Welcome to the NSF Workshop on the Future of AI for the Mathematical and Physical Sciences (MPS)

March 24–26, 2025

Sponsors and Organizers

This event is supported by the **National Science Foundation (NSF)** under Award Number 2512945.

Additional funding for this event is provided by the **MIT School of Science**, **MIT Department of Physics**, **MIT Department of Chemistry**, and **MIT Department of Mathematics**.

Workshop Organizers

Jesse Thaler
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Physics

Andrew Ferguson
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Emory University
Mathematical Sciences

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The Ohio State University
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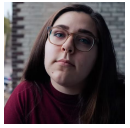
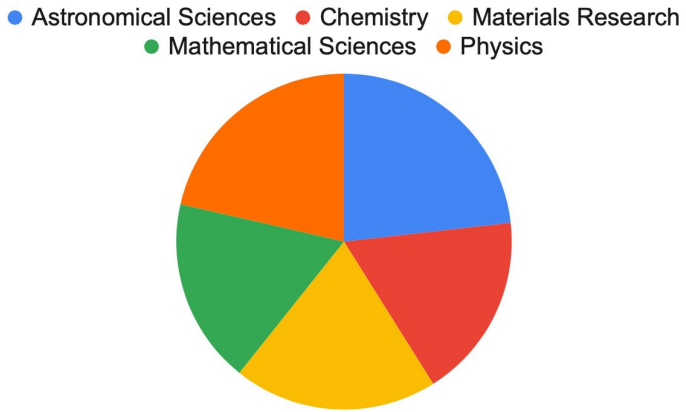
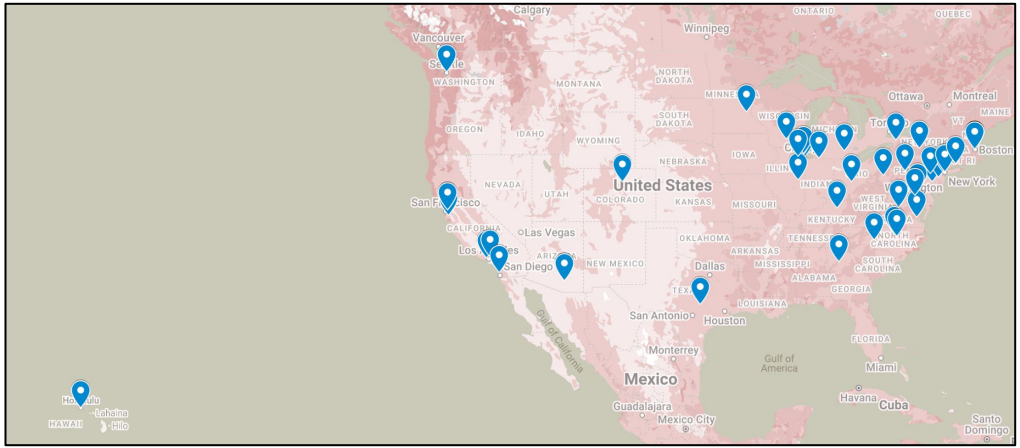


Sarah Wells
Science Writer

Who is here

Invited Participants (white paper authors)





Attendees/Observers (feedback welcome!)

- Virtual and in person
- From institutions in almost 30 states
- Includes representatives from NSF and other funding agencies
- The meeting is being recorded for reference only and will not be shared

AI+MPS

- The MPS domains have long **used and developed techniques in machine learning, statistics, and data science** to drive scientific innovation.
- Starting about a decade ago, the rise of **deep learning enabled exciting new strategies to analyze scientific datasets and perform scientific calculations**.
- Today, the widespread availability of powerful generative AI models is poised to **fundamentally change the ways scientists pursue groundbreaking discoveries**.
- **AI is now ubiquitous**, in the sciences and in society more generally, and there are no signs of AI progress slowing down. If anything, there is a sense that **AI is advancing at an ever accelerating pace**, with some AI systems exhibiting human-like levels of reasoning that were previously only seen in speculative fiction.

Jesse's Personal Flashback to 2020

The New York Times

By Dennis Overbye Nov. 23, 2020

Can a Computer Devise a Theory of Everything?

"In five to 10 years from now, I'm going to want to do exactly what you're getting at: Here's the data, here's a very rough tool kit; find the equation I could put on a T-shirt, the equation that replaces the Standard Model of particle physics. What's the equation that replaces Einstein's general relativity?"

In 2020, this could be dismissed as just another trip around the AI hype cycle.
In 2022, you could joke: "why ChatGPT hasn't already solved it for you?"
In 2025, you can have a lucid conversation about this topic with GPT-4o…

Possible Future: “Centaur Science”

GPT-4o Version:

Could a Computer Discover a ToE?

- If physics is ultimately a **solvable** problem (with a well-defined mathematical structure), then an AI, given enough computational power, could potentially **discover** it.
- If, however, the ToE requires **a fundamentally new paradigm**, AI may struggle without human intuition guiding it.

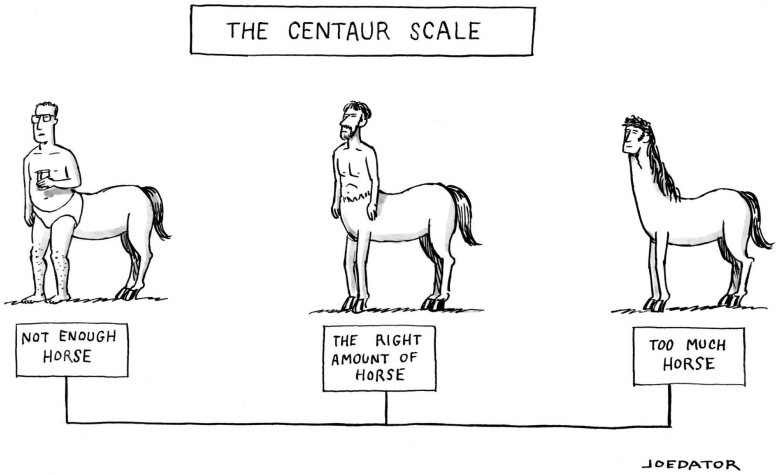
Possible Future Scenario

A hybrid approach is most likely:

- AI assists physicists in refining theories, running simulations, and discovering mathematical structures.
- Humans provide the creative insights, interpretation, and experimental validation.

This collaboration could one day lead to the elusive **theory of everything**, possibly faster than human effort alone.

New Yorker Cartoon Version:



Not only is AI-enabled science a reality, but many researchers (especially early-career) are passionate about **simultaneously advancing MPS and pursuing cutting-edge AI**.

NSF AI+MPS Workshop: Goals

- Understand the **interdisciplinary landscape of AI+Science**, while recognizing and engaging the specific methods, culture, and drivers for each disciplinary field
- Identify the **potential opportunities and challenges for integration and impact of AI** within and among the MPS domains
- **Write a white paper outlining next steps and needs** for integrating MPS research within the interdisciplinary field of AI+Science and positioning MPS to both harness and build on the advances and tools driving the AI revolution
    - *N.B. The zeroth draft white paper is supposed to spark discussion not stifle it!*

Driving Question: How can the MPS domains best capitalize on, and contribute to, the future of AI?

NSF Perspective

Dave Berkowitz
NSF, Assistant Director for the Mathematical and Physical Sciences

Questions to Consider

- What **key drivers are advancing science** in the world of AI?
- What are **common enablers and barriers** in each MPS discipline?
- What are the **key gaps between the current use/development of AI technologies and the needs** of the MPS scientific community?
- What are the **opportunities for bridging the gap** between AI advances and scientific discovery?
- What is the need for **education and training to advance science** with AI tools?

Driving Question: How can the MPS domains best capitalize on, and contribute to, the future of AI?

Workshop Plan

Morning Sessions (9:00am–12:30pm):

- Presentations and full-group discussions
  - Monday: Introductory
  - Tuesday and Wednesday: Reports from breakout group discussions
- Broadcast on Zoom

Afternoon Sessions (2:00–5:30pm):

- Breakout discussions *in person only*
  - Monday: by theme
  - Tuesday: by domain
- Invited participants have been assigned breakout groups
- Attendees/observers may join any breakout group

Domains

- Astronomical Sciences (AST)
- Chemistry (CHE)
- Materials Research (DMR)
- Mathematical Sciences (DMS)
- Physics (PHY)

Themes

- Interdisciplinary Research: Opportunities and Challenges
- Interdisciplinary Research: Resources Needed
- Education & Workforce Development
- Responsible AI

Today's Schedule (Monday)

9:00–9:30 am: Welcome and Overview

9:30–10:30 am: Theme Overviews

- Interdisciplinary Research: Opportunities and Challenges: Lars Ruthotto
- Interdisciplinary Research: Resources Needed: Andrew Ferguson
- Education & Workforce Development: Yuan-Sen Ting
- Responsible AI: Pratyush Tiwary

10:30–11:00 am: Break

11:00 am–12:30 pm: Domain Overviews

- AST: Yuan-Sen Ting
- CHE: Pratyush Tiwary
- DMR: Andrew Ferguson
- DMS: Soledad Villar
- PHY: Jesse Thaler

12:30–2:00 pm: Lunch

2:00–5:30 pm: Theme Breakouts

- Interdisciplinary Research: Opportunities and Challenges: Room 801 North (here)
- Interdisciplinary Research: Resources Needed: Room 801 South
- Education & Workforce Development: Room 804
- Responsible AI: Room 812