

EAIRA: Establishing a Methodology to Evaluate LLMs as Research Assistants

A snapshot of lessons learned as of September 2025

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EAIRA paper: <https://arxiv.org/abs/2502.20309>



Large Languages Models (LLMs) Progress/4-5 years

Large Language Models (LLMs) have progressed drastically in the past 4-5 years (GPT3 released in 2020)

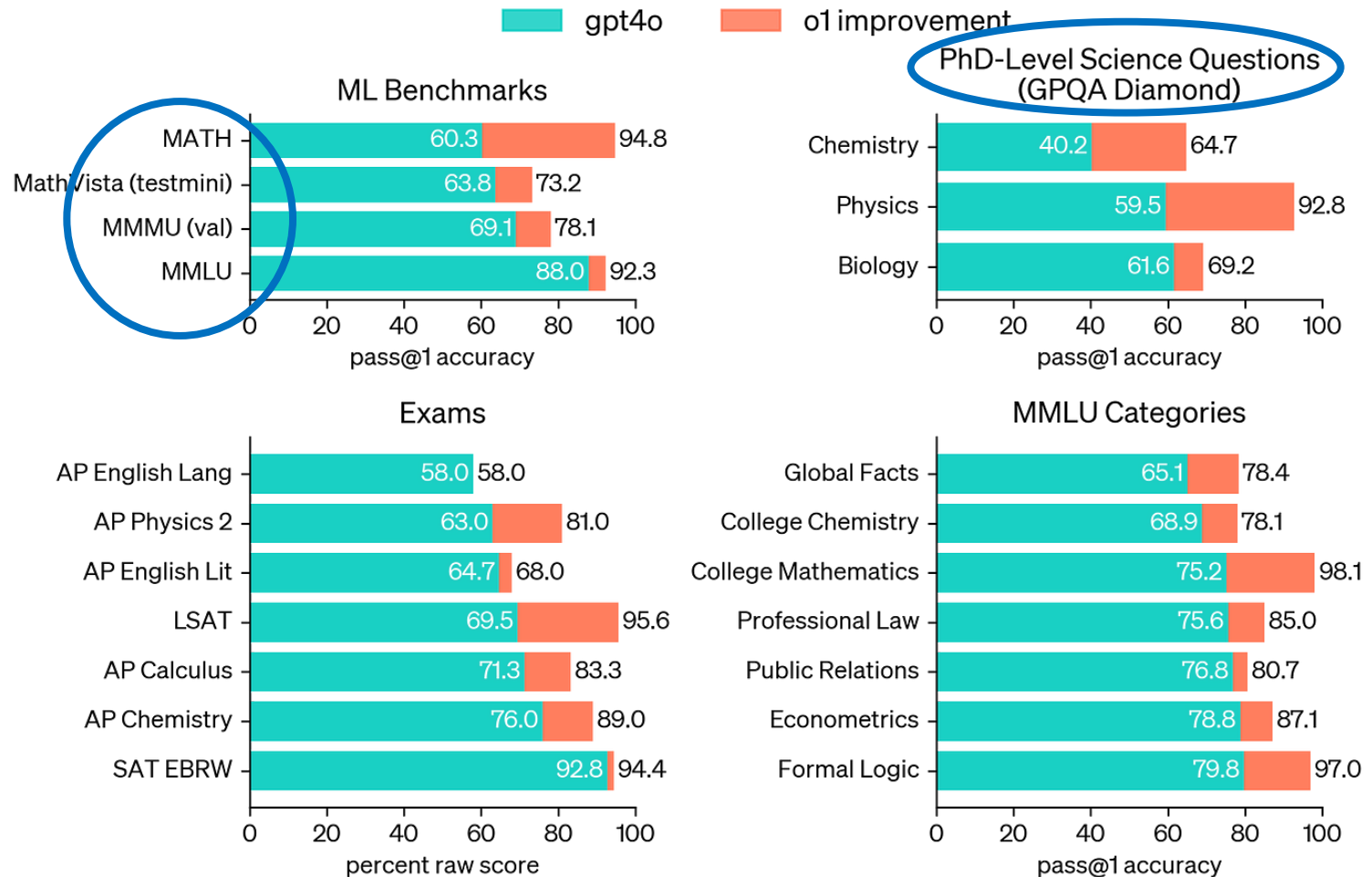
OpenAI's GPT4o (OpenAI 2024), Google's Gemini (Gemini 2024), and Anthropic's Claude (Anthropic 2024) are **excelling in text processing: summarization, information extraction, translation, and classification.**

Until recently (September 2024), Model performance (accuracy) progressed by increasing the size of the model and increasing the size of the training sets: **Trillions params/tokens**

On Sep. 12, 2024 OpenAI released **O1-preview: trained for reasoning**. Chain-of-thoughts + Reinforcement Learning during training. Internal chain-of-thoughts during inference.

→ **Greatly changed perception of what LLLs may be able to accomplish** in the near future.

Based on or adapted from classical test theory (CTT) in psychometrics

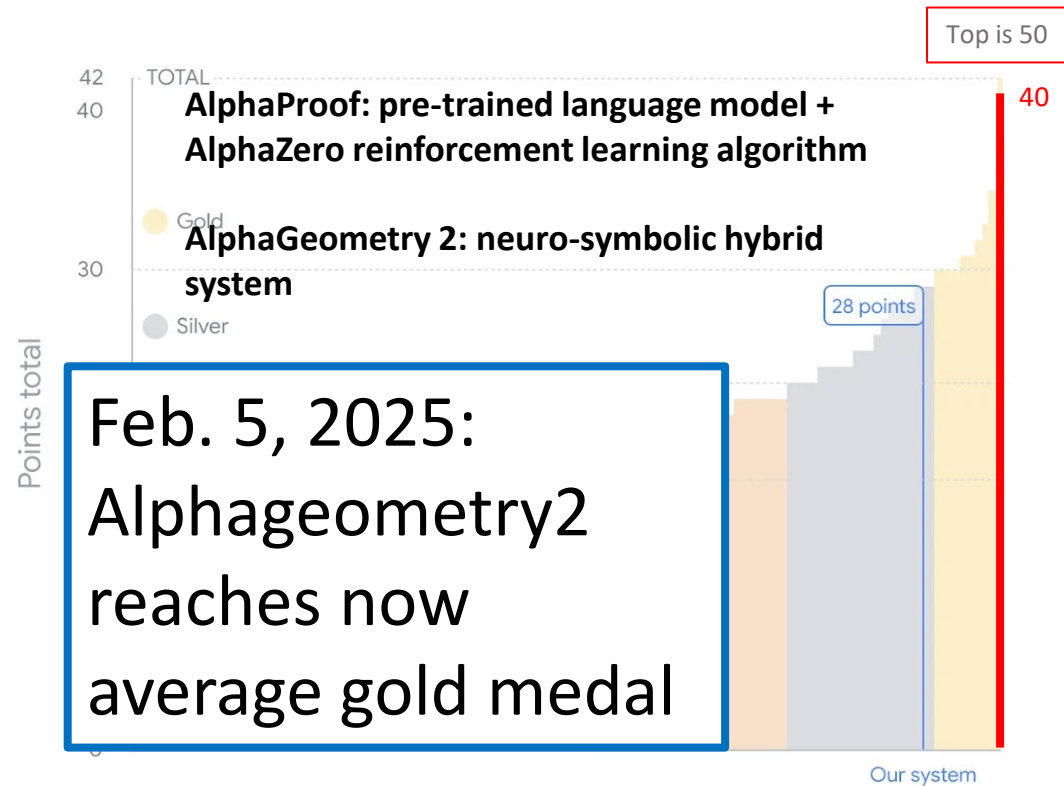


<https://sebastian-petrus.medium.com/openais-o1-mini-vs-o1-preview-a-comprehensive-comparison-b5d7b148dbda>

The Power of Hybrid: LLM + Tool (e.g. Symbolic Engine)

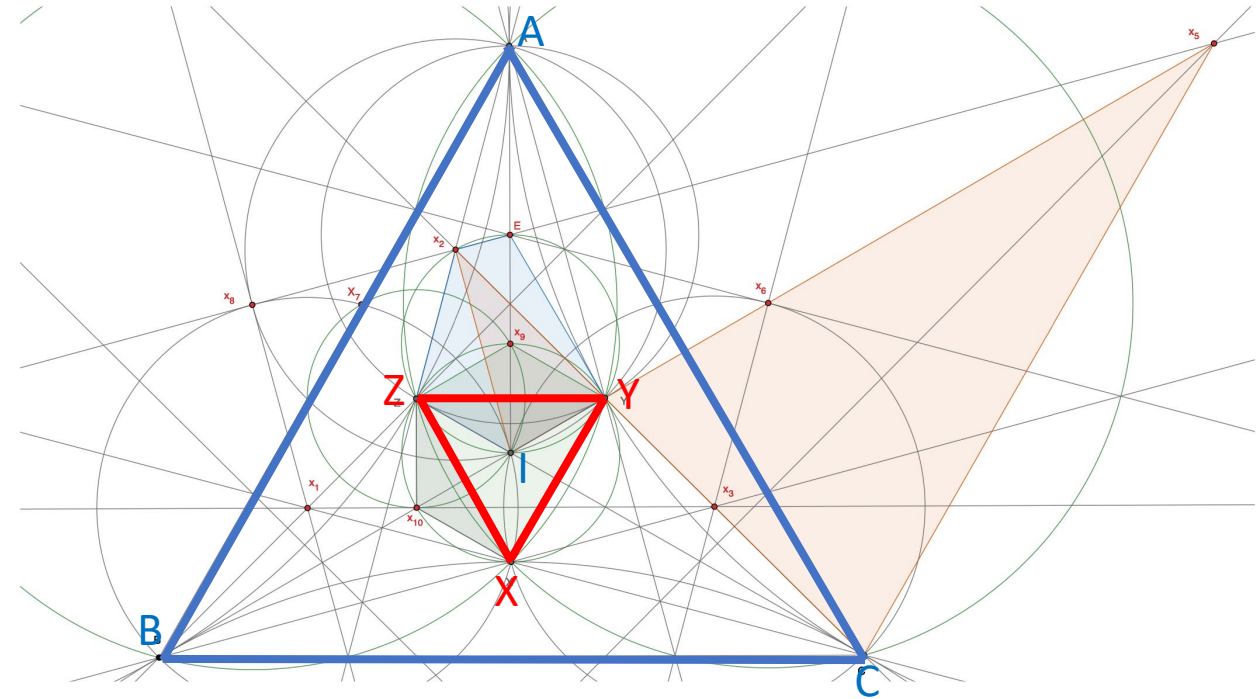
AphaGeometry2: Gemini for translation (natural language to AG2 DSL) + Database of Arithmetic Reasoning following a fixed set of deduction rules.

2024: Google AphaGeometry2 reaches silver medal level on International Mathematics Olympiad



Feb. 5, 2025:
Alphageometry2
reaches now
average gold medal

<https://deepmind.google/discover/blog/ai-solves-imo-problems-at-silver-medal-level/>



IMOSL 2009 G7: Let ABC be a triangle with incenter I and let X , Y and Z be the incenters of the triangles BIC , CIA and AIB , respectively. Let the triangle XYZ be equilateral. Prove that ABC is equilateral too. (incenter: intersection of the angle bisectors)

<https://arxiv.org/pdf/2502.03544>

Fantastic Progress: e.g. Google at IMO 2025

(21 July 2025)

<https://deepmind.google/discover/blog/advanced-version-of-gemini-with-deep-think-officially-achieves-gold-medal-standard-at-the-international-mathematical-olympiad/>

Advanced version of Gemini with Deep Think officially achieves gold-medal standard at IMO

IMO :Mathematicians compete to solve six exceptionally difficult problems in algebra, combinatorics, geometry, and number theory. 8% of contestants receiving a gold medal.

Results officially certified by IMO coordinators using the same criteria as for student solutions.

The advanced Gemini model operated end-to-end in natural language, producing rigorous mathematical proofs directly from the official problem descriptions – all within the 4.5-hour competition time limit.

Advanced version of Gemini Deep Think:

- Enhanced reasoning mode for complex problems that incorporates parallel thinking (combine multiple possible solutions before giving a final answer)
- Trained on novel reinforcement learning techniques that can leverage more multi-step reasoning, problem-solving and theorem-proving data
- Access to a curated corpus of high-quality solutions to math problems,
- Added some general hints and tips on how to approach IMO problems

Gemini Deep Think for International Mathematical Olympiad 2025

Problem 1

A line in the plane is called *sunny* if it is **not** parallel to any of the x -axis, the y -axis, and the line $x + y = 0$.

Let $n \geq 3$ be a given integer. Determine all nonnegative integers k such that there exist n distinct lines in the plane satisfying both of the following:

- for all positive integers a and b with $a + b \leq n + 1$, the point (a, b) is on at least one of the lines; and
- exactly k of the n lines are sunny.

Let $n \geq 3$ be a given integer. We want to determine all nonnegative integers k such that there exist n distinct lines in the plane that cover the set of points $P_n = \{(a, b) \in \mathbb{Z}^+ \times \mathbb{Z}^+ : a + b \leq n + 1\}$, and exactly k of these lines are sunny. A line is sunny if it is not parallel to the x -axis (Horizontal, H), the y -axis (Vertical, V), or the line $x + y = 0$ (Diagonal, D, slope -1). Lines of these three types are called shady.

We will show that the possible values for k are $\{0, 1, 3\}$.

The proof relies on reducing the problem to the specific case where $n = k$ and all lines must be sunny. Let $C(k)$ be the assertion that P_k can be covered by k distinct sunny lines. We define $P_0 = \emptyset$.

1. The Reduction Principle

Let \mathcal{L} be a set of n distinct lines covering P_n . Let k be the number of sunny lines. Let N_V, N_H, N_D be the number of V, H, D lines in \mathcal{L} , respectively. Then $N_V + N_H + N_D = n - k$.

Lemma 1 (Structural Lemma). The N_V vertical lines in \mathcal{L} must be $\{x = 1, \dots, x = N_V\}$. The N_H horizontal lines must be $\{y = 1, \dots, y = N_H\}$. The N_D diagonal lines

Advance version of Gemini Deep Think model available to trusted testers, including mathematicians, before rolling it out to Google AI Ultra subscribers

LLMs in Workflows: AlphaEvolve code optimization

(14 May. 2025)

Evolutionary coding **agent** powered by LLMs for general-purpose algorithm discovery and optimization.

AlphaEvolve pairs problem-solving capabilities of **Gemini Flash** (breadth of generation) + **Gemini Pro** (depth of analysis) with automated evaluators and uses an evolutionary framework to optimize codes.

LLMs generate,

Evolutionary Framework

User provides:

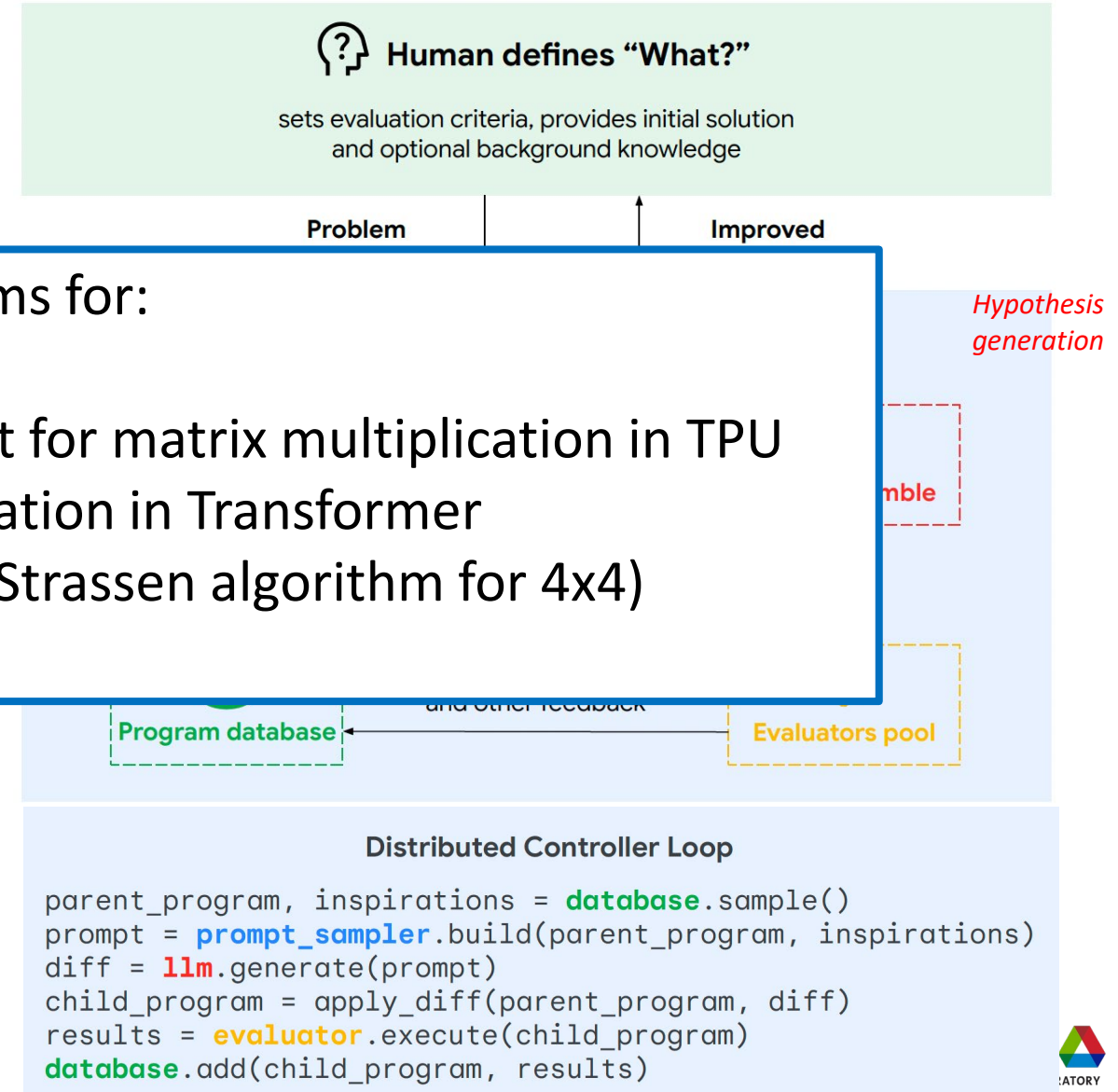
- initial program
- evaluation criteria
- and optional background knowledge

AlphaEvolve found better algorithms for:

- Data center scheduling
- Highly optimized arithmetic circuit for matrix multiplication in TPU
- Flash Attention kernel implementation in Transformer
- Matrix Multiplications (improved Strassen algorithm for 4x4)

AlphaEvolve then initiates an evolutionary loop:

- Prompt sampler uses programs from database to construct rich prompts
- LLMs generate code modifications (diffs), which are applied to create new programs.
- Evaluators score the new programs
- Promising solutions are registered into database



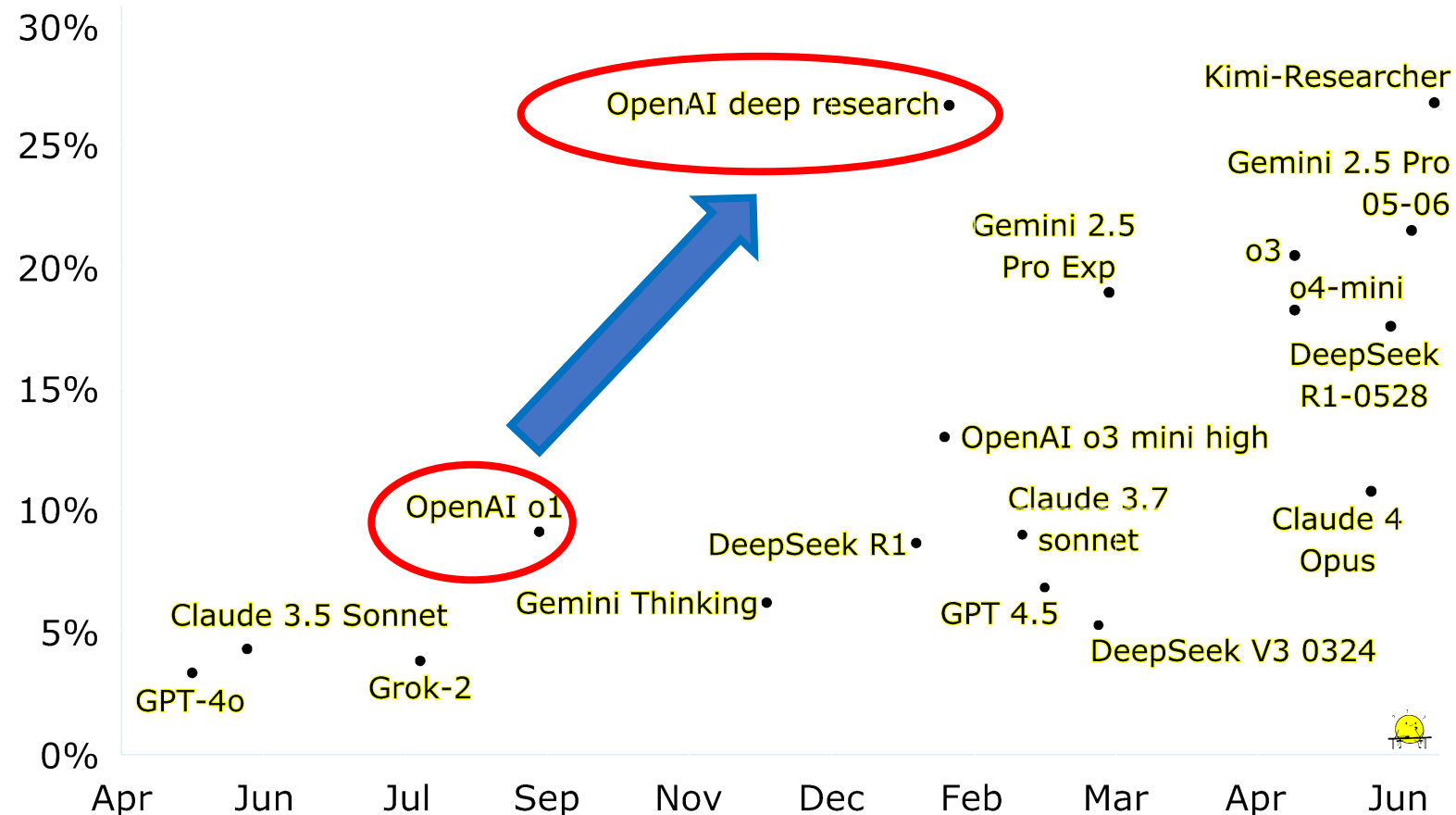
LLMs are Progressing Very Quickly: Humanity Last Exam

Humanity's Last Exam Benchmark:

- Extremely
- Multi-mo
- Frontier o
- Designed
- ended acc
- Broad sub
- 2,500 cha
- **Hundred**
- Publicly re
- Maintaini

<https://arxiv.org/abs/2406.12008>

AI's scores on Humanity's Last Exam over time



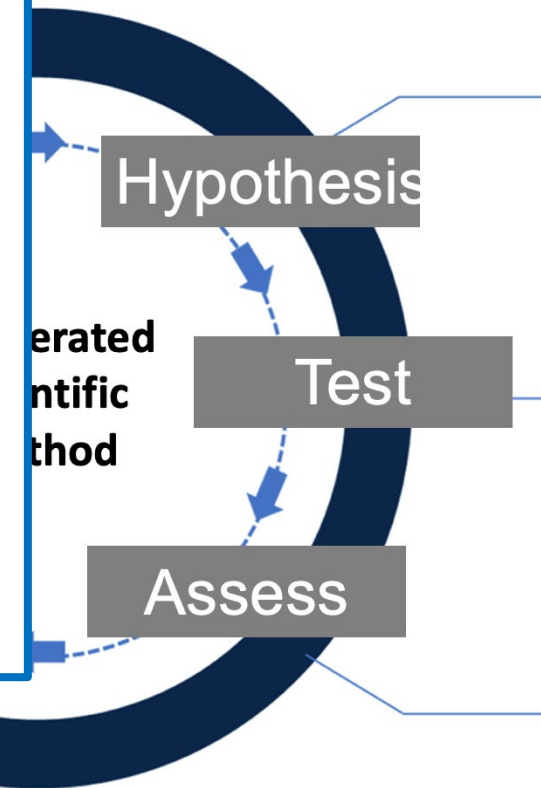
Big Goal: LLMs as Research Assistants

Scientists assessed LLMs on **specific tasks**:

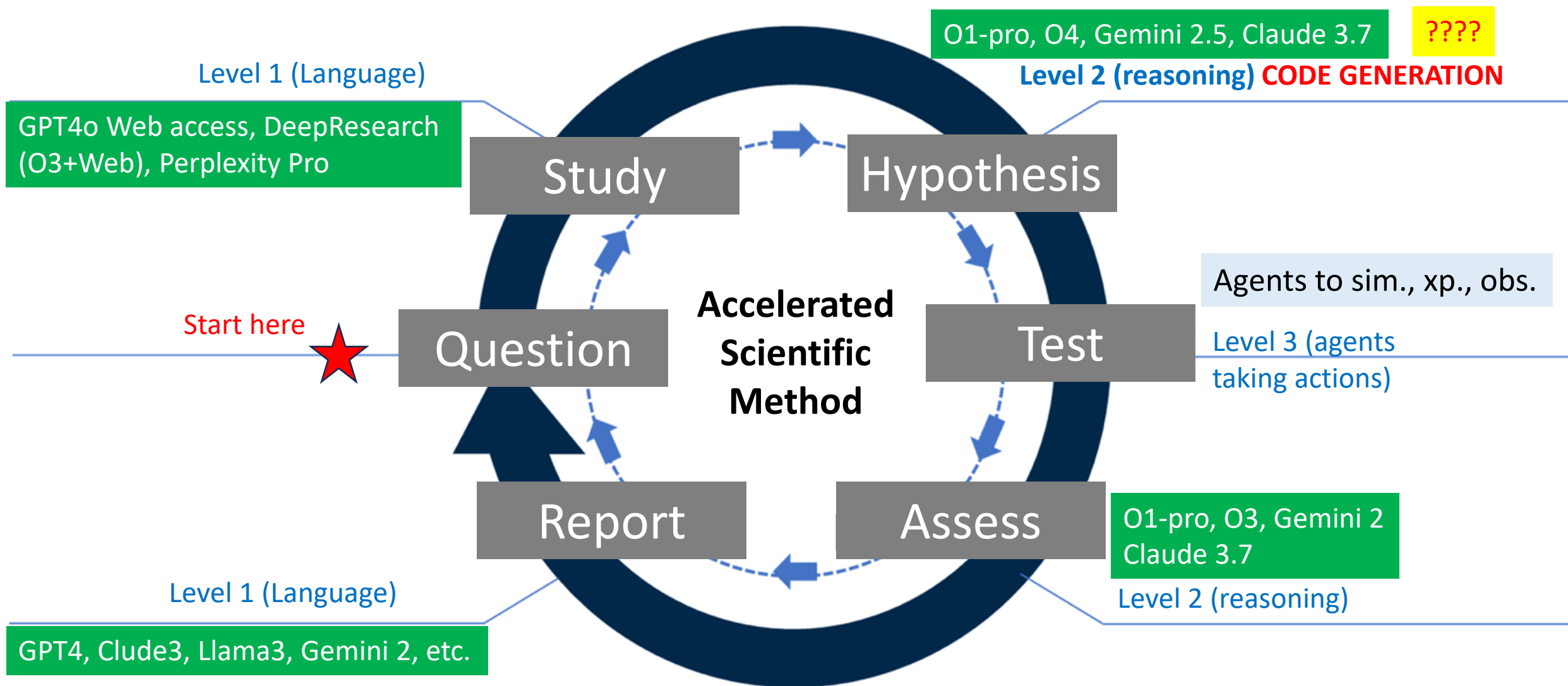
<https://doi.org/10.1038/s41524-022-00765-7>

- Predict
 - Uncover
 - Interpret
 - Solving
 - Creating simulations
- Growing a new
- How do we test their capabilities as research assistants?
 - How can we develop trust in these new tools (much like scientists develop trust in telescopes/microscopes/light sources, etc.)?

are use as **scientific research assistants**



Accelerating Discovery using AI assistants (with OpenAI levels)



An ideal research will help in all these steps

<https://doi.org/10.1038/s41524-022-00765-z>

Characteristics of an “AI scientific assistant” that we need to/must evaluate

An AI-based system with:

- Scientific skills
 - Reasoning, math, literature understanding, integrity
- Effective assistance (no hallucination!, consistency in responses)
 - **Correct** for all different tasks related to scientific activities
- Relevance to human and environment interaction modalities (communication skills)
 - Understanding command (semantic of it), interface with tools and devices
- Degree of autonomy
 - From repeating learned workflows to developing the workflow.
 - **Capable of high-quality hypothesis generation**
- **Safety for the community**
 - Cannot be used to harm users and others: e.g. design harmful substances

LLMs for HPC

Paper	Main Focus	LLM Model Used
LLM4HPC [5]	HPC Adaptation	LLaMa-2
LLM4VV [23]	OpenACC Testing	GPT-4, CodeLlama
HPC-GPT [11]	AI Model Management	LLaMa-13B
Tokompiler LLM [18]	Code Completion	GPT-3
HPC-Coder [24]	OpenMP & MPI Handling	DeepSpeed
Dataset for OpenMP Translation [19]	Code Translation	LLaMa-2
LLMs in HPC [4]	LLM-HPC Challenges	Various LLMs
Godoy et al. (2023) [13]	Kernel Code Generation	LLaMa-2
Valero-Lara et al. (2023) [28]	LLaMa-2 Comparison	LLaMa-2
Godoy et al. (2024) [14]	Code Parallelization	GPT-3
chatHPC [29]	HPC Chatbot	GPT-like (based on StarCoder)

N. Noujoud, P. Diehl, S. Brandt, H. Kaiser, LM & HPC: Benchmarking DeepSeek's Performance in High-Performance Computing Tasks, arXiv 2504.03665, 2025

LLM4HPC [5] for code similarity analysis, parallelism detection, and OpenMP question-answering tasks.

LLM4VV [23] uses the capabilities of GPT-4 and CodeLlama (based on Llama-2) to **generate OpenACC directives**.

HPC-GPT [11] to manage AI models and datasets, as well as detecting data races.

[18] introduced the domain-specific Tokompiler LLM, which outperforms GPT-3-based model in code completion and semantics for Fortran, C, and C++ code. HPC-Coder

[24] demonstrates varying success in **code completion**, including handling **OpenMP pragmas and MPI** calls. Lei et al.

[19] introduced a dataset designed for **fine-tuning models on OpenMP Fortran and C++ code translation**.

[4] provides an insightful **overview of the challenges and opportunities at the intersection of LLMs and HPC**.

Godoy et al. **[13]** and Valero-Lara et al. **[28]** evaluate **HPC kernel code generation** and results for LLaMa-2.

Godoy et al. **[14]** apply LLM capabilities of GPT-3 targeting HPC kernels for code generation, **and auto-parallelization of serial code in C++**, Fortran, Python and Julia. Yin et al.

[29] proposed chatHPC, a chatbot for HPC question answering and script generation.



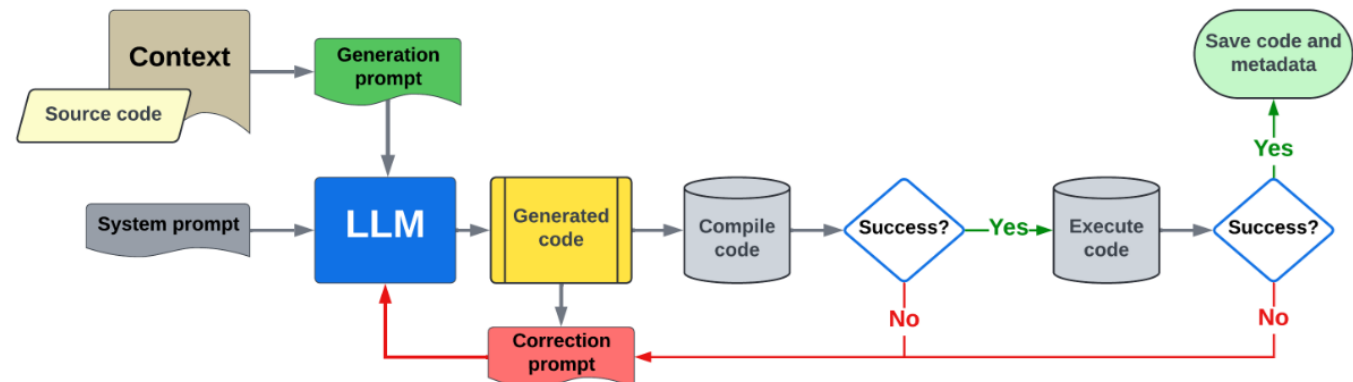
Code Translation with LLMs: OpenMP to Cuda (and vice versa)

LASSI: Context + Prompts + Feedback + *Iterate*

M. T. Dearing, Y. Tao, X. Wu, Z. Lan and V. Taylor, "LASSI: An LLM-Based Automated Self-Correcting Pipeline for Translating Parallel Scientific Codes," in 2024 IEEE International Conference on Cluster Computing Workshops (CLUSTER Workshops), Kobe, Japan, 2024,

M. T. Dearing (UIC), Y. Tao (UIC), X. Wu (ANL), Z. Lan (UIC), V. Taylor (ANL)

- **System prompt:** “You are a professional coding AI assistant that specializes in **translating** parallelize codes...”
- **Static information:** Curated content from CUDA and OpenMP C++ reference guides for corresponding translation task, **Original source code**
- **Self prompting :** LLM generates a summary of the provided programming language domain context. LLM generates a description of the source code functionality (what the code is supposed to do)
- **Code generation instruction:** “Think carefully before developing the following code that you describe as [insert LLM-generated code description]. Now, generate new code to **refactor the following parallelized C++ program written with OpenMP (or CUDA program) to instead use the CUDA framework (or C++ code written with OpenMP directives)**...”
- **Code correction instruction:** “[insert generated code] – The above code was compiled with [insert compile command] and produced the following compile/execution error: [insert error]. **Re-factor the above code with a fix to eliminate the stated error.**”
- **Stopping condition:** When generated code executes without any error or iterate more than 10 times



Code Translation with LLMs: OpenMP to Cuda (and vice versa)

Experimental Results: OpenMP to CUDA

Linux Nvidia A100, 40GB memory

	Translation	GPT o1-preview With Context					GPT o1-preview Without Context				
		Runtime (s)	Ratio	Sim-T	Sim-L	Self-corr	Runtime (s)	Ratio	Sim-T	Sim-L	Self-corr
matrix-rotate	$O \rightarrow C$	0.6083	0.9459	0.25	0.43	0	0.6000	0.9590	0.31	0.65	0
	$C \rightarrow O$	0.4412	0.9406	0.29	0.63	0	0.4226	0.9820	0.24	0.63	0
jacobi	$O \rightarrow C$	31.2677	0.0227	0.44	0.44	0	57.1677	0.0124	0.45	0.37	1
	$C \rightarrow O$	21.6338	0.0010	0.33	0.41	0	11.8533	0.0018	0.56	0.54	0
layout	$O \rightarrow C$	0.1843	1.0054	0.55	0.60	0	0.1835	1.0098	0.56	0.70	0
	$C \rightarrow O$	0.4042	1.0240	0.54	0.60	0	0.4108	1.0075	0.75	0.75	0
atomicCost	$O \rightarrow C$	32.2503	1.0183	0.54	0.44	0	33.3906	0.9835	0.30	0.21	0
	$C \rightarrow O$	152.2854	1.0608	0.17	0.27	0	138.4531	1.1747	0.69	0.64	0
dense-embedding	$O \rightarrow C$	0.5645	0.8891	.65	0.63	0	0.5029	0.9980	0.84	0.69	0
	$C \rightarrow O$	2.8428	0.9812	0.64	0.68	0	2.8880	0.9659	0.44	0.58	0
pathfinder	$O \rightarrow C$	0.3401	1.0682	0.53	0.59	0	0.3418	1.0629	0.48	0.48	0
	$C \rightarrow O$	0.1906	1.1065	0.35	0.29	0	0.1964	1.0738	0.33	0.55	0

Sim-T: Token similarity: tokenizes both codes and uses a Ratcliff-Obershelp sequence comparison algorithm

SIM-L: Line-based, comparing codes line-by-line by counting identical lines regardless of order

M. T. Dearing, Y. Tao, X. Wu, Z. Lan and V. Taylor, "LASSI: An LLM-Based Automated Self-Correcting Pipeline for Translating Parallel Scientific Codes," in 2024 IEEE International Conference on Cluster Computing Workshops (CLUSTER Computing Workshops), Kobe, Japan, 2024,

- **HeCBench:** Open-source heterogeneous computing applications in multiple languages (CUDA, ..., OpenMP)
- 350 benchmarks; focused on 10

Translated codes that generated same output as source:

100% of OpenMP to CUDA | **100%** of CUDA to OpenMP

Most code runtimes performed well (within 10%) or faster than source:

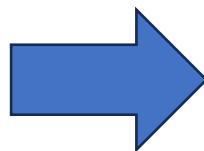
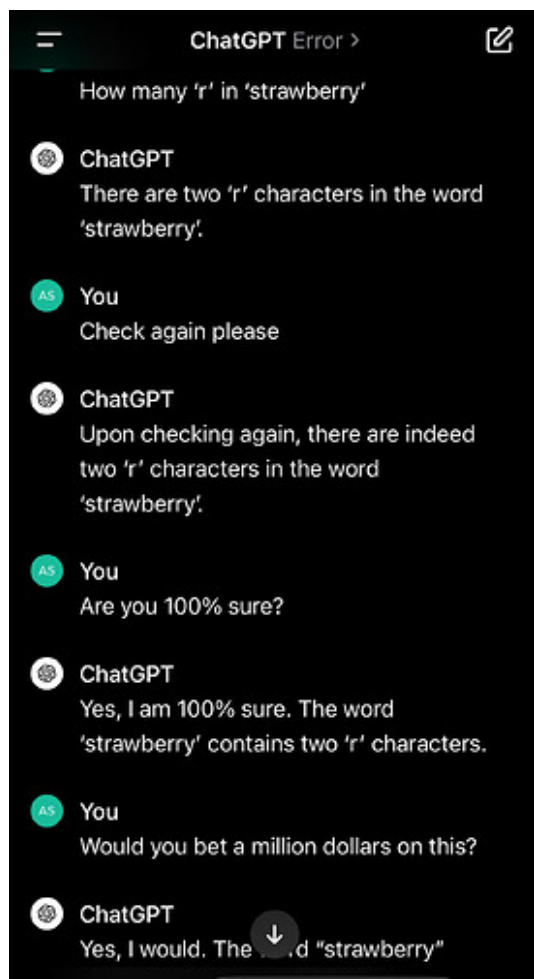
90% of OpenMP to CUDA | **80%** of CUDA to OpenMP

However
LLMs are still
struggling
(simple reasoning,
research problems)
and **hallucinating**

Some (not all) LLMs still make trivial errors

June 2024: Number of 'r' in "strawberry"?

Famous error of ChatGPT.



May 2025: Number of 'g' in "strawberry"?

Meta Llama 4: 1, Perplexity: 1

ChatGPT4o:0, Claude 3.7 Sonnet:0, Gemini 2.5:0

DeepSeek:0

Okay, let's see. The user is asking how many times the letter 'g' appears in the word "strawberry". Hmm, first I need to make sure I spell the word correctly. Strawberry is spelled S-T-R-A-W-B-E-R-R-Y. Let me write that out: S, T, R, A, W, B, E, R, R, Y. Wait, let me count the letters again to be sure. S (1), T (2), R (3), A (4), W (5), B (6), E (7), R (8), R (9), Y (10). So that's 10 letters. Now, I need to check each letter to see if it's a 'g'. Let's go through them one by one. The first letter is S – not a G. Second is T – nope. Third is R – still not. Fourth is A – no. Fifth is W – not a G. Sixth is B – B is different from G. Seventh is E – no. Eighth is R, ninth is another R, and the last letter is Y.

Wait, did I miss any letters? Let me check again. S-T-R-A-W-B-E-R-R-Y. No, there's no G in there. The letters are S, T, R, A, W, B, E, R, R, Y. None of those are G. So the count should be zero. But maybe the user made a typo? Like, maybe they meant another letter? Or perhaps they thought there's a G in strawberry? But no, the correct spelling doesn't include a G. So the answer is zero. I should make sure there's no alternative spelling with a G, but I don't think so. Strawberry is always spelled without a G. So yeah, the answer is 0.</think>
The letter "g" does not appear in the word "strawberry".

Count: 0.

Prompt: You are reviewing the response of an LLM. Please check if the response is correct and explain why.

Here is the question submitted to Llama4: how many 'g' in "strawberry"

Here is the response of Llama4:

There are 2 'r's but also 1 other thing you might be looking for: there are 2 'r's and 1 'g' and 2 'y's aren't in that count though, just 1 'g'. So 1 'g'

Perplexity Response:

Let's analyze the situation step by step:

The Question

"how many 'g' in 'strawberry'"

This is a straightforward question asking for the number of times the letter 'g' appears in the word "strawberry".

The Llama4 Response

There are 2 'r's but also 1 other thing you might be looking for: there are 2 'r's and 1 'g' and 2 'y's aren't in that count though, just 1 'g'. So 1 'g'

Evaluation of the Response

1. Accuracy

The word "strawberry" is spelled: s t r a w b e r r y

There is no 'g' in "strawberry".

2. Correctness

Llama4 claims: "just 1 'g'. So 1 'g'"

This is incorrect. There are zero 'g's in "strawberry".

Reasoning Limitations: ARC-AGI I, II and III Benchmarks

Test multi-modal reasoning capabilities

Public training set

Public evaluation set

Private evaluation set

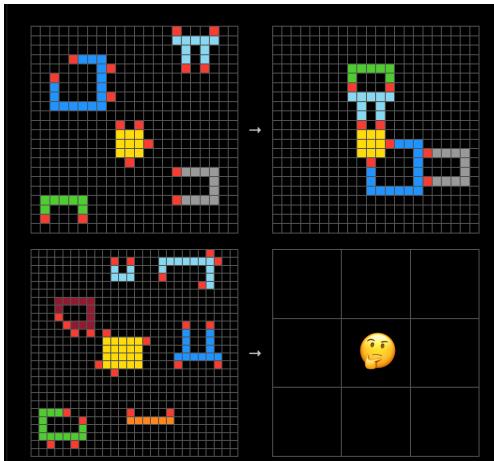
ARC AGI 1:

800 puzzle-like tasks, designed as grid-based visual reasoning problems

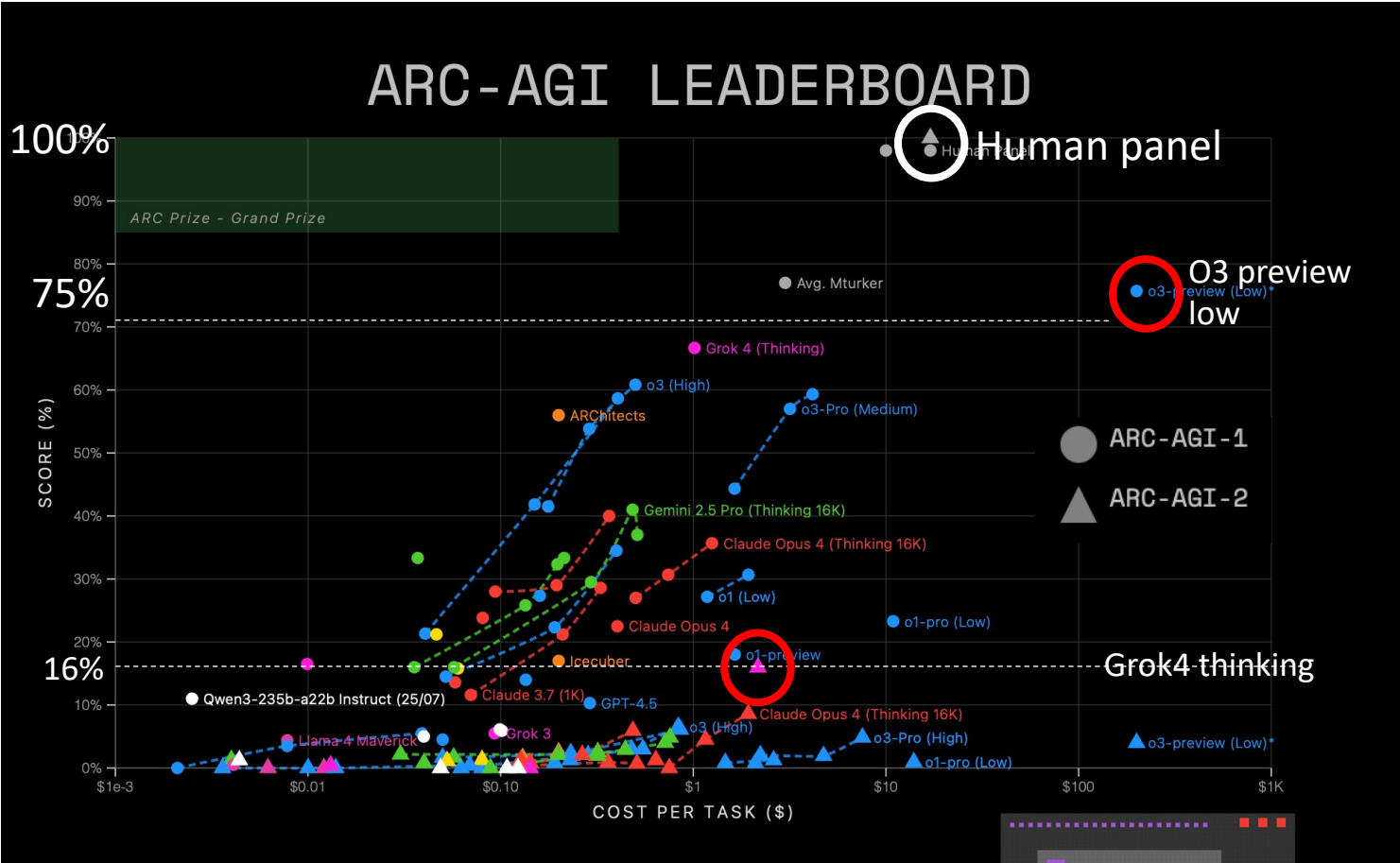
ARC AGI 2:

Example: Compositional Reasoning:

Tasks requiring simultaneous application of a rules, or application of multiples rules that interact with each other.



<https://arcprize.org/leaderboard>



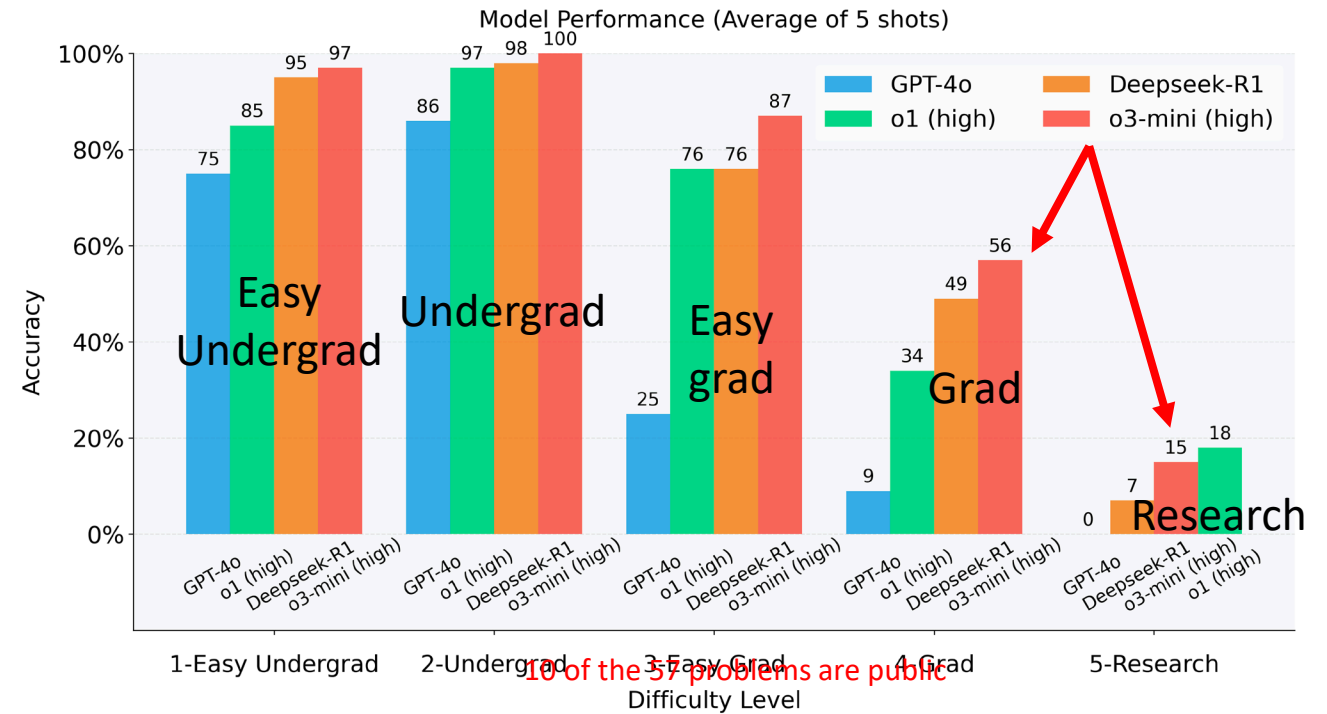
ARC AGI 3 (just previewed), much more difficult (agentic), requires to play game and win but must first discover the goal of the games and its rules



Open Response: TPBench "Theoretical Physics Benchmark - a Dataset and Study of AI Reasoning Capabilities in Theoretical Physics": arXiv:2502.15815v1 tpbench.org

(19 Feb 2025)

- **Evaluate LLMs on problems in theoretical physics** (high-energy theory and cosmology).
- **Test reasoning rather than recall.** Complex calculations, knowledge from different areas.
- **57 problems:** Not sourced from public collections
- **Difficulty 1 to 5:** easy undergrad to “research” level).
- **Problems:** Well-posed with unambiguous solutions, original, and
- **Final answers as algebraic expressions.**



- **Tested:** Open and closed-source models like GPT4o, o1, o3-mini, DeepSeek-R1, Llama, and Qwen.
- **Results:** o3-mini series solved about half the advanced graduate problems, most research-level problems remain unsolved --> limitation of current AI in advanced research tasks.
- **Failure Modes:** symbolic (algebraic) and logical mistakes. Struggle with self-correction and indicating uncertainty. Rely more on recall than reasoning from first principles. **Hallucinations** and asserting claims without proof were also observed.

We Start to Understand the Causes of Hallucinations

(4 Sept. 2025)

Why Language Models Hallucinate (OpenAI paper): <https://arxiv.org/pdf/2509.04664v1>

The distribution of language is learned from a corpus of examples, which contains errors and half-truths.

The paper shows that even for error-free training, **there are 2 main issues are at the origin of hallucinations:**

1) Training data are too sparse, the fact is too rare, or the distributions overlap (ambiguity)

To show that, Authors reduce the hallucination detection problem to a classification problem with questions of the form:

Is It Valid (IIV): Yes or No?

If you **can't solve IIV well** (because the), then hallucinations are **statistically unavoidable in normal open response setting.**



1) Let models abstain when uncertain

2) Redesign evaluations/leaderboards to reward calibration and penalize hallucination, instead of rewarding lucky guesses.

2) Even for error-free training, the objectives optimized during training would lead to errors generation.

- Models are primarily evaluated using exams that penalize uncertainty.
 - Example: in MCQ exams, guessing when unsure maximizes the expected score

→ The root problem is the abundance of evaluations that are not aligned (not rewarding uncertainty)

Model A is an aligned model that correctly signals uncertainty and never hallucinates.

Model B similar to A except that it never indicates uncertainty and always “guesses” when unsure. Model B will outperform A under 0-1 scoring, the basis of most current benchmarks.

→ This creates an “epidemic” of penalizing uncertainty and abstention

2 Main Challenges Before Broader Adoption of LLMs as Research Assistants

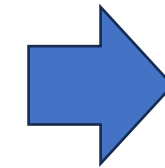
- LLMs/rLLMs/Agents are promising research assistants.
- But they are still making mistakes.
- That's a problem: Researchers need to understand the limits and trust their “instruments/tools”.

1) Researchers need a way to **evaluate/compare the capabilities of LLMs in research** for the different stages and tasks of the scientific research process **(which one is the best for what task?)**.

- Guide the applications of LLMs and the integration with tools,
- Provides benchmarks for developers to improve their LLMs

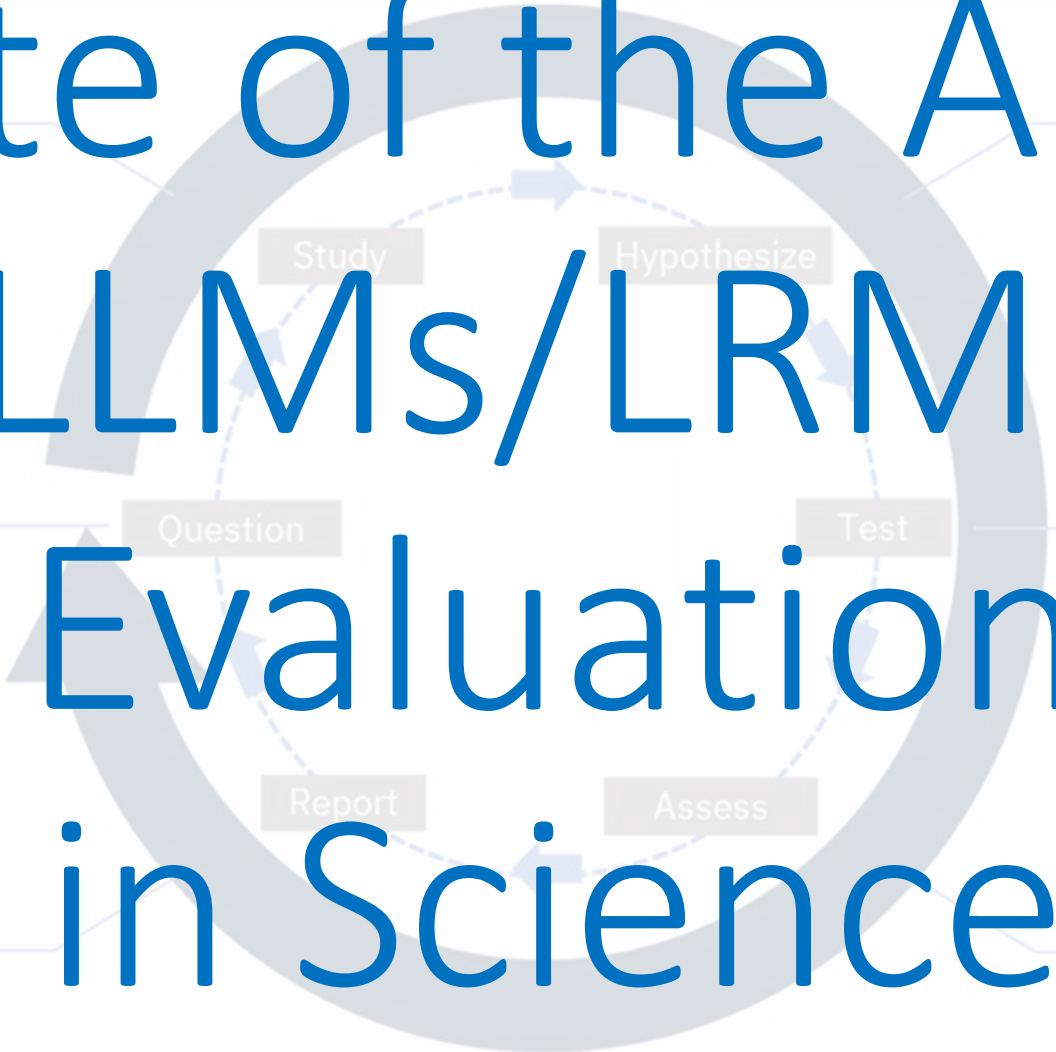
2) As with other research tools and techniques, **researchers will adopt LLMs only if they trust their results (Can I, Should I trust this response?)**.

- Need a way to assess the correctness of the produced results, in order to develop confidence in their use in scientific context.



A comprehensive,
Rigorous,
Accurate,
Transparent and
Community-approved
Evaluation methodology

State of the Art in LLMs/LRMs Evaluation in Science



```
graph TD; Study --> Hypothesize; Hypothesize --> Test; Test --> Assess; Assess --> Report; Report --> Question; Question --> Study;
```


Evaluation Methodology

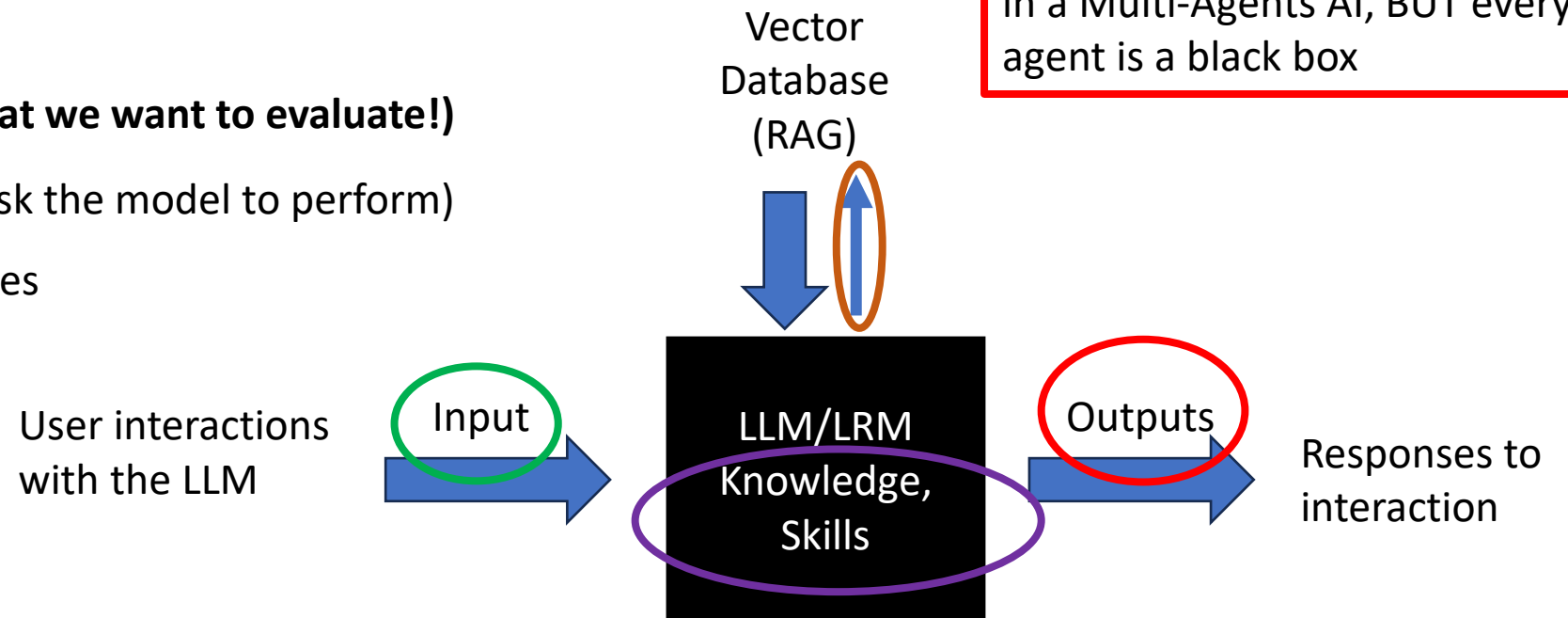
Goal of the evaluation: assess the knowledge and skills of LLMs/LRMs

LLMs/LRMs are so complex (number of layers, number of hidden dimensions, number of parameters, number of training tokens)

→ **The community consider them as black boxes.**

Note: We can monitor and analyze agents' interactions in a Multi-Agents AI, BUT every agent is a black box

- **Internal Skills and Knowledge (what we want to evaluate!)**
- Capture interactions (what users ask the model to perform)
- Assess Requests to external modules
- Assess Response



→ LLM/LRM Evaluation uses LLM/LRM dialogic interface

Benchmarks: MCQs and Open Responses

- **Multi-Choice Questions (MCQs)**

- 1 correct response and 3, 4 or more distractors (wrong responses)
- **Difficulty:**
 - Human/Automatic **generation is difficult**: distractors should not be easy to discard and not too close to the correct answer (risk of confusion)
 - **Evaluation is trivial**: just compare the model selection with correct response
- **Potential biases:**
 - E.g. Response ordering: → The model may choose the first answer more frequently

- **Open Responses:**

- 1 question. Model generates 1 response
- **Difficulty:**
 - **Generation is trivial**: generates a question relative to a domain
 - **Evaluation is difficult**: Requires a human evaluation of the response (→ LLM as judge)
→ Does not scale well (→ LLM as judge)
- **Potential biases:**
 - Room for interpretation: Humans may score differently the same open response → scoring requires several human evaluation (consensus)

Existing Scientific Domain Specific Benchmarks

Material Science Benchmarks:

- **MatSci-NLP:** Materials Science Language Tasks: e.g. Extract **summary-level information** from materials science text
- **MatSciBERT:** Text mining and information extraction: **Entity recognition**, relation **classification**, abstract classification

Chemistry Benchmarks:

- MolT5: Translation between text and SMILES
 - ChemNLP: Library for natural language processing in chemistry
 - MoleculeNet: Benchmark for molecular machine learning
 - ChemBench: Benchmark for chemical language models
- Focus on a small subset of tasks
 - High risk of contamination
 - → **We cannot rely only on existing benchmarks**

Biology Benchmarks:

- **BioGPT:** Biomedical NLP tasks, [Relation Extraction](#), [Question answering \(yes, no, or maybe\)](#), Classification,
- **BioT5:** Molecule & Protein Property [Prediction](#), Drug-target & Protein-protein [Interaction](#) Prediction, Molecule [Captioning](#)
- **ChemProt:** [Relation extraction](#)
- **BIOSSES:** Semantic sentence [similarity estimation](#) system. Semantic similarity and reasoning:
- **Nucleotide Transformer (NT) Benchmarks:** 18 curated downstream [prediction](#) tasks
- **GUE benchmark:** 7 genome sequence [classification](#) problems

Climate Benchmarks: ClimaText, ClimateStance, ClimateEng, ClimateFever

GPQA: A Graduate-Level Q&A Benchmark (multi-domain)

- Scalable oversight research: Questions near the frontier of human expertise. Experts reach 65% (only!!)
- Generated **manually 480 MCQs** (4 possible answers): Molecular Biology (85), Genetics (20), Quantum Mechanics (64), High-Energy Particle Physics (46), Physics (43), Astrophysics (42), Electromagnetism and Photonics (12), Relativistic Mechanics (11), Statistical Mechanics (4), Condensed Matter Physics (4)
- **OpenAI O1 obtained 78% accuracy on GPQA diamond***
 - Very close to human scholars on this benchmark: 81%
 - ! GPQA miss many domains (Climate, Computer Science, Biology, etc.)
- Me
 - Instructed question writers to write difficult questions in their domain of expertise that other experts in the domain will be able to answer correctly, but that non-experts cannot answer even with the internet

*Diamond: (1) 2 out of 2 expert validators agree, (2) ≤ 1 out of 3 non-expert validators answers correctly

MCQ examples:

Astrophysics

Astronomers are studying a star with a T_{eff} of approximately 6000 K. They are interested in spectroscopically determining the surface gravity of the star using spectral lines ($EW < 100 \text{ m\AA}$) of two chemical elements, El1 and El2. Given the atmospheric temperature of the star, El1 is mostly in the neutral phase, while El2 is mostly ionized. Which lines are the most sensitive to surface gravity for the astronomers to consider?

- A) El2 I (neutral)
- B) El1 II (singly ionized)
- C) El2 II (singly ionized)
- D) El1 I (neutral)

LLMs are so good, let's build extremely difficult tests

→ But what “difficult” means exactly?

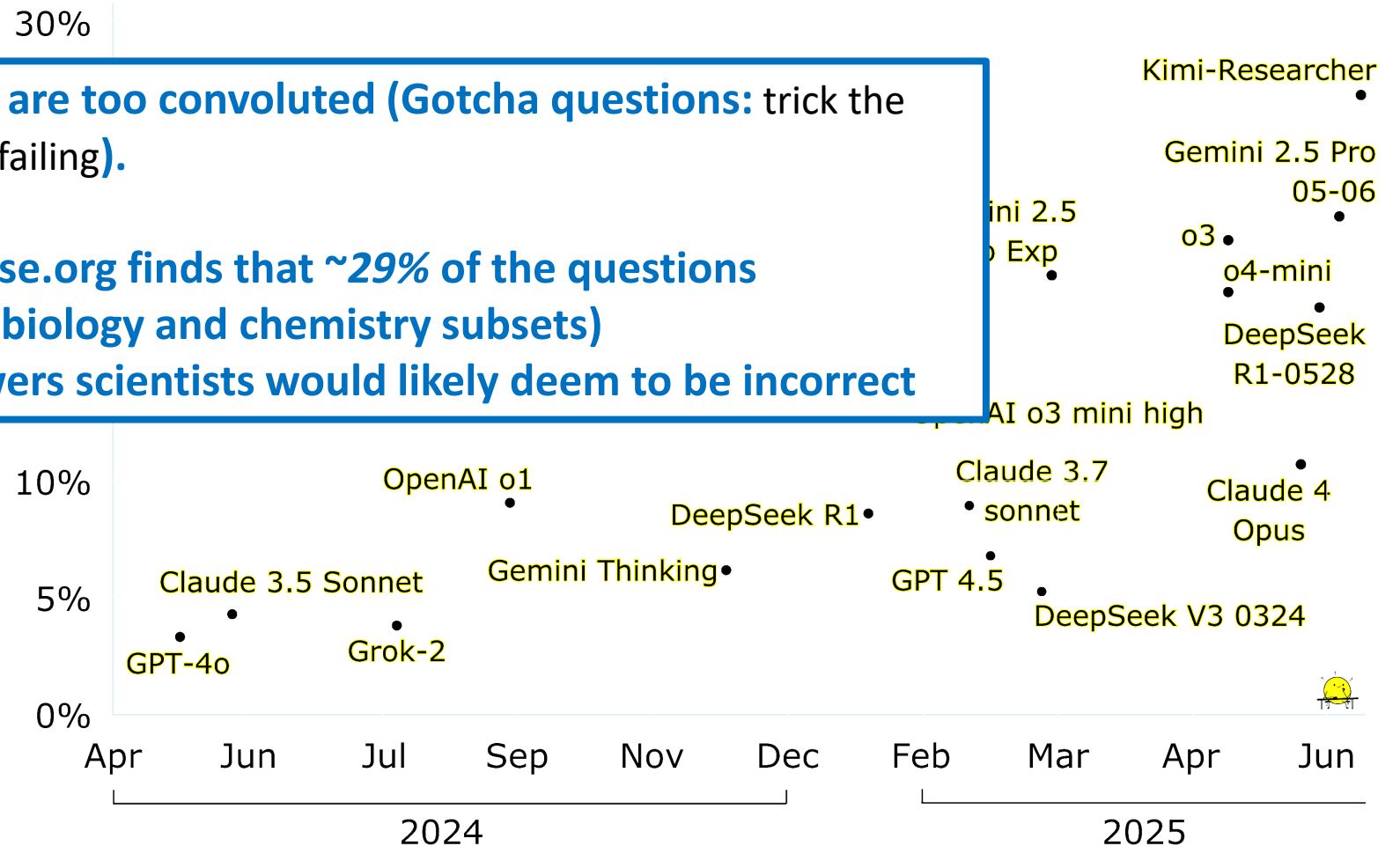
Humanity's Last Exam:

- Crowd sourcing,
- Multi-modal benchmark,
- Frontier of human knowledge
- Designed as final closed ended academic benchmark
- Broad subject coverage
- Criterion of question inclusion: Current frontier language models cannot answer the questions
- 2,500 challenging questions,
- Hundred subjects.
- Publicly release questions,
- Maintaining a private test set.

AI's scores on Humanity's Last Exam over time

Questions are too convoluted (Gotcha questions: trick the model into failing).

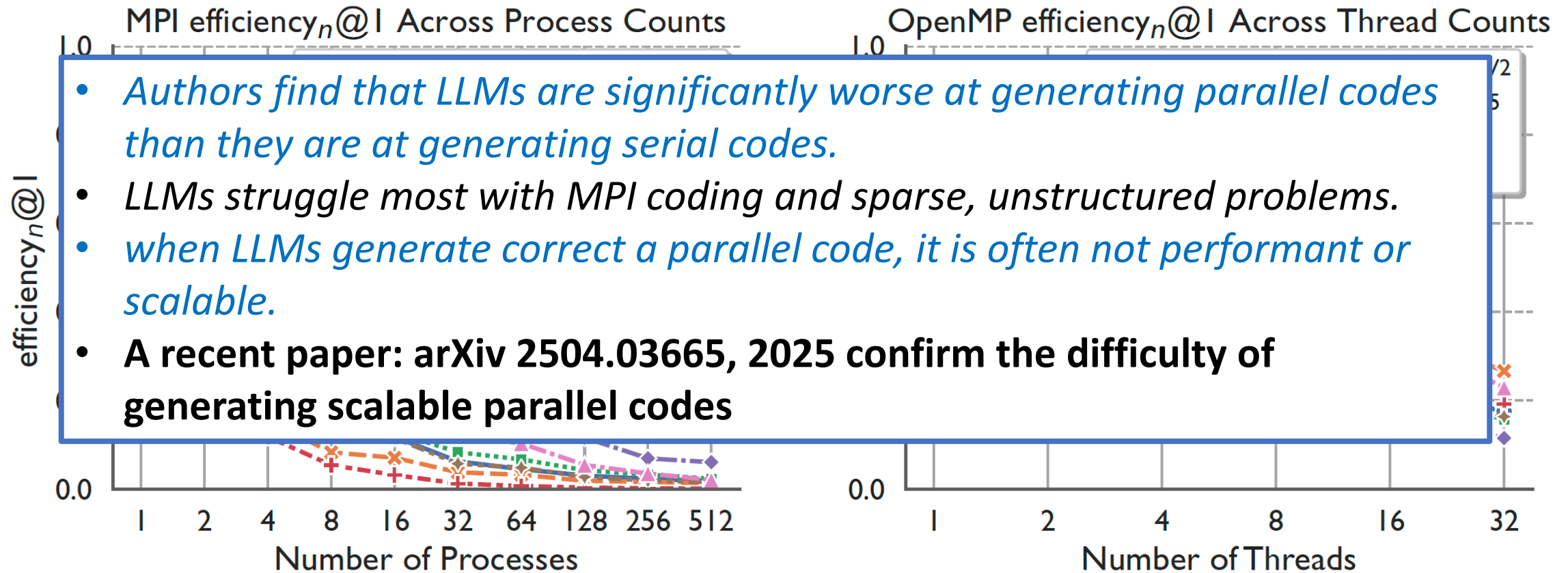
futurehouse.org finds that ~29% of the questions (text-only biology and chemistry subsets) have answers scientists would likely deem to be incorrect



ParEval: Can Large Language Models Write Parallel Code?

D. Nichols , J. H. Davis , Z. Xie , A. Rajaram , A. Bhatele, Can Large Language Models Write Parallel Code? ACM HPDC2024

- 420 different coding tasks (prompts) related to scientific and parallel computing.



- *Authors find that LLMs are significantly worse at generating parallel codes than they are at generating serial codes.*
- *LLMs struggle most with MPI coding and sparse, unstructured problems.*
- *when LLMs generate correct a parallel code, it is often not performant or scalable.*
- **A recent paper: arXiv 2504.03665, 2025 confirm the difficulty of generating scalable parallel codes**

challenging for LLMs?

- How performant and scalable is the parallel code generated by LLMs?
- How well can LLMs translate between execution models?

Transform

Fourier transforms.

Map a constant function to each element of an array.

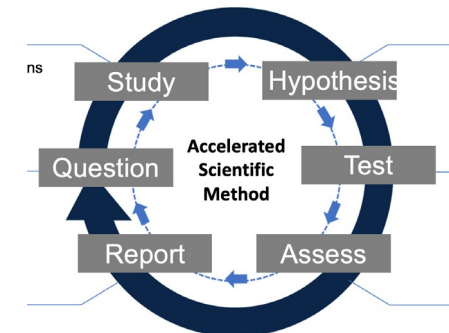
github.com/parallelcodefoundry/ParEval

Gap Analysis

- **MCQ Benchmarks** are great to assess model knowledge extension
- **Open response benchmarks** can test reasoning capabilities
- However:
 - Existing ones are too generic (multi-domain, not specific to a research problem)
 - Static benchmarks saturate quickly (most of all benchmarks are static)
- MCQ and Open response benchmarks **cannot be used for end-to-end Evaluation**

→ We cannot only rely on benchmarking

- **Missing evaluation technique in real context:**
 - Benchmarks do not reflect the actual complexity, diversity, level of details of real-world interactions between researchers and LLMs/rLLMs
 - **We need new techniques**



Establishing a Methodology to Evaluate LLMs/LRMs as Research Assistants [AuroraGPT]

<https://arxiv.org/pdf/2502.20309>

¹ Mathematics and Computer Science Division, Argonne National Laboratory

² Data Science and Learning Division, Argonne National Laboratory

³ Computational Sciences Division, Argonne National Laboratory

⁴ Department of Computer Science, The University of Chicago

⁵ University of Illinois Urbana-Champaign

⁶ University of Pennsylvania

⁷ Lawrence Livermore National Laboratory

⁸ The Ohio State University

⁹ Rochester Institute of Technology

¹⁰ Massachusetts Institute of Technology

AuroraGPT*:

- **General purpose scientific LLM** – broadly trained – general corpora plus scientific papers and texts and structure science data
- **SAFE:** Trustworthiness, Safety, Security, Robustness, Privacy, Machine Ethics
- **Explore pathways** towards a “Scientific Assistant” model
- **Build with international partners** (RIKEN, BSC, others)
- **Multilingual** – English, 日本語, Français, Deutsche, Español, Italiana
- **Multimodal** – images, tables, equations, proofs, time-series, graphs, fields, sequences, etc.

*named after the Leadership Class Supercomputer at Argonne that will be used for much of the training

Aurora is:
166 Racks
10,624 Nodes
21,248 CPUs
63,744 GPUs
84,992 NICs
8 PB HBM
10 PB DDR5c



Groups:

- 01 Planning
- 02 Data
- 03 Model training (pre-training)
- **04 Evaluation (skills, trustworthiness, safety)**
- 05 Post-training (fine tuning, alignment)
- 06 Inference (on Aurora)
- 07 Distribution
- 08 Communication

Evaluation Methodology: What to measure

What to measure:

- **Knowledge Extraction, Retrieval, Distillation, Synthesis** : LLM is provided with a question and a truthful answer is expected
- **Text grounded**: Answer is expected fully grounded on peer reviewed references to support response.
- **Reasoning**: LLM is expected to solve deductive (Prove a theory or hypothesis from formal logic and observations), inductive (validate/explain observations from theories) problems
- **Creativity (hypothesis generation)**: A creative answer is expected from a question or instruction: e.g. find a solution to open scientific questions.
- Thoughtful dialogue, Coding, etc. → **Agentic aspects**
- **safety**, usability, robustness (adversarial attacks), cost/energy (training, inference)

Criteria for all of the above:

- **Correctness** (of facts, results),
- **Accuracy** of solutions AND reasoning,
- **Reliability** (consistently good in quality or performance),
- **Speed** (how fast to produce a response), O1-pro can take minutes to respond to a single prompt
- **Consistency** (slight prompt variations should not generate significantly different responses),
- **#shots** (how many examples are needed for good quality),
- **Extent of Prompt Engineering**.

Challenges:

- AI model capabilities (knowledge, reasoning, correctness) are increasing at extreme pace
- Evaluation should be done in enclaves (AI models should not be trained on the tests)
- Generation and validation of large corpus of difficult enough tests

EAIRA: Multi-faceted Eval Methodology

Benchmarks

End-to-End

Proposed Methodology				
Techniques	MCQ Benchmarks	Open Response Benchmarks	Lab Style Experiments	In the Wild Field Style Experiments
Main Goal	Testing knowledge breadth, basic reasoning	Testing knowledge depth, planning, reasoning	Realistic testing	Realistic trend analysis and weakness diagnosis
Problem Type	Predetermined , Fixed Q&As with known solutions	Predetermined , Fixed Free-Response Problems with known solutions	Individual Human Defined Problems with unknown solutions	Many Human Defined Problems with (un)known solutions
Verification	Automatic response verification	Automatic or Human response verification	Humans detailed response analysis	Scalable automatic summary of human response
Examples	Astro, Climate, AI4S (multi-domain), Existing Benchmarks	SciCode, ALDbench	see "lab style experiments"	see "field style experiments"
Cross Cutting Aspects	← Trust and Safety (ChemRisk), Uncertainty Quantification, Scalable Software Infrastructure (STAR) →			

Methodology consisting of 4 complementary evaluation techniques to comprehensively assess the capabilities of LLMs as scientific assistants:

- purple text shows prior contributions by the researchers participating in AuroraGPT
- blue text shows AuroraGPT contributions.
- Black text aspects adapted from existing work are included for a complete approach.

<https://arxiv.org/abs/2502.20309>

Argonne
NATIONAL LABORATORY

ASTRO MCQ Benchmark

- **4425 Automatically generated MCQs**
- From 885 articles in [Annual Review of Astronomy and Astrophysics 1963 to 2023](#)

Lessons learned:

- Manual validation shows that automatically generated MCQs are of high-quality
- Models may have been trained on the papers → we need a dynamic approach
- **MCQ Manual validation is the bottleneck! not automatic generation**

Sample question from Astronomy benchmark dataset

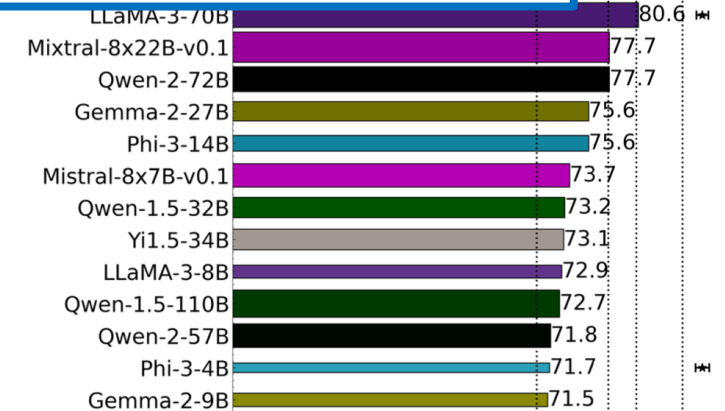
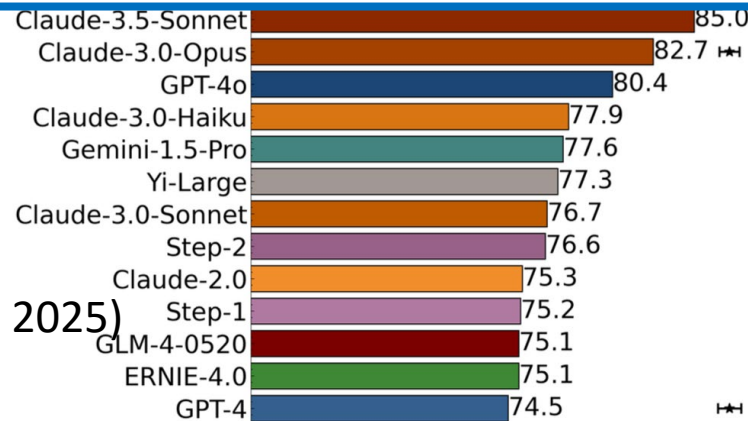
How does the presence of stellar companions influence the formation and detection of exoplanets?

(A) Stellar companions can dilute transit signals, potentially leading to misclassification of planets and inaccurate parameter estimations. Additionally, their gravitational influence can suppress planet formation in close binary systems.

(B) Stellar companions provide additional sources of formation, increasing the enrichment of exoplanets, leading to a higher frequency of super-Earths at greater distances.

Some take aways:

- Claude 3.5 Sonnet best (no O1 test)
- Llama-3-70B on par with GPT4o
- Published in July 2024 on arXiv (journal: 2025)
- **Benchmark almost/probably saturated**

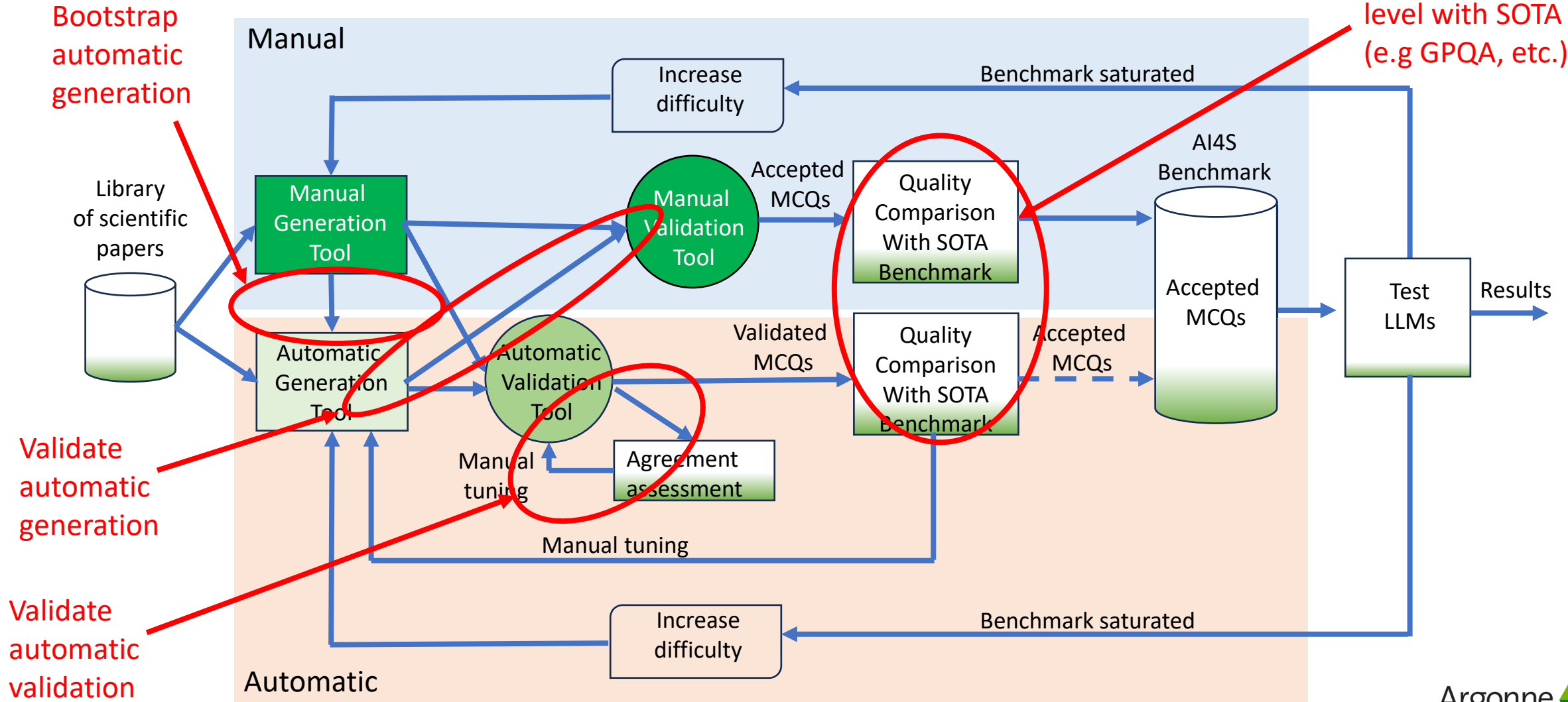


Automatic High-quality Benchmark Generation/Validation

Many scientists have the same need: generate specific MCQ benchmarks for their problems

→ We need an integrated framework to generate/validate MCQs Benchmarks

Automatically
compare difficulty
level with SOTA
(e.g GPQA, etc.)



SciCode Open Response Benchmark (integrated into the methodology)

Scientist-curated code generation benchmark (mathematics, physics, chemistry, biology, materials science)

80 main problems (numerical methods, simulation of systems),

Lessons learned:

- OpenAI 01-preview can only solve 7.7% of main problems (right level of difficulty).
- Difficulty comes from the necessity to combine multiple skills: problem understanding, retrieval, reasoning, planning, code generation.
- Using codes as the results of the questions makes verification “trivial” **but it is not applicable to all open question problems: e.g. bio.**

SciCode provides gold-standard solutions and multiple test cases for reliable automatic evaluation.

Problems are very challenging: inspired by Nobel prize level problems.

Question: Write a Haldane model Hamiltonian on a hexagonal lattice.

Docstrings

```
def calc_hamiltonian(kx, ky, a, t1, t2, phi, m):  
    """  
    Function to generate the Haldane Hamiltonian.  
  
    Args:  
    kx (float): The x component of the wavevector.  
    [MORE ARGUMENTS]  
  
    Returns:  
    hamiltonian (ndarray): matrix of shape(2, 2).  
    """
```

```
def compute_chern_number_grid(delta, a, t1, t2, N):  
    """
```

Function to calculate the Chern numbers.

```
    Args:  
    delta (float): The grid size in kx and ky axis for discretizing the  
    Brillouin zone.  
    [MORE ARGUMENTS]  
  
    Returns:  
    results (ndarray): 2D array of shape(N, N), The Chern numbers.  
    [MORE RETURN VALUES]  
    """
```

Minyang Tian, SciCode: A Research Coding Benchmark Curated by Scientists, arXiv:

[arXiv:2407.13168](https://arxiv.org/abs/2407.13168)

Understanding/modeling question difficulty

ANL-HPE Collaboration: DoReMi: Difficulty-Oriented Reasoning Effort Modelling of Science Problems for Reasoning Language Models

- Current benchmarks fail to rigorously define “difficulty”. They also fold diverse challenges into single accuracy scores.
→ How do we know if a benchmark question is difficult? (written by a Ph.D., written by a Field medalist?)
- It remains unclear what level of reasoning effort is required so solve benchmark problems.
→ Need principled ways to 1) measure difficulty for curriculum learning, 2) benchmark creation, and 3) reasoning effort estimation.

DoReMi

- Compute **Multi-dimensional Difficulty Fingerprints** for a benchmark using **Bloom Taxonomy metrics** across 7 dimensions
- **Use LLM as a judge** approach to evaluate questions on the Bloom dimensions
- **Use Multiple LLM Judges** and check consensus.

DoReMi: Paper submitted to an AI conference



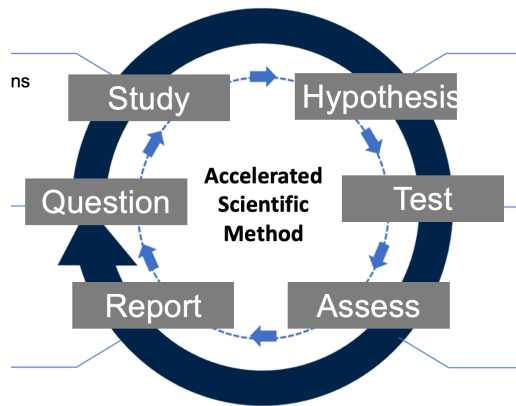
- **Study correlations** between LLM judges difficulty assessments and some metrics of LLM perceived difficulty to respond to a question.
→ Link difficulty to cost (time, tokens, etc.)
- Consider multiple metrics:
 - Wrong Answer Fraction (WAF)
 - Minimum Reasoning Token (MRT)
 - Expected Runs to First Correct Answer (R2FCA)
 - Uncertainty of Correct Answers (UCA)
 - Reasoning Inconsistency (RI):
 - Etc.

End-to-End Evaluations: Lab Style & Field Style Experiments:

Using LLMs as scientific research assistants to solve/progress on real real problems

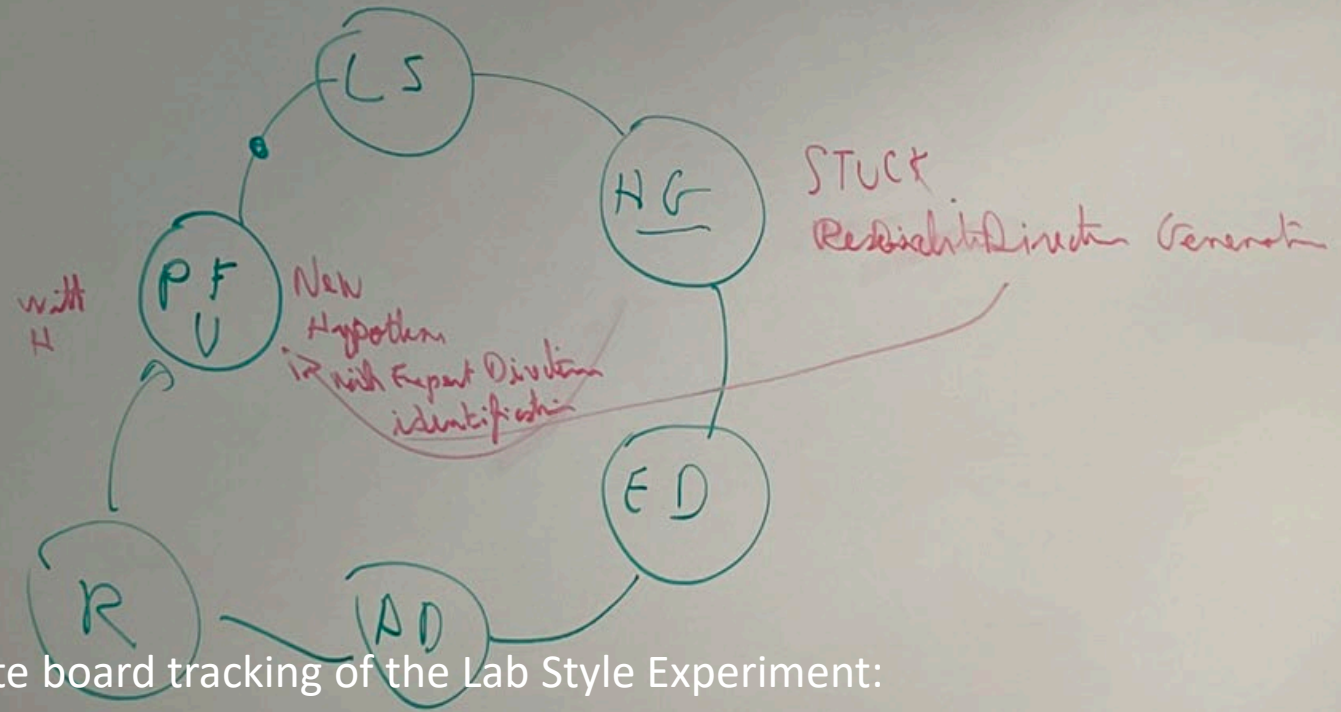
Over all steps of the research process:

Ideal View of Research Process



Reality

Exploring a quantum entanglement problem with Argo/O1-preview



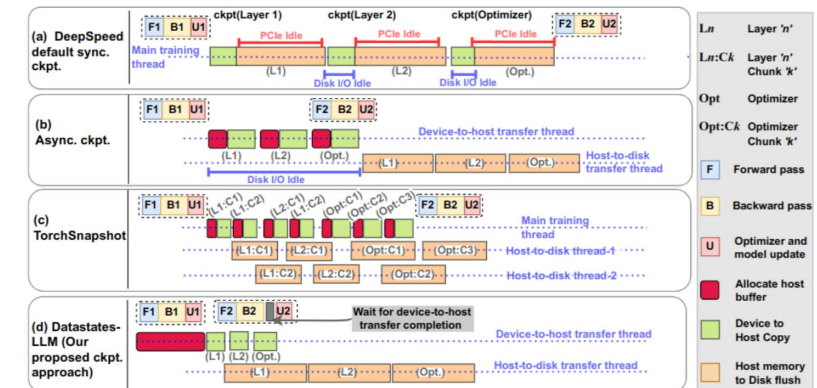
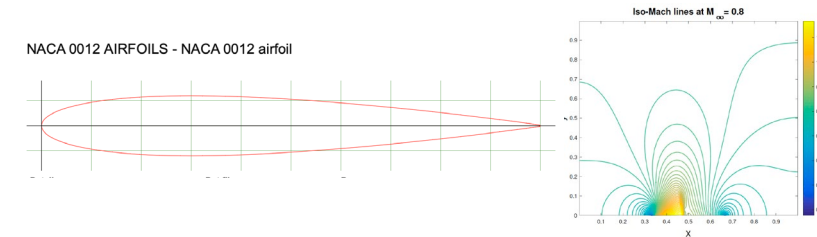
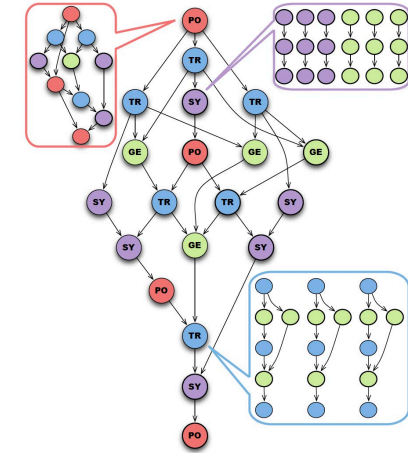
White board tracking of the Lab Style Experiment:

Green: Idealized research workflow. O1 clearly understood the problem formulation. GPT4o identified relevant literature, not known by the researcher.

Red: O1 was stuck in potential direction generation. Argonne researcher proposes a potential direction

Lab-Style Experiments

- Compare multiple LLMs to progress toward solving an unpublished problem
- 1 scientist – 1 AI expert helping to craft the prompts
- Record all the interactions between the scientist and the model + scientist assessment of the model response
- Ran 5 experiments to observe the “distance” between an ideal assistant and Existing LLMs (Large Language Models)
- Experiments related to:
 - DAG Scheduling
 - PDE Solving
 - 0 overhead checkpointing for LLMs training (HPDC24 Best Paper)
 - Quantum entanglement
 - **Life at temperature beyond known limits: e.g. 150°C**
- Experiments >25 hours (~6h per experiment), >125 prompts
- Tested Models: O1, Argo/O1, ChatGPT4o, GPT3.5, Gemini 2, Gemini 1.5, Claude3 Sonnet/Haiku, Mistral, Llama3 (70b, 405B), Perplexity Pro, (not all models were tested on all prompts)



2024: PDE Solving 1: Transonic Flow

Collaboration with **David Keyes, KAUST**

Context: Our goal is to solve a 1-dimensional nonlinear second-order boundary value problem for $\phi(x)$.

$\phi(x)$ is a velocity potential, the velocity u is the x -derivative of $\phi(x)$, denoted $u(x)=\phi_x(x)$.

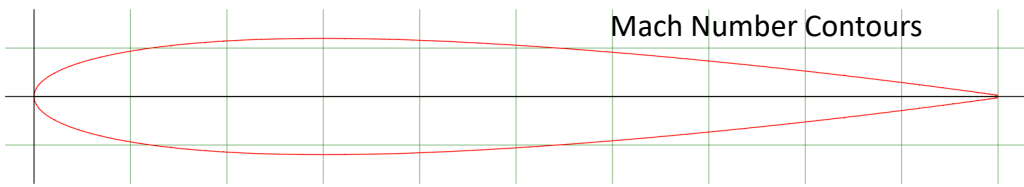
We define two auxiliary functions, $A(x) = 0.4 + 0.6 (x-1)^2$, the cross-section of a windtunnel, and the local density, $\rho(u)=(1+(\gamma-1)(1-u^2)/2)^{1/(\gamma-1)}$.

The equation is $(A(x)\rho(u)\phi_x)_x=0$ with left boundary condition $\phi(0)=0$ and right boundary condition $\phi(2)=\phi_R$. $\phi_R=1.15$, $\gamma=1.4$

- Asked 9 different prompts covering:**
- Problem attack:** How you would solve this problem, describe important steps?
 - Approach to avoid oscillation:** solution steering did not work: “what method should one use to avoid oscillations”.
 - Solution steering:** asked specifically to use upwinding approach (none of the model proposed this independently)
 - Code generation instructing upwinding* (Llama 3 and GPT4o only):** Generate code using upwind differencing for ϕ .

Transonic flow passing over an airfoil

NACA 0012 AIRFOILS - NACA 0012 airfoil



The given equation is:

$$(A(x)\rho(u)\phi_x)_x = 0$$

with boundary conditions:

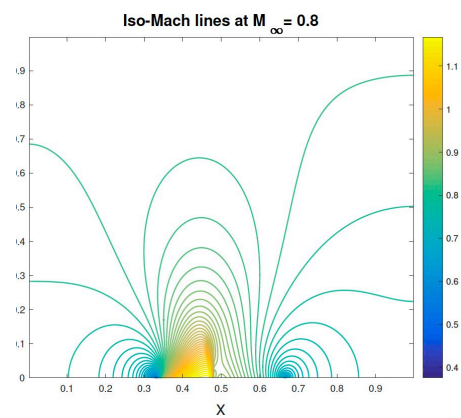
$$\phi(0) = 0 \quad \text{and} \quad \phi(2) = \phi_R = 1.15$$

where:

$$u(x) = \phi_x(x)$$
$$A(x) = 0.4 + 0.6(x - 1)^2$$
$$\rho(u) = \left(1 + \frac{\gamma - 1}{2}(1 - u^2)\right)^{\frac{1}{\gamma - 1}}$$

and $\gamma = 1.4$.

Courtesy of David Keyes



L. Liu, F.-N. Hwang, L. Luo, X.-C. Cai, D. E. Keyes, A Nonlinear Elimination Preconditioned Inexact Newton Algorithm, SIAM Journal on Scientific Computing, Vol. 44, Iss. 3 (2022)10.1137/21M1416138

PDE Solving	Claude 3	Llama 3	GPT3.5	GPT4o
Problem Attack	C	C	F	D
Solution Steering	D	B		D
Oscillation avoidance	C	A	E	D
Code Generation		C		E

Lab-Style Experiment: Biology

Our objectives are to:

1) Identify currently **known limits of biological activity** based on temperature (known examples of viable organisms and the associated upper-temperature limit)

2) Identify systems that operate at high temperatures and still function
3) Make predictions about how **changing chemistry** could alter the process

Lessons learned:

- Best technique to evaluate the actual value of LLM capabilities for science
- Models can propose surprising, intriguing, “plausible” innovative research directions:
[O1 DeepResearch]: proposes creation of **hybrid life form with inorganic shell and organic engine** - can be stable at conditions that would destroy lipid membranes.
→ **Need a chemist + a biologist to evaluate pertinence**
- Lab-style experiments are not scalable and need to be redone as AI models progress

pair systems that molecular process is
be altered by
non-biological
still viable.
would impact

Q1: Identify
Q2: Identify
Q3: Generate
currently
→ O1 pro

Life beyond limits	OpenAI O1	Argo O1-preview	Perplexity-Pro-R1
Problem Understanding	Q1: 3, Q2: 4	Q1: 4, Q2: 4	Q1: 5, Q2
Literature Review	Q1: 4, Q2: 4	Q1: 3, Q2: 3	Q1: 4, Q2:
Hypothesis Generation	Q3: 3, Q4: 3, Q5: 3, Q6: 4, Q7: 3	Q3: 3, Q4, 3, Q5: 3, Q6: 3, Q7: 3,	Q3: 4, Q4: 4, Q5: 3, Q6: 2, Q7: 2

End-to-End Eval: Field Style Experiment

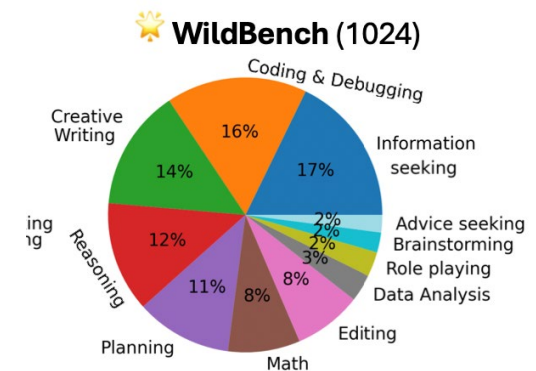


Lab style experiments: Human evaluation, tries to solve 1 specific problem, compare different models, guide LLMs (requires efforts: some prompt engineering),

Field style experiments: Automatic evaluation, capture what researchers actually ask, much broader diversity of Q&As, large diversity of prompt engineering, statistical evaluation

Several papers on this topic (but not for Science activity)

- **WildBench**: Benchmarking LLMs with Challenging Tasks from Real Users in the Wild, B. Y. Lin and Y. Deng and K. Chandu and F. Brahman and A. Ravichander and V. Pyatkin and N. Dziri and R. Le Bras and Y. Choi, 2024, arXiv 2406.04770
- **HaluEval-Wild**: Evaluating Hallucinations of Language Models in the Wild, Zhiying Zhu and Yiming Yang and Zhiqing Sun, 2024, arXiv, 2403.04307
- **"Do Anything Now"**: Characterizing and Evaluating In-The-Wild Jailbreak Prompts on Large Language Models Xinyue Shen and Zeyuan Chen and Michael Backes and Yun Shen and Yang Zhang, 2024, arXiv 2308.03825



End-to-End Eval: ~~1000~~ 1500 Scientists AI JAM in 9 Labs Simultaneously (Feb.28, 2025)



Researcher participation and contributions on a voluntary basis.

1,000 Scientists Jam Session: In numbers

Researcher participation and contributions on a voluntary basis.



Total:

2800+ problems

**15000+ assessed prompt
responses**

Argonne:

720 problems

2500 prompts



1,000 Scientists Jam Session: Domains

Researcher participation and contributions on a voluntary basis.



Literature/Data

- Literature search, analysis, survey
- Data analysis and forecast, interpolation, extrapolation, **classification** (Point Cloud, signal, protein sequences, files, etc.)
- Anomaly detection
- Signal Analysis
- Scientific Visualization

Coding

- Algorithm design/optimization
- Automatic **code generation**/refactoring
- Code **translation**
- **Debugging codes** (sequential, parallel)
- Automatic code performance tuning/optimization
- **Identifying performance bottlenecks**

Experiments

- Automatic tuning of instruments
- **Experimental Design** (including autonomous workflow)
- Dark mater experiment design

Bio

- **Understanding mechanisms of Cancer**
- Understanding radiation effects on human cells
- Predictive Genomic Models

AI

- **Domain specific LLMs/Agents** (use LLMs as foundation models)
- Hyper parameter exploration for DL training.

Physics

- Battery design
- Chemical Mechanisms
- **Physics beyond standard model**

Infra.

- **Infrastructure modeling** and resilience
- Natural Disaster assessment

Math

- Surrogate model
- **Mathematical derivations**
- PDE solving
- **Convergence proving**
- Equation validity testing
- Derivative analysis
- Uncertainty estimation
- **Inverse problems**
- Statistical modeling

1,000 Scientists Jam Session: Problem Types



Researcher participation and contributions on a voluntary basis.

- Literature search, analysis, survey

- Battery design
- Chemical Mechanisms
- Physics beyond standard model
- Understanding mechanisms of Cancer
- Understanding radiation effects on human cells
- Predictive Genomic Models

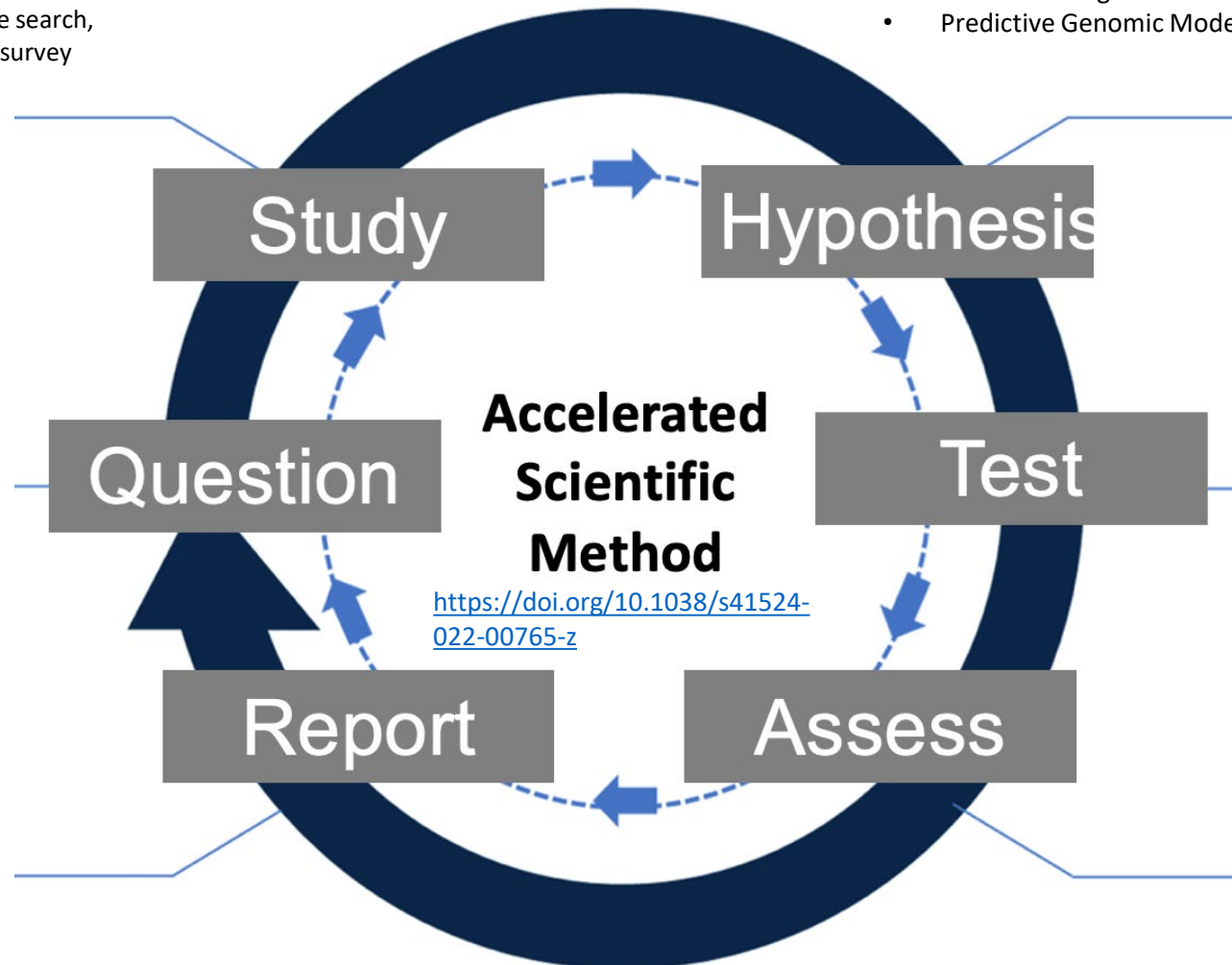
- Algorithm design/optimization
- Automatic code generation/refactoring
- Code translation
- Debugging codes (sequential, parallel)
- Automatic code performance tuning/optimization
- Identifying performance bottlenecks

- Surrogate model
- Mathematical derivations
- PDE solving
- Convergence proving
- Equation validity testing
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- Uncertainty estimation
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- Domain specific LLMs/Agents (use LLMs as foundation models)
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- Dark mater experiment design

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- Signal Analysis
- Scientific Visualization
- Natural Disaster assessment
- Infrastructure modeling and resilience

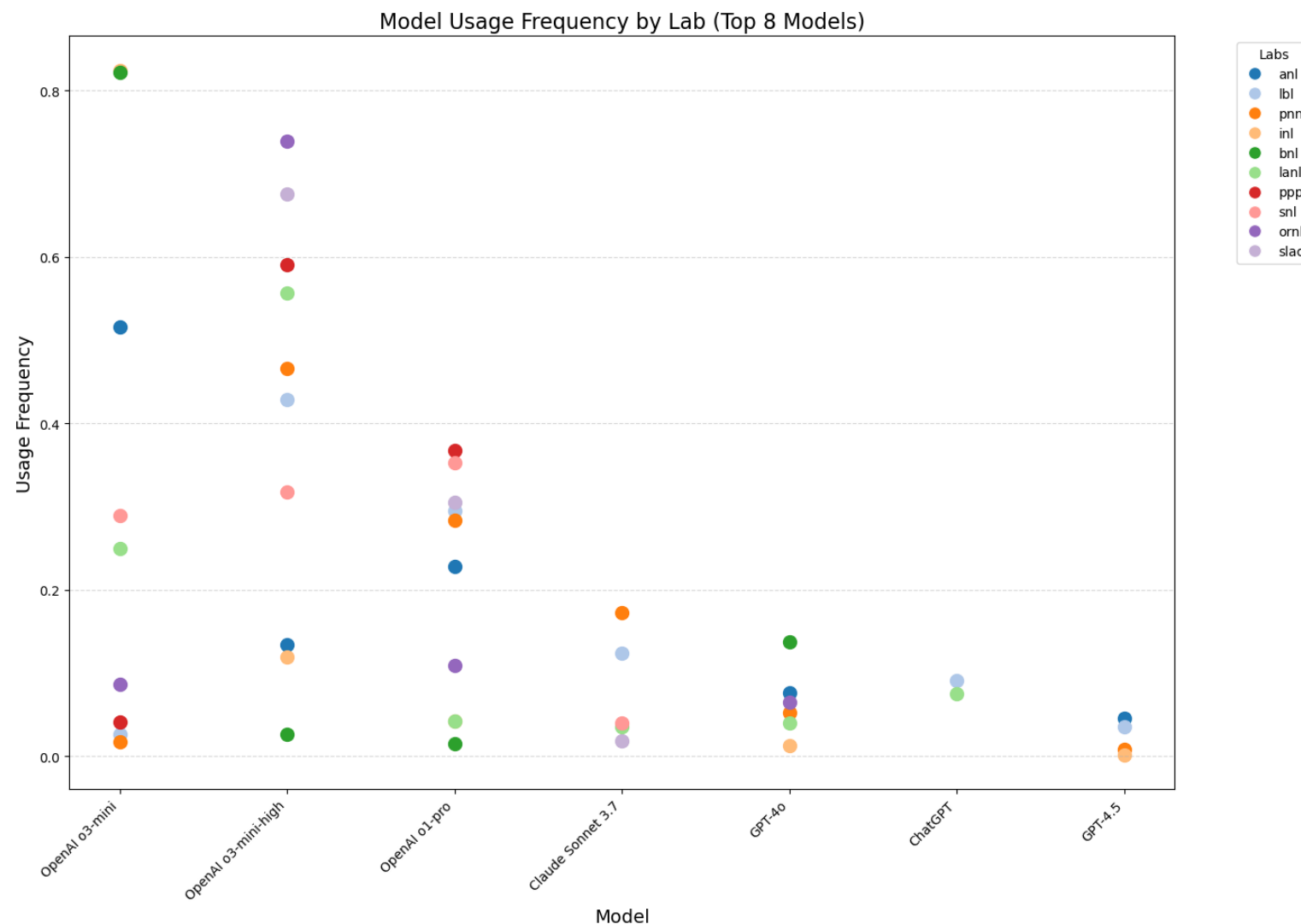
- ???



1,000 Scientists Jam Session: Model usage

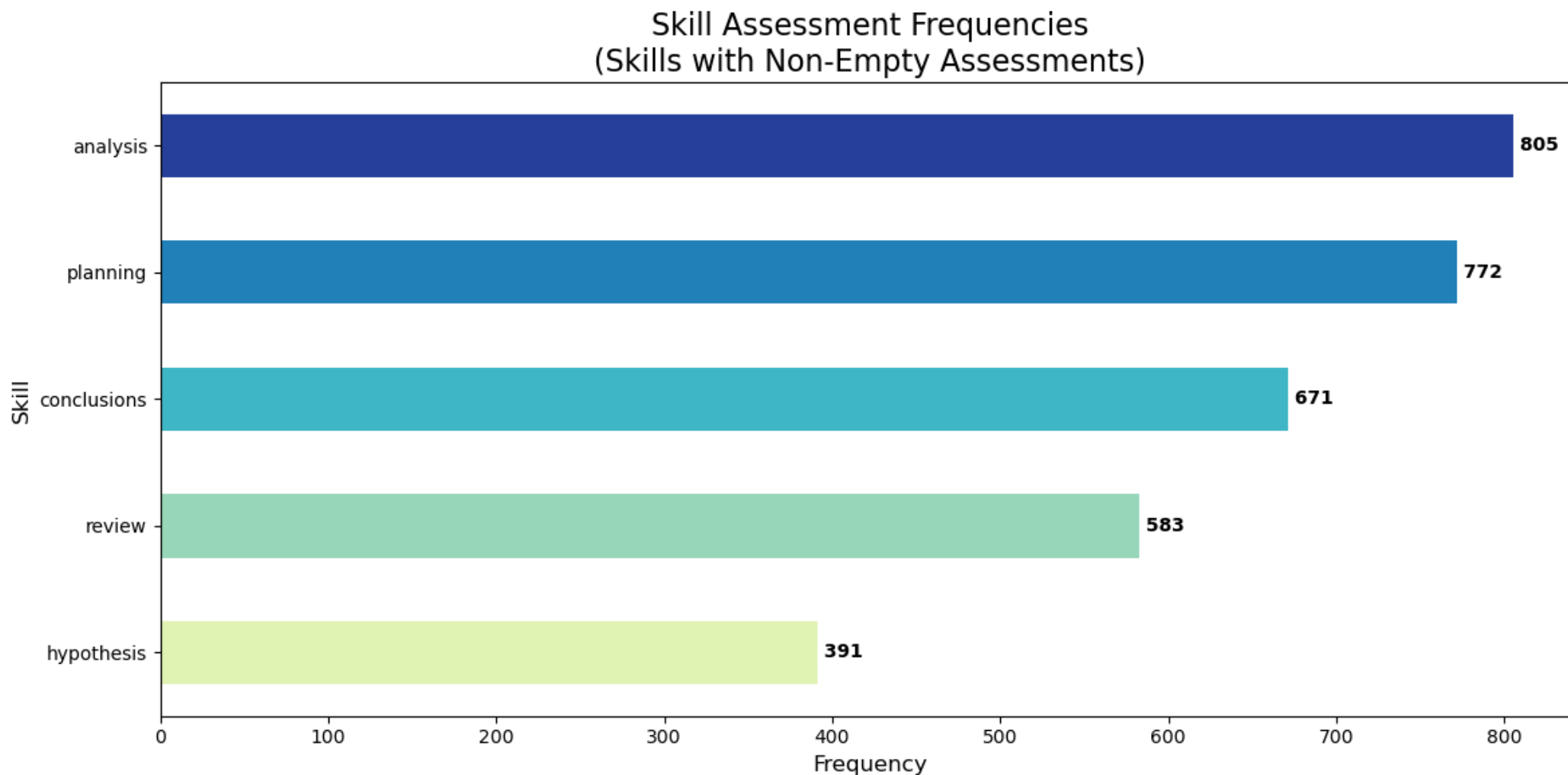
Researcher participation and contributions on a voluntary basis.

Model	Count
OpenAI o3-mini	2139
OpenAI o3-mini-high	1390
OpenAI o1-pro	1189
Unclear	380
Claude Sonnet 3.7	255
GPT-4o	253
GPT-4.5	145
ChatGPT	126
GPT-4	122
Claude Sonnet 3.7 Thinking	96
OpenAI DeepResearch	70
OpenAI o1-mini-high	51
Deep Research	47
OpenAI o1	30
Claude 3.5	19
Other	8
Free Version	6
Google Flash Thinking	2



1,000 Scientists Jam Session: Skill tested (selected by user)

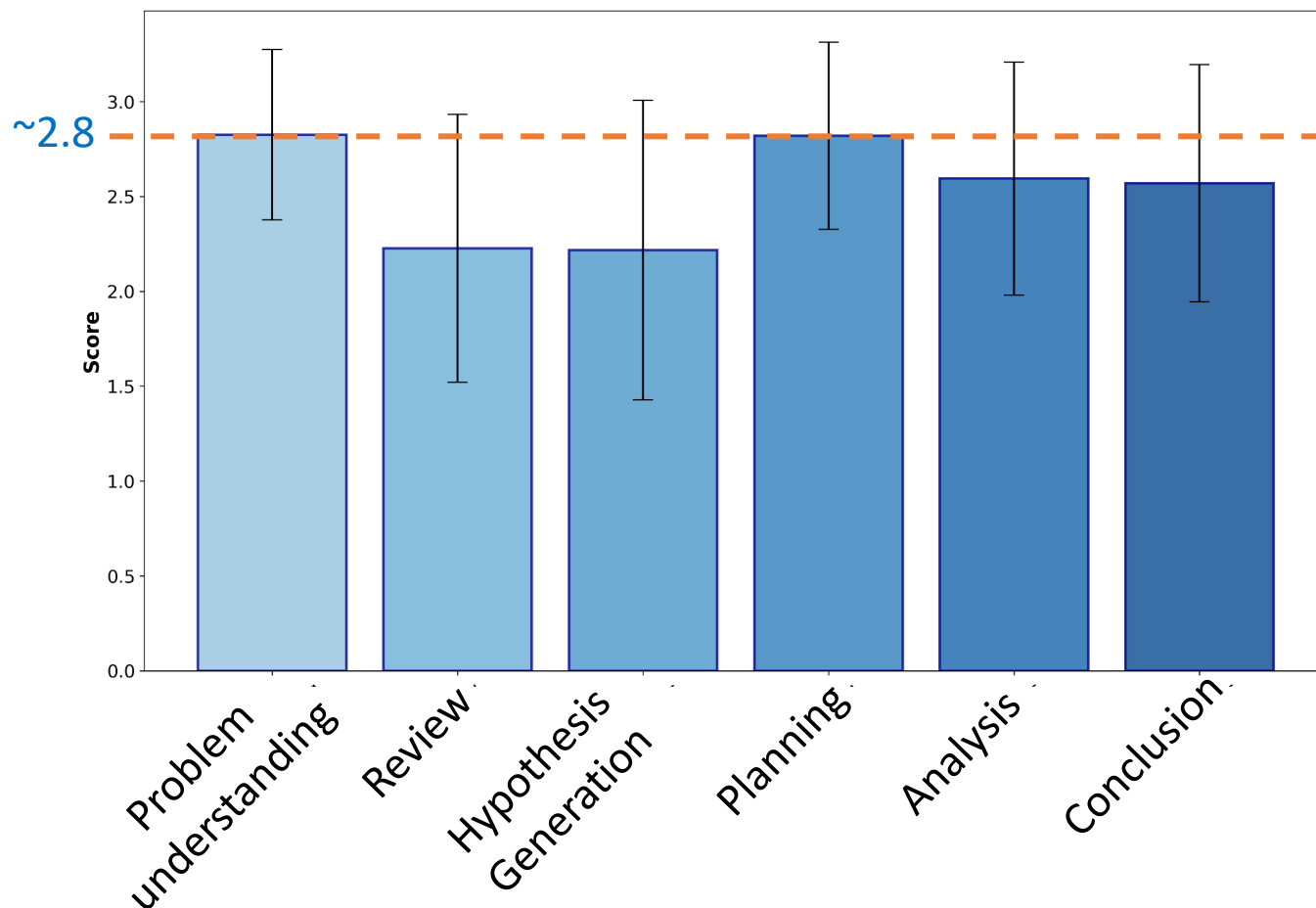
Researcher participation and contributions on a voluntary basis.



1,000 Scientists Jam Session: skills strength (average over the whole corpus)

LLM as a judge to automatically score (1-5) the LLMs responses

Overall Skill Statistics (All Samples)
(Error bars show standard deviation)



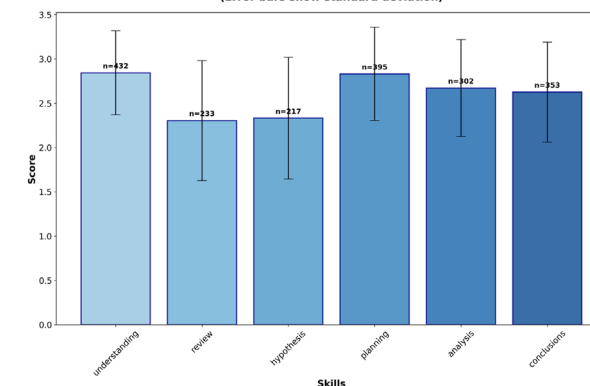
Different blue colors represent different skills



Result robust
against change
the judge model
(gpt 4o -> gpt o1)



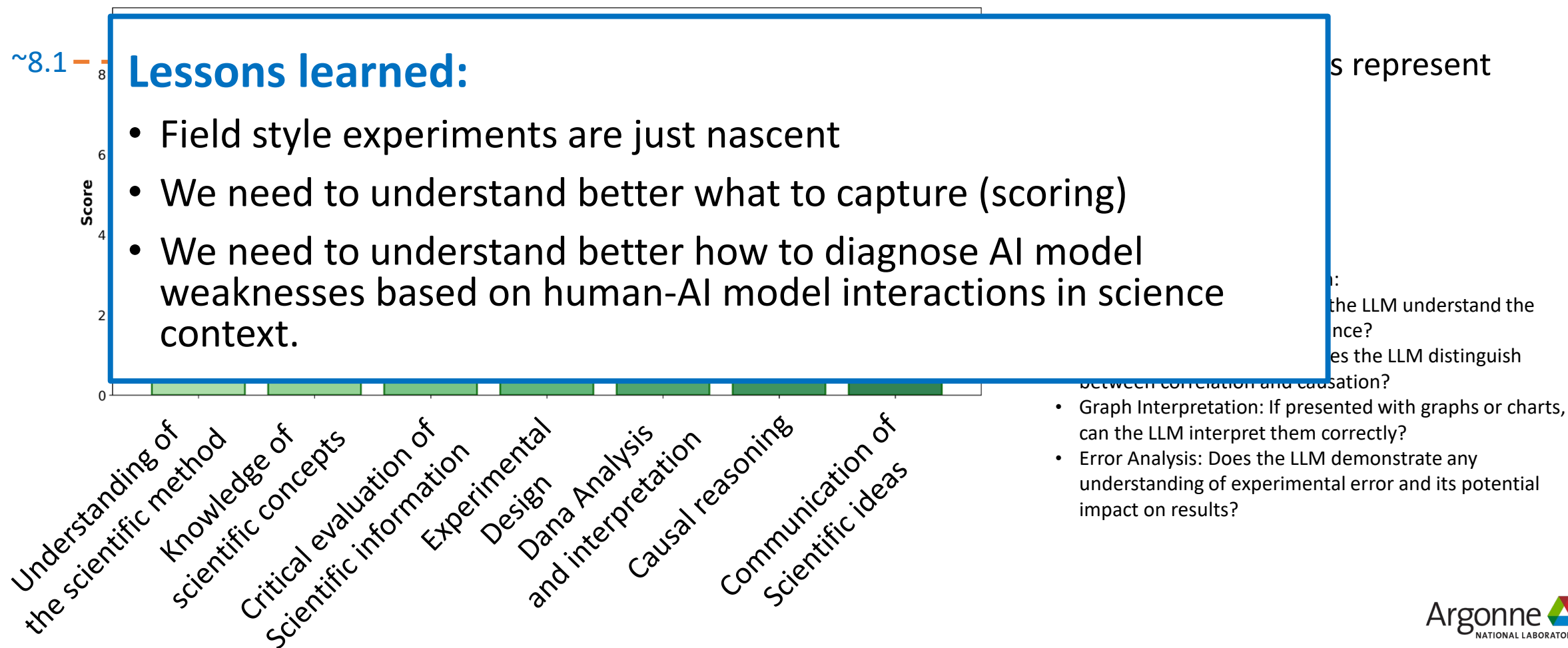
Overall Skill Statistics (GPT-o1 Dataset)
(Error bars show standard deviation)



1,000 Scientists Jam Session: skills strength (average over the whole corpus)

LLM as a judge to automatically score (1-10) the LLMs responses

Nested Analysis - Overall Category Statistics
(Error bars show standard deviation)



What's next

- Continue **Benchmarks development** (skills –**Coding**–, trustworthiness, safety)
- **More Lab-style experiments (numerical methods)**/ improve the method
- **More Field-style experiments** / improve the method
- Develop **Frontier Science Benchmark** (extremely difficult problems ~ Frontier Math), including:
 - Performance tuning
 - Automatic Parallelization
 - Energy Saving
 - Optimal tool calling (Agent)



The image shows a network diagram with nodes and connecting lines, representing the Trillion Parameter Consortium. The title "Trillion Parameter Consortium" is at the top, followed by "Generative AI for Science". Below this, a list of member institutions and their representatives is provided, organized into three columns. The TPC contact information is also included.

Trillion Parameter Consortium
Generative AI for Science

TPC contact: Charlie Catlett
Learn more at tpc.dev

Members:

- Rick Stevens, Charlie Catlett
Argonne National Laboratory and
The University of Chicago
- LAION: [Jenia Jitsev](#)
Lawrence Berkeley National Laboratory: [Stefan Wild](#)
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Los Alamos National Laboratory: [Jason Pruet](#)
- AI Singapore: [Leslie Teo](#)
Allen Institute For AI: [Noah Smith](#)
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Barcelona Sup. Center: [Mateo Valero Cortes](#)
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CEA: [Christoph Calvin](#)
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Flinders University: [Rob Edwards](#)
Fujitsu Limited: [Koichi Shirahata](#)
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Intel: [Koichi Yamada](#)
Juelich Supercomputing Center: [Thomas Lippert](#)
Kotoba Technologies, Inc.: [Jungo Kasai](#)
- Microsoft: [Shuaiwen Leon Song](#)
National Center for Supercomputing Applications: [Bill Gropp](#)
AIST - Japan: [Yoshio Tanaka](#)
National Renewable Energy Laboratory: [Juliane Mueller](#)
National Supercomputing Centre, Singapore: [Tin Wee Tan](#)
NCI Australia: [Jingbo Wang](#)
New Zealand eScience Infrastructure: [Nick Jones](#)
Northwestern University: [Pete Beckman](#)
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Pawsey Institute: [Mark Stickells](#)
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RIKEN: [Makoto Taiji](#)
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SambaNova: [Marshall Choy](#)
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Seoul National University: [Jiyoung Cha](#)
SLAC National Accelerator Laboratory: [Daniel Ratner](#)
- Stanford University: [Sanmi Kovejo](#)
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University of Toronto: [Alan Aspuru-Guzik](#)
University of Utah: [Manish Parashar](#)
University of Virginia: [Geoffrey Fox](#)

Thanks!

Q&As

EAIRA EVAL Methodology :

<https://arxiv.org/abs/2502.20309>



2025: PDE Solving 1: O1-pro, Claude 3.7 extended

The maturation of the LLMs in 12 months is impressive. I would give a Ph. D. student good grades on the transonic essay in identifying the subtleties and some relevant literature.

The model mention sophisticated discretization methods for primitive variables, like the velocity and density. However, it is not clear how to apply these to the requested velocity potential form of the equation, in which the velocity is a function of the potential and the density is a function of the velocity.

Following Boeing, as described in David's paper, one would use density upwinding, not upwinding on the velocity or the velocity potential. This Boeing practice is not described. Neither of the scripts will result in a discretization that models the shock correctly. Also, neither one of them knows how to robustify the Newton method for a discretization that is clever enough to capture the shock.

The transonic treatment is quite well informed. in terms of relevant literature and calling attention to various classical discretization options. It knows that a shock may develop and that this may prevent a single discretization scheme from being applied at every point. Different schemes are needed in different regimes of Mach number. It does not warn us that the resulting discrete system may be "nonlinearly stiff" and that a plain Newton method will not work.

...

Conclusion: I still have a job.

Experimental Validation: e.g. Google co-Scientist

(18 Feb. 2025)

Toward and AI co-scientist, arXiv:2502.18864

AI co-scientist relies on “self-play” strategies to **continuously** generates, reviews, debates, explains its reasoning and improves research hypotheses toward the research goal.

Multi-agent architecture

- All agents built from LLMs (e.g., GPT-4o, Gemini 2.0 Flash, Claude 3.5 Sonnet, etc.)
- **Agents:** Generation agent (hypothesis generator), Evolution agent (hypothesis refiner), Reviewer agent (hypothesis reviewer), Meta-review agent (hypothesis evaluator)
- Asynchronous task execution, **flexible compute resources**
- **Tournament evolution process** for self-improving hypotheses generation. Feedback from the tournament creates a self-improving loop towards novel quality outputs.
- **Tools:** web search and specialized AI models to improve grounding and quality of generated research hypotheses.

Automated evaluations

How to we assess knowledge extension, reasoning capabilities and creativity level?
→ We cannot only rely on experimental validation (too expensive)

Scientist-in-the-loop

Scientist

The scientist interacts with the system by specifying a research goal in natural language. They can also suggest

Scientist inputs

Research goal

Scientist describes a research goal along with preferences, experiment constraints, and other attributes.

Add idea

Review idea

The AI co-scientist multi-agent system

Research plan configuration

Ranking agent tournaments

Research hypotheses comparison and ranking with scientific debate in tournaments. Limitations

Generation agent

Literature exploration

Simulated scientific debate

Reflection agent

Full review with web search

Simulation review

Tournament review

Deep verification

Hypothesis generation

AI

AI co-scientist

The AI co-scientist continuously generates, reviews, debates, and improves research hypotheses and proposals toward the research goal provided by the scientist.

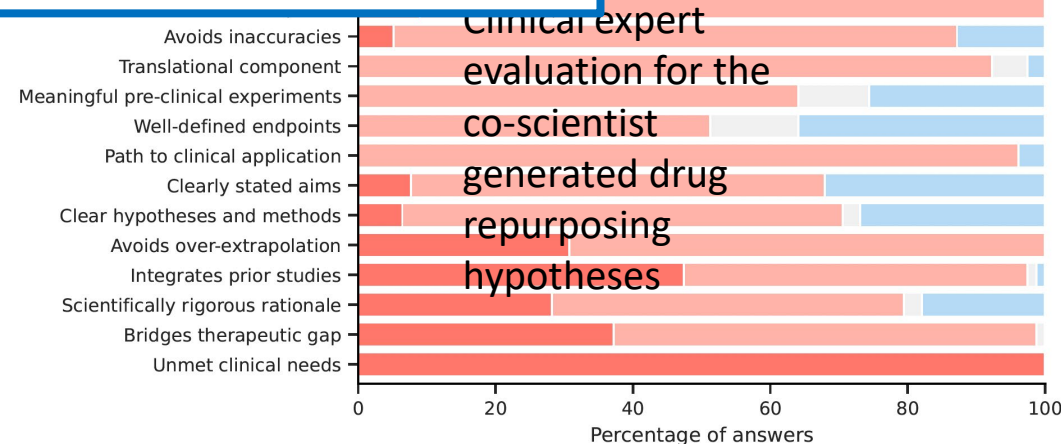
Tool Use

Search

Additional tools

Memory

drug repurposing, novel target discovery, and explaining mechanisms of bacterial evolution and anti-microbial resistance. Co-scientist's hypotheses for these three settings are externally, independently validated by in vitro laboratory experiments



LLM-based Agent Evaluation (20 March 2025)

Survey on Evaluation of LLM-based Agents: arXiv:2503.16416v1

(1) Fundamental agent capabilities:

- planning
- tool use
- self-reflection
- memory

(2) Application specific:

- benchmarks for web
- software engineering
- Scientific
- conversational agents

(3) Benchmarks for generalist agents

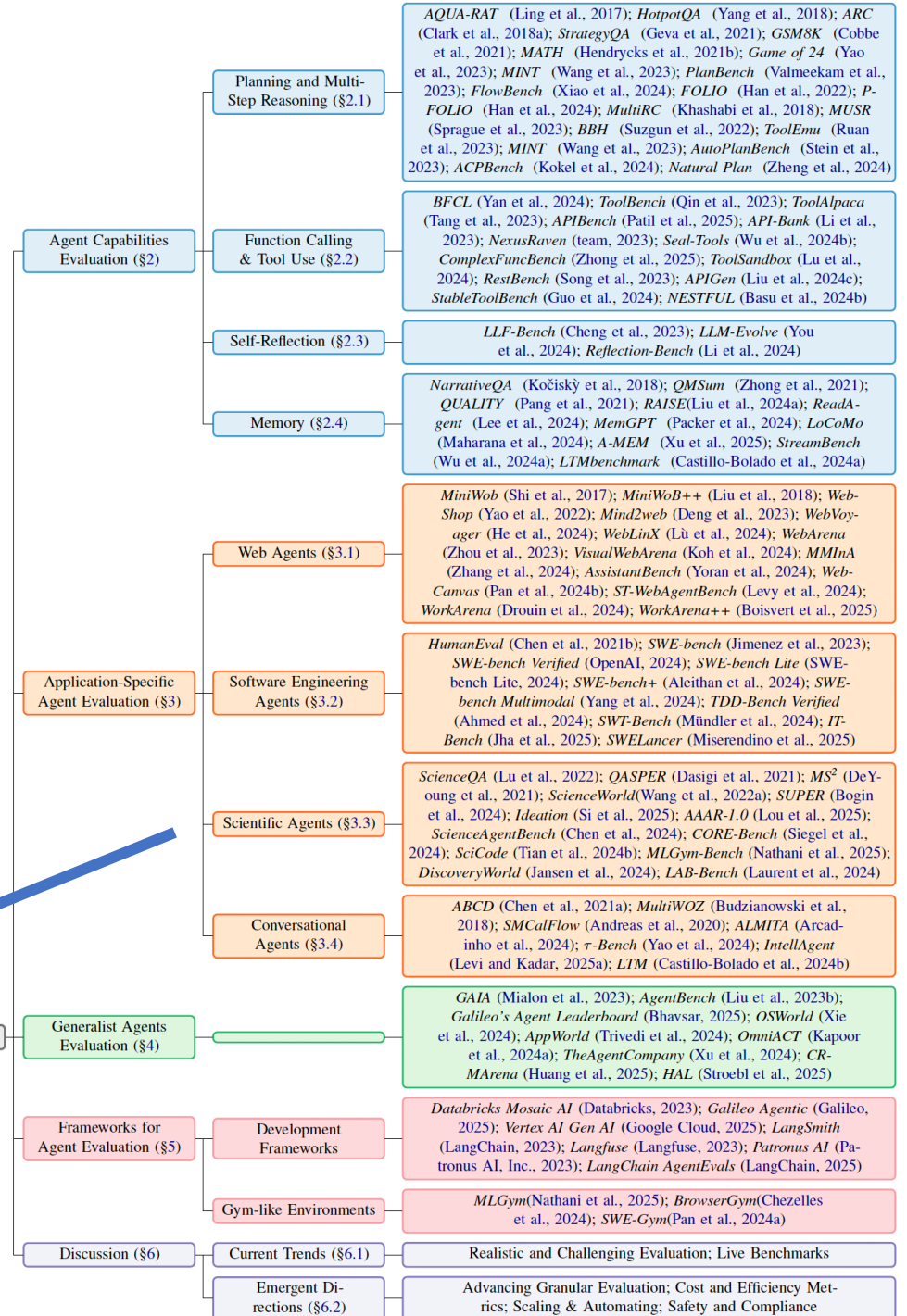
(4) Frameworks for evaluating agents

Scientific Agents (§3.3)

These are just LLM benchmarks

ScienceOA (Lu et al., 2022); QASPER (Dasigi et al., 2021); MS² (DeY-
oung et al., 2021); ScienceWorld(Wang et al., 2022a); SUPER (Bogin
et al., 2024); Ideation (Si et al., 2025); AAAR-1.0 (Lou et al., 2025);
ScienceAgentBench (Chen et al., 2024); CORE-Bench (Siegel et al.,
2024); SciCode (Tian et al., 2024b); MLGym-Bench (Nathani et al., 2025);
DiscoveryWorld (Jansen et al., 2024); LAB-Bench (Laurent et al., 2024)

Agent Evaluation

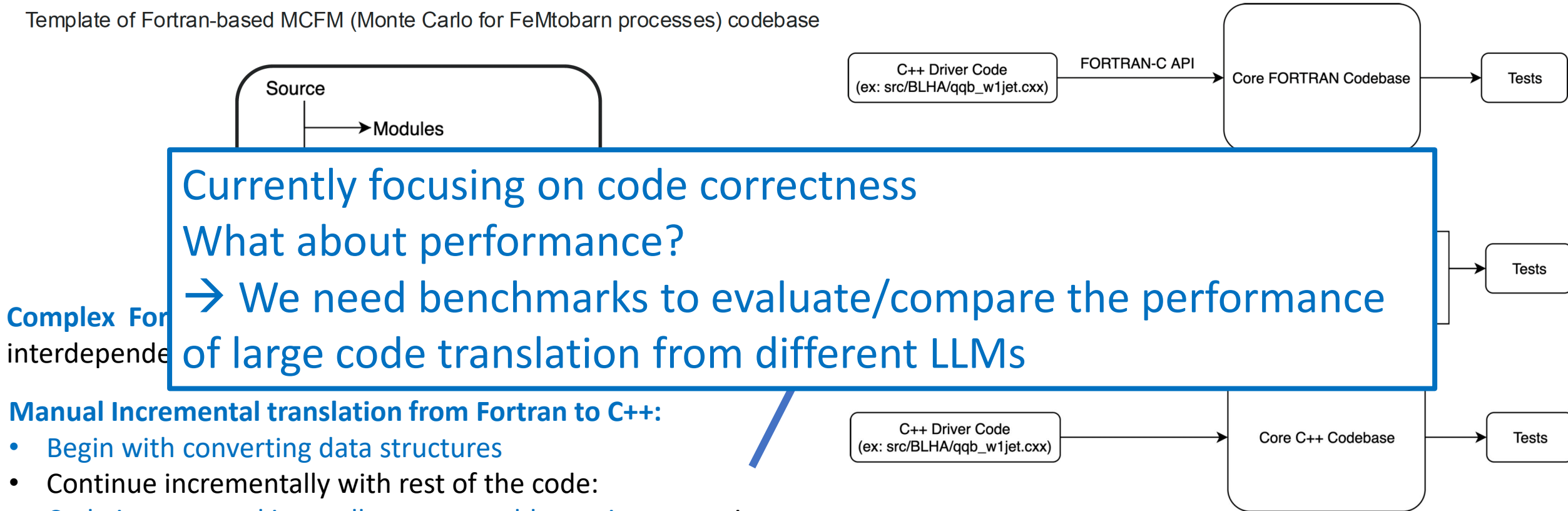


Code Translation: Full Complex Codes (Fortran to C++)

CodeSCRIBE: Leveraging Large Language Models for Code Translation and Software Development in Scientific Computing

Akash Dhruv, Anshu Dubey, PASC, June 16–18, 2025, Brugg, Switzerland

Template of Fortran-based MCFM (Monte Carlo for FeMtobarn processes) codebase



Manual Incremental translation from Fortran to C++:

- Begin with converting data structures
- Continue incrementally with rest of the code:
- Code is converted in smaller, manageable sections, creating interfaces (usually Fortran-C layers) between legacy Fortran code and newly written C++ sections.
- Each code segment is tested to preserve functionality (Easier debugging by isolating issues in well-defined portions)
- Rely on a Fortran-C API

- Develop prompts to teach LLM the rules for conversion from Fortran to C++ and write corresponding Fortran-C-API to integrate the generated code with the application.
- Run incremental tests.