- Context
- Why we did it
- Organizational challenges
- What we learn from it

Idea and lead organizer: Rick Stevens

DOE Labs experience exploring large AI models for science

Franck Cappello

Lead of AuroraGPT/Eval

Argonne National Laboratory

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

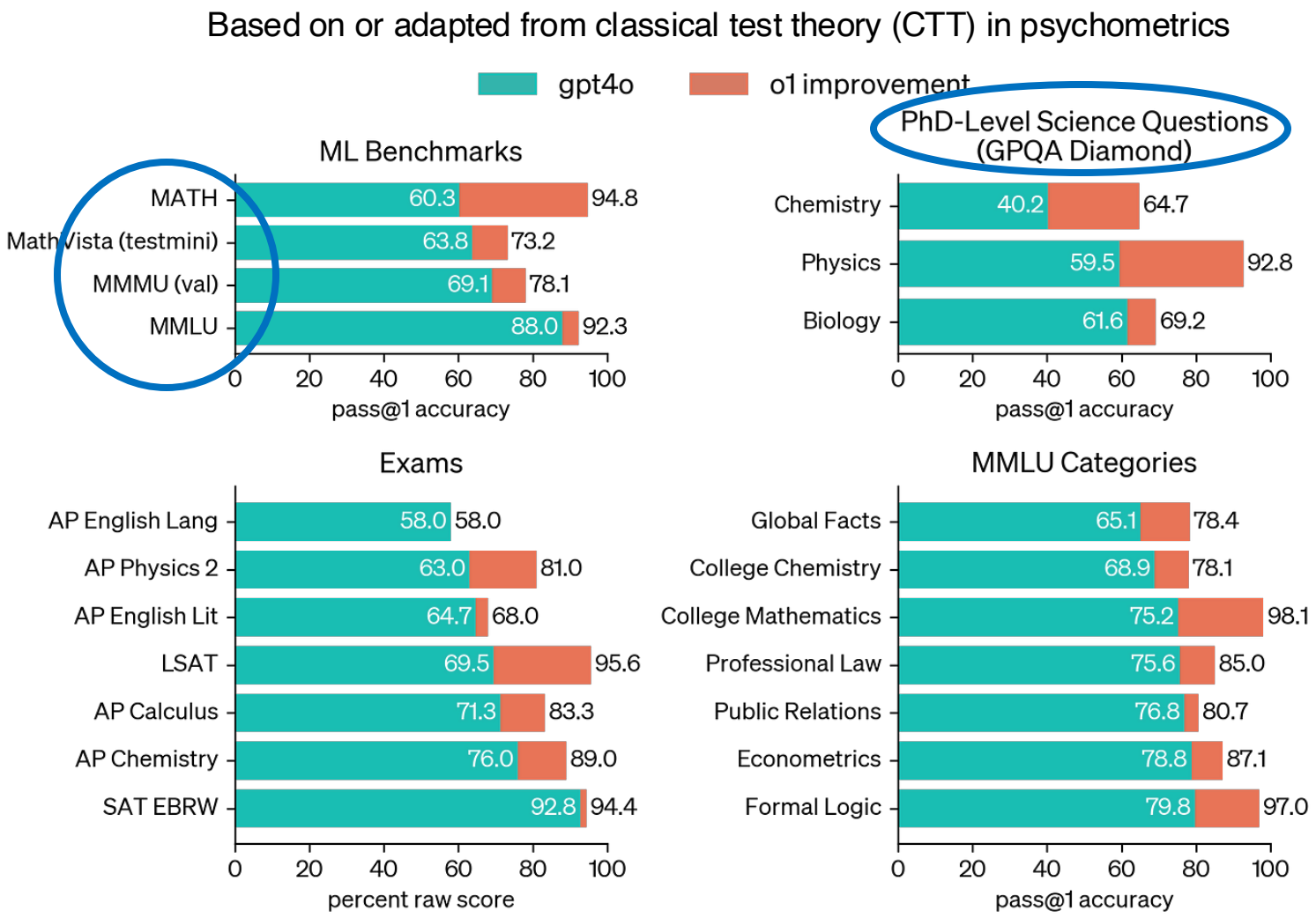
Large Language Models (LLMs) have progressed drastically in the past 4-5 years (GPT3 released in 2020)

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.



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

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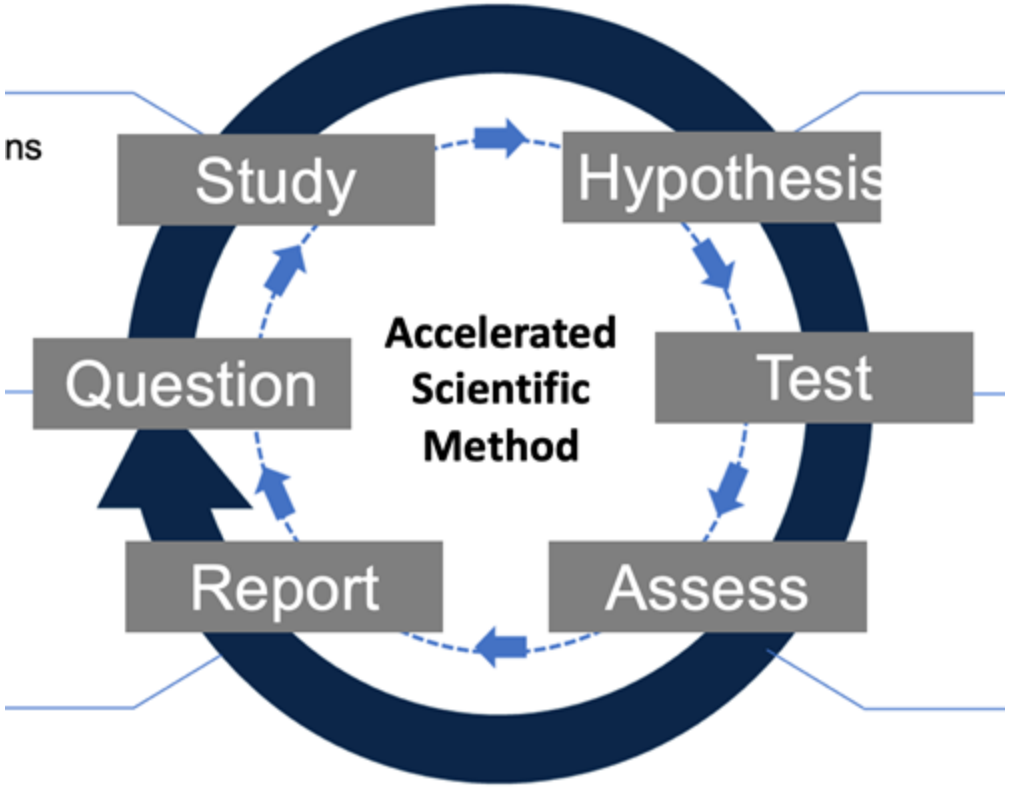
LLMs/rLLMs as Research Assistants?

Scientists assessed LLMs on **specific tasks**:

- Predicting molecular properties
- Uncovering genomic patterns
- Solving mathematical problems
- Creating and manipulating tools for simulations and analysis
- Etc.

→ Diversity and strength of skills and capabilities (Knowledge, Reasoning, Web search, Tools) **Suggest a new holistic approach** where LLMs/rLLMs are use as **scientific research assistants**

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



Three Main Challenges **Before Broad Adoption**

1) Encourage/Recommend Researcher to test LLMs for the different steps of the research circle **(Can LLMs accelerate research?)**

→ Many researchers are aware of these models but barely tried to use them for their research

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

→ Need methods to evaluate and compare LLMs in research context

3) 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.

The EAIRA Evaluation Methodology for the Evaluation of LLMs

End-to-End

New

New

In the Wild

Proposed Methodology				
Techniques	**MCQ Benchmarks**	**Open Response Benchmarks**	**Lab Style Experiments**	**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)** →			

https://arxiv.org/abs/2502.20309

or search EAIRA on Google

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Argonne Jam Sessions

Argonne researcher participation and contribution on a voluntary basis.

First session: November 1, 2024

Argo/O1-Preview JAM Session
Introducing LRM to researchers + training session
200 researchers from across Argonne
spent two hours tackling a "staff-level" problem
with Argo/O1-preview

- Asked researchers to solve a research problem (1h-1h30)
- Used O1-preview Chat interface (different "system" prompt compared to OpenAI O1-preview web version)
- 180 experiments in total
- 134 Experiments from various scientific domains (after removing non non-scientific questions and experiments requiring only recall capabilities)
- Use the same 5 criteria and questions as the ones used by LANL in their recent report
- Collected in addition, scoring explanations and full conversations
- Total of 19 questions/boxes

By the end of March 2025, All Argonne Directorates organized a JAM Session

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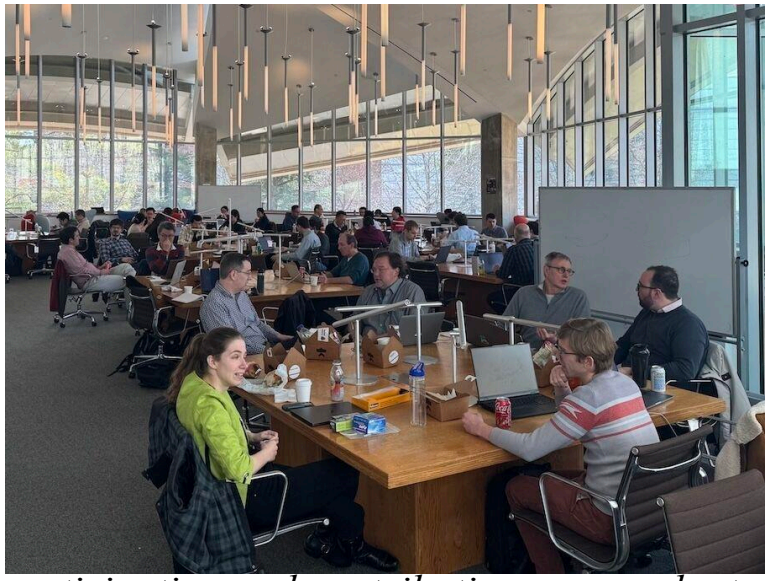
~~1000~~ 1500 Scientists AI JAM in 9 Labs Simultaneously (Feb.28, 2025)



Researcher participation and contributions on a voluntary basis.

1000 Scientists AI JAM Session: Goal and Rules of engagement

Researcher participation and contribution on a voluntary basis.

Goals:

- Give Lab researchers an opportunity to test the best available LLMs
- Build a large corpus of interactions between researchers and AI models
  - Will help Labs understand how researchers will use reasoning models LLMs for Science → **How AI models may accelerate discoveries**
  - Will help AI labs (OpenAI, Anthropic) to improve their model → to improve our research

Rules:

- Explore advanced AI models on **challenging scientific problems**,
- Better understand the potential impact of AI reasoning models on **national security and science**,
- **In-person event** hosted at Argonne, Berkeley, Brookhaven, Idaho, Livermore, Los Alamos, Oak Ridge, Pacific Northwest, and Princeton Plasma Physics national laboratories. Scientists from other DOE labs are also participating,
- Explore models from OpenAI (**o1-pro, o1-deepresearch, o3-mini-high**) and Anthropic (**Claude 3.7 extended**),
- **OpenAI people in the rooms**.

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1000 Scientists AI JAM Session: Rules of engagement (cont.)

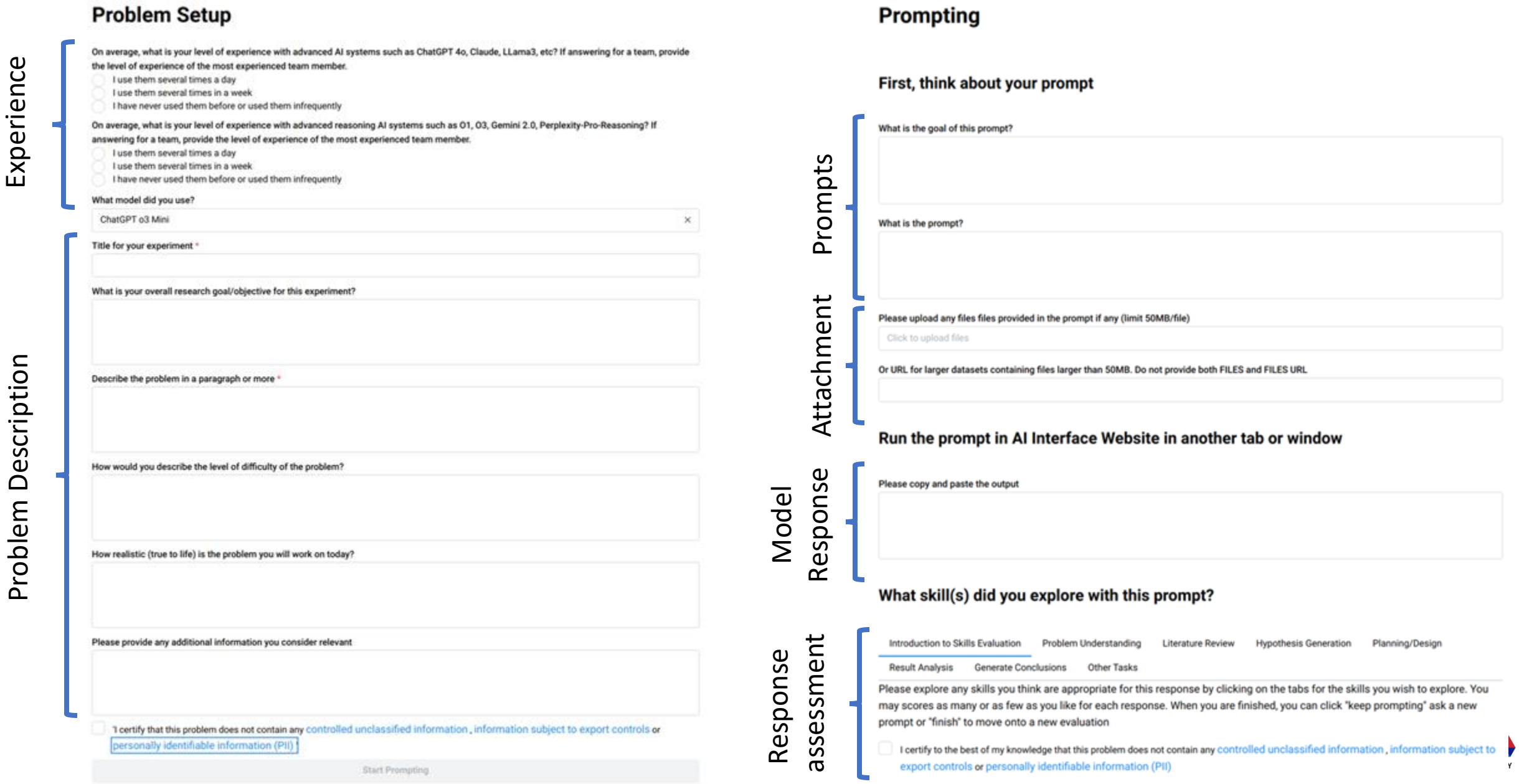
Researcher participation and contributions on a voluntary basis.

Rules (cont.):

- **Each participant brough 2-3 problems** from their scientific domain,
- Diverse range of realistic, representative tasks in scientific research and development,
- **Spend the day** using the latest capabilities of AI reasoning models,
- Participants can work in small teams to avoid getting stuck and to help observe or analyze the performance of the models,
- **All prompts, model responses and participant assessments are recorded --> the AI JAM Corpus,**
- The results will give an early estimate of how these tools could benefit the scientific community,
- The AI JAM Corpus is **shared with all participating DOE labs and AI labs (industry),**
- **Future sessions** will feature models from different AI companies (XAI, Nvidia, Google).

1000 Scientists AI JAM Session: Collection

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

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What we learn from the 1000 Scientists AI JAM

- **Benchmarking is not enough** (we knew it, but real-life JAMs affirm it)
- Demonstrating AI models' capabilities to researchers is **important for adoption**
- **Organization was very challenging** (legal aspects)
- **Participants tested all aspects** of the research circle (except text processing…)
- The corpus represents the **largest existing collection of scientists/AI models' interactions**
- **Mining this corpus will help understand what researchers need and the gaps between the current situation and effective AI research assistants**

First large scale collaboration with AI Industry

- **AI labs (OpenAI, Anthropic) are very interested** in scientific research (reasoning)
- What's our added value:
  - **1) We produce/have the scientific data AND we know how to transform it for injection.**
  - **2) We have the scientific knowledge/skills in many science domains**
  - **3) We will use LLMs for science only if we trust them.**

Thanks!

Q&As

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