The Future of Artificial Intelligence and the Mathematical and Physical Sciences (AI+MPS)

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NASA AI/ML Science and Technology Interest Group — November 3, 2025

Based on [arXiv:2509.02661] supported by NSF Award Number 2512945
Thanks to Marisa LaFleur (NSF AI+MPS Workshop Project Manager) for essential contributions to these slides!

Motivation

The MPS domains have long **used and developed techniques in machine learning, statistics, and data science** to drive scientific innovation. The rise of **deep learning has enabled exciting new strategies to analyze scientific datasets and perform scientific calculations**. The widespread availability of powerful AI models is poised to **fundamentally change the ways scientists pursue groundbreaking discoveries**.

The NSF MPS-AI Working Group convened a group of researchers to gather and synthesize perspectives from the MPS community about the impact and potential of AI in the Mathematical and Physical Sciences:

Jesse Thaler
MIT
Physics

Andrew Ferguson
University of Chicago
Materials Research

Lars Ruthotto
Emory University
Mathematical Sciences

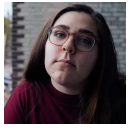
Yuan-Sen Ting
The Ohio State University
Astronomical Sciences

Pratyush Tiwary
University of Maryland
Chemistry

Soledad Villar
Johns Hopkins University
Mathematical Sciences

Additional support from:

Marisa LaFleur
Project Manager

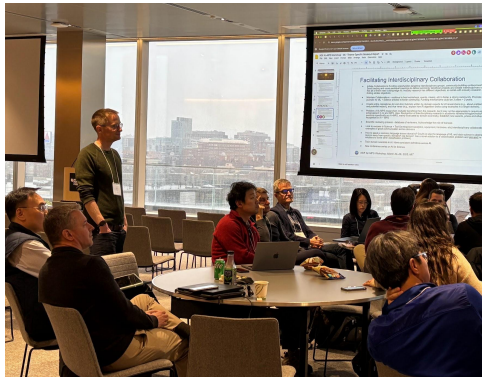


Sarah Wells
Science Writer

NSF Workshop on the Future of AI+MPS

- March 24–26, 2025 at MIT
- Invited ~60 experts from across MPS domains to participate and provide insights via a survey in advance
- Organized presentations + breakout discussions by domain and on the following interdisciplinary topics:
  - Interdisciplinary Research: Challenges & Opportunities
  - Interdisciplinary Research: Resources Needed
  - Education & Workforce Development
  - Responsible AI

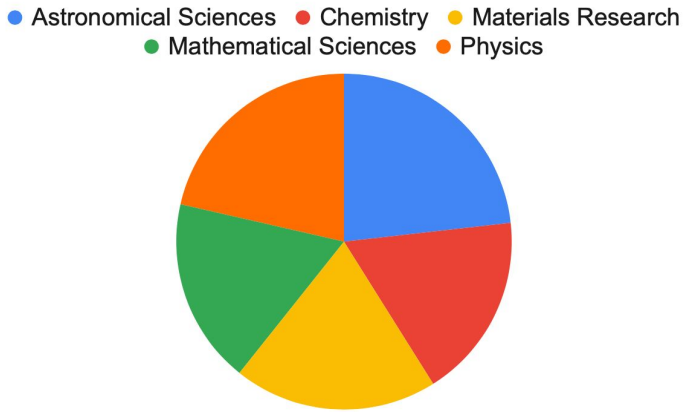
White paper now available on arXiv!
https://arxiv.org/abs/2509.02661

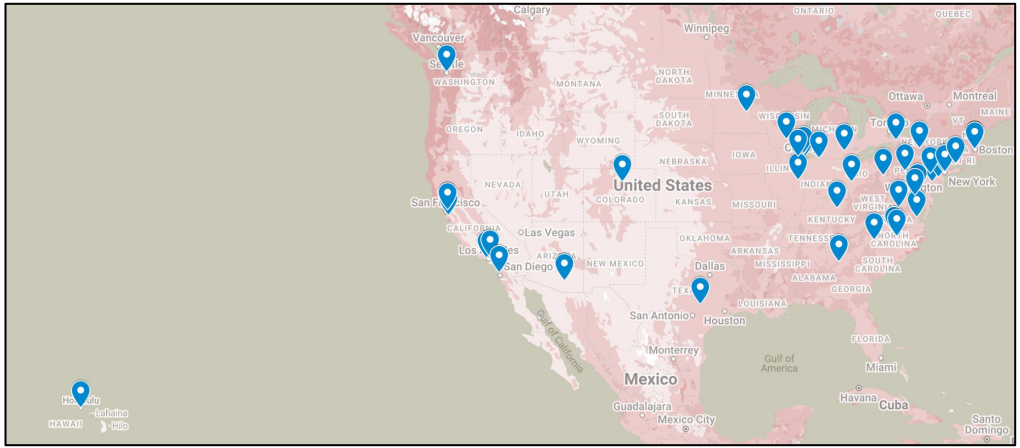


Supported by the **National Science Foundation (NSF)** under Award Number 2512945

Workshop Participants

Invited Participants





- Virtual and in person observers also attended from institutions in almost 30 states, including representatives from the NSF and other funding agencies
- By default, invited participants were white paper authors, but attendees/observers could become authors as well if they provided substantial feedback

Current State of AI+MPS

*In this context, we treat **AI as a broad umbrella** that encompasses a wide range of computational, mathematical, and statistical innovations, including machine learning.*

AI accelerating scientific discovery in MPS

- Enabling **simulation-based inference**
- Accelerating **simulations**
- Facilitating **pattern recognition** and **anomaly detection**
- Leveraging **representation learning**
- Enhancing **predictions**
- Streamlining the **scientific workflow**
- Enhancing **communication**

MPS driving AI understanding

- Incorporating **fundamental physical laws** into AI
- Improving **interpretability** and **transparency**
- Improving **efficiency** and reducing **data dependency**
- Creating **benchmark** problems and datasets
- Quantifying **uncertainty** and ensuring **reliability**
- Enhancing **reinforcement learning** for sparse rewards
- Providing a **safe ecosystem** of development

Future of AI+MPS

*We found many **commonalities across MPS disciplines** in the way they are approaching AI, which point to opportunities for **establishing an AI strategy for the broad MPS community**.*

We anticipate that combining AI with domain sciences will lead to **significant, transformational outcomes**, including:

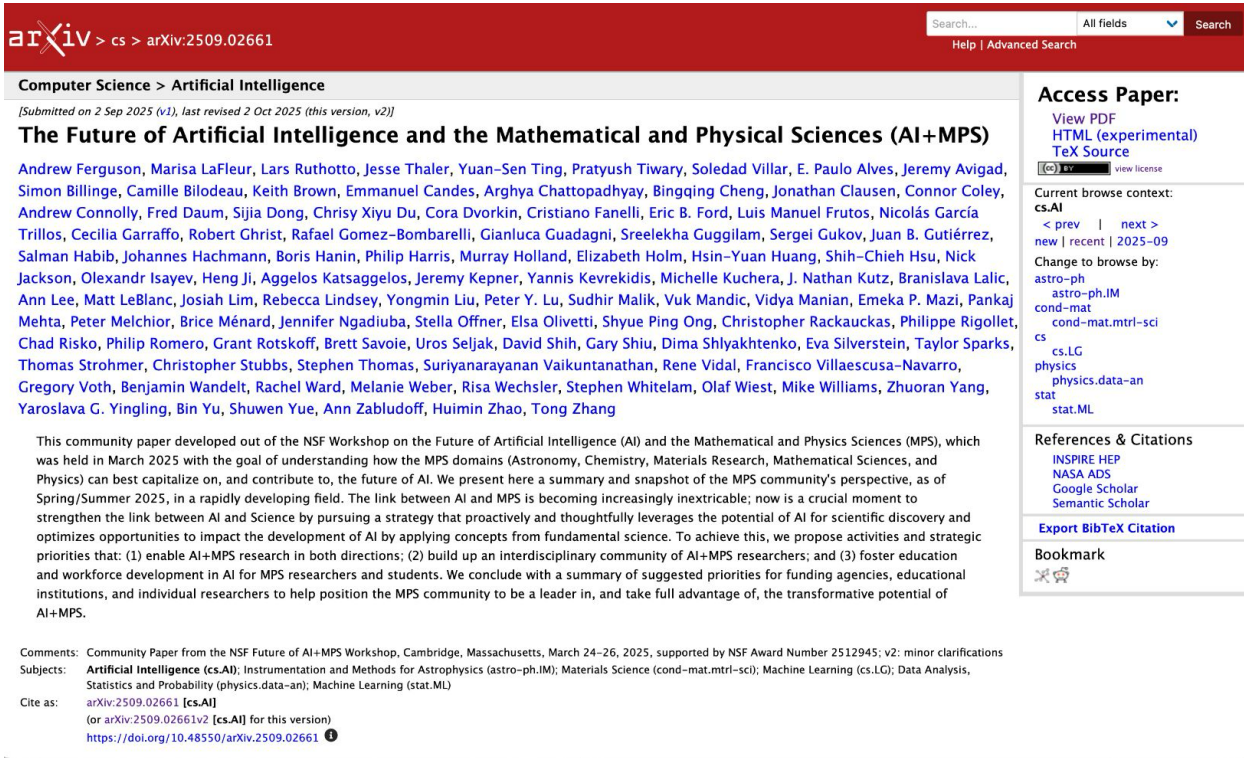
- Establishing a new scientific domain at the intersection of AI and science
- Breaking open the AI “black box”
- Accelerating the pace of scientific discovery

I found myself surprised by the commonality I felt with researchers across very different domains

The workshop was extremely useful in establishing contacts between different areas of MPS. It can hopefully provide some guidance in the challenging and changing research landscape ahead.

[The workshop] had the feeling of an excellent community of like-minded investigators across broad disciplines.

Our Report!



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Computer Science > Artificial Intelligence

[Submitted on 2 Sep 2025 (v1), last revised 2 Oct 2025 (this version, v2)]

The Future of Artificial Intelligence and the Mathematical and Physical Sciences (AI+MPS)

Andrew Ferguson, Marisa LaFleur, Lars Ruthotto, Jesse Thaler, Yuan-Sen Ting, Pratyush Tiwary, Soledad Villar, E. Paulo Alves, Jeremy Avigad, Simon Billinge, Camille Bilodeau, Keith Brown, Emmanuel Candes, Arghya Chattopadhyay, Bingqing Cheng, Jonathan Clausen, Connor Coley, Andrew Connolly, Fred Daum, Sijia Dong, Chrisy Xiyu Du, Cora Dvorkin, Cristiano Fanelli, Eric B. Ford, Luis Manuel Frutos, Nicolás García Trillos, Cecilia Garraffo, Robert Ghrist, Rafael Gomez-Bombarelli, Gianluca Guadagni, Sreelekha Guggilam, Sergei Gukov, Juan B. Gutiérrez, Salman Habib, Johannes Hachmann, Boris Hanin, Philip Harris, Murray Holland, Elizabeth Holm, Hsin-Yuan Huang, Shih-Chieh Hsu, Nick Jackson, Olexandr Isayev, Heng Ji, Aggelos Katsaggelos, Jeremy Kepner, Yannis Kevrekidis, Michelle Kuchera, J. Nathan Kutz, Branislava Lalic, Ann Lee, Matt LeBlanc, Josiah Lim, Rebecca Lindsey, Yongmin Liu, Peter Y. Lu, Sudhir Malik, Vuk Mandic, Vidya Manian, Emeka P. Mazi, Pankaj Mehta, Peter Melchior, Brice Ménard, Jennifer Ngadiuba, Stella Offner, Elsa Olivetti, Shyue Ping Ong, Christopher Rackauckas, Philippe Rigollet, Chad Risko, Philip Romero, Grant Rotskoff, Brett Savoie, Uros Seljak, David Shih, Gary Shiu, Dima Shlyakhtenko, Eva Silverstein, Taylor Sparks, Thomas Strohmer, Christopher Stubbs, Stephen Thomas, Suriyanarayanan Vaikuntanathan, Rene Vidal, Francisco Villaescusa-Navarro, Gregory Voth, Benjamin Wandelt, Rachel Ward, Melanie Weber, Risa Wechsler, Stephen Whitelam, Olaf Wiest, Mike Williams, Zhuoran Yang, Yaroslava G. Yingling, Bin Yu, Shuwen Yue, Ann Zabludoff, Huimin Zhao, Tong Zhang

This community paper developed out of the NSF Workshop on the Future of Artificial Intelligence (AI) and the Mathematical and Physics Sciences (MPS), which was held in March 2025 with the goal of understanding how the MPS domains (Astronomy, Chemistry, Materials Research, Mathematical Sciences, and Physics) can best capitalize on, and contribute to, the future of AI. We present here a summary and snapshot of the MPS community's perspective, as of Spring/Summer 2025, in a rapidly developing field. The link between AI and MPS is becoming increasingly inextricable; now is a crucial moment to strengthen the link between AI and Science by pursuing a strategy that proactively and thoughtfully leverages the potential of AI for scientific discovery and optimizes opportunities to impact the development of AI by applying concepts from fundamental science. To achieve this, we propose activities and strategic priorities that: (1) enable AI+MPS research in both directions; (2) build up an interdisciplinary community of AI+MPS researchers; and (3) foster education and workforce development in AI for MPS researchers and students. We conclude with a summary of suggested priorities for funding agencies, educational institutions, and individual researchers to help position the MPS community to be a leader in, and take full advantage of, the transformative potential of AI+MPS.

Comments: Community Paper from the NSF Future of AI+MPS Workshop, Cambridge, Massachusetts, March 24-26, 2025, supported by NSF Award Number 2512945; v2: minor clarifications

Subjects: **Artificial Intelligence (cs.AI)**; Instrumentation and Methods for Astrophysics (astro-ph.IM); Materials Science (cond-mat.mtrl-sci); Machine Learning (cs.LG); Data Analysis, Statistics and Probability (physics.data-an); Machine Learning (stat.ML)

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Contents

Strategic Vision for AI+MPS

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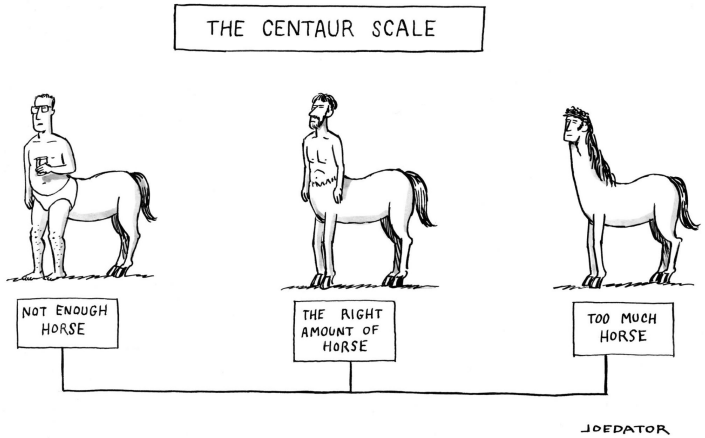
Strategic Vision for AI+MPS

Developing a strategy that builds a **mutually beneficial bridge** between MPS and AI research and recognizes the “two-way street” between science and AI.



New Yorker Cartoon, Feb 2025

Enable AI+MPS research in both directions

Build up an interdisciplinary community of AI+MPS researchers

Foster education and workforce development in AI for MPS researchers and students

Enable AI+MPS Research in Both Directions

AI is a powerful tool for advancing scientific discovery

- Leverage key AI techniques that already show promise for scientific applications
- Use AI as a partner for conducting research
- Take advantage of AI to accelerate research and provide new insights

AND

MPS insights are essential for enhancing AI innovation and understanding

- Need for further research in the “Science of AI” to generate AI innovations, enhance our understanding of AI, and support the development of robust AI techniques
- Empower AI innovation by helping make AI research more cost-efficient, improving the scientific integrity of AI, and communicating the impact of AI.

Resources should be allocated to efforts with impact in both MPS domains and AI development

Build up an interdisciplinary community of AI+MPS researchers

Cross-disciplinary AI collaborations facilitate knowledge sharing and broad applications

- Fund various types of interdisciplinary efforts
- Provide scalable resources
- Facilitate collaborations through workshops, conferences, and other events

AND

MPS domain-specific science leads to novel AI development for various scales and rigor

- Leverage solutions currently in development to address domain-specific problems
- Build AI-enabled communities and enable knowledge sharing within and across domains
- Collaborate with AI researchers interested in scientific applications

It is essential to identify ways to facilitate interdisciplinary research collaboration and establish community hubs for knowledge exchange, both within and across MPS domains

Foster education and workforce development in AI for MPS researchers and students

Broad AI education and training is needed for researchers at the AI+MPS intersection

- Provide training for senior researchers who may be using AI in their research for the first time
- Develop training for early career researchers with varying levels of experience using AI

AND

MPS has unique opportunities to integrate AI literacy into all levels of education

- Opportunity to strengthen the future AI+MPS talent pool and shape public perception of AI
- Establish credentials in AI+MPS to attract more students and researchers
- Maintain focus in MPS on developing the experience and intuition necessary to use AI productively

By proactively integrating AI into education and training, the MPS community can more effectively demonstrate and maintain its leadership in AI.

Cross-Disciplinary AI+MPS Opportunities

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Cross-Disciplinary MPS Opportunities

MPS will have the biggest impact in these areas if the domains collaborate to develop strategies, transfer knowledge, and innovate.

Advocate for Diverse Funding Streams

- Institute-Scale Activities
- Project-Scale Activities
- Individual Investigators
- Industry Collaborations

Pursue the Science of AI

- AI Innovations from Science
- Understanding AI
- Robust and Interpretable AI

Establish Scalable AI Infrastructures

- Computing Resources
- Data Management and Access
- Benchmarking and Reproducibility

Facilitate Interdisciplinary Collaborations

- Knowledge Transfer
- Workshops and Conferences
- Collaborating beyond MPS

I'll only have time to cover some of these, so please ask in Q&A if I skip your favorite topic!

Cultivate Key AI Techniques for Science

- Simulation-Based Inference
- Multi-scale Simulations
- Uncertainty Quantification
- Foundation Models
- AI for Experimental Control
- Data-Efficient Methods
- Additional Research Opportunities

Leverage AI for Conducting Research

- AI Co-Pilot
- Self-Driving Labs
- Digital Twins

Educate and Train an AI+MPS Workforce

- Faculty and Leadership Training
- Postdoctoral Training and Research Scientists
- Graduate Education
- Undergraduate Education
- K-12 and Public Education

Empower AI Innovation

- Cost-Efficient Computing
- Scientific Integrity
- Public Engagement on AI+Science

Advocate for Diverse Funding Streams

*AI and interdisciplinary expertise is causing a paradigm shift in how research is conducted, which would benefit from **nimbleness in the opportunities and structures** made available.*

Institute-Scale

- *Example: NSF AI Institutes*
- Provides **essential infrastructure** where researchers can meet across disciplines and forge collaborative ties across institutions
- Key recommendations:
  - Build on success of existing high-profile centers and share resources/best practices
  - Continue to seek collaborations with funding partners for new efforts

Project-Scale

- *Example: NSF Cyberinfrastructure for Sustained Scientific Innovation program*
- **Targeted research opportunities** with multiple PIs **combining AI and domain science**
- Key recommendations:
  - Adjust novelty requirements for review of proposals applying AI methods to domains
  - Include AI technology in project solicitations and proposals
  - Fund projects that encourage collaboration between AI developers and domain experts

Advocate for Diverse Funding Streams

*AI and interdisciplinary expertise is causing a paradigm shift in how research is conducted, which would benefit from **nimbleness in the opportunities and structures** made available.*

Individual Investigators

- *Example: MPS-ASCEND*
- Nurtures **interdisciplinary experts** who thoughtfully integrate deep domain knowledge with advanced AI skills
- Key recommendations:
  - Offer incentives for universities to train or hire individuals in a dedicated connector role (a “centaur” or polymath)
  - Fund opportunities for upskilling faculty and establishing interdisciplinary postdoctoral/graduate fellowships
  - Provide multi-year funding

Industry Collaborations

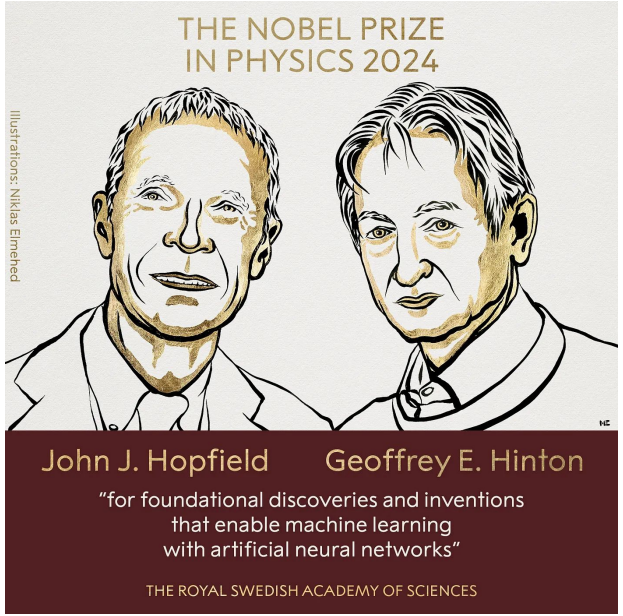
- *Example: NSF Industry-University Cooperative Research Centers*
- Engages **corporate partners to collaborate** on MPS problems, increasing real-world impact and opening a career pipeline for young researchers
- Key recommendations:
  - Leverage existing industry investments in AI and its applications
  - Encourage partnerships with industry
  - Support “reverse sabbaticals” to bring industry experts to academia

Pursue the Science of AI

*Developing a "**Science of AI**" would advance efforts toward powerful and robust AI models that are rigorous, interpretable, and firmly rooted in scientific understanding*

AI Innovations from Science

- MPS researchers are developing **AI innovations infused with scientific principles**, due to requirements for models to adhere to fundamental laws and/or limitations in data.
- Key opportunities:
  - New AI architectures developed using scientific principles
  - Efficient computing and alternative computing platforms
  - Physics-based AI simulations
  - Raising the bar for AI to recognize scientifically impactful results



Pursue the Science of AI

*Developing a "**Science of AI**" would advance efforts toward powerful and robust AI models that are rigorous, interpretable, and firmly rooted in scientific understanding*

Understanding AI Behaviors

- Can improve **trust and usability**, and develop a **theoretical understanding** of learning
- Key opportunities:
  - Apply scientific frameworks to AI
  - Extrapolate from behavioral patterns of agentic systems
  - Perform interpretability experiments on black-box models

Example:
https://www.anthropic.com/research/tracing-thoughts-language-model
(Anthropic)

Robust and Reproducible AI

- Can **improve confidence** in AI tools as effective ways to solve a given problem
- Key opportunities:
  - Develop systematic verification procedures
  - Expand the scope of uncertainty quantification to AI-based approaches
  - Keep mathematical understanding and rigor central to the scientific process

Establish Scalable AI Infrastructures

*With the exponentially increasing use of AI, the need for scalable infrastructure, including **accessible resources, data management, and guidelines**, are crucial.*

Computing Resources

- **Can offset the growing cost of AI tools** with shared moderate-scale GPU clusters, open-source data, and tool repositories.
- Key opportunities:
  - Accessible cloud computing
  - Software development and maintenance
  - Funding for API services
  - Software/hardware interface development
  - Testing unique resources
  - Computing investment from funding agencies

NAIRR Pilot National Artificial Intelligence Research Resource Pilot

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Establish Scalable AI Infrastructures

*With the exponentially increasing use of AI, the need for scalable infrastructure, including **accessible resources, data management, and guidelines**, are crucial.*

Data Management and Access

- Better data is required to build models that can **perform reliably** enough for scientific applications
- Key opportunities:
  - Domain-specific data generation and availability
  - Centralized data facility
  - Curated data archives
  - Public access to data
  - AI-ready data and connecting to computing

Benchmarking and Reproducibility

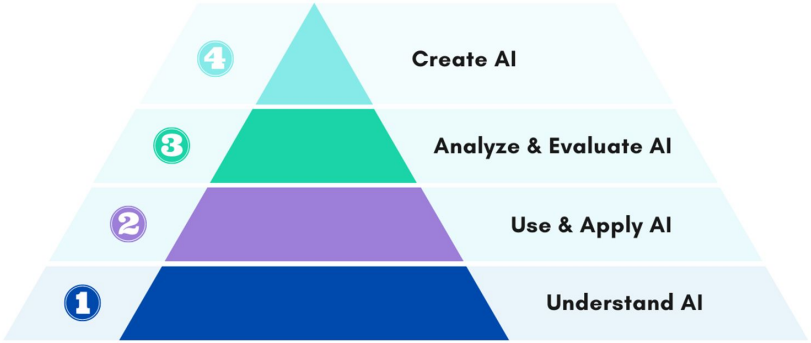
- Can **improve the quality of AI tools** using accessible, scalable training data that is augmented with domain knowledge
- Key opportunities:
  - Documentation incentives and standards
  - Community-wide agreement on data standards, policies, definitions, and benchmarks
  - Evaluation frameworks

Facilitate Interdisciplinary Collaborations

***AI is a common language** between scientific domains that can open lines of communication.*

Knowledge Transfer

- Helps to match the right **scientific questions** with the right **AI approach** and **reduces barriers** to entry to AI
- Key opportunities:
  - Recruit cross-disciplinary experts
  - Conduct trainings
  - Establish an AI literacy framework
  - Improve the quality of AI tools by establishing community standards
  - Develop a shared scientific language, potentially using AI systems to translate



Example AI literacy framework

Facilitate Interdisciplinary Collaborations

***AI is a common language** between scientific domains that can open lines of communication.*

Workshops and Conferences

- Offer **valuable opportunities for AI+MPS researchers to collaborate**, share resources, exchange insights, and discuss challenges (e.g. Kavli Workshops)
- Key opportunities:
  - Science at AI conferences
  - Coding camps/hackathons
  - National joint working group of AI researchers and MPS scientists

Collaborating beyond MPS

- Important to encourage such opportunities as **AI becomes ever more pervasive** and continues to blur disciplinary lines
- Key opportunities:
  - Create a new language/science to understand AI
  - Generate radically new models of AI
  - Understand the broad implications of using AI
  - Define regulations and best practices for ethical use with ethicists and philosophers

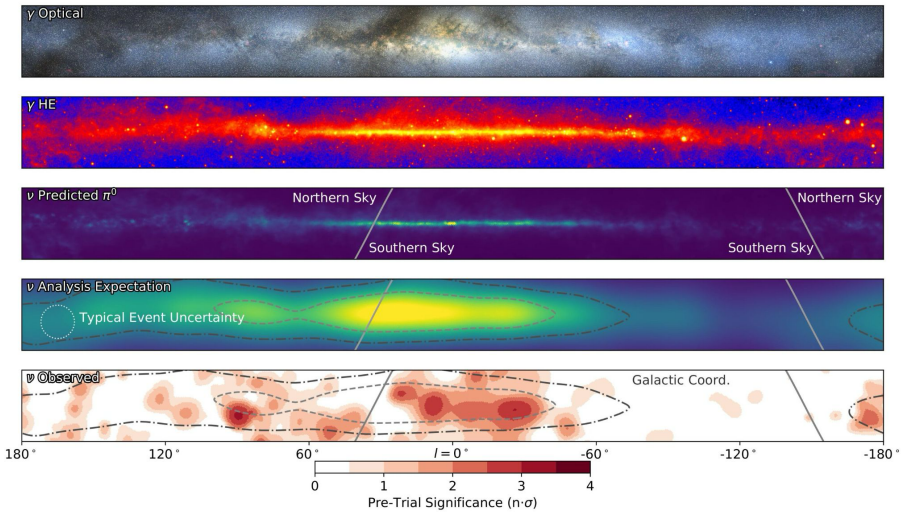
Cultivate Key AI Techniques for Science

*AI serves as a **common language** across various subfields within MPS, providing a **unifying framework** that fosters **holistic understanding**.*

Cross-Cutting Research Opportunities

- Organizing **collaborative efforts** around common AI techniques can be a catalyst for progress
- Key topics:
  - **Simulation-Based Inference**
  - **Multi-Scale Simulations**
  - **Uncertainty Quantification**
  - **Foundation Models**
  - **AI for Experimental Control**
  - **Data-Efficient Methods**

IceCube Neutrino Observatory



https://phys.org/news/2023-06-ghost-particle-image-milky-galaxy.html

Cultivate Key AI Techniques for Science

*AI serves as a **common language** across various subfields within MPS, providing a **unifying framework** that fosters **holistic understanding**.*

Additional Research Opportunities

- Other examples relevant across multiple domains but perhaps less pervasive:
  - **Inverse problems**
  - **Anomaly detection**
  - **Heterogeneous data**
  - **Balancing physical insights**
  - **Improving simulations**
  - **Accounting for bias**
  - **Transfer learning and domain adaptation**
  - **High-throughput experiments**

Leverage AI for Conducting Research

*AI can be used as a tool for **streamlining the way research is conducted** by supporting automation, synthesis, and even at times act as a thought partner in hypothesis generation and scientific workflows.*

AI Co-Pilot

- **Interactive AI** that assists with performing complex tasks
- Key opportunities:
  - Literature search and visualization
  - Hypothesis generation
  - Translate technical content for a broad audience
  - Speed up hypothesis testing and validation

Self-Driving Labs

- Ingest data and determine what experiments to conduct to **advance a scientific objective**
- Key opportunities:
  - Utilize expertise from domain science, data science, and robotics
  - Consider transferability, modularity, and flexibility

Digital Twins

- Incorporate feedback loops to synchronize simulations with real-world counterparts and **perform real-time actions** in response to predictions
- Key opportunities:
  - Literature search and visualization
  - Hypothesis generation, testing, and validation
  - Translate technical content

Educate and Train an AI+MPS Workforce

*The advancement of AI+MPS heavily depends on **strategic workforce development** that addresses both training in the use and development of AI methods, and leveraging AI to transform how we teach and learn.*

Faculty and Leadership Training

- Can help **overcome hesitations** and **create pathways** for broader adoption
- Key opportunities:
  - Support interdisciplinary faculty in tenure and promotion
  - Recruit and hire innovative AI pioneers in MPS domains
  - Upskill faculty to integrate AI
  - Incentivize development of courses with AI components
  - Address AI concerns directly

Postdocs and Research Scientists

- Leveraging interdisciplinary expertise will be crucial for **maintaining global leadership** in the academic workforce
- Key opportunities:
  - Fund interdisciplinary postdoctoral fellowships
  - Co-sponsor postdoctoral positions with industry
  - Provide specialized training opportunities for research scientists

Educate and Train an AI+MPS Workforce

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Graduate Education

- Develop students' ability to identify **AI-based solutions** and **opportunities for innovation**
- Key opportunities:
  - Establish interdisciplinary PhD programs
  - Implement graduate certificates with modular, stackable credentials
  - Utilize graduate admissions to identify future interdisciplinary leaders
  - Create online masters programs in AI+Science
  - Develop formal internship programs in partnership with industry

Undergraduate Education

- Students who **effectively leverage AI tools** will have significant advantages over those who do not
- Key opportunities:
  - Integrate AI and computational skills into curriculum
  - Enhance teaching with AI tools
  - Provide access to public domain AI tools, resources, and pedagogy
  - Combine expertise to develop educational infrastructure

Educate and Train an AI+MPS Workforce

*The advancement of AI+MPS heavily depends on **strategic workforce development** that addresses both training in the use and development of AI methods, and leveraging AI to transform how we teach and learn.*

K-12 and Public Education

- Cultivate a **strong pipeline of researchers** to join the MPS community in the coming years
- Key opportunities:
  - Educate about AI, especially in relation to STEM, through press releases, user-friendly web applications, science fairs, open houses, and community events
  - Establish a system of stackable modules for core AI competencies
  - Establish standard definitions for AI literacy and proficiency
  - Invest in AI education for community colleges and technical schools
  - Train K-12 educators to utilize AI technologies to enhance K-12 learning

Empower AI Innovation

*By removing barriers for AI adoption, we can help **empower more researchers** to integrate AI into their work and contribute their domain expertise to innovation.*

Cost-Efficient Computing

- Costs of compute and data storage resources to **support modern AI-enabled science** are substantial
- Key opportunities:
  - Leverage scientific innovation for more efficient computing solutions
  - Increase adoption of smaller, more structured models
  - Utilize model distillation
  - Prioritize well-designed code and professional software development

Scientific Integrity

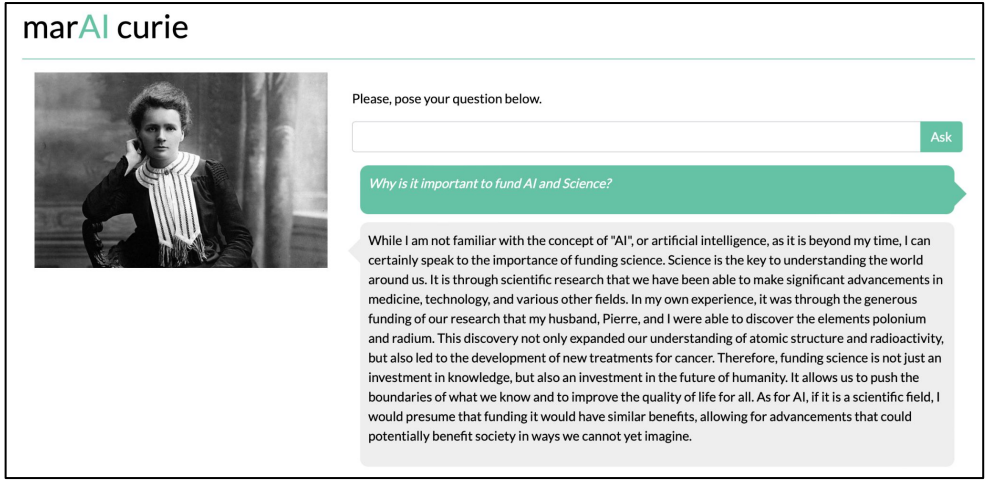
- Given AI's influence, we must reconsider **what defines our contributions** to scientific knowledge and **what gives meaning** to scientific work.
- Key considerations:
  - Protect academic integrity
  - Address AI skepticism
  - Provide interpretable and/or reproducible results
  - Advocate for the disclosure of training data
  - Maintain data provenance
  - Make AI accessible

Empower AI Innovation

*By removing barriers for AI adoption, we can help **empower more researchers** to integrate AI into their work and contribute their domain expertise to innovation.*

Public Engagement on AI+Science

- Proactive public engagement can help **foster public trust** in scientific research
- Key opportunities:
  - Establish programs to increase AI literacy
  - Emphasize the connection between AI and national interests/economic competitiveness
  - Address ethical considerations important to the public



https://github.com/GaiaGrosso/ChatXYZ

Domain-Specific Opportunities

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Domain-Specific Opportunities

*It is important to recognize and engage the specific **methods, culture, and drivers** for each MPS domain*

Astronomical Sciences

The Vera C. Rubin Observatory and the Nancy Grace Roman Space Telescope will generate **unprecedented data volumes** that far exceed traditional analysis capacities, presenting **substantial computational and analytical challenges** and making them ideal candidates for AI applications.

Chemistry

AI is helping chemists predict reactions, design molecules, and analyze complex datasets with **speed and precision**, and theoretical chemistry has inspired some of today's **most powerful generative models**.

Materials Science

AI is **accelerating the pace** of molecular and materials discovery and enabling the development of new design, discovery, and engineering modalities, and materials science presents the opportunity to **build robust AI/ML models** in the face of uncertain and sparse data.

Mathematical Sciences

Mathematics and statistics form the **foundational backbone of AI**, supplying essential techniques, tools, and theoretical frameworks. AI allows for **tackling previously intractable problems** such as high-dimensional statistics and differential equations, data-driven simulation, surrogate modeling, theorem proving, and discovery of mathematical objects.

Physics

AI is being used to **accelerate theoretical calculations**, **improve the operations** of frontier experiments, and **analyze and interpret** rich and unique datasets. Physics involves various unique data types and data requirements that **push the boundaries** of AI.

Recommendations to AI+MPS Stakeholders

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Recommendations for Funding Agencies

Through solicitations and strategic planning, **funding agencies play a crucial role in helping shape the direction of future research** and providing guidance to the scientific community about outcomes that will be most impactful

- **Support interdisciplinary projects, institutes, and researchers**
- **Centralize and scale access to computing resources and data**
- **Fund research in high-priority, cross-cutting areas**

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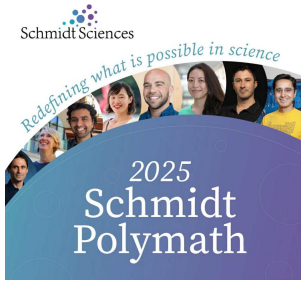
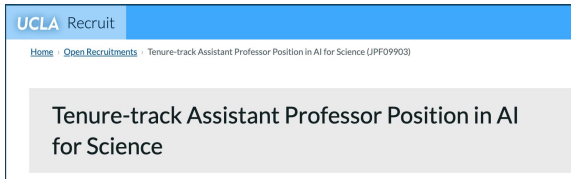


Recommendations for Educational Institutions

Educational institutions will play an important role in **optimizing the integration of AI** into teaching, learning, and training

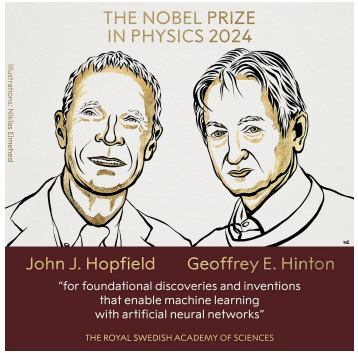
- **Hire and support interdisciplinary researchers**
- **Establish AI+Science degree programs**
- **Build relationships with industry**

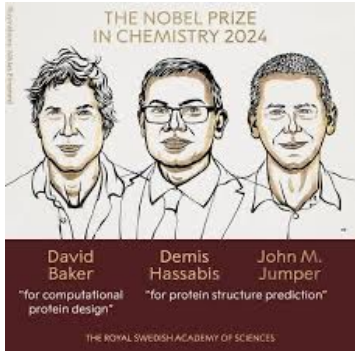


Recommendations for Individual Researchers

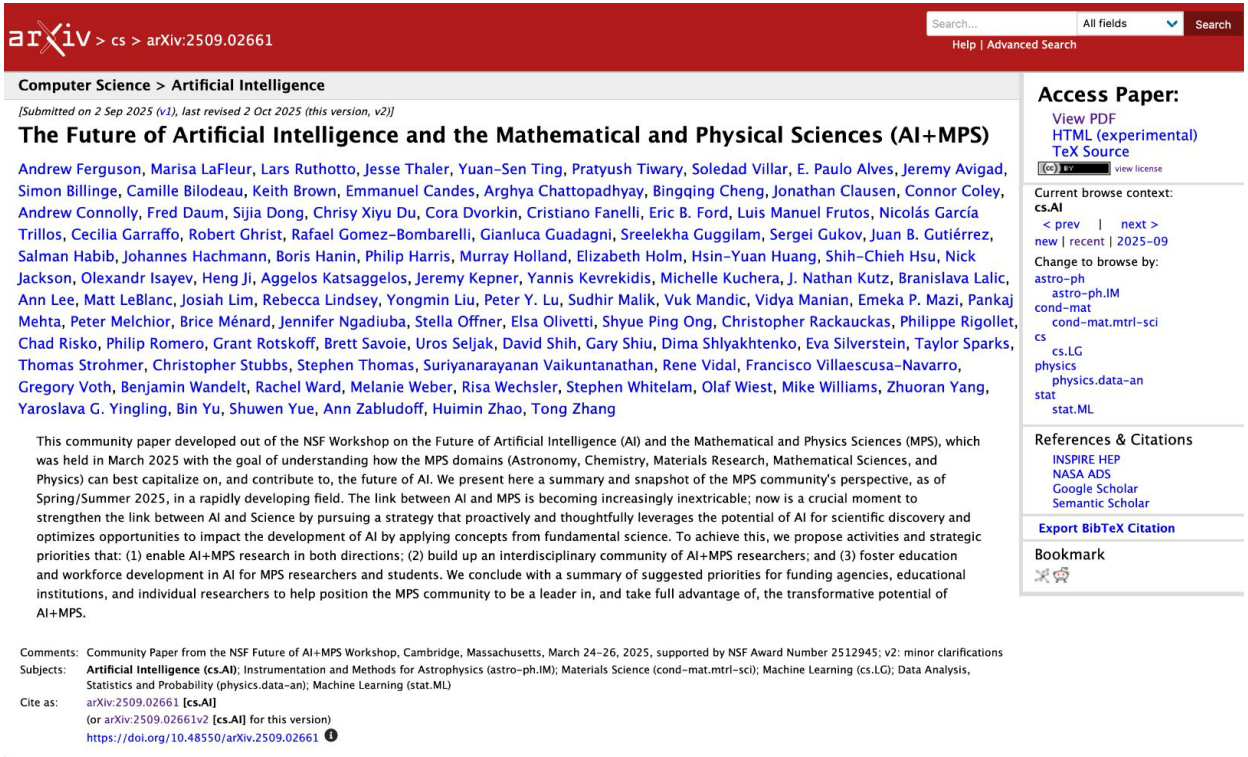
At the heart of **scientific discovery and AI innovation** are individual researchers, as they explore and develop new tools, build connections across disciplines, and apply scientific principles to understanding AI.

- **Leverage scientific insights to improve, understand, and test AI tools**
- **Explore opportunities for using both off-the-shelf AI tools and bespoke tools**
- **Collaborate across disciplines to broaden applications, reduce redundancy, and accelerate scientific discovery**





We hope our report is a valuable resource and advocacy tool for the AI+MPS community!



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[Submitted on 2 Sep 2025 (v1), last revised 2 Oct 2025 (this version, v2)]

The Future of Artificial Intelligence and the Mathematical and Physical Sciences (AI+MPS)

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This community paper developed out of the NSF Workshop on the Future of Artificial Intelligence (AI) and the Mathematical and Physics Sciences (MPS), which was held in March 2025 with the goal of understanding how the MPS domains (Astronomy, Chemistry, Materials Research, Mathematical Sciences, and Physics) can best capitalize on, and contribute to, the future of AI. We present here a summary and snapshot of the MPS community's perspective, as of Spring/Summer 2025, in a rapidly developing field. The link between AI and MPS is becoming increasingly inextricable; now is a crucial moment to strengthen the link between AI and Science by pursuing a strategy that proactively and thoughtfully leverages the potential of AI for scientific discovery and optimizes opportunities to impact the development of AI by applying concepts from fundamental science. To achieve this, we propose activities and strategic priorities that: (1) enable AI+MPS research in both directions; (2) build up an interdisciplinary community of AI+MPS researchers; and (3) foster education and workforce development in AI for MPS researchers and students. We conclude with a summary of suggested priorities for funding agencies, educational institutions, and individual researchers to help position the MPS community to be a leader in, and take full advantage of, the transformative potential of AI+MPS.

Comments: Community Paper from the NSF Future of AI+MPS Workshop, Cambridge, Massachusetts, March 24–26, 2025, supported by NSF Award Number 2512945; v2: minor clarifications

Subjects: **Artificial Intelligence (cs.AI)**; Instrumentation and Methods for Astrophysics (astro-ph.IM); Materials Science (cond-mat.mtrl-sci); Machine Learning (cs.LG); Data Analysis, Statistics and Probability (physics.data-an); Machine Learning (stat.ML)

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Summary and Conclusions

*The opportunities in AI+MPS are vast, so now is the time to ensure that the MPS domains **capitalize on, and contribute to**, the future of AI.*

- AI could achieve a real moon-shot in an MPS domain, so we encourage MPS researchers to **keep sight of the big questions** that AI (and perhaps only AI) could potentially answer.
- The virtuous cycle of AI+MPS has the potential to be transformative for both---offering **insight into AI**, **accelerating the pace of scientific discovery**, and **developing robust science and AI** tools.
- By developing an **intentional strategy**, the MPS community is well positioned to be a leader in, and take full advantage of, the coming waves of AI.

Thanks to the NSF AI+MPS workshop co-organizers and participants for their thoughtful contributions!
I look forward to your questions, comments, and suggestions!