

Open Discussion

1 hour



Final Questions and Feedback

- What is something that **has not** been said thus far that you want to make sure we capture?
- What is something that **has** been said already that you feel is particularly important and you would like to amplify?



To provide any additional thoughts (including general thoughts):

<https://bit.ly/ai-mps-whitepaper-feedback>

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



Closeout: NSF Workshop on the Future of AI for the Mathematical and Physical Sciences (MPS)



March 24–26, 2025



Thanks again to our sponsors!



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Troy Van Voorhis (Chem)
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Carol Cuesta-Lazaro (IAIFI Fellow)
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Valerie Alleyne (LNS)
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We (still) welcome your feedback!

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Mathematical Sciences



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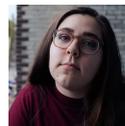
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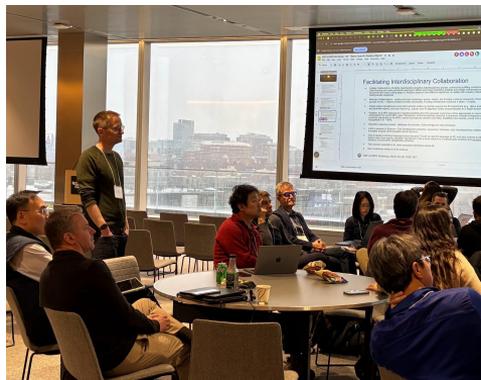
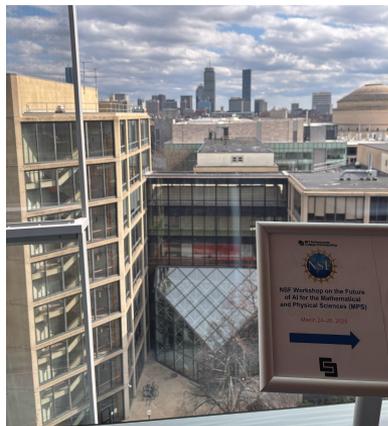
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Thank you for thoughtful discussion!

- It is invigorating to be surrounded by people who are **passionate** about the transformative potential of AI + MPS...
- ...while also **thoughtful and forthright** about the challenges we face as an interdisciplinary community.
- Let's hope that these strategic conversations will turn into scientific opportunities!
- Perhaps we'll meet again...



Related Recent and Upcoming Events

- Dimensionality reduction techniques for molecular dynamics, Univ. of Edinburgh, June 2025;
- Recent Advances in Modeling Rare Events (RARE): Methods and Applications, Khajuraho, India, March 2025;
- Data-driven, low-dimensional, and generative models for molecular and materials discovery and design, Paris, June 2025;
- Biomolecular Dynamics in the Age of Machine Learning,' CECAM-US-CENTRAL at UW Madison, July 2025;
- Machine Learning Advances for Molecular and Materials Property Prediction, CECAM-US-CENTRAL at University of Notre Dame, 2025;
- IAIFI Summer Workshop, Harvard University, August 2025

Email Marisa if you know of other events, and we'll update this slide!



Planned Next Steps

- **Friday, March 28, 2025:** Deadline to submit feedback on the current white paper draft: <https://bit.ly/ai-mps-whitepaper-feedback>
- **Friday, April 11, 2025:** Revised white paper draft sent for review/feedback
- **Friday, April 18, 2025:** Deadline to submit feedback on revised draft
- **Friday, May 2, 2025:** Final(ish) draft send to the NSF and MPS community
- **TBA:** Additional rounds of feedback? Peer review? Authorship/endorsement? ArXiv posting?

Reminder: The end goal is a public report to the MPS community that will be posted (at minimum) on the arXiv

