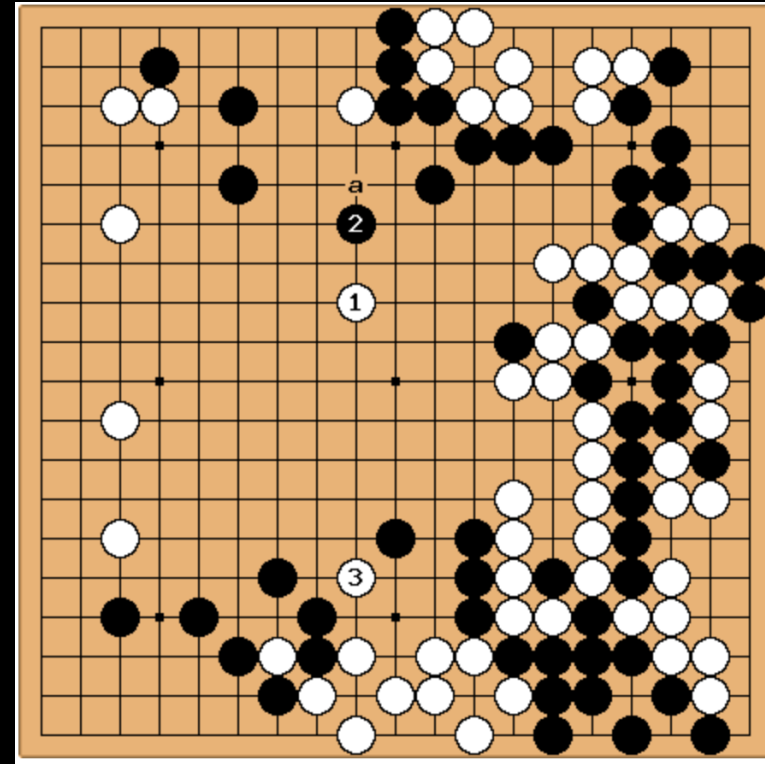
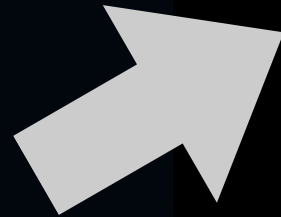


State of the research

Research is essentially a *reinforcement learning* process

Evaluate the state

propose new theory or data



State of the research

But most *"state" of research* cannot be
mathematically defined

But most *"state" of research* cannot be
mathematically defined



Human *"intuition"* +
experience

Perform "reinforcement learning" (*policy learning*)
without a reward function

Perform "reinforcement learning" (*policy learning*)
without a reward function

Enabling LLM agents to *learn through real-world exploration* and interaction.

Automating Astronomical Research with Large Language Model Agents: A Case Study with Galaxy Spectral Energy Distribution Fitting

Zechang Sun¹ Yuan-Sen Ting^{2,3} Yaobo Liang⁴ Nan Duan⁴ Song Huang¹ Zheng Cai¹

Abstract

The application of AI has generated significant interest in astrophysics; however, most studies have been limited to using AI for specific predefined tasks. In contrast, real-life astronomical research involves a complex series of reasoning processes that researchers develop through years of training and experience. In this study, we explore the use of large language model-based collaboration agents to distill knowledge and experience by interacting with actual astronomical questions and

Bubeck et al., 2023). This has led to a myriad of perform tasks beyond including applications robotics (Wang et al., 2023) and mathematics (Azhar et al., 2023). There has been a growing trend of using large language models to design and conduct experiments both in chemistry and physics (Liu et al., 2023; Lei et al., 2024;



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Abstract

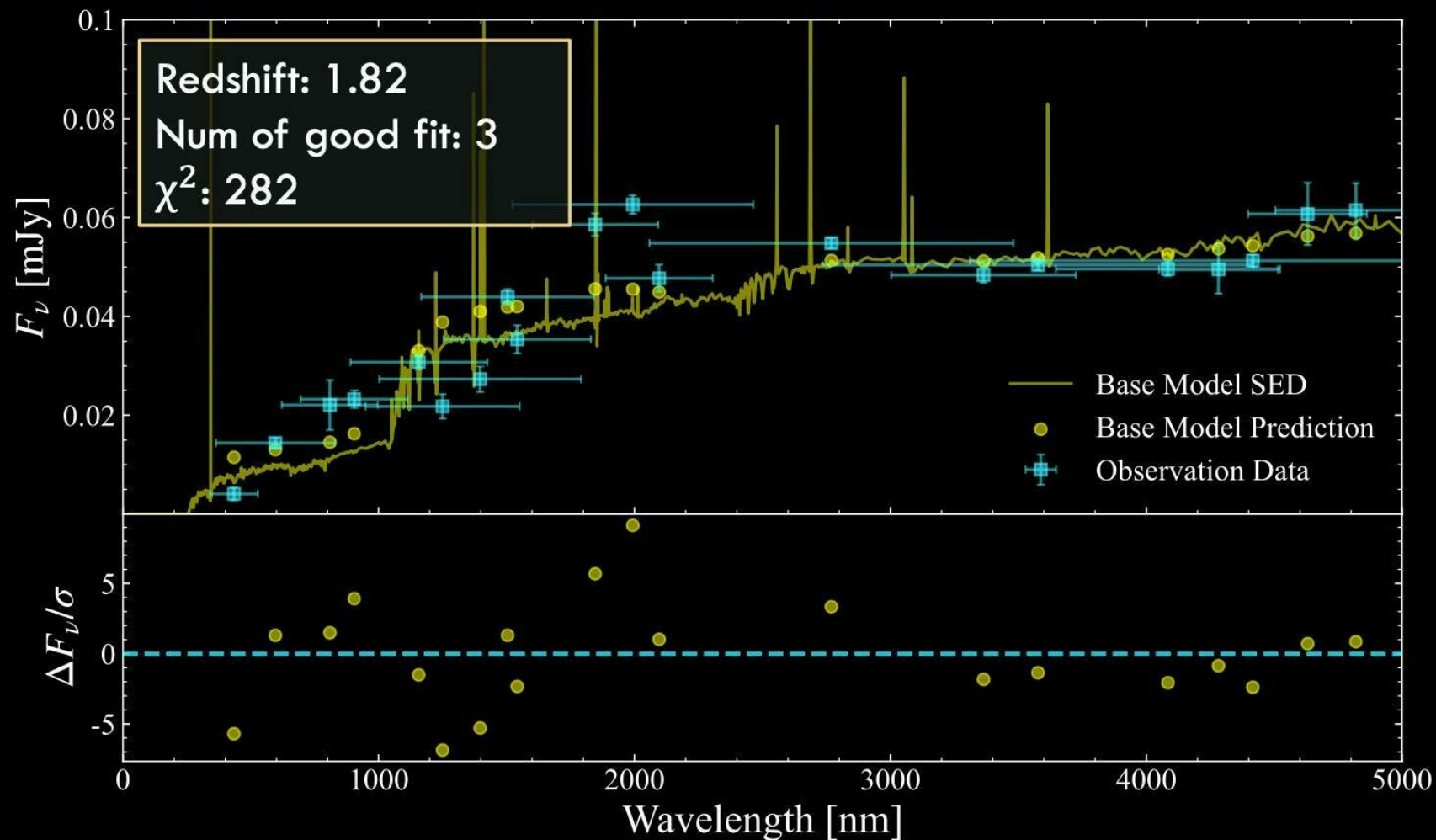
The application of AI has generated significant interest in astrophysics; however, most studies have been limited to using AI for specific predefined tasks. In contrast, real-life astronomical research involves a complex series of reasoning processes that researchers develop through years of training and experience. In this study, we explore the use of large language model-based collaboration agents to distill knowledge and experience by interacting with actual astronomical questions and

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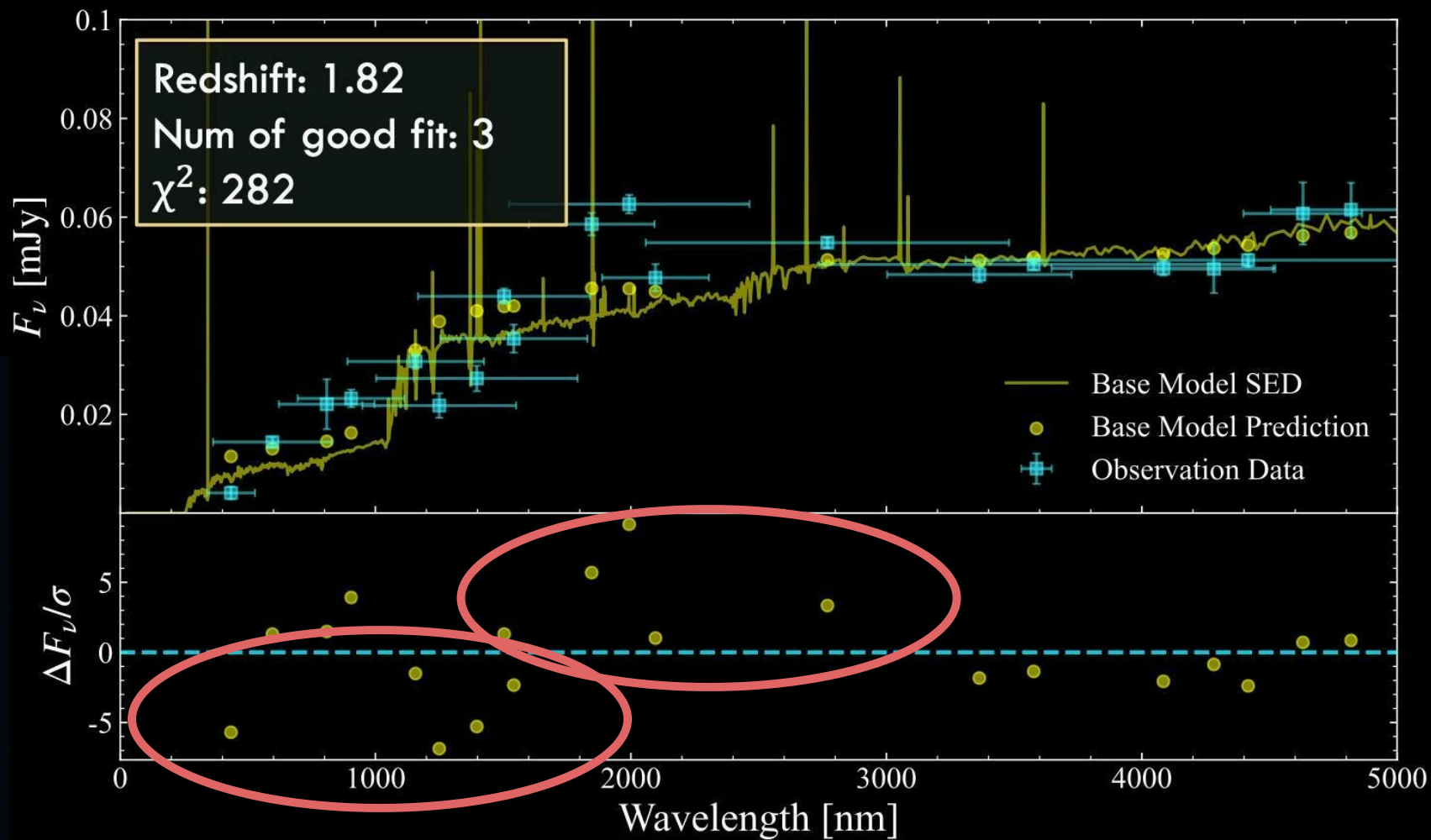
Action space is vast and transcends mathematical formalism

A default fit with
an SED model

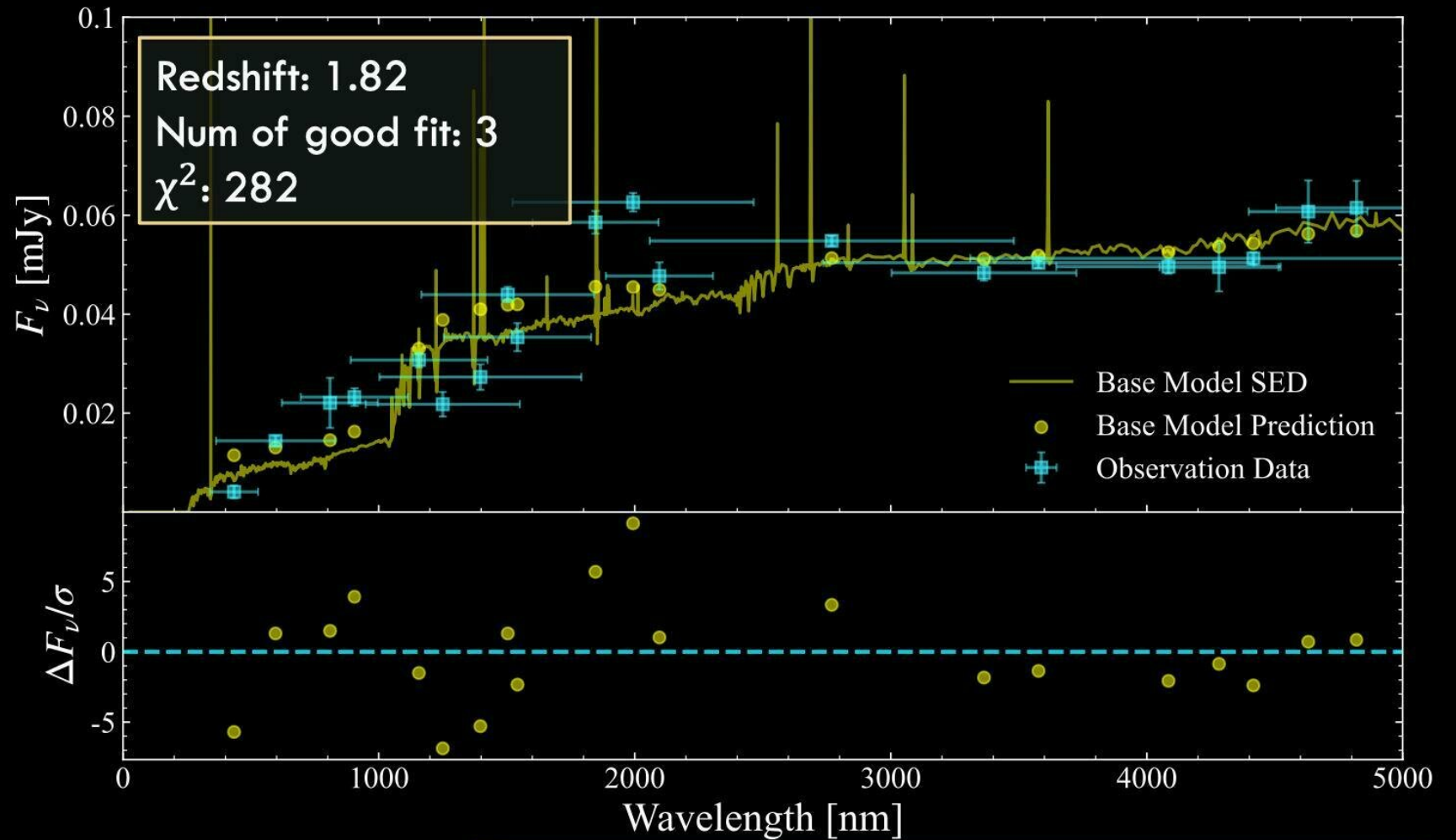


Action space is vast and transcends mathematical formalism

A default fit with
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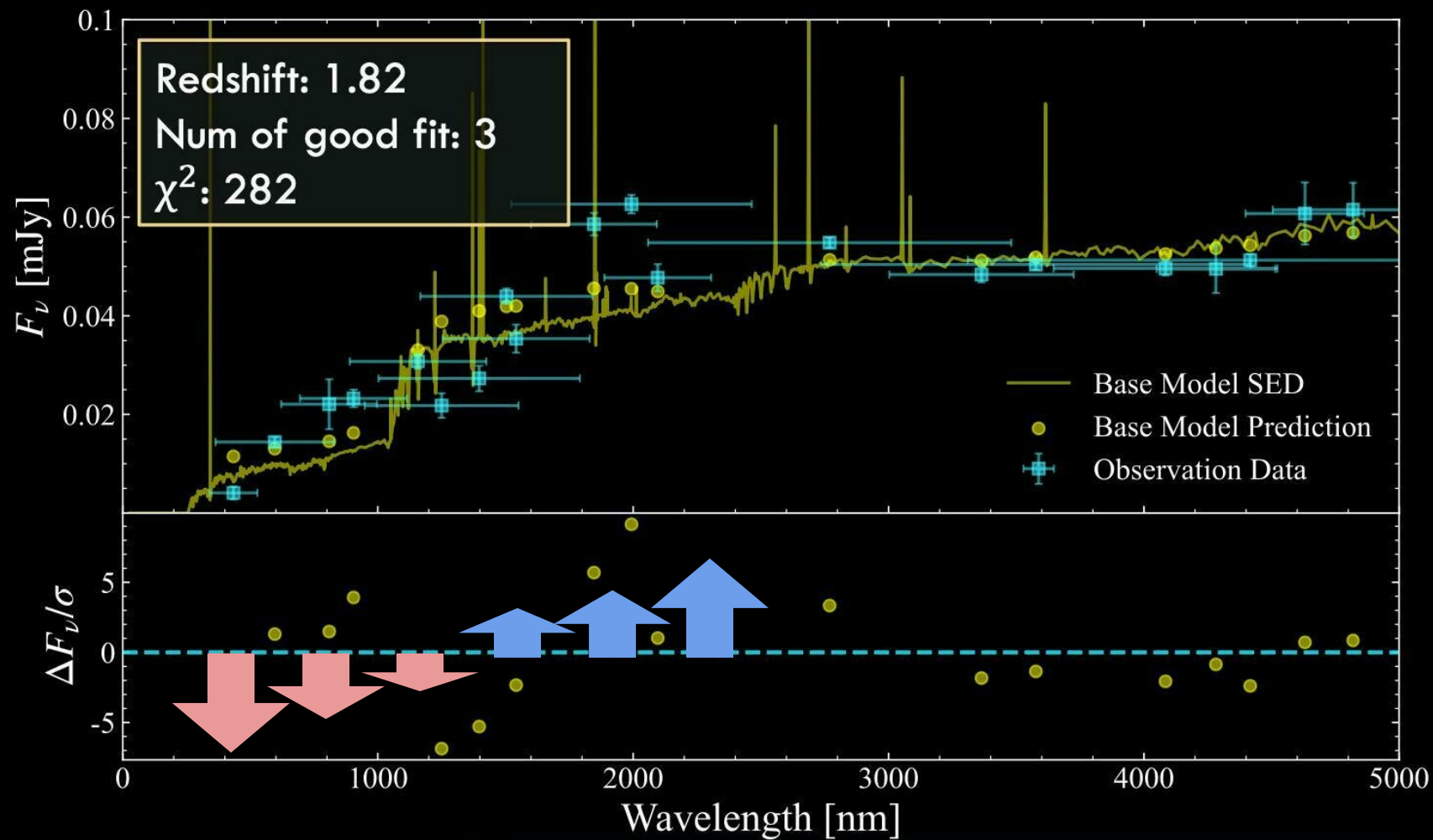


Action space is vast and transcends mathematical formalism



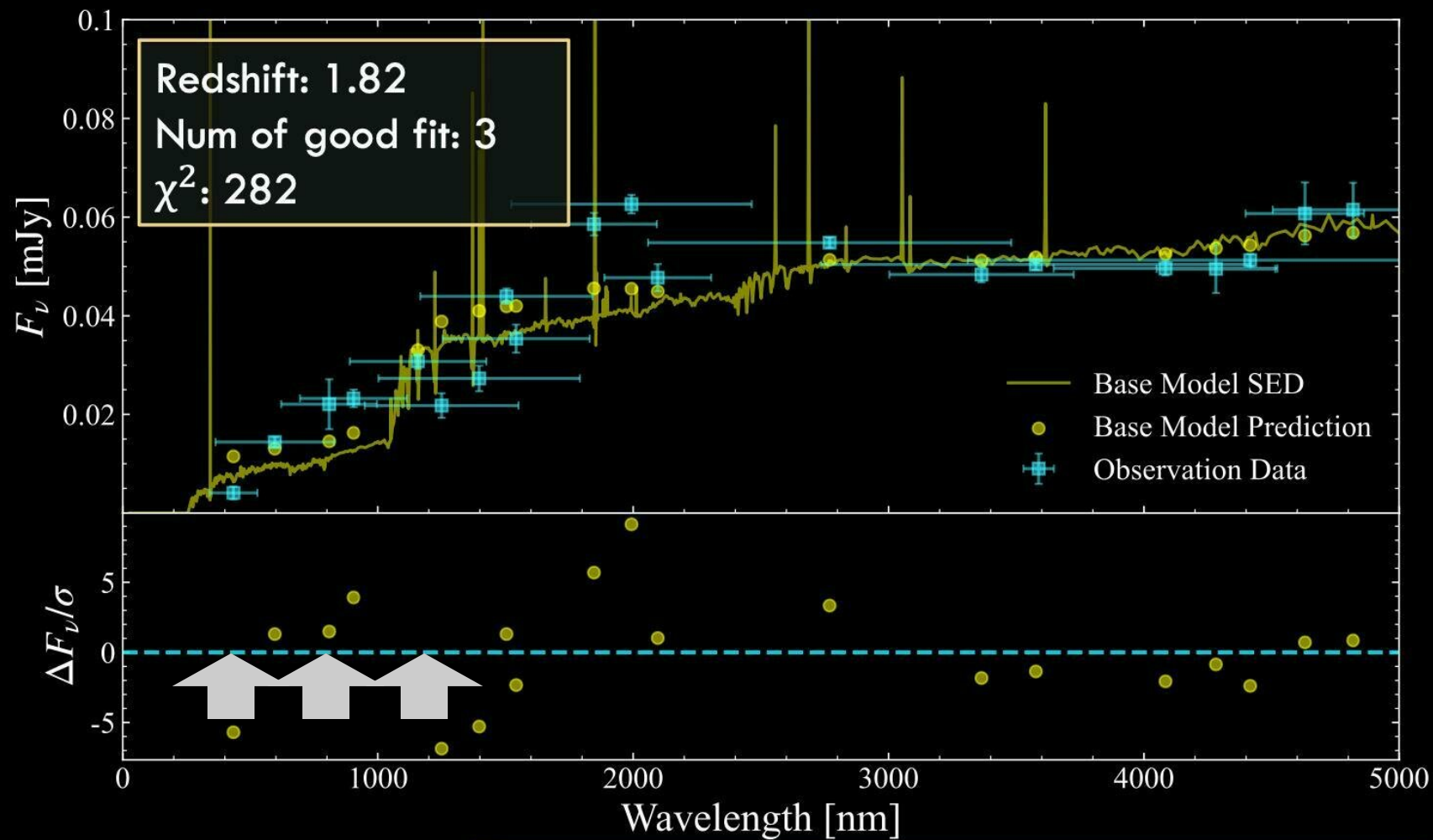
Action space is vast and transcends mathematical formalism

Extinction model ?



Action space is vast and transcends mathematical formalism

Young stellar population?



Introducing *Mephisto**



* In the classic tale of Faust, Mephisto is a demon who tempts the scholar Faust with *knowledge* and power in exchange for his soul.

A *collaboration* of multiple AI agents (LLM models)

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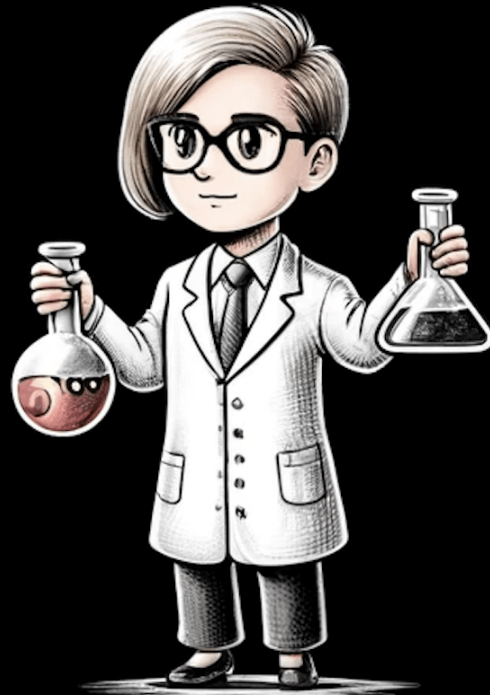


Proposing actions

A *collaboration* of multiple AI agents (LLM models)



Proposing actions

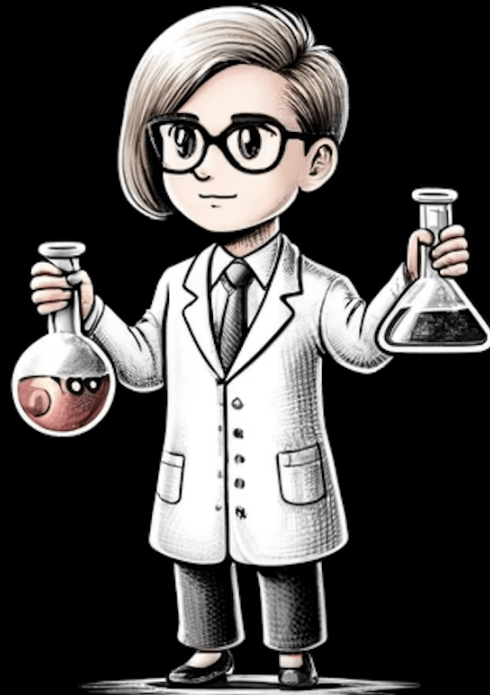


Execute actions

A *collaboration* of multiple AI agents (LLM models)



Proposing actions



Execute actions

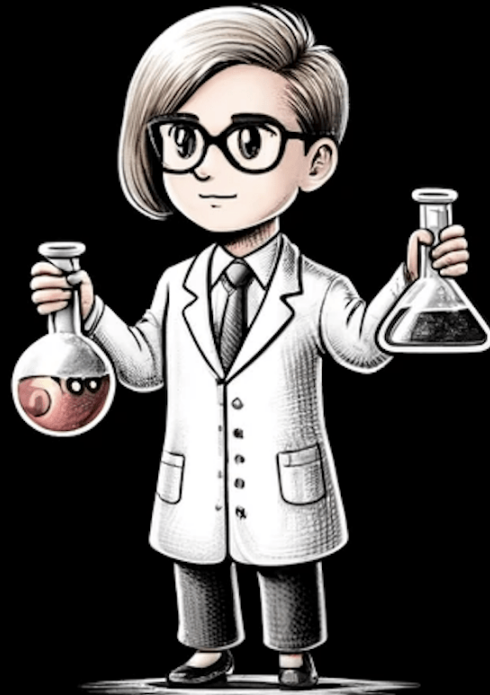


State evolution

A *collaboration* of multiple AI agents (LLM models)



Proposing actions



Execute actions



State evolution



Knowledge
distillation

A *collaboration* of multiple AI agents (LLM models)



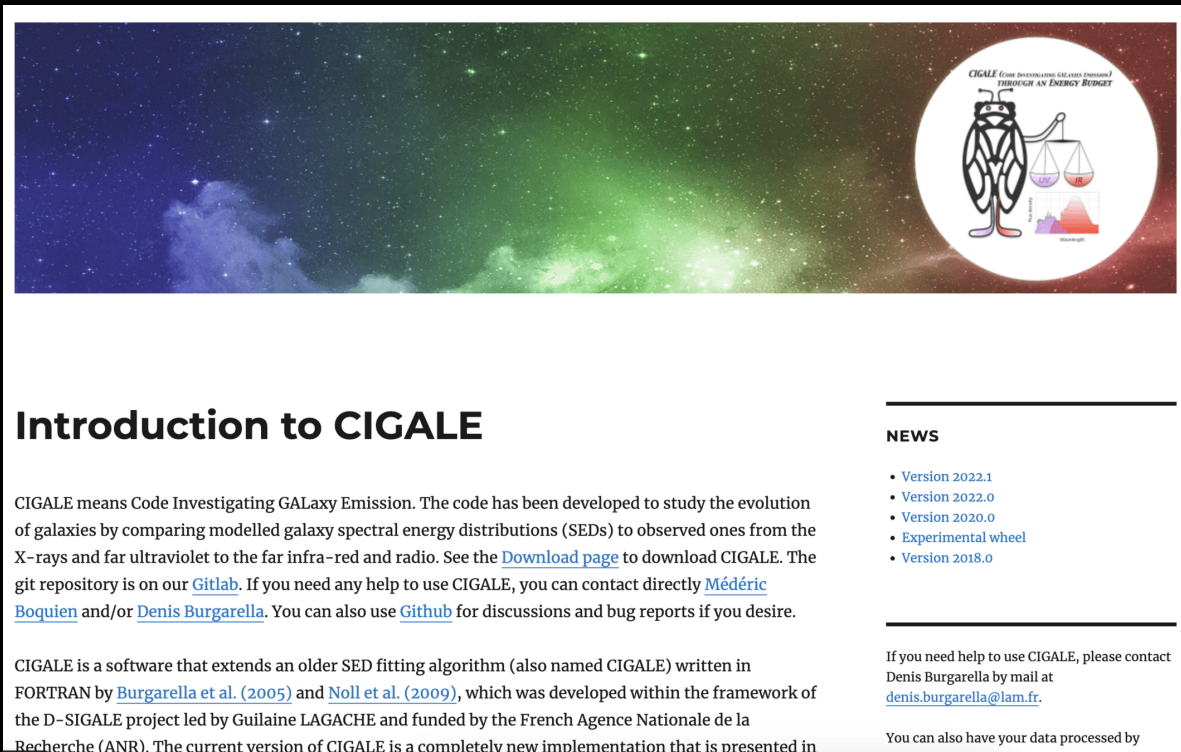
Proposing actions

Execute actions

State evolution

Knowledge
distillation

A case study: Fitting galaxy spectral energy distributions



Introduction to CIGALE

CIGALE means Code Investigating GALaxy Emission. The code has been developed to study the evolution of galaxies by comparing modelled galaxy spectral energy distributions (SEDs) to observed ones from the X-rays and far ultraviolet to the far infra-red and radio. See the [Download page](#) to download CIGALE. The git repository is on our [Gitlab](#). If you need any help to use CIGALE, you can contact directly [Médéric Boquien](#) and/or [Denis Burgarella](#). You can also use [Github](#) for discussions and bug reports if you desire.

CIGALE is a software that extends an older SED fitting algorithm (also named CIGALE) written in FORTRAN by [Burgarella et al. \(2005\)](#) and [Noll et al. \(2009\)](#), which was developed within the framework of the D-SIGALE project led by Guilaine LAGACHE and funded by the French Agence Nationale de la Recherche (ANR). The current version of CIGALE is a completely new implementation that is presented in

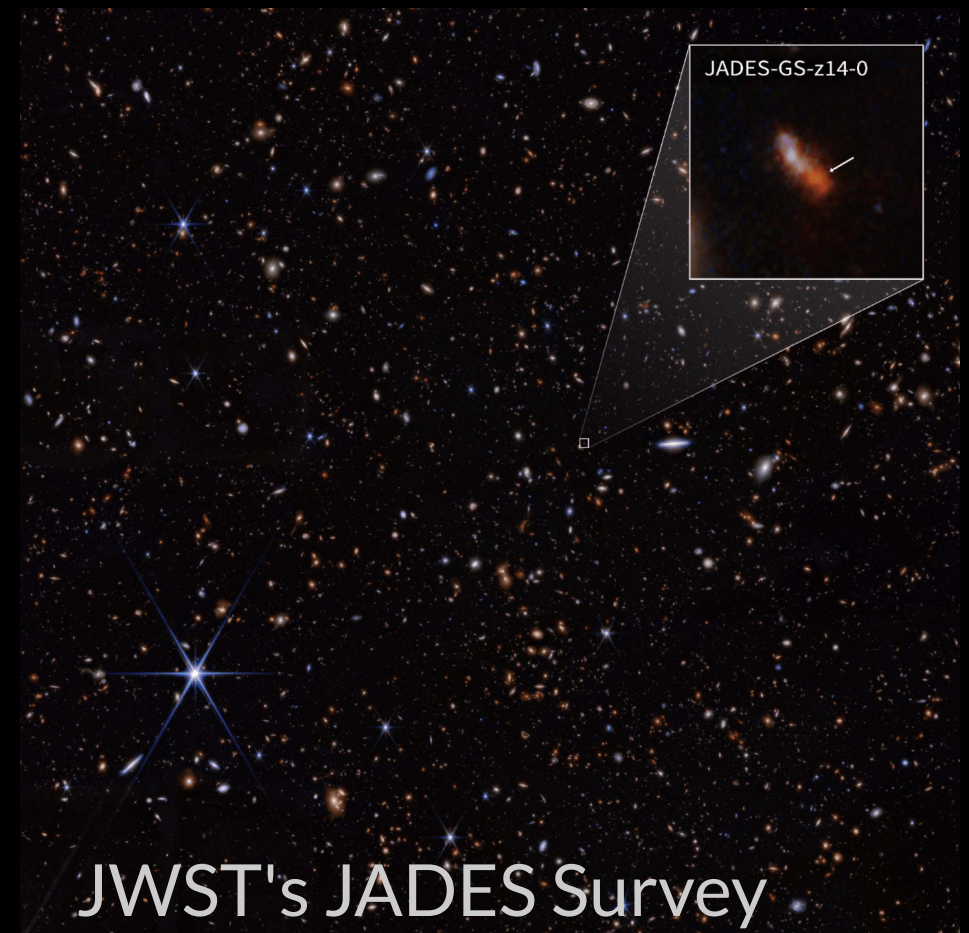
NEWS

- [Version 2022.1](#)
- [Version 2022.0](#)
- [Version 2020.0](#)
- [Experimental wheel](#)
- [Version 2018.0](#)

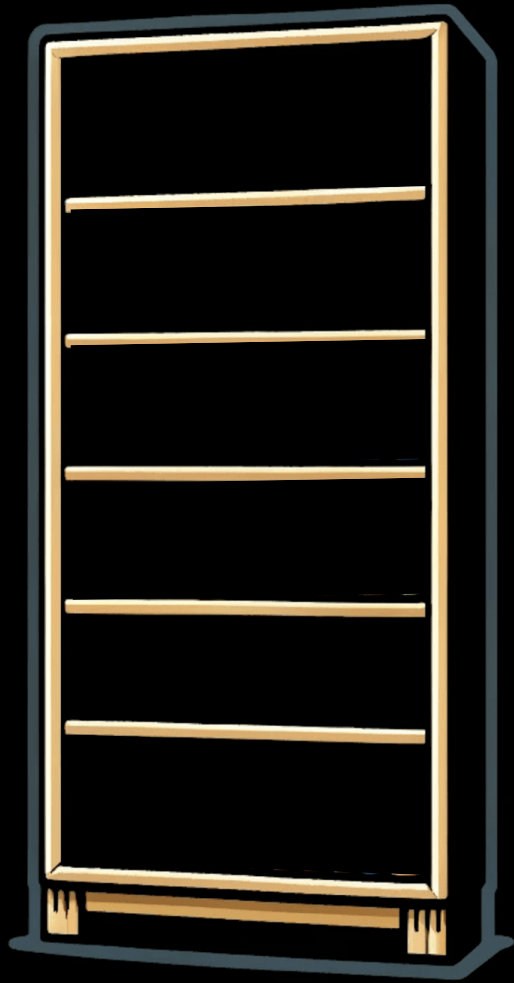
If you need help to use CIGALE, please contact Denis Burgarella by mail at denis.burgarella@lam.fr.

You can also have your data processed by CIGALE with our online tool [SED fitting](#).

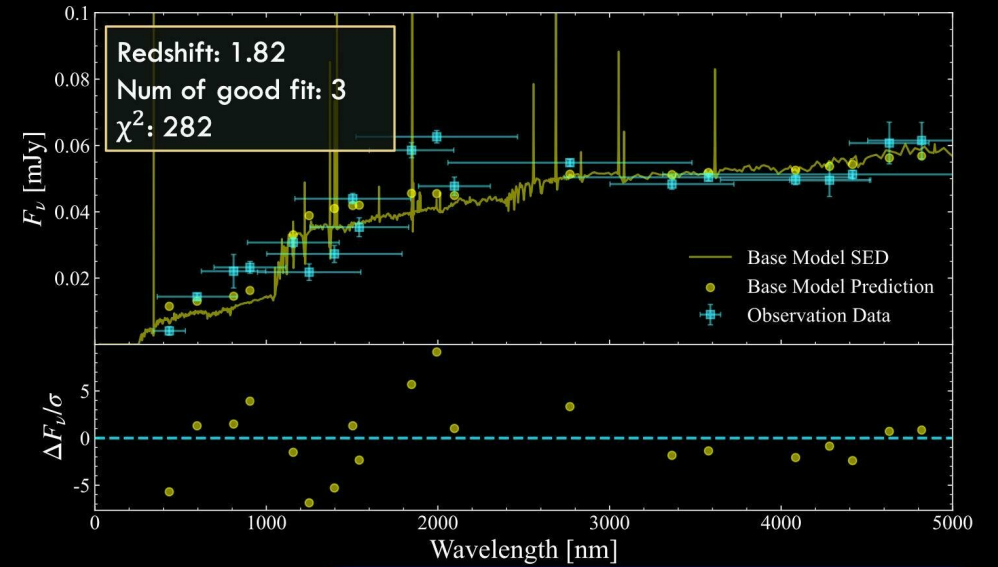
CIGALE SED Fitting Codes



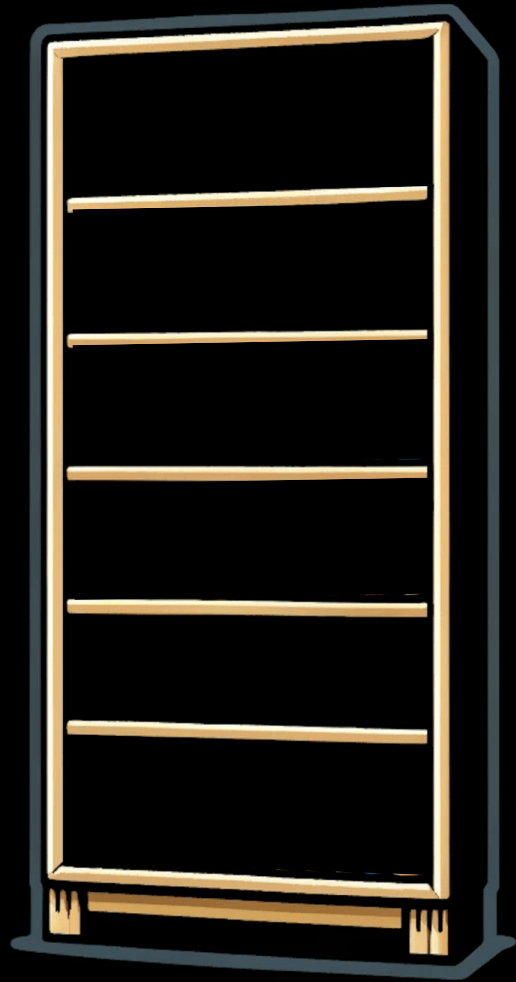
Enabling AI to collect "*knowledge*" through exploration



Knowledge base



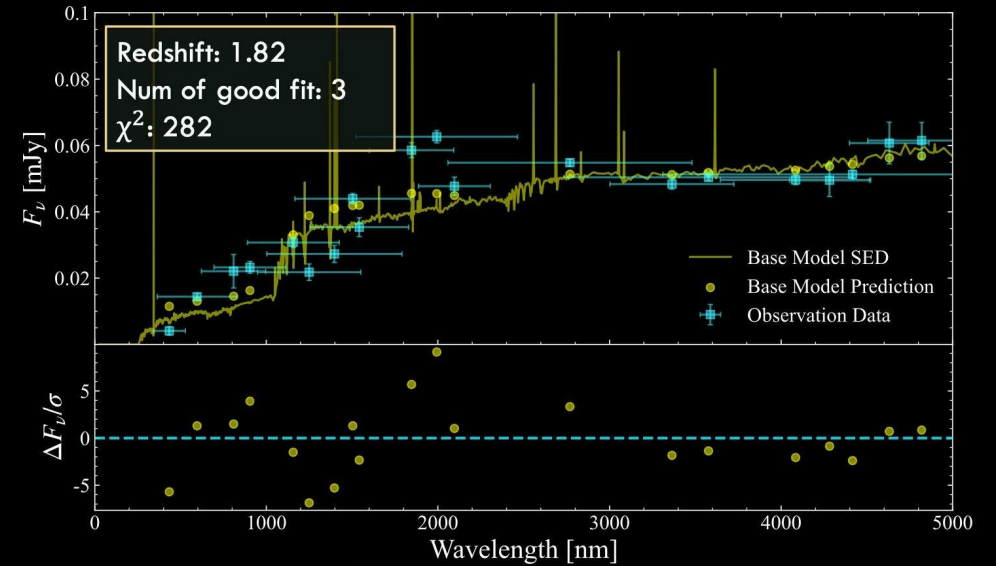
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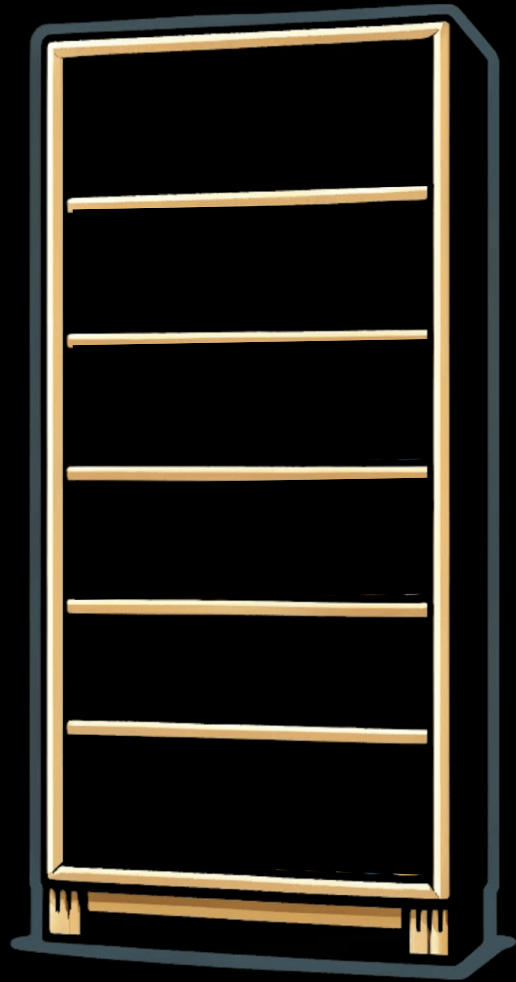
Knowledge base



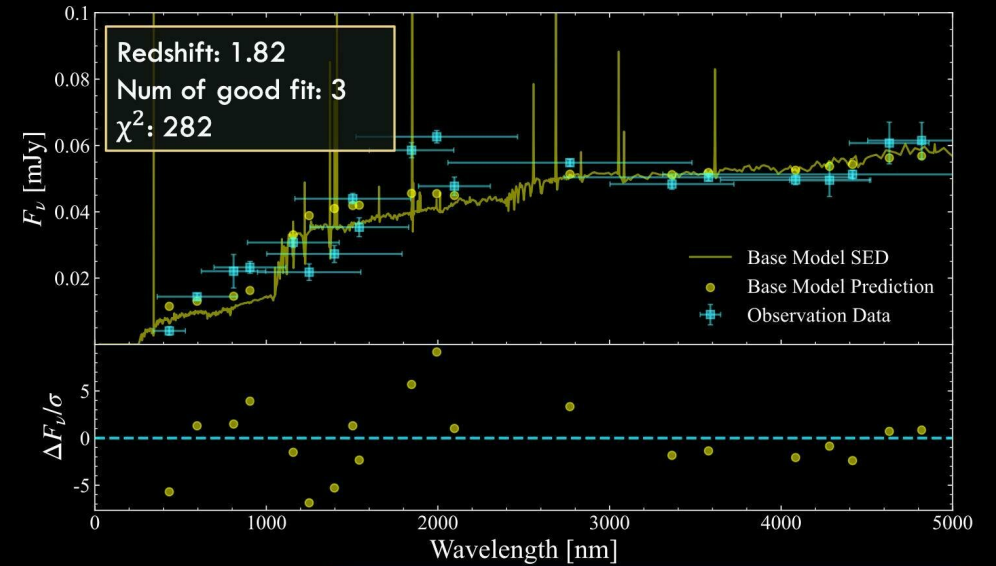
Proposing Actions - e.g., different physical models / parameter range



Enabling AI to collect "*knowledge*" through exploration



Knowledge base



1

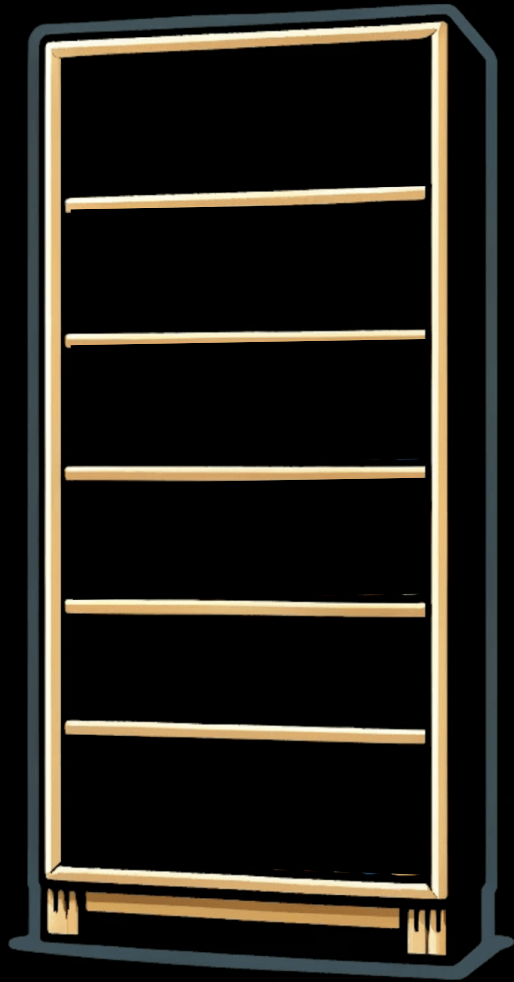
2

3

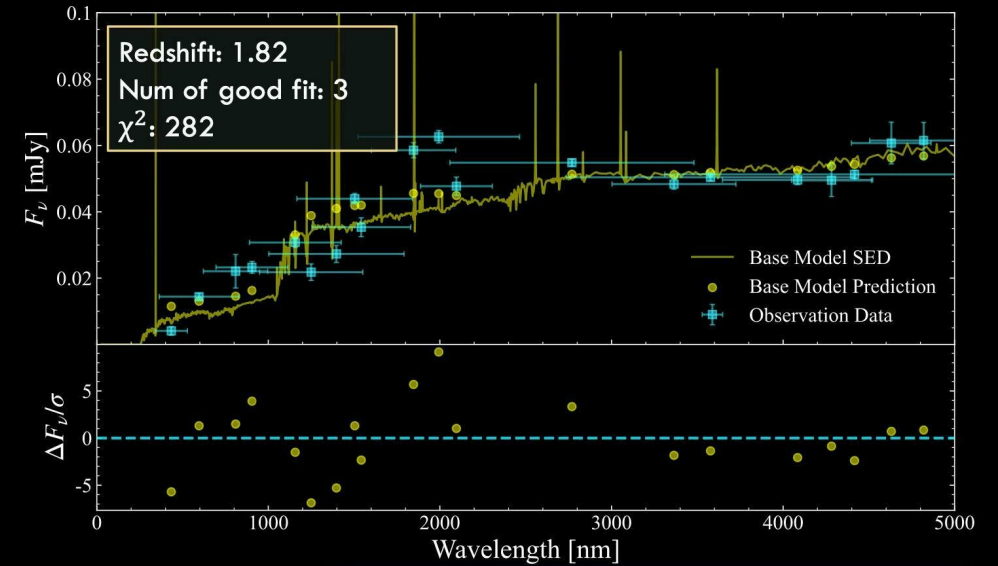
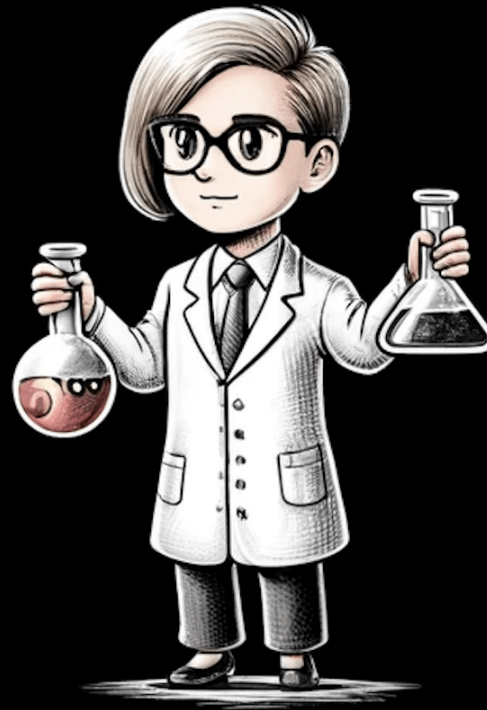
4

Proposing Actions - e.g., different physical models / parameter range

Enabling AI to collect "*knowledge*" through exploration



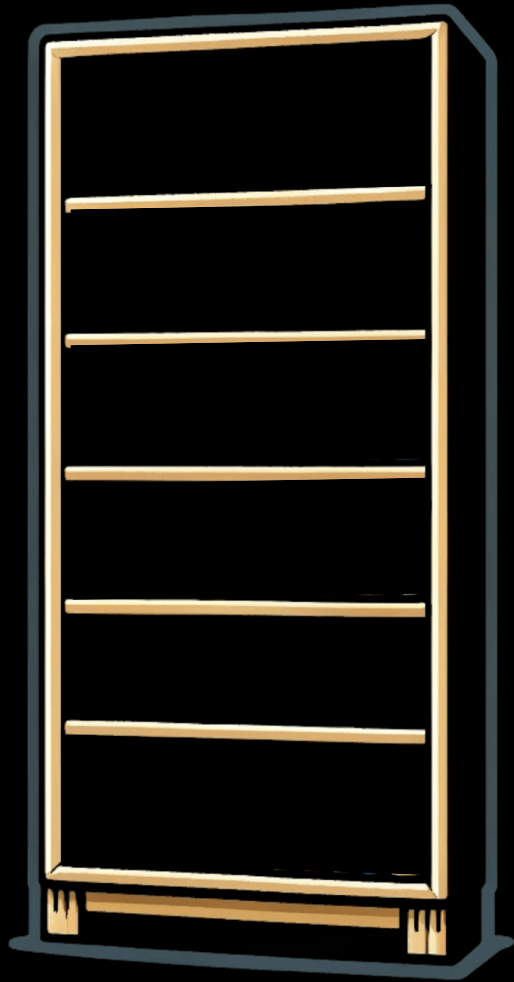
Knowledge base



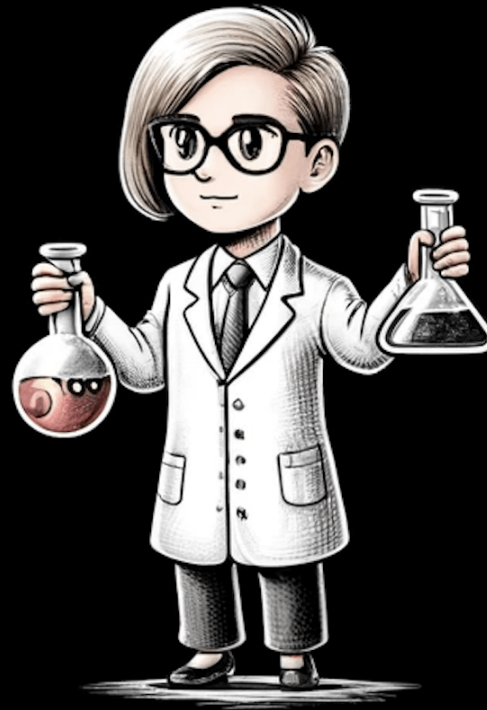
- 1
- 2
- 3
- 4

Execute Actions - write configuration files, run the codes, autonomously

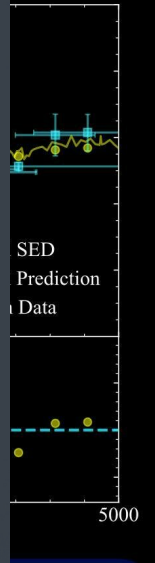
Enabling AI to collect "*knowledge*" through exploration



Knowledge base



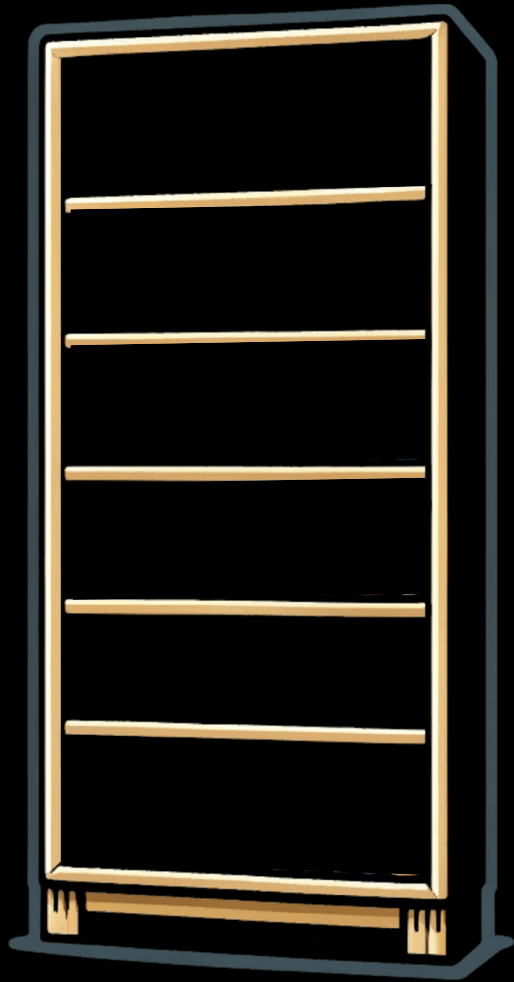
```
25
26 def check_db():
27     if not os.path.isfile(FILE_URI):
28         db.create_all()
29
30 @app.route("/")
31 def home():
32     check_db()
33     all_books = db.session.query(Book).all()
34     return render_template("index.html", books=all_books)
35
36 @app.route("/edit", methods=["GET", "POST"])
37 def edit():
38
39     if request.method == "POST":
40         book_id = request.form["id"]
41         book_to_update = Book.query.get(book_id)
42         book_to_update.rating = request.form["rating"]
43         db.session.commit()
44         return redirect(url_for("home"))
```



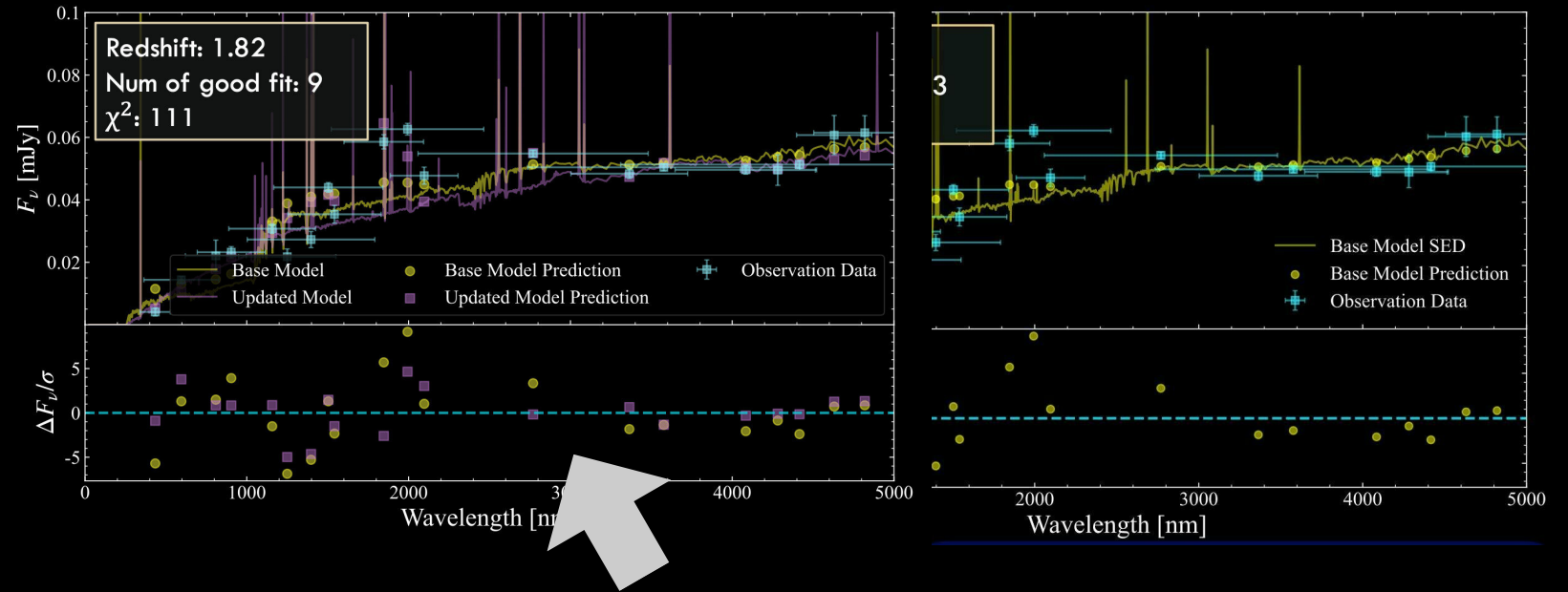
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Execute Actions - write configuration files, run the codes, autonomously

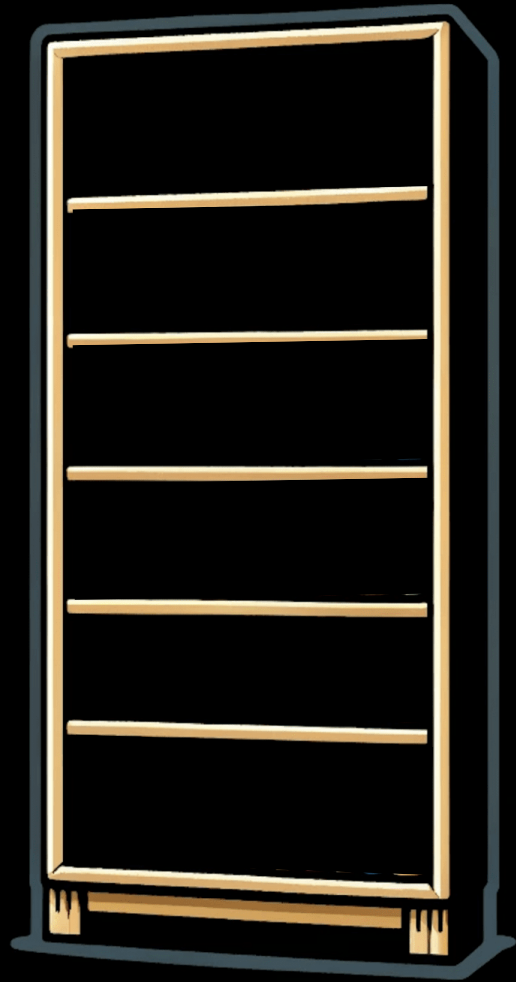
Enabling AI to collect "*knowledge*" through exploration



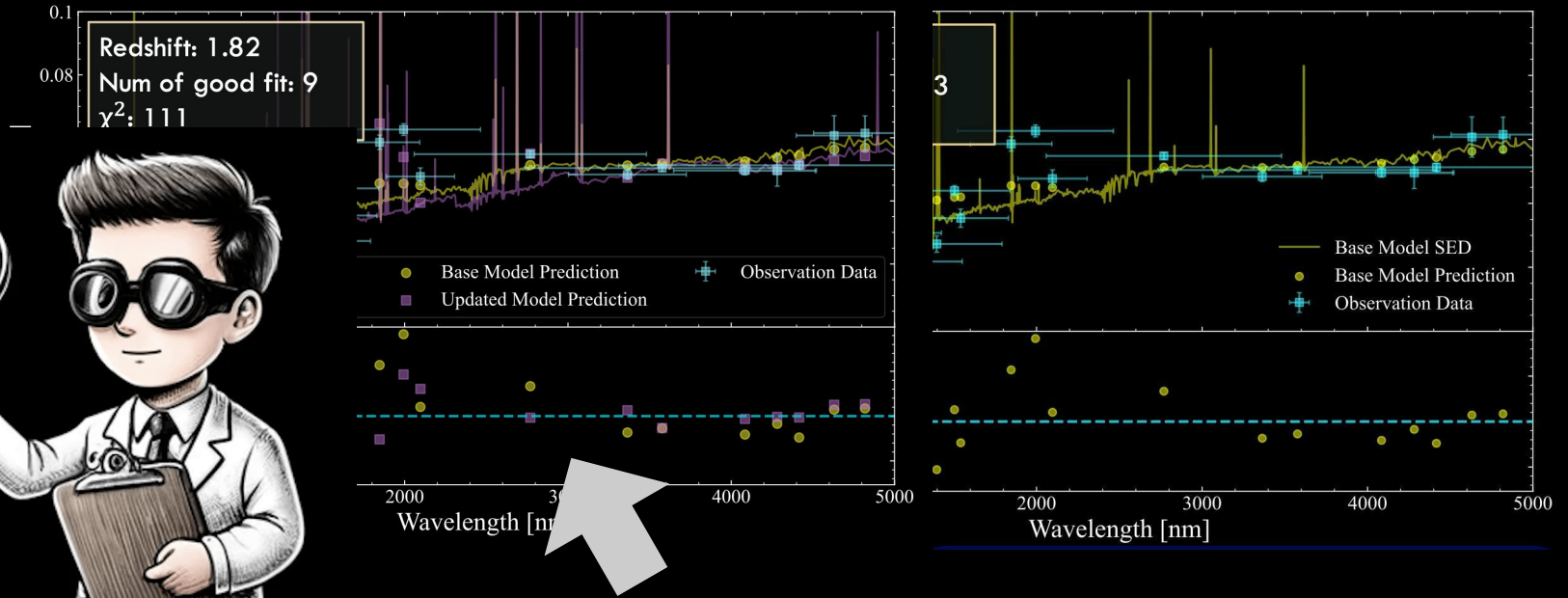
Knowledge base



Enabling AI to collect "*knowledge*" through exploration



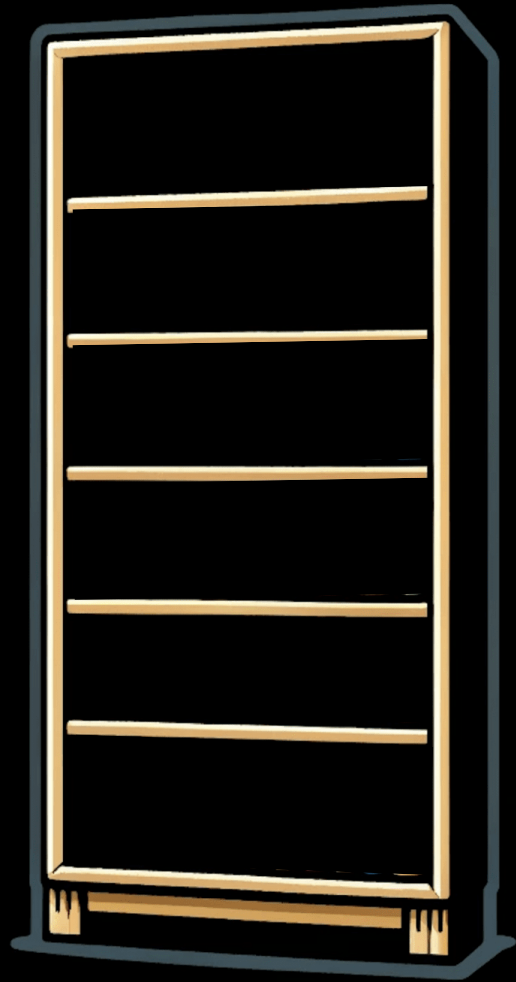
Knowledge base



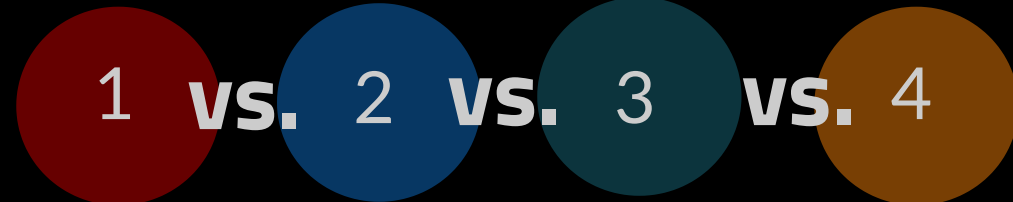
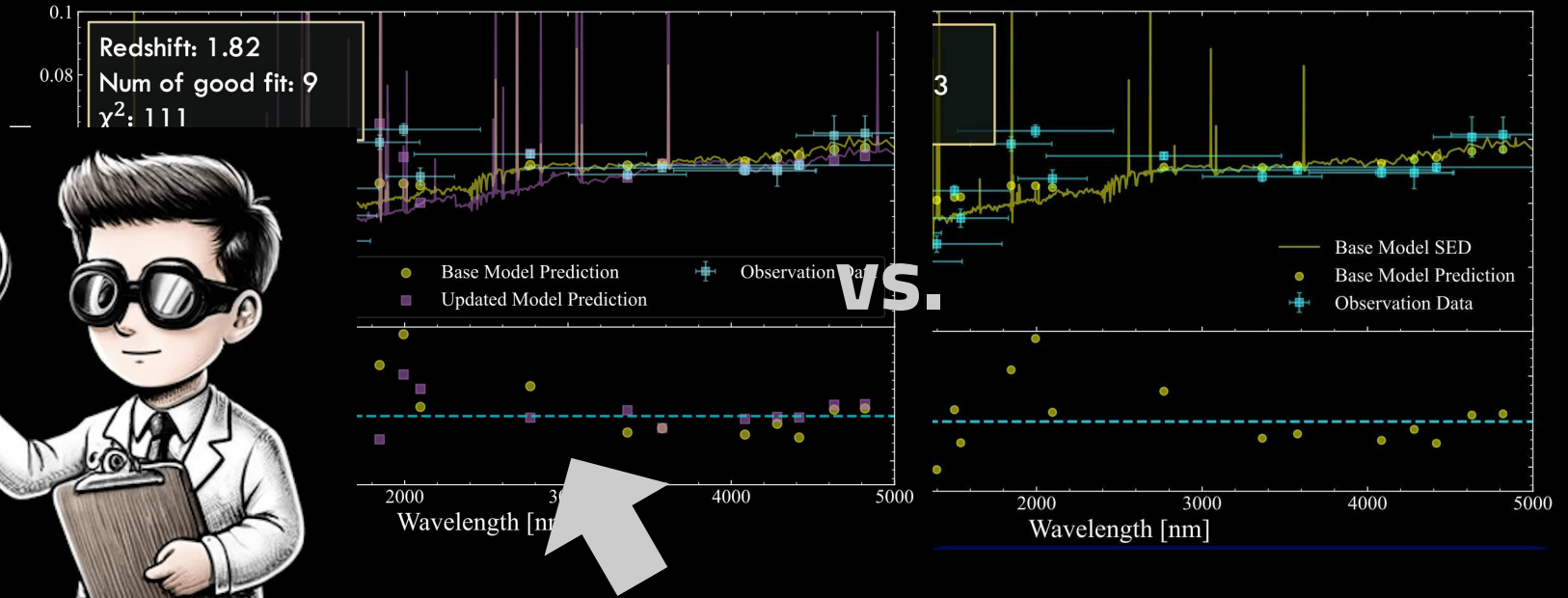
- 1
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- 3
- 4

State Evaluation - evaluate the results (beyond a single error metric)

Enabling AI to collect "*knowledge*" through exploration

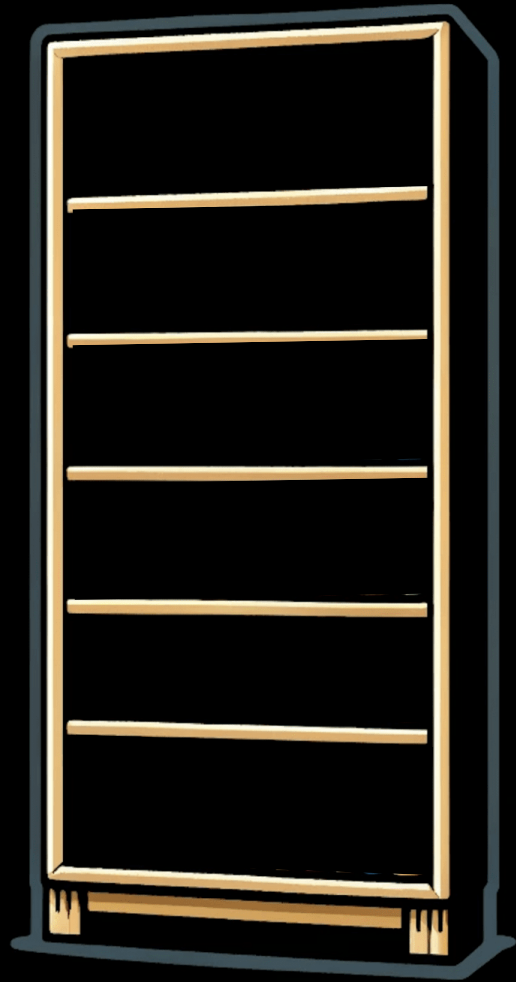


Knowledge base



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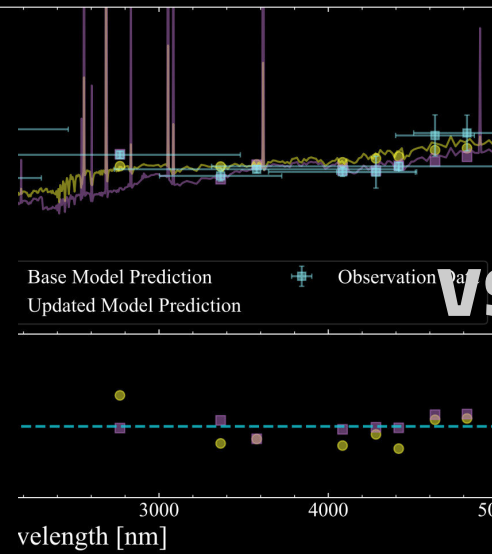
Enabling AI to collect "*knowledge*" through exploration



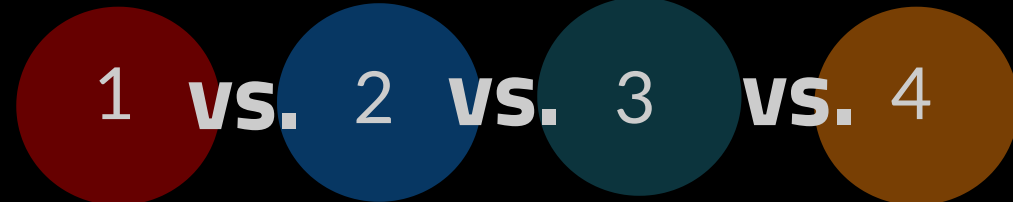
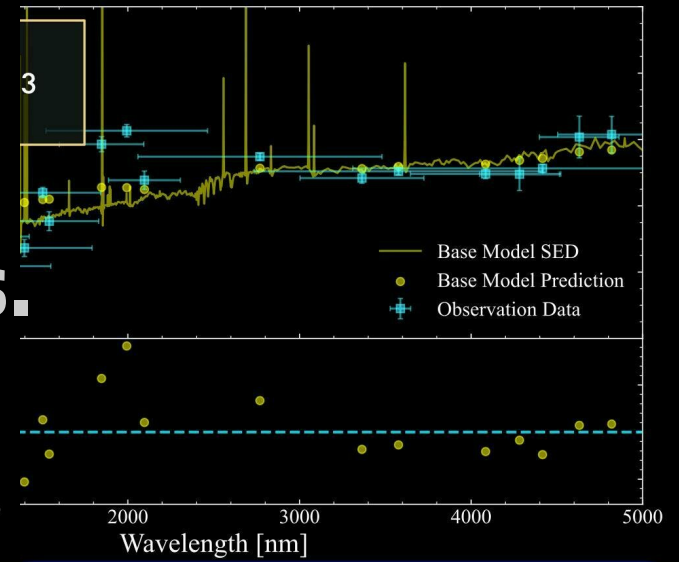
Knowledge base



Redshift: 1.82
Num of good fit: 9

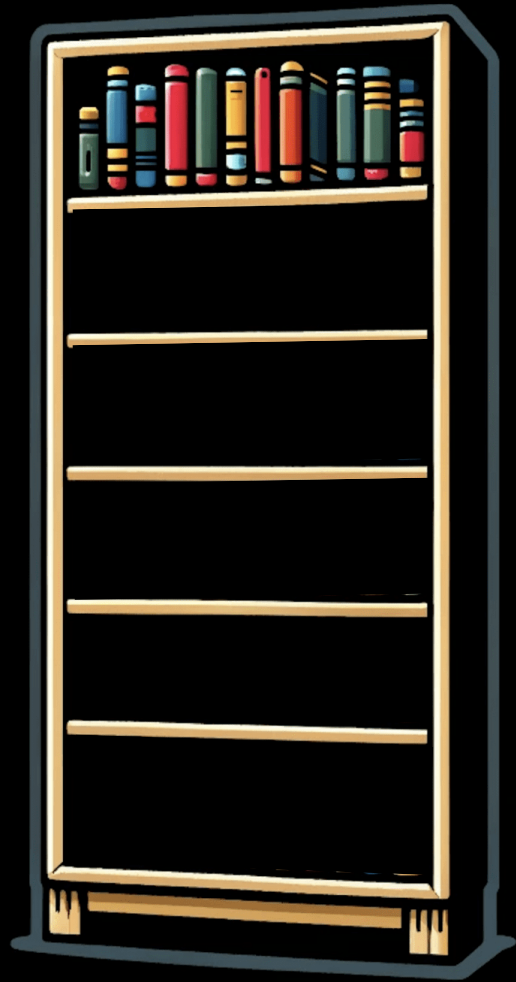


vs.



Knowledge Distillation - summarise useful actions given the previous state

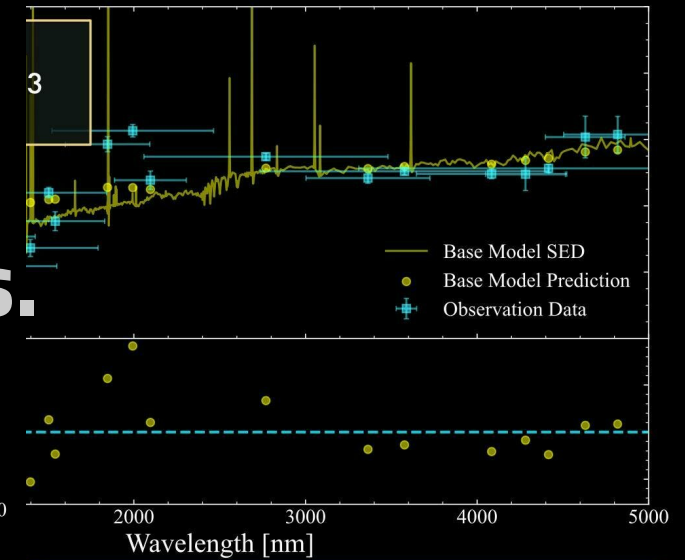
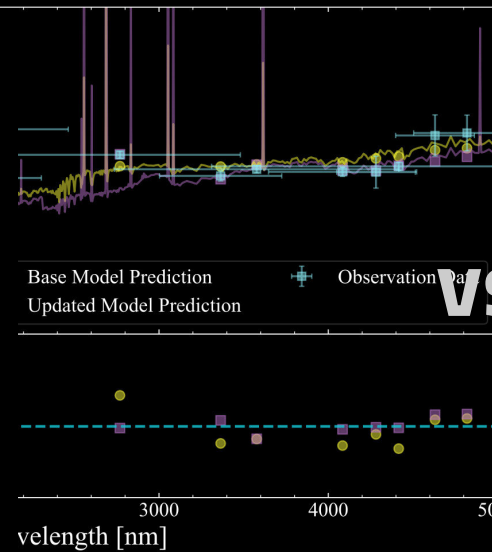
Enabling AI to collect "*knowledge*" through exploration



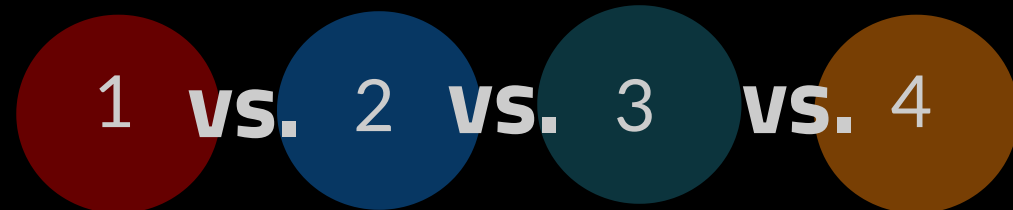
Knowledge base



Redshift: 1.82
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vs.



Knowledge Distillation - summarise useful actions given the previous state

Example of learned "knowledge"

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" If the fit is *overestimated in the UV and optical* bands,

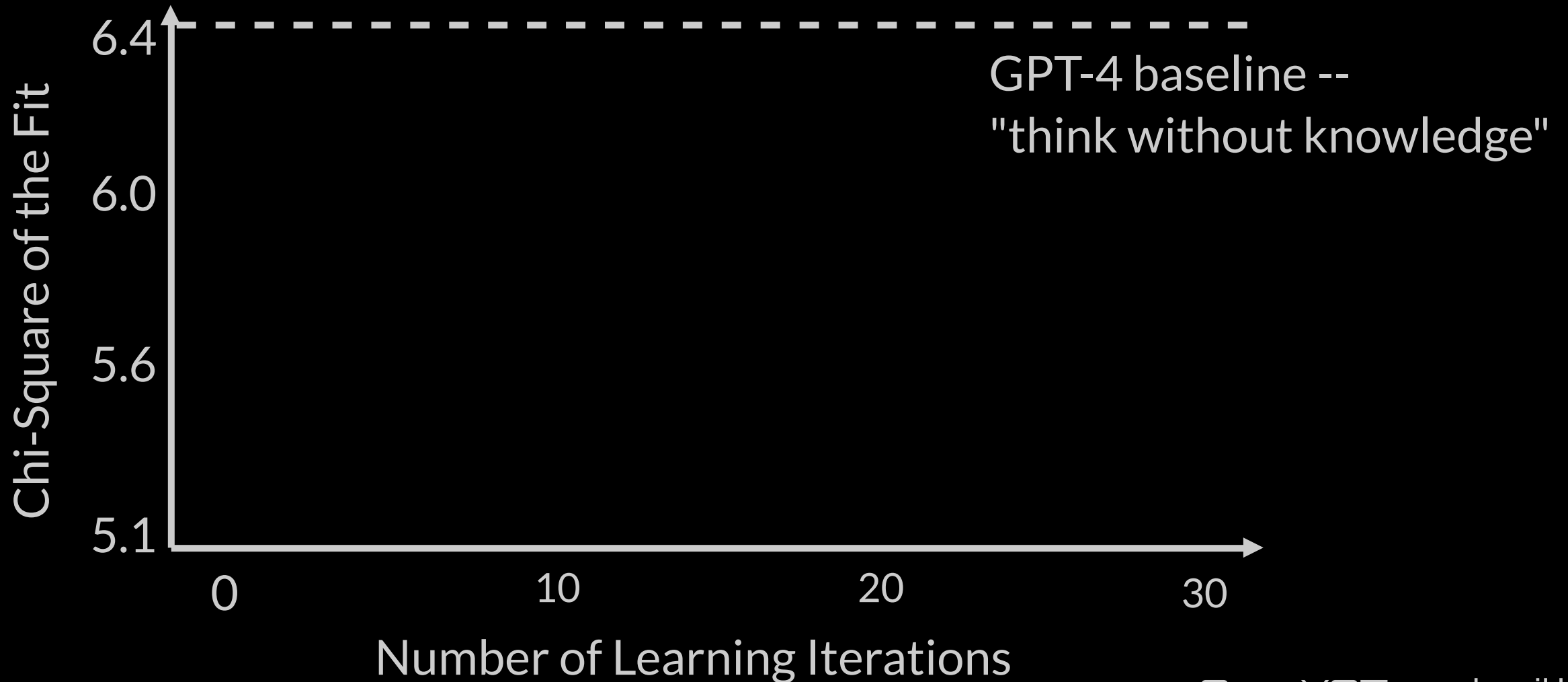
Example of learned "knowledge"

" If the fit is *overestimated in the UV and optical* bands,

increasing the E_{BV_lines} parameter may lead to a better fit by accounting for more *dust attenuation* in these bands. "

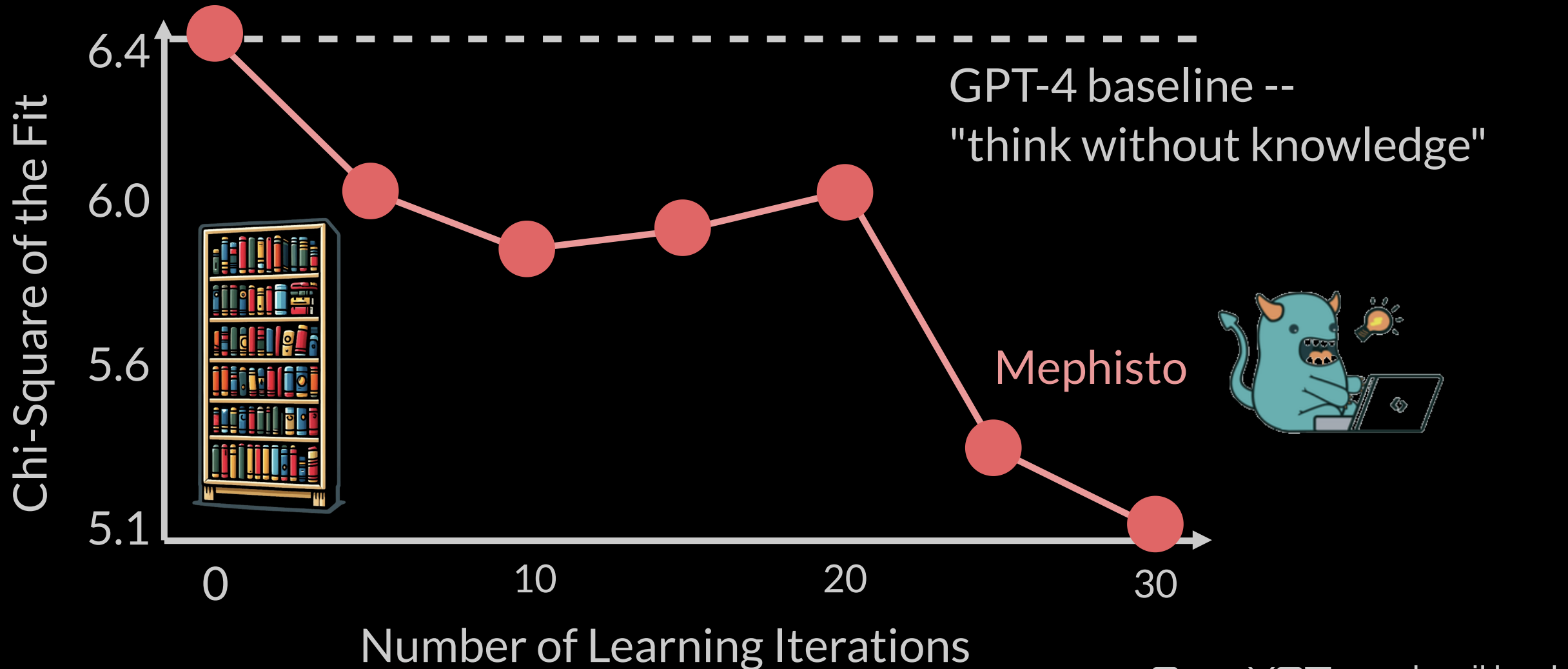


Reinforcement learning with LLM *outperforms* native LLMs



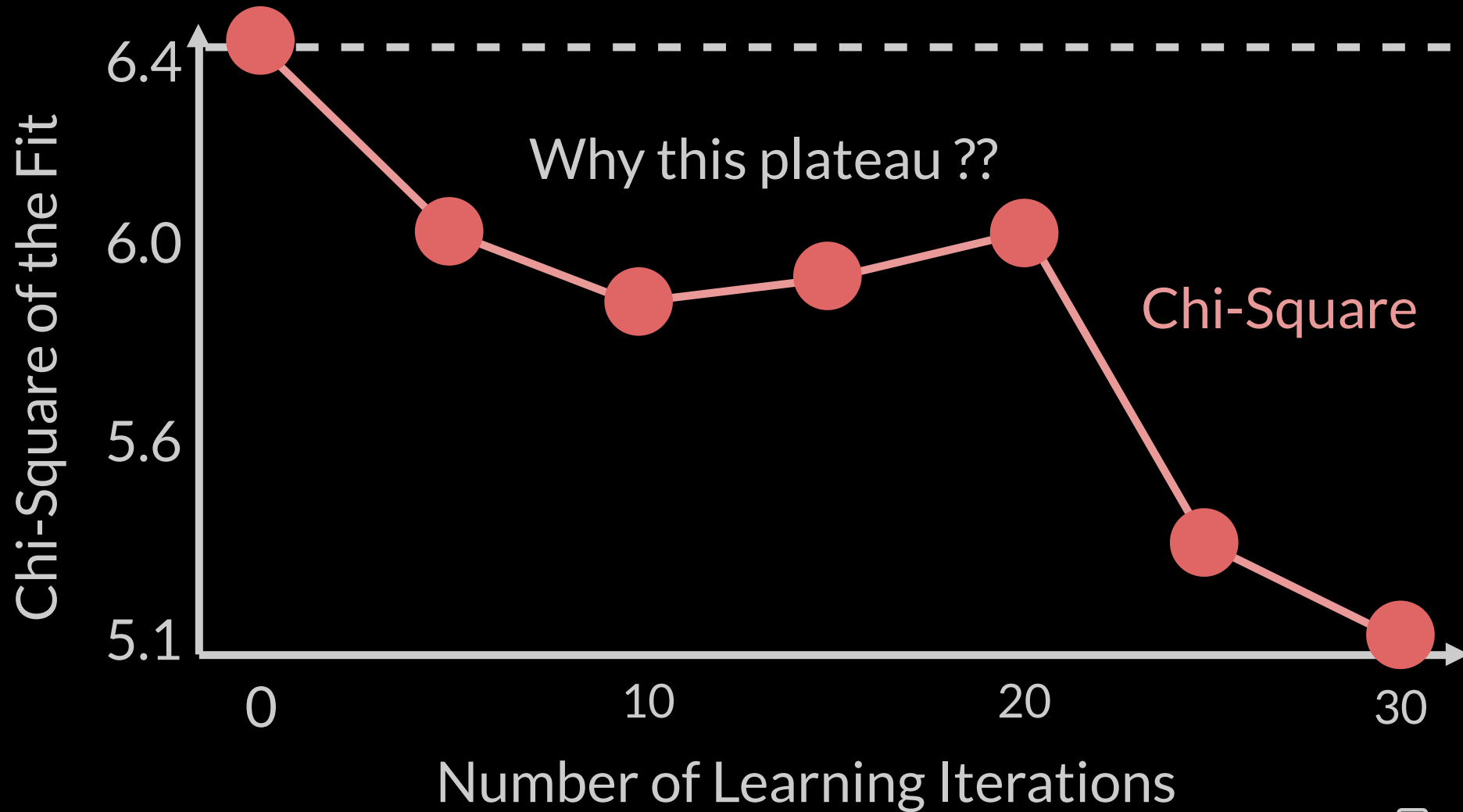
Sun, YST+, submitted

Reinforcement learning with LLM *outperforms* native LLMs

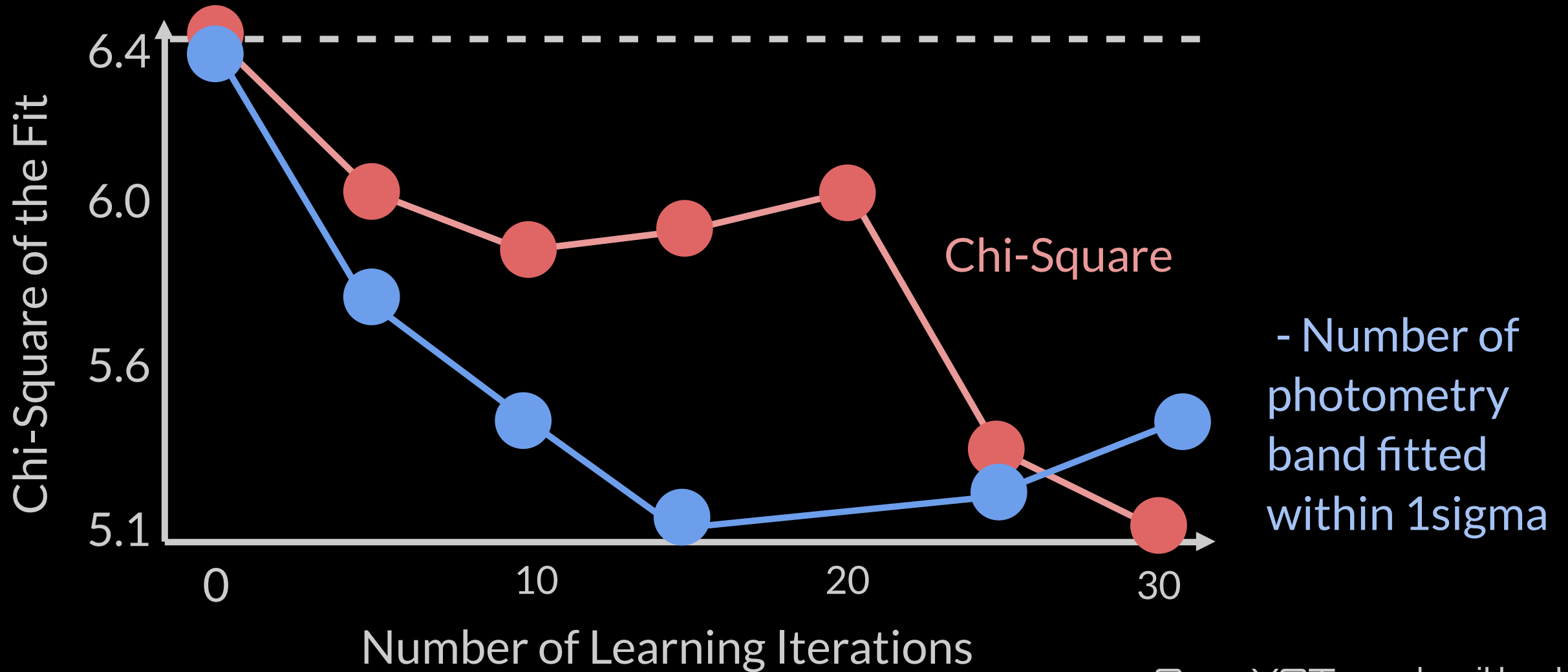


Sun, YST+, submitted

Reinforcement learning with LLM *outperforms* native LLMs

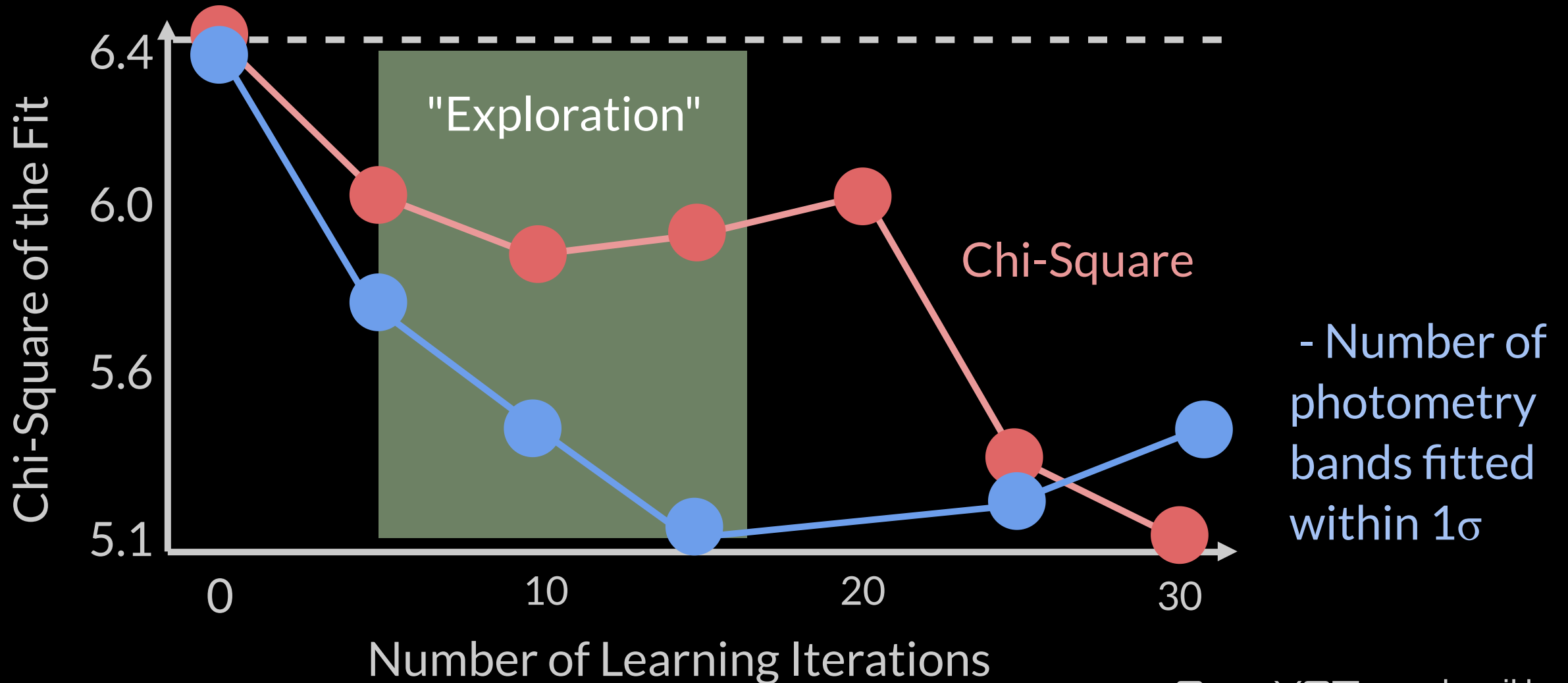


Reinforcement learning with LLM *outperforms* native LLMs

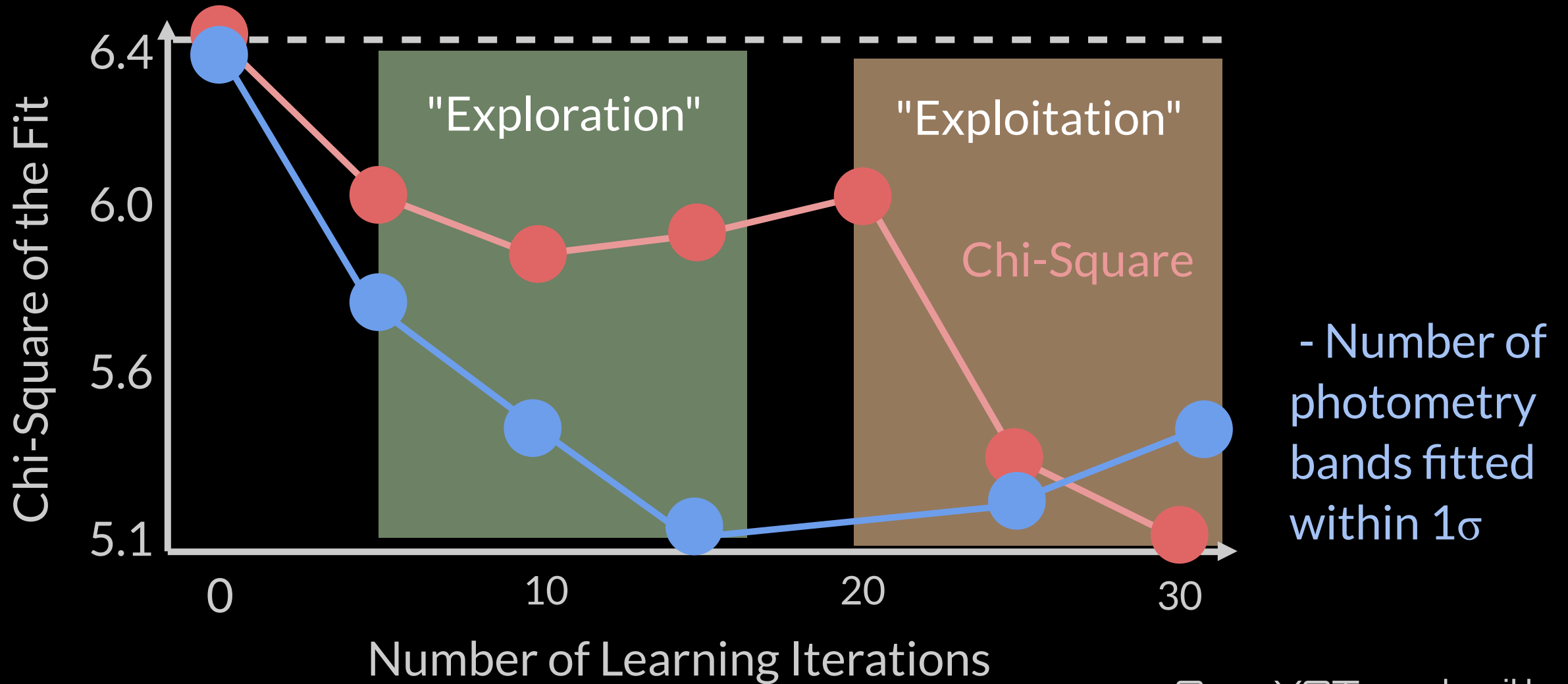


Sun, YST+, submitted

Reinforcement learning with LLM *outperforms* native LLMs



Reinforcement learning with LLM *outperforms* native LLMs



While we are far from AGI, LLMs are
prolific enough to understand
basic causality through actions



Reason about all astronomical objects in the cosmos



Provided that we have *a capable model* that can generate inference quickly and *cost efficiently*....



Provided that we have *a capable model* that can generate inference quickly and *cost efficiently*....



capable model

vs.

cost efficiency



In the SED case study, we need *~0.1M tokens* per source

capable model

vs.

cost efficiency

e.g., GPT-4o (this study)



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capable model

vs.

cost efficiency

e.g., GPT-4o (this study)



Model	Input	Output
gpt-4o	\$5.00 / 1M tokens	\$15.00 / 1M tokens
gpt-4o-2024-05-13	\$5.00 / 1M tokens	\$15.00 / 1M tokens

In the SED case study, we need *~0.1M tokens* per source

capable model

vs.

cost efficiency

e.g., GPT-4o (this study)

= USD 1 *per source*



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1B sources = \$1 billion

e.g., *Roman* Space Telescope, *Euclid* Space Telescope

1B sources = \$1 billion

e.g., *Roman* Space Telescope, *Euclid* Space Telescope

~ approximately the build cost

- Where are we in AI for Astronomy - What's the problem?

- What could be the AlphaFold moment for astronomy?

- How do we get there in a cost-effective way?

- Where are we in AI for Astronomy - What's the problem?
- What could be the AlphaFold moment for astronomy?
- How do we get there in a cost-effective way?

The curation of an astronomy *benchmark* dataset



The screenshot shows the website for the Annual Review of Astronomy and Astrophysics. The header includes the logo and navigation links for 'Publications A-Z' and 'Journal Information'. The main content area features a navigation bar with 'Home', 'About', 'Current', 'Early Publication', 'Previous Volumes', and 'Editorial Committee'. Below this is a section titled 'Annual Review of Astronomy and Astrophysics' with a description of the journal's scope and a table of key statistics.

Home / A-Z Publications / [Annual Review of Astronomy and Astrophysics](#)

Annual Review of Astronomy and Astrophysics

Home About Current Early Publication Previous Volumes Editorial Committee

AIMS AND SCOPE OF JOURNAL: The *Annual Review of Astronomy and Astrophysics* covers the significant developments in the field of astronomy and astrophysics, including: the sun; solar system and extrasolar planets; stars; the interstellar medium; galaxy and galaxies; active galactic nuclei; cosmology; and instrumentation and techniques, and the history of the development of new areas of research.

Published Since	1963
Journal Status	Active
DOI:	https://doi.org/10.1146/astro.683
Impact Factor	33.3

ISSN: 0066-4146
eISSN: 1545-4282

Current Volume is OA 

Latest Articles 



(i.e. as part of the Aurora-GPT effort with the Argonne National Laboratory)

But how do we know which model is better?



WHO WINS THE ASTRONOMY JEOPARDY!

YUAN-SEN TING, ET AL.

Submitted to ApJL

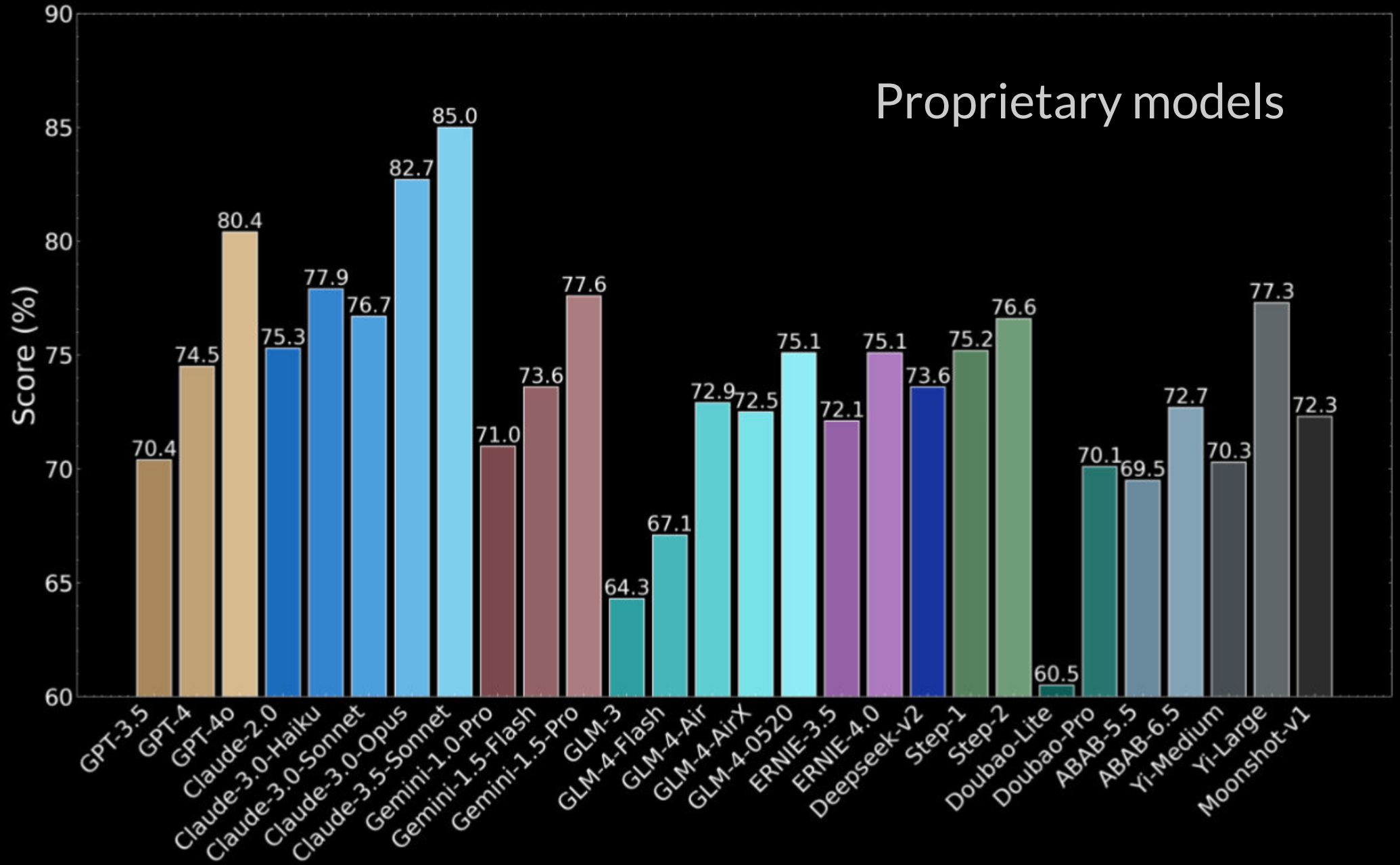
ABSTRACT

We present a comprehensive evaluation of proprietary and open-weights large language models (LLMs) using the first astronomy-specific benchmarking dataset. This dataset comprises 4,425 multiple-choice questions curated from the Annual Review of Astronomy and Astrophysics, covering a broad range of astrophysical topics. Our analysis examines model performance across various astronomical subfields and assesses response calibration, crucial for potential deployment in research environments. Claude-3.5-Sonnet outperforms competitors by up to 4.6 percentage points, achieving 85.0% accuracy. We observed a universal trade-off in proprietary models: a 10-fold cost increase yields a 3.5-point accuracy improvement. This suggests a 10-fold reduction in cost every 3 months to a year, offering optimistic prospects for LLM deployment in astronomy research. Open-source models have rapidly improved, with LLaMA-3-70b (80.6%) and Qwen-2-72b (77.7%) now competing with some proprietary models. We identify significant performance variations across topics, with models generally struggling more in exoplanet-related fields, recent stellar astrophysics, and observational techniques. These challenges likely stem from less abundant training data, limited historical context, and rapid recent developments in these areas. This pattern is observed across both open-weights and proprietary models, with regional dependencies evident, highlighting the impact of training data diversity on model performance in specialized scientific domains. Top-performing models demonstrate well-calibrated confidence, with correlations above 0.9 between confidence and correctness, though they tend to be slightly underconfident. The development for fast, low-cost inference of open-weights models presents new opportunities for affordable deployment in astronomy. The rapid progress observed suggests that LLM-driven research in astronomy may become feasible in the near future, potentially revolutionizing how we approach large-scale data analysis in the field.

40 pages of all you
need to know about
LLM for astronomy

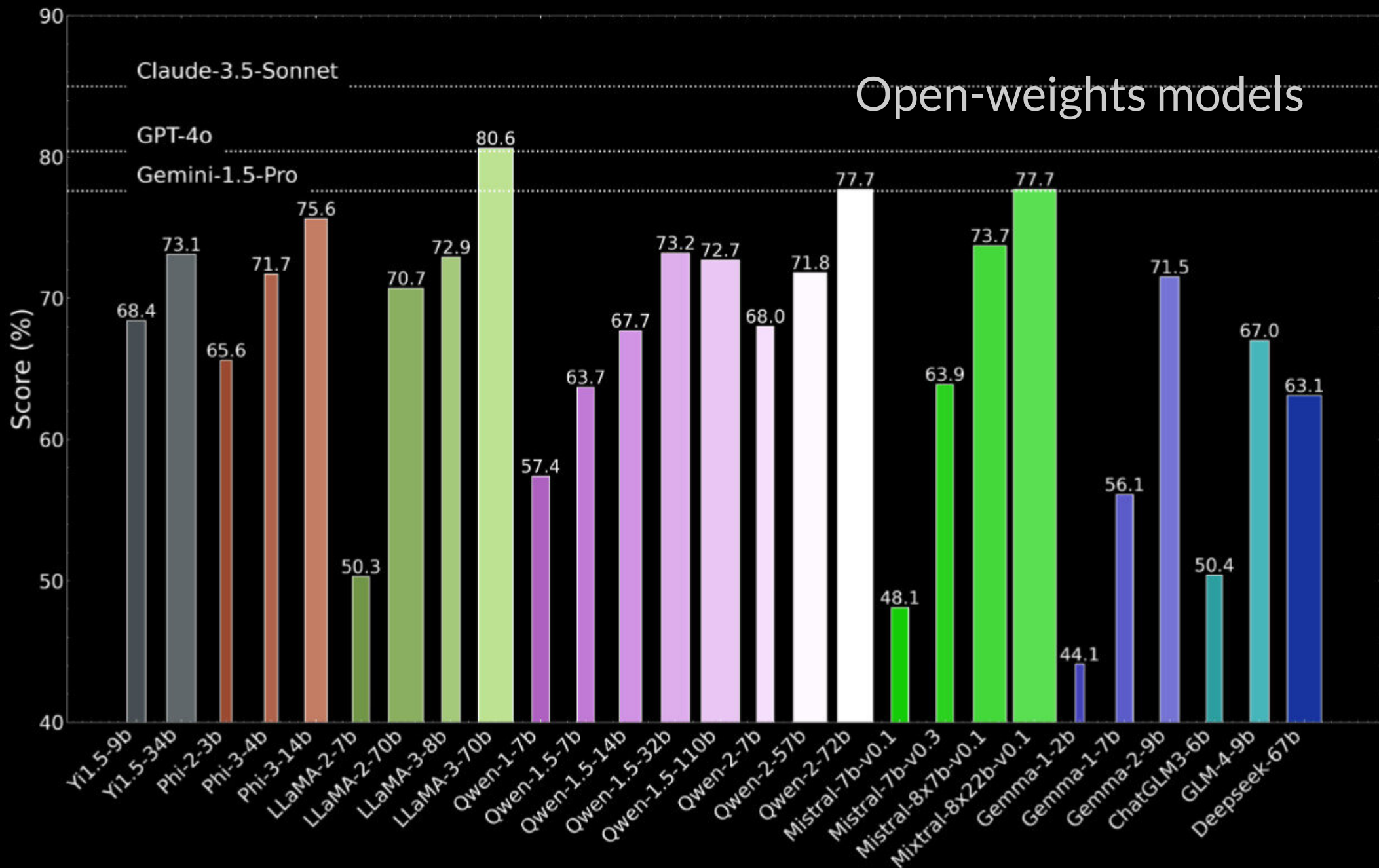
Model Series

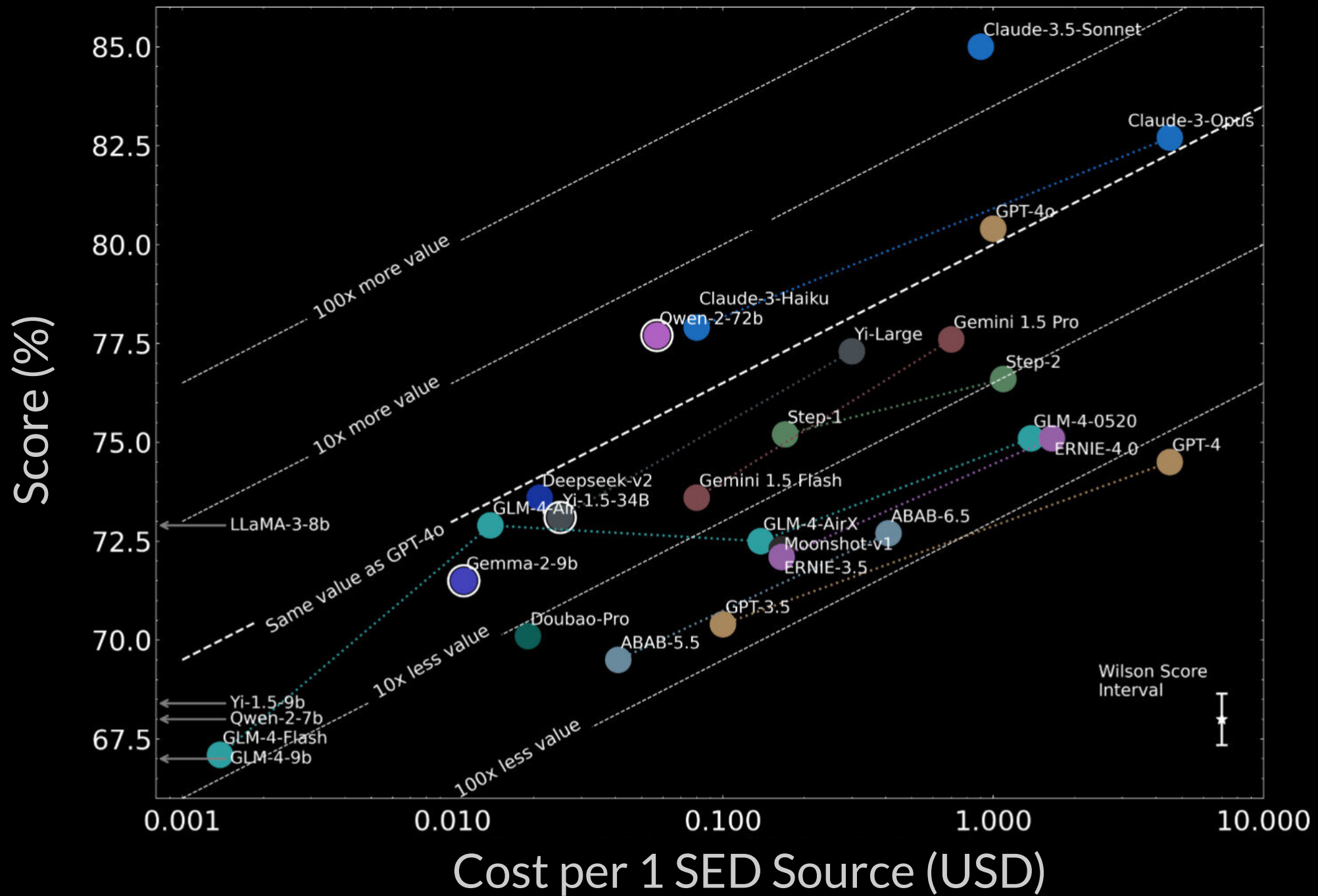
- GPT
- Claude
- Gemini
- GLM
- ERNIE
- Deepseek
- Step
- Doubao
- ABAB
- Yi
- Moonshot

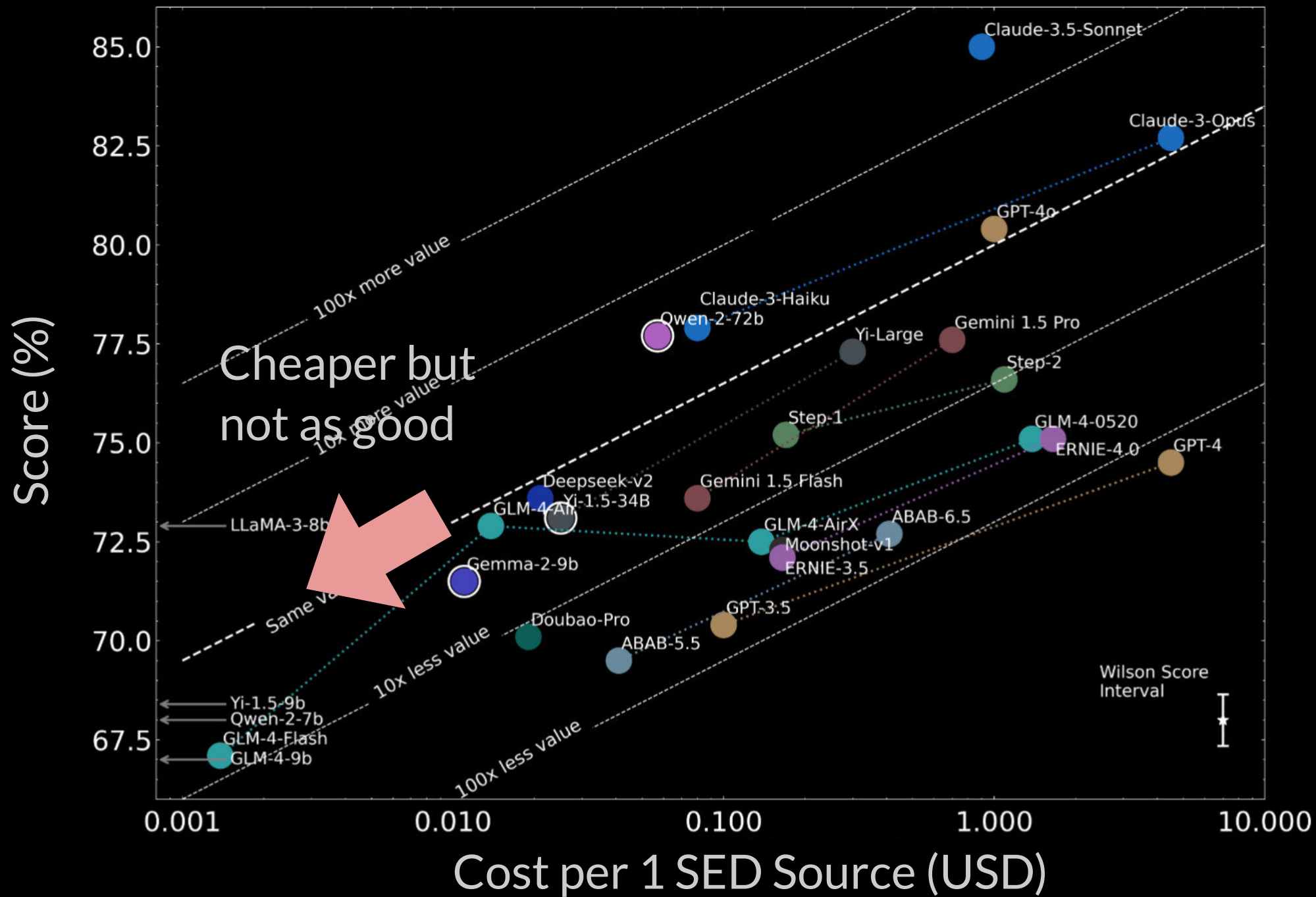


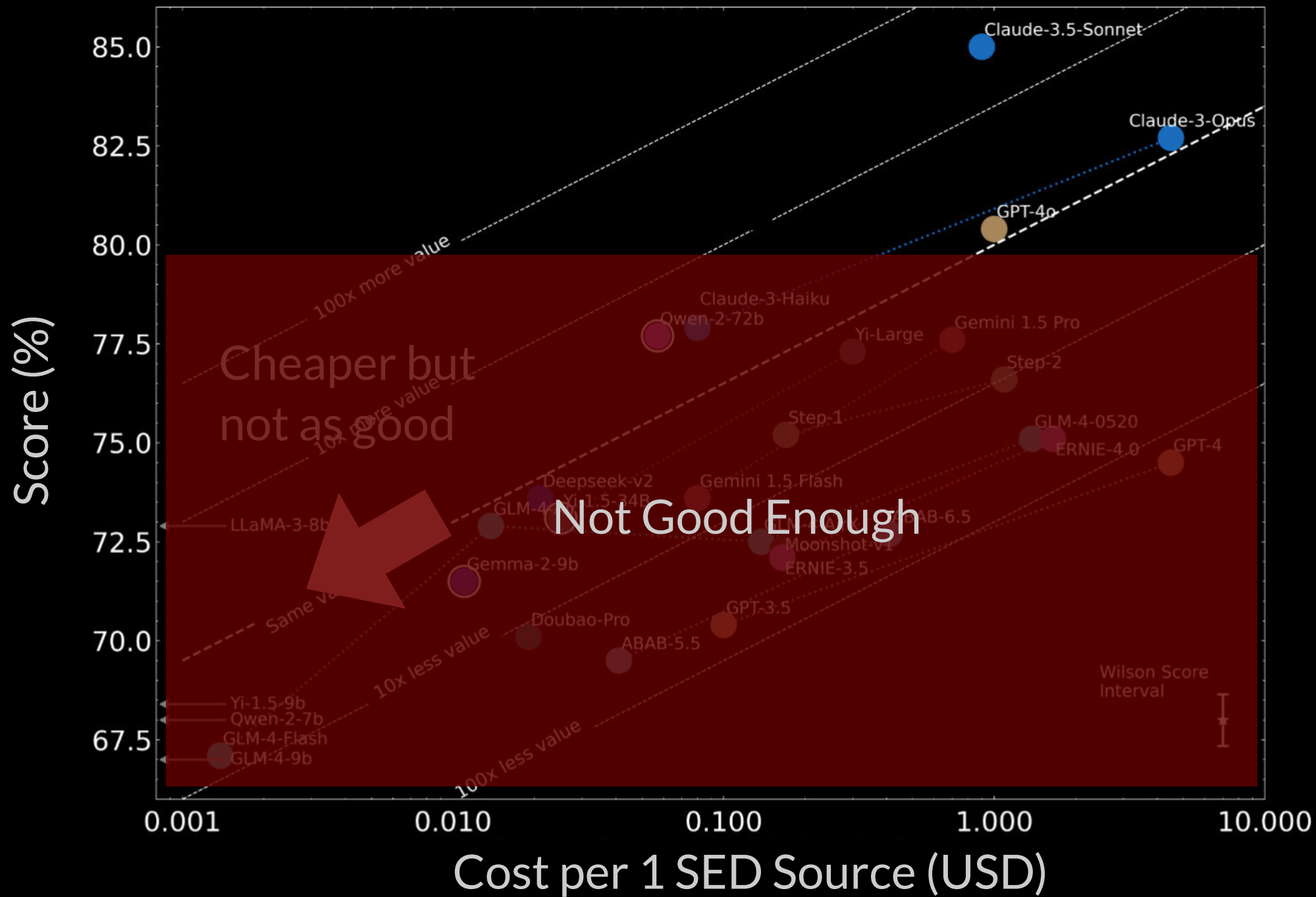
Model Series

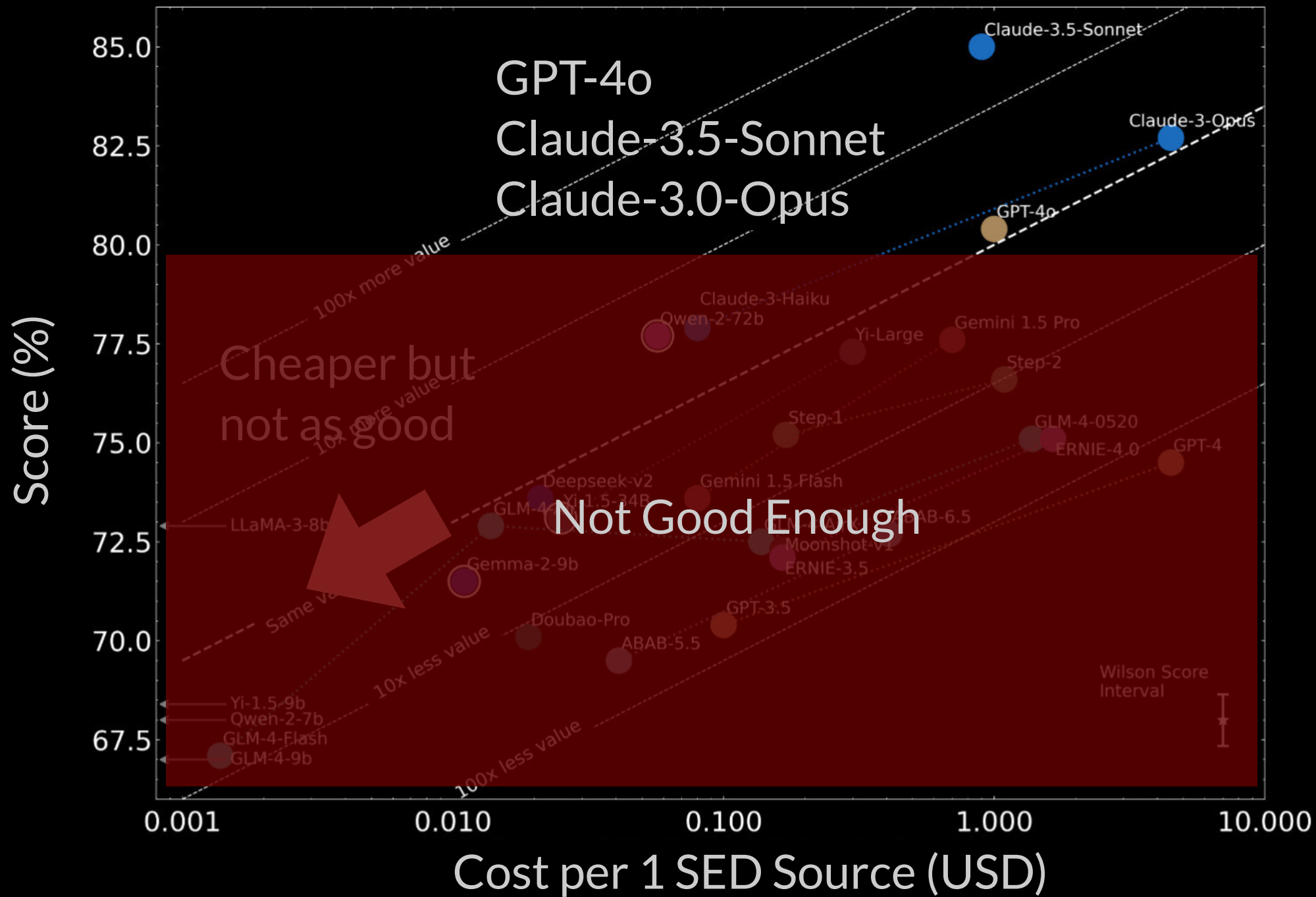
- Yi
- Phi
- LLaMA
- Qwen
- Mistral
- Gemma
- GLM
- Deepseek
- Closed







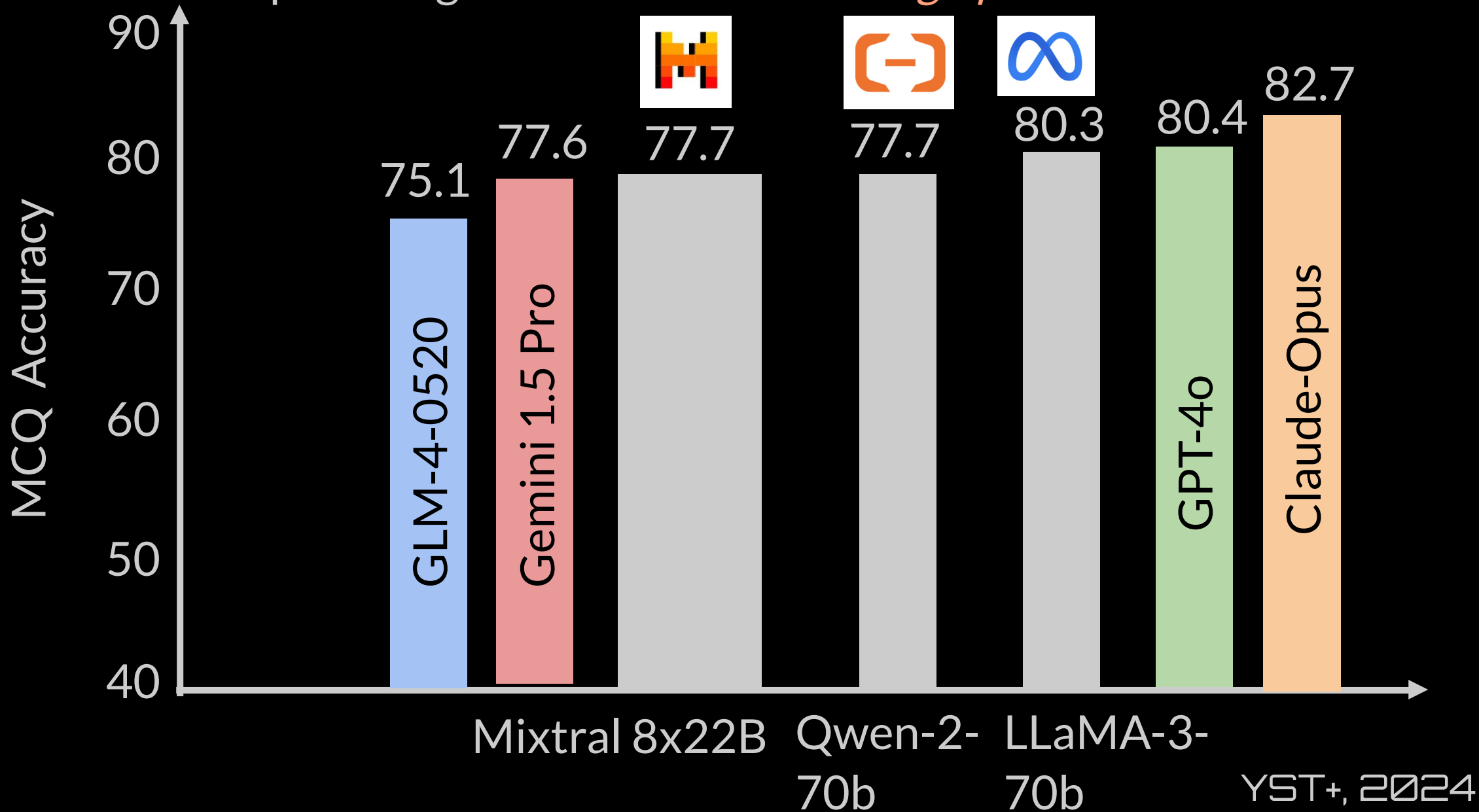




Open-weights large language models?



Open-weights models *are catching up* in 2024



Open-source large language models
are *as good as* the closed-source models



Open-source large language models
are *as good as* the closed-source models

at the ~70B level



Still it is *not very scalable*



Still it is *not very scalable*



LLaMA-3 70b throughput on *four A100 GPUs*

= ~ 100 tokens / second



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1 SED source = 15 GPU minutes



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1B sources = 10M GPU days



LLaMA-3 70b throughput on *four A100 GPUs*

= ~ 100 tokens / second

1 SED source = 15 GPU minutes

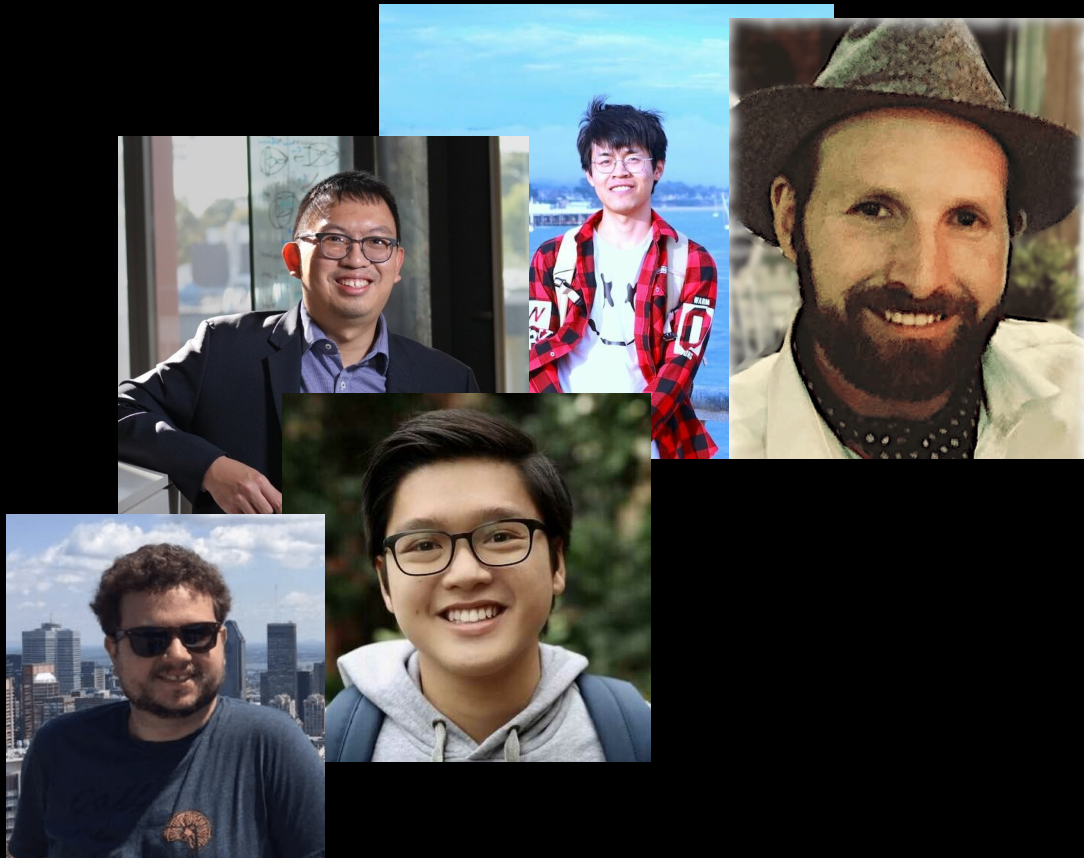
1B sources = 10M GPU days

A cluster with *1000 A100 GPUs*
running for *30 years*

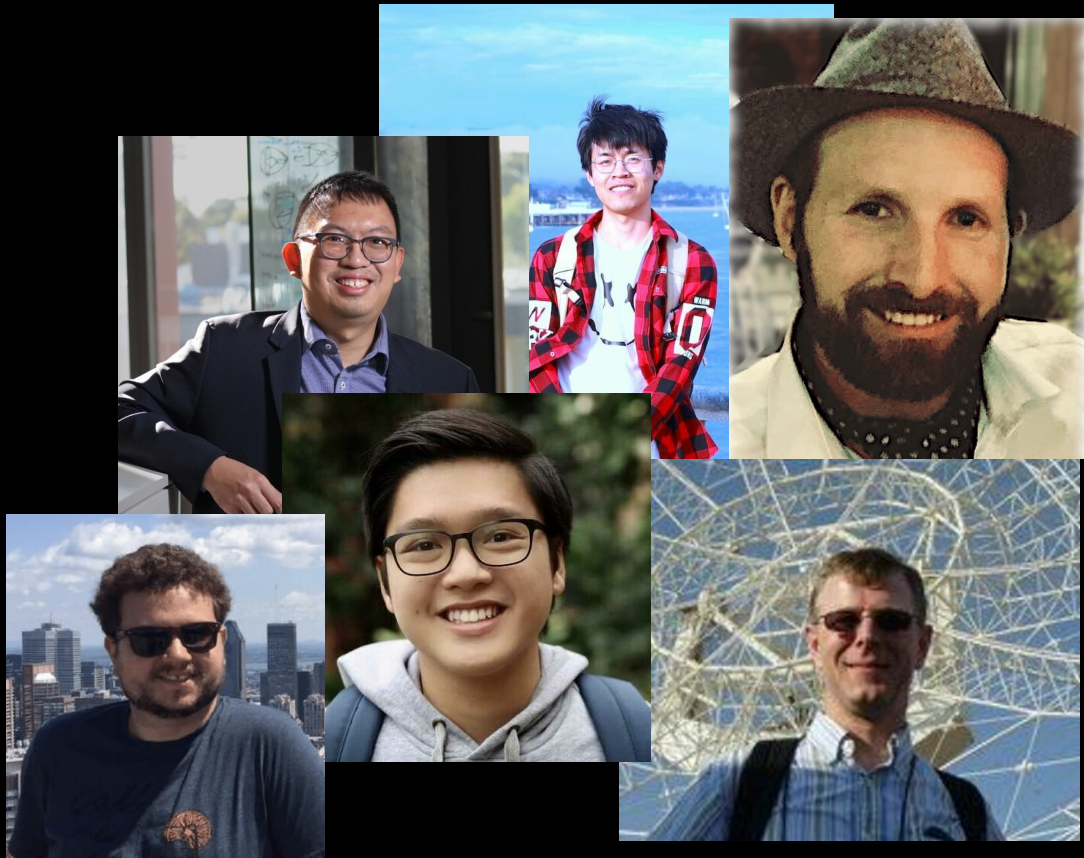


Can the light-weight $\sim 7B$ open-source models
perform equally with some "fine-tuning" ?

Previously UniverseTBD -> now *AstroMLab* (astromlab.org)



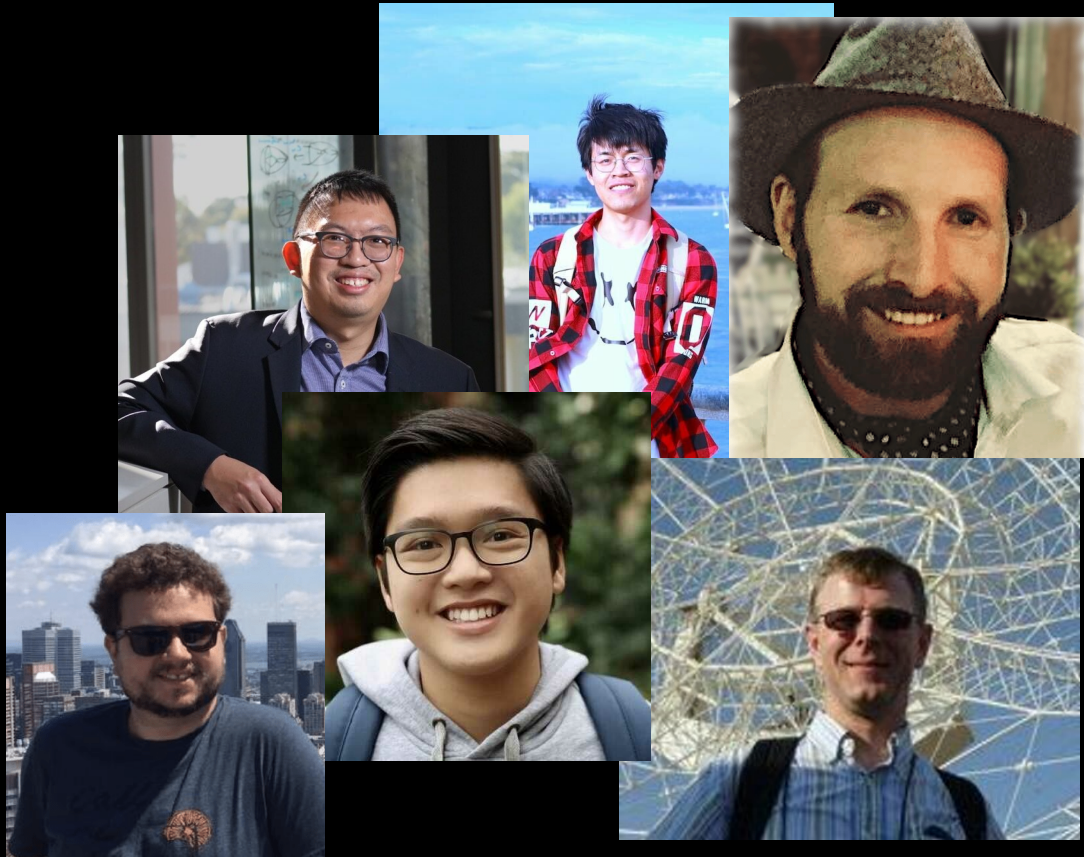
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Harvard-Smithsonian ADS

Previously UniverseTBD -> now *AstroMLab* (astromlab.org)

Natural Language Processing
experts



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U. Illinois
Urbana-
Champaign

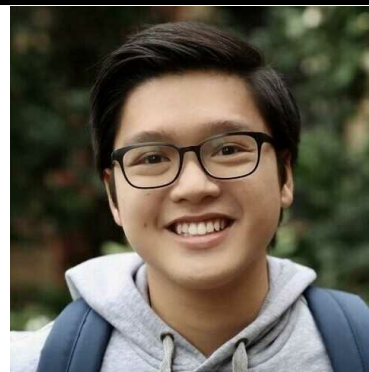













Harvard-Smithsonian ADS

Continual pre-training on all the *330K astronomy papers*

AstroLLaMA: Towards Specialized Foundation Models in Astronomy

Published on Sep 12 · ★ Featured in [Daily Papers](#) on Sep 13





Authors:  [Tuan Dung Nguyen](#),  [Yuan-Sen Ting](#),  [Ioana Ciucă](#), [Charlie O'Neill](#), [Ze-Chang Sun](#), [Maja Jabłońska](#), [Sandor Kruk](#), [Ernest Perkowski](#), [Jack Miller](#),  [Jason Li](#), [Josh Peek](#),  [Kartheik Iyer](#),  [Tomasz Róžański](#),  [Pranav Khetarpal](#), [Sharaf Zaman](#),  [David Brodrick](#),  [Sergio J. Rodríguez Méndez](#),  [Thang Bui](#), [Alyssa Goodman](#), [Alberto Accomazzi](#), [Jill Naiman](#),  [Jesse Cranney](#) + 2 authors



Continual pre-training on all the *330K astronomy papers*

OPEN ACCESS

AstroLLaMA-Chat: Scaling AstroLLaMA with Conversational and Diverse Datasets

Ernest Perkowski^{15,1}, Rui Pan^{15,2}, Tuan Dung Nguyen³, Yuan-Sen Ting^{4,5,6,7} , Sandor Kruk¹ ,
Tong Zhang⁸, Charlie O'Neill⁹, Maja Jablonska⁴, Zechang Sun¹⁰, Michael J. Smith¹¹

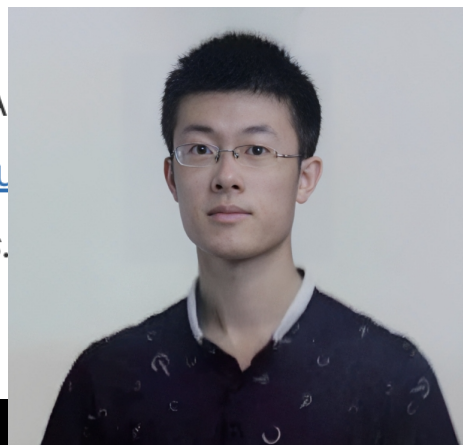
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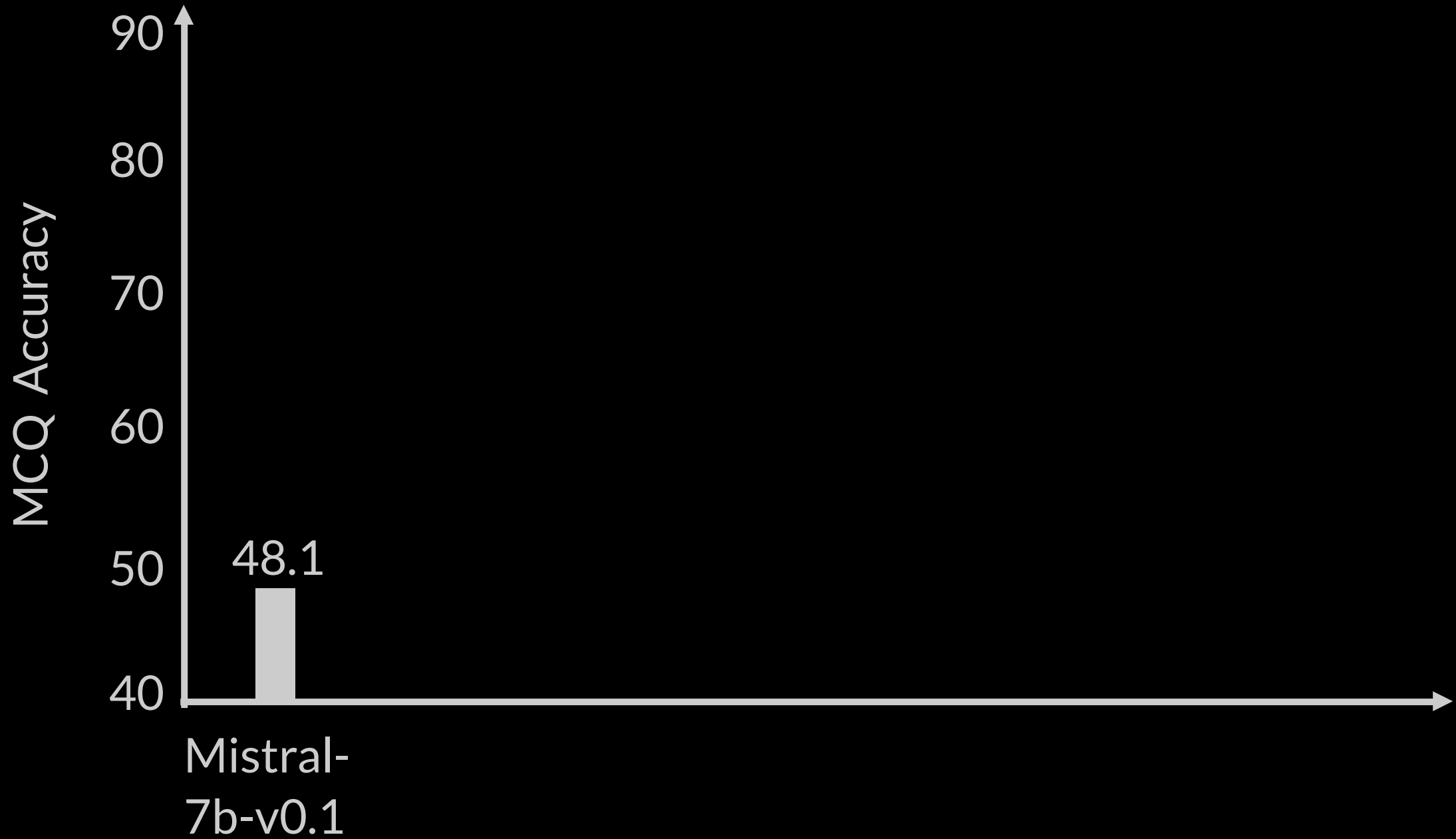
Published Jan 2024

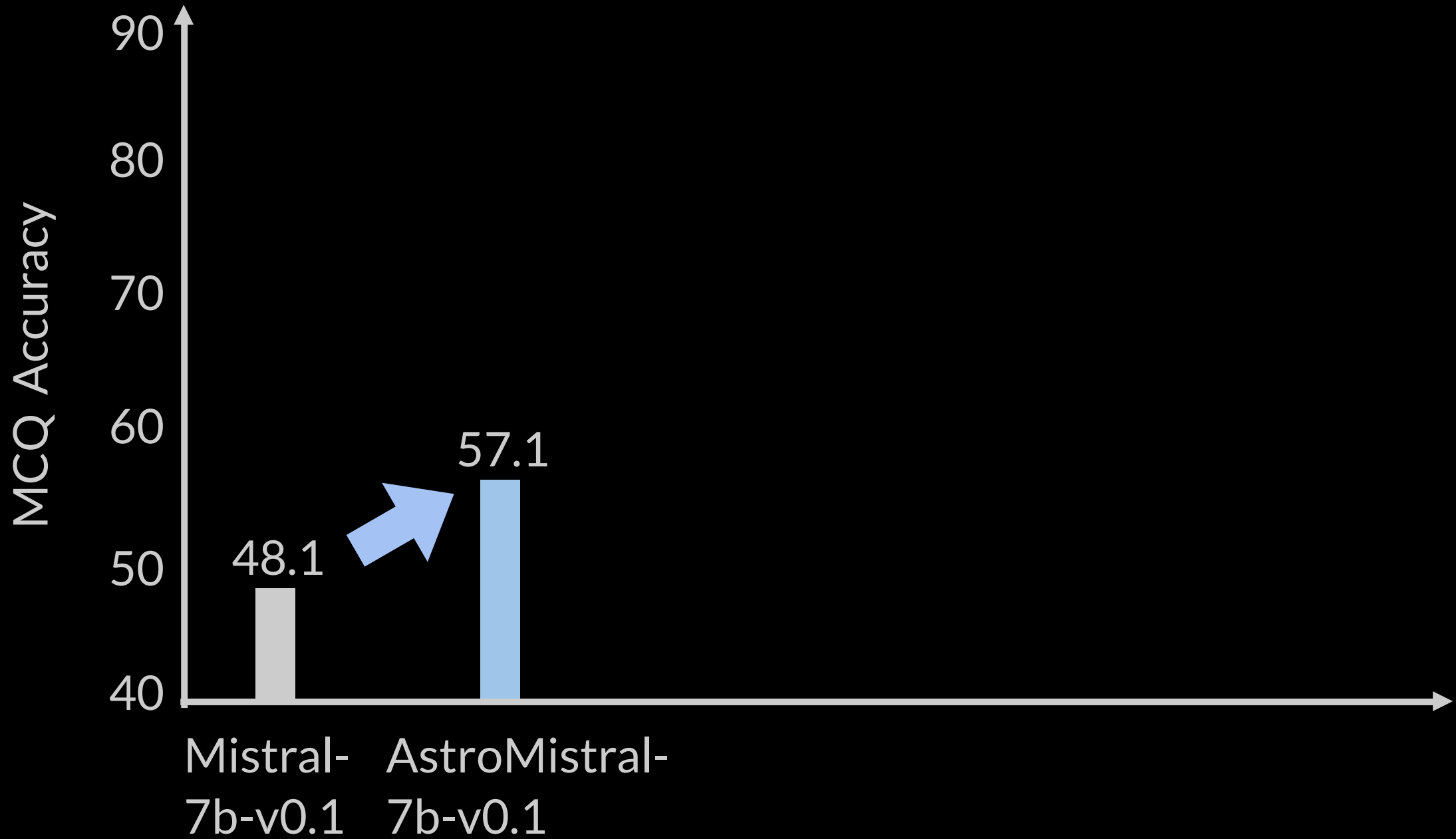
[Research Note](#)

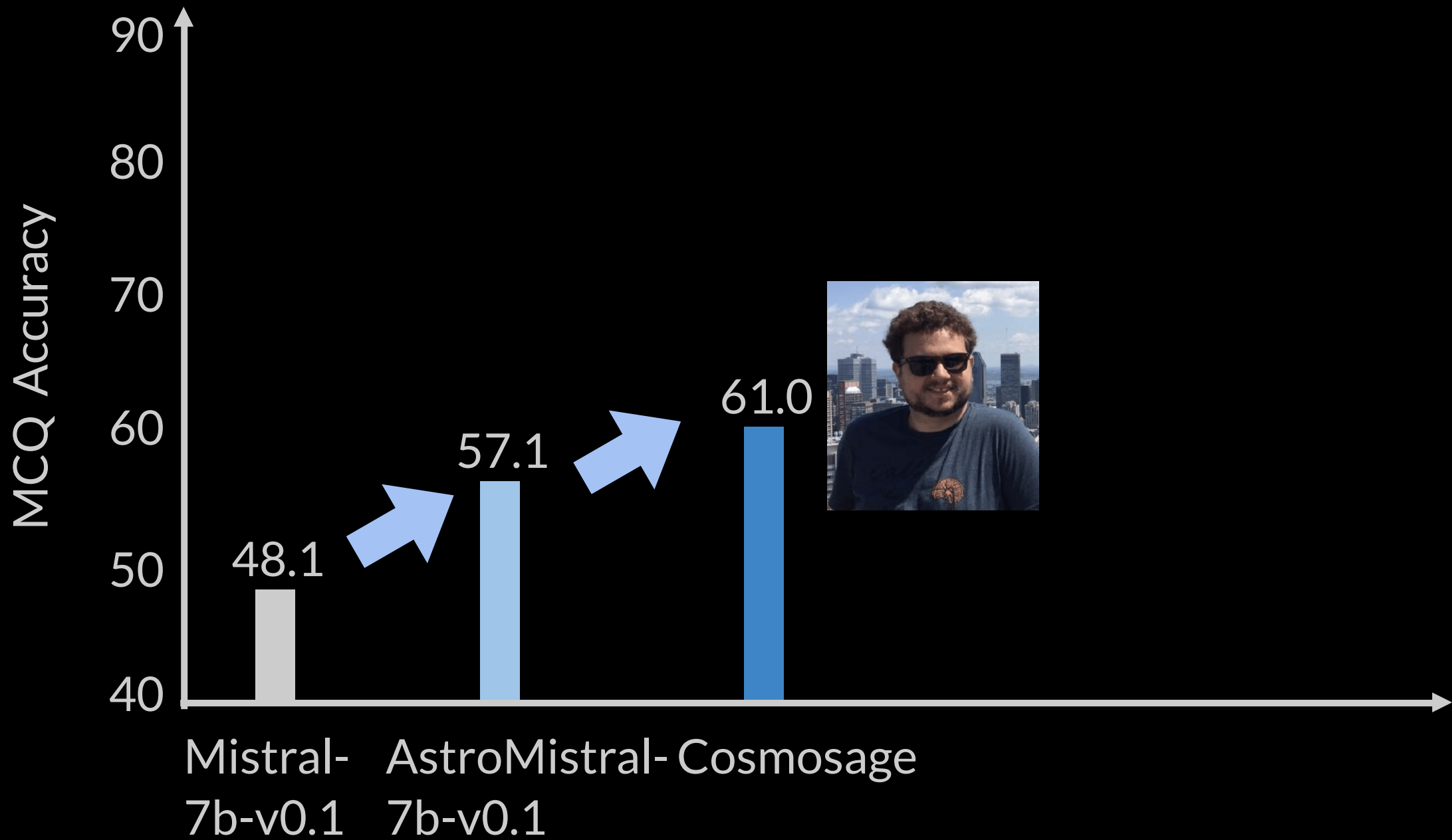
Citation Ernest Perkowski et al.

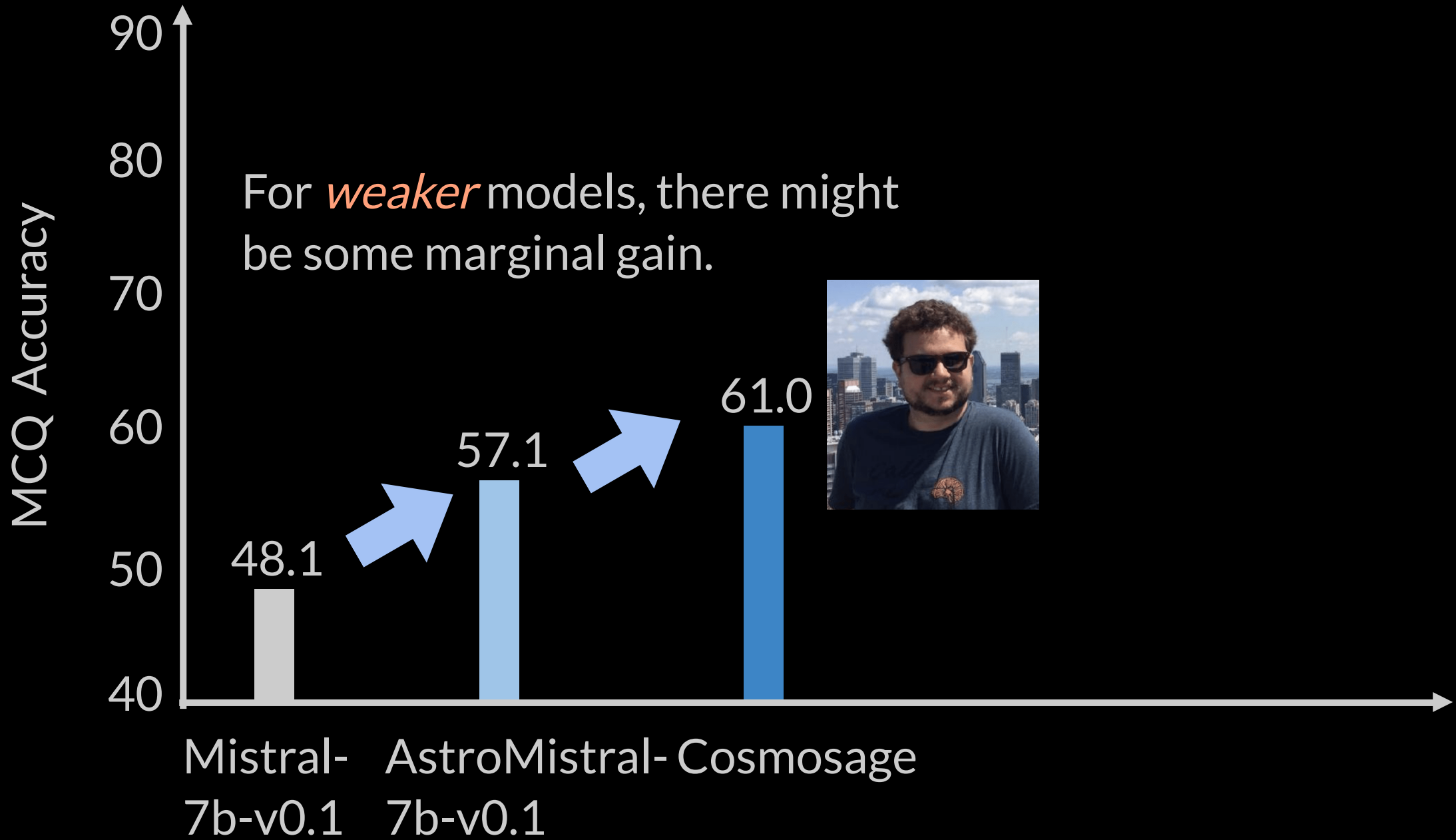
DOI 10.3847/1538-4357/511/1/1

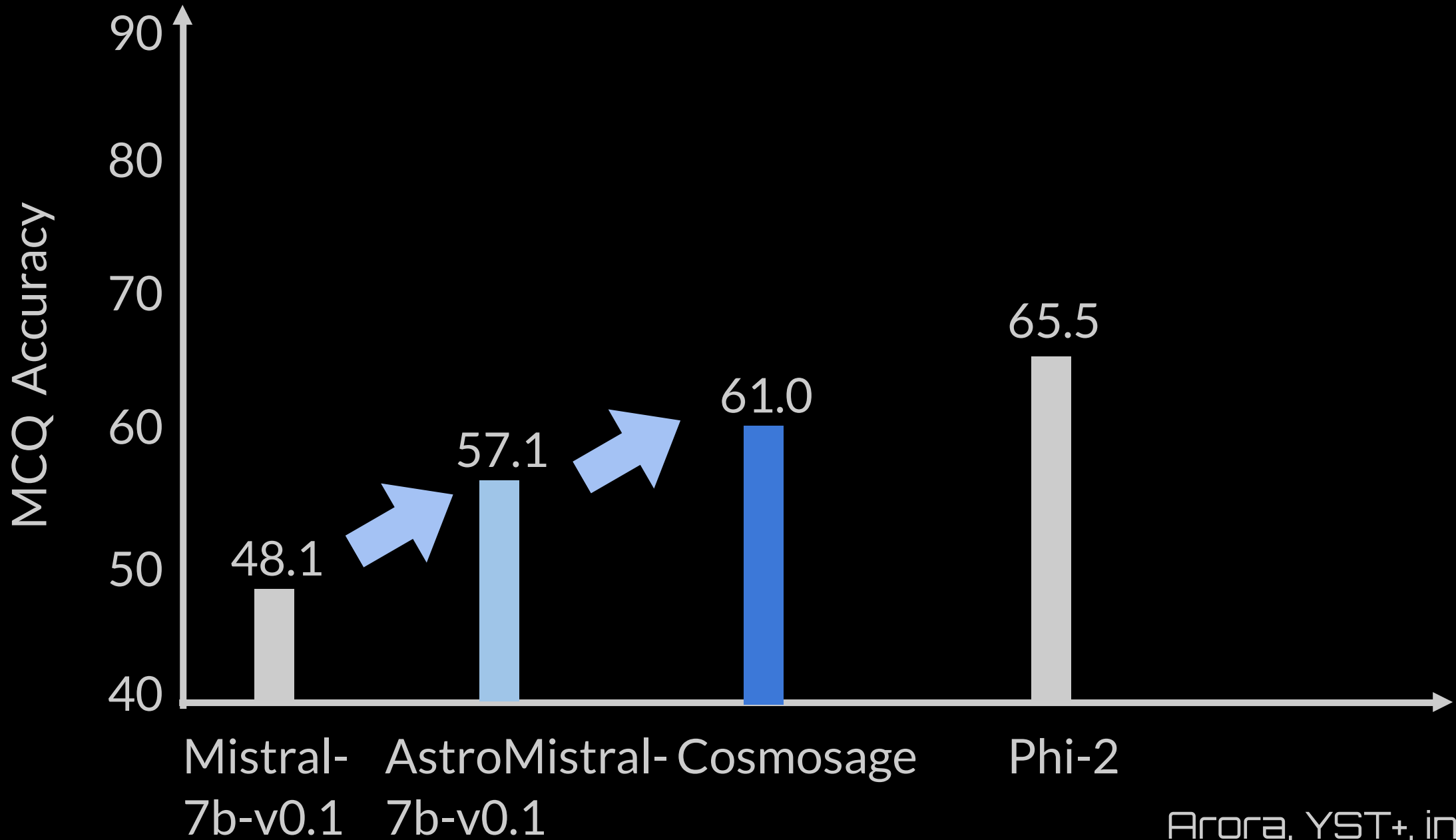




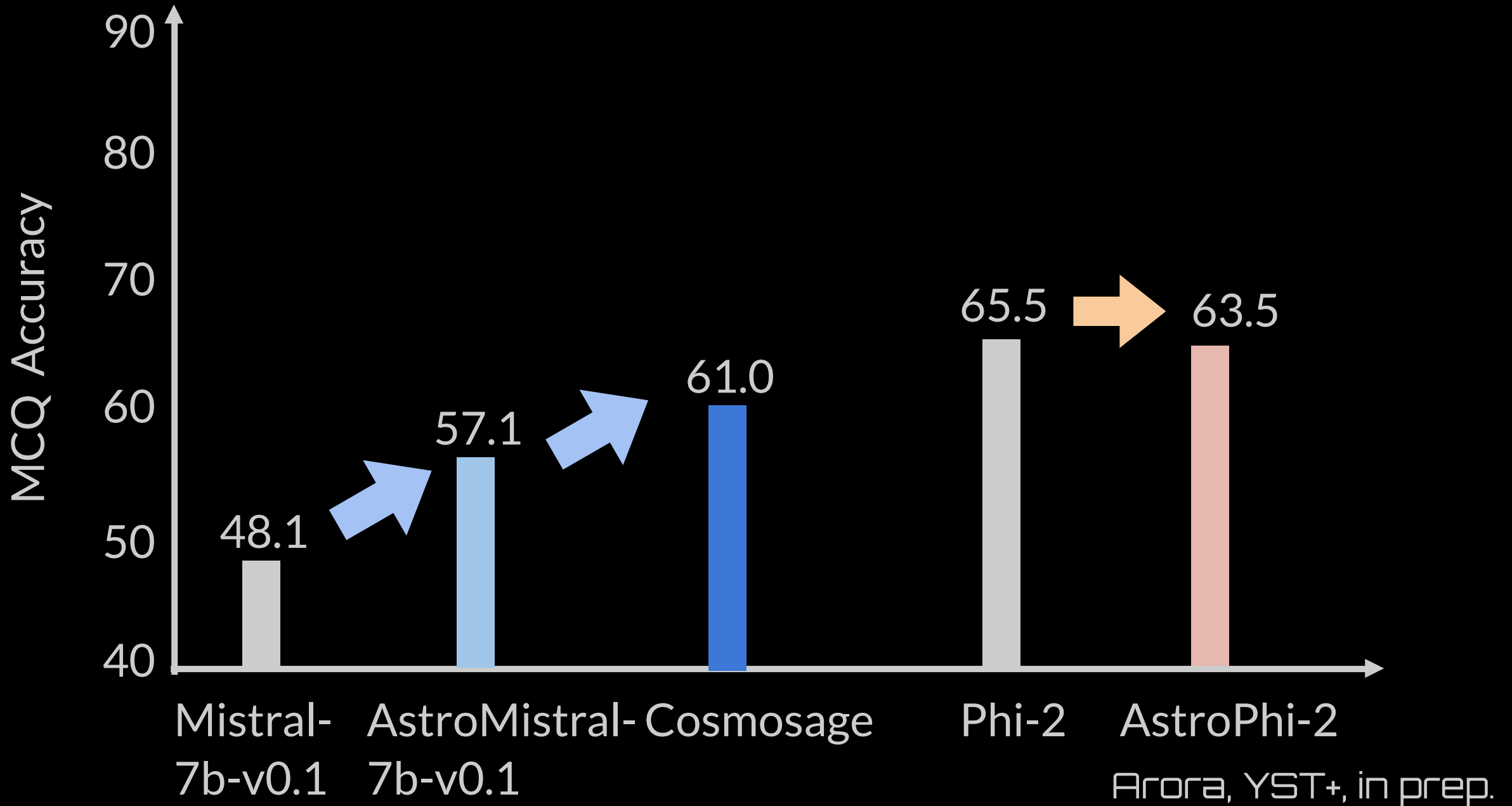


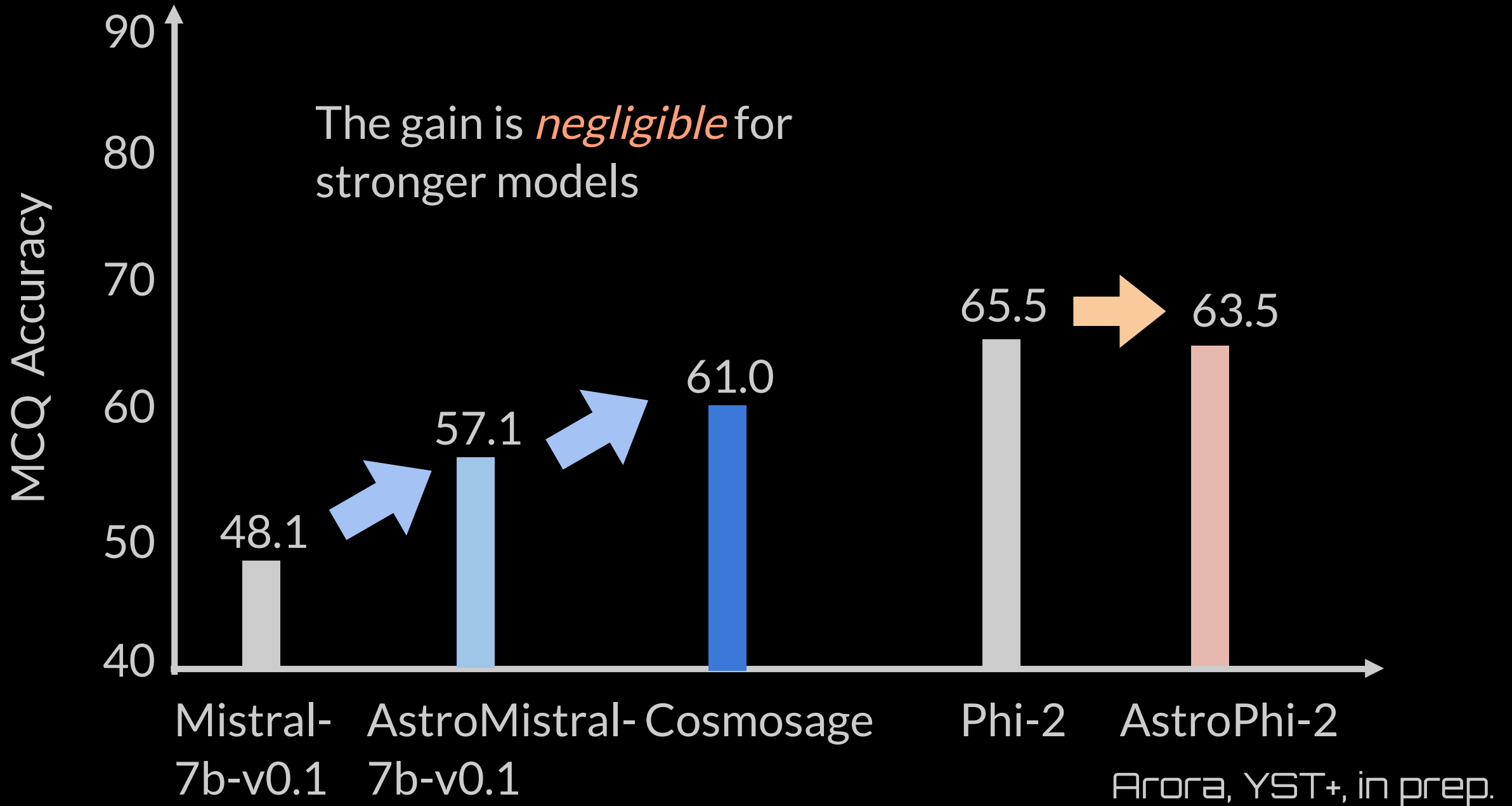






Arora, YST+, in prep.





Current LLMs remain *brittle*, and efforts to improve them through continual pretraining *have yet* to yield significant gains.

So what should we do ?

Warren Buffet :

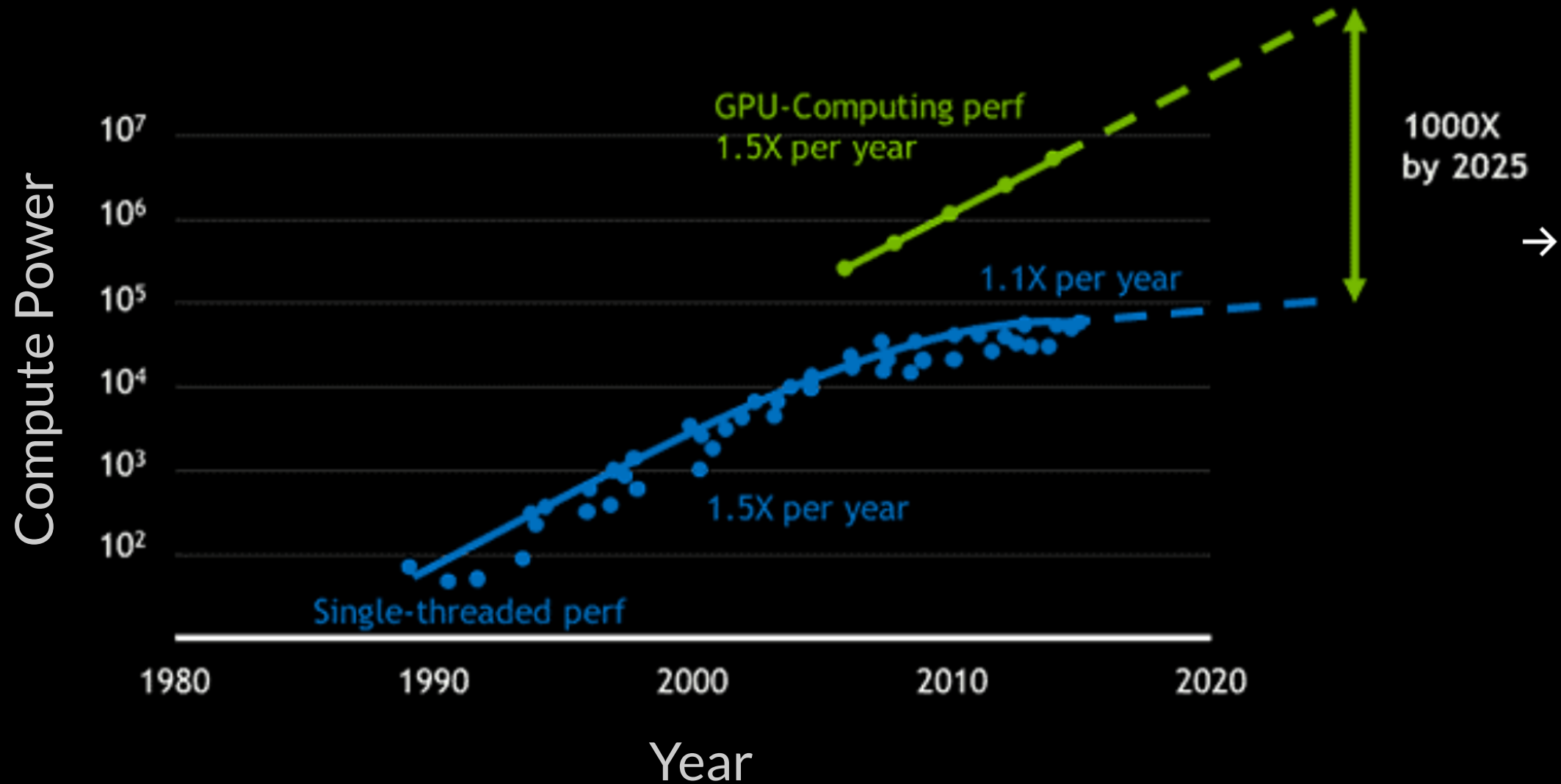
"The trick is, when there is nothing to do, *do nothing*."

Warren Buffet :

"The trick is, when there is nothing to do, *do nothing*."

"The stock market is designed to transfer money from the Active to the *Patient*."

Huang's Law



Tech / Tech Trends

Tech unicorn Zhipu AI joins China's LLM price war amid new funding round

- Zhipu AI's GLM series of large language models now costs 90 per cent less than the current industry average of 1 yuan per 1 million tokens



0.1 Yuan
per 1 million tokens

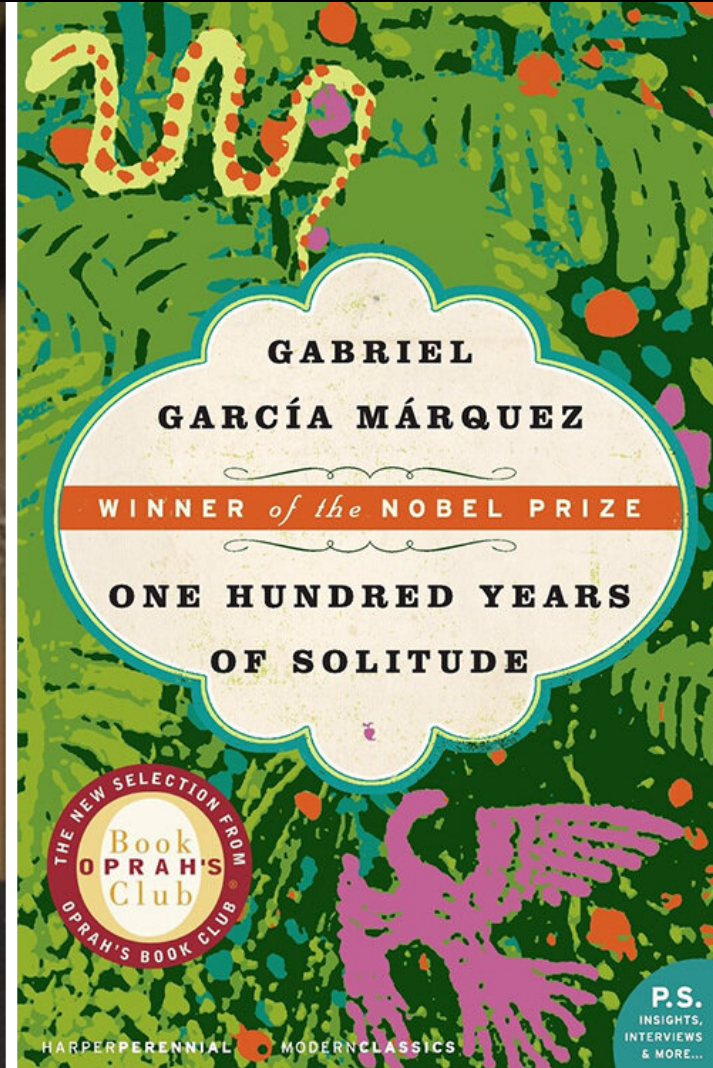
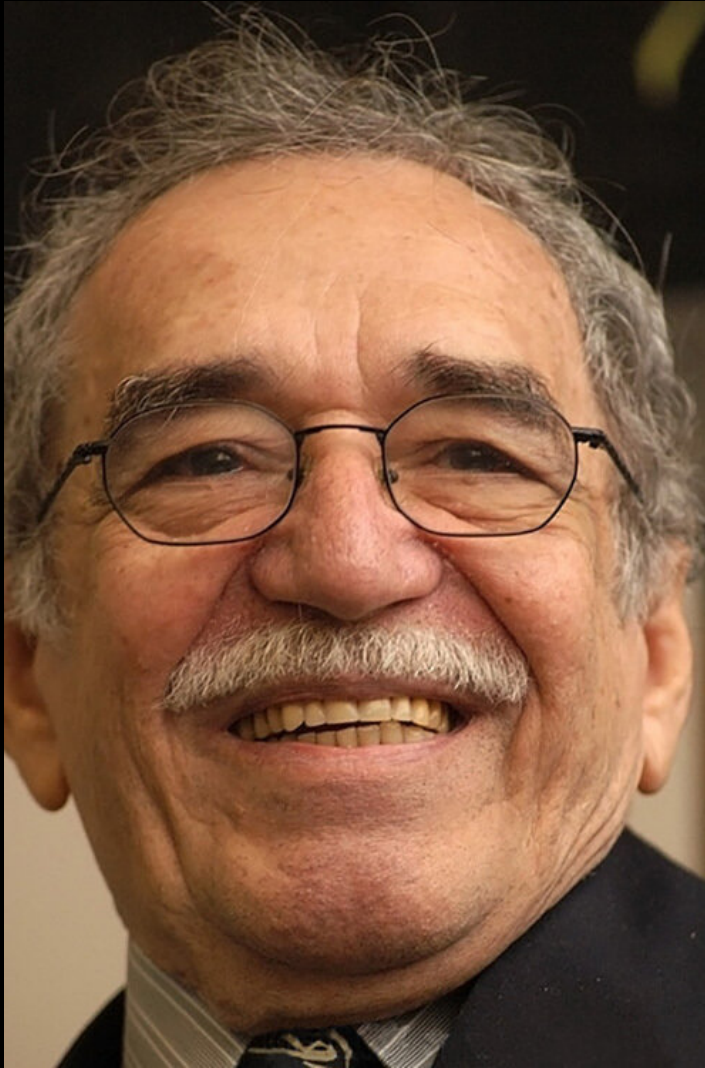


Ben Jiang in Beijing

+ FOLLOW

Published: 8:00pm, 5 Jun 2024

 [Why you can trust SCMP](#)



= 0.03 Euro





Cornell University

arXiv > astro-ph

Astrophysics (since April 1992)

= 40 Euro





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EVERYONE
CAN FLY**

LLM

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Fly Now!**

Summary :

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- Current research prioritizes tool development over *creating meta-methods* that could accelerate the discovery of 'unknown unknowns'!
- By interacting with real-world data, *LLM agents* can distill causal relationships, conducting end-to-end research autonomously.
- The astronomical cost of *applying at scale* limits our progress, but the growth in GPU computing power will inevitably overcome this.