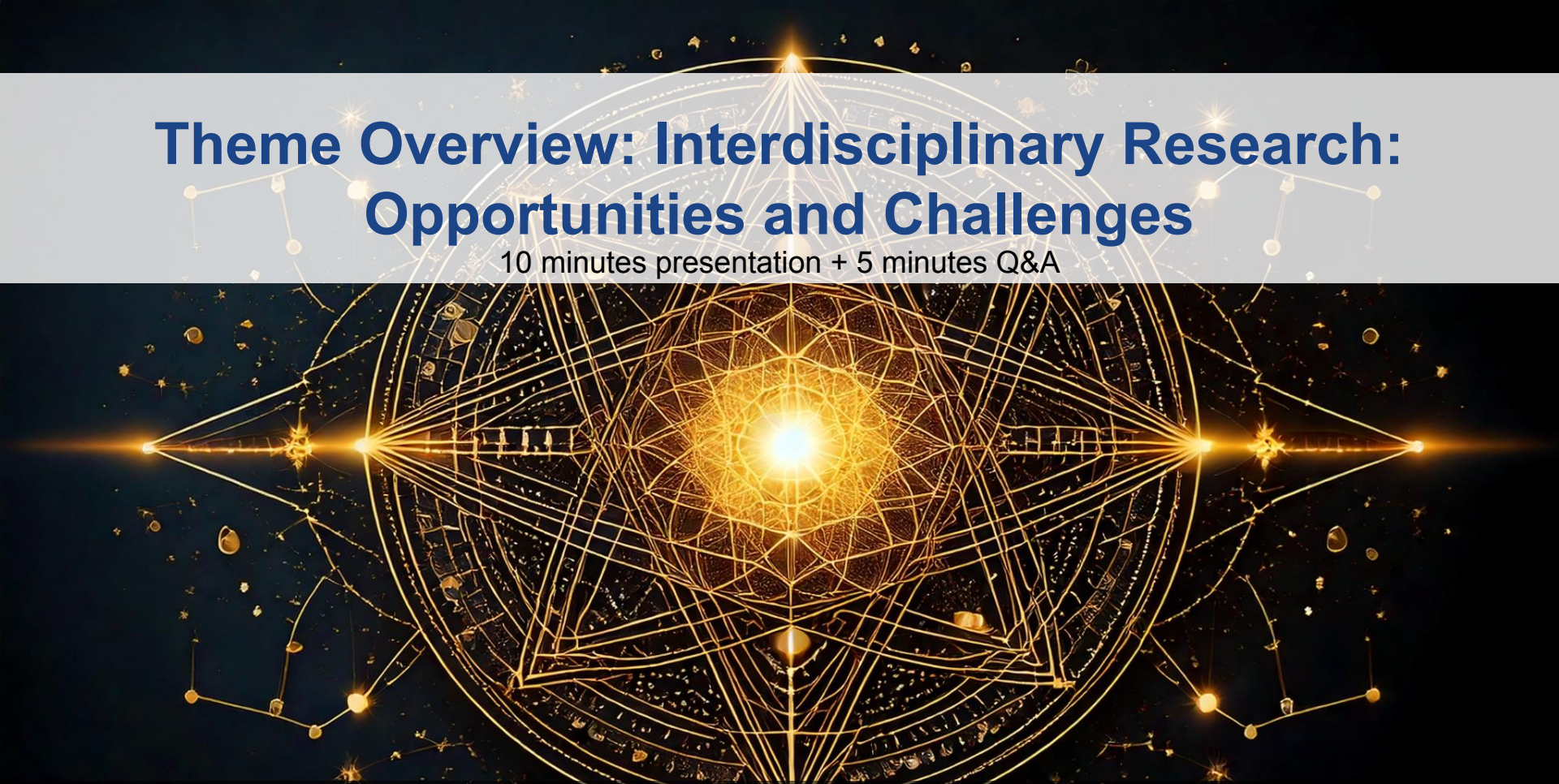
Theme Overview: Interdisciplinary Research: Opportunities and Challenges

10 minutes presentation + 5 minutes Q&A



Lars Ruthotto, Emory University

Theme Charge

- For many MPS researchers, AI represents a fundamental shift in the way they carry out their research and the resources they need. To **overcome shared barriers** to AI integration, the MPS community should work together to **develop solutions** and **enable research collaboration**.
- This theme outlines specific **recommendations for the MPS community** to address challenges, suggests **opportunities for shared research directions,** and outlines ways for **funding agencies and researchers to facilitate interdisciplinary collaboration**.

Common Interdisciplinary Opportunities

- **Research:**
  - Data processing and imaging
  - Predictions, simulations, and discovery
  - Pattern recognition and anomaly detection
  - Multimodal, science-informed models
  - High-dimensional statistics
  - Inverse problems
- **Automation**:
  - Self-driving labs
  - Hypothesis and research workflow generation
  - Experiment design, control, and optimization
- **Advancing AI:**
  - Industry collaboration
  - Evaluating different approaches
  - Boot camps with CS community
  - Frameworks for when to use AI
- **Science of AI**:
  - Incorporating scientific insights
  - Accounting for bias/quantifying uncertainty
  - Robust/interpretable AI
  - AI as a common language

These opportunities are summarized from responses to the survey–more to be discussed in the breakout groups!

Common Interdisciplinary Challenges/Barriers

- **Data Quality and Size:** MPS researchers require better data to build models that can perform reliably enough for scientific applications.
- **Data Management:** Each domain has different expectations for data distribution and access. The lack of a federal or national data infrastructure impedes the development of data-intensive AI systems.
- **Learning Curves:** A common concern among MPS researchers is a lack of time to effectively integrate AI tools into existing workflows and there can be a steep learning curve for researchers looking to integrate AI into their research.
- **Ability to Generalize:** While many MPS domains have achieved state-of-the-art results using AI tools, these results do not typically generalize well to new questions.
- **Reproducibility and Accuracy:** MPS researchers are concerned about AI's heuristic nature and that it may lack mathematical rigor necessary.
- **Trust and Interpretability:** The MPS community increasingly demands explainable AI methods that not only make predictions but also reveal the physical relationships and features driving those predictions.
- **Communication Gaps:** A lack of AI/statistical inclination in domain experts leads to false assumptions, negative biases that are difficult to overcome, and a negative feedback loop in hiring. While some domain experts may harbor skepticism about AI, other researchers in the field sometimes superficially apply basic ML algorithms and label it as AI research, which further reinforces the skepticism among domain specialists.

Facilitating Interdisciplinary Collaboration

- **Challenges to Interdisciplinary Collaboration:**
  - Learning barriers across scientific domains and with AI
  - Communication and cultural barriers across disciplines and subdomains
  - Difficulty identifying opportunities amenable to AI
  - Challenges in implementation and generalizing across domains
- **Opportunities for Facilitating Interdisciplinary Collaboration**
  - Simplify the operational aspects of AI tools
  - Hold workshops to familiarize faculty with these tools
  - Utilize AI systems to facilitate knowledge exchange across traditionally separate domains
  - Develop systematic verification procedures for AI predictions
  - Improve the quality of AI tools with accessible, scalable training data that is augmented with domain knowledge
  - Embed physical principles into ML models to make predictions more interpretable and accurate

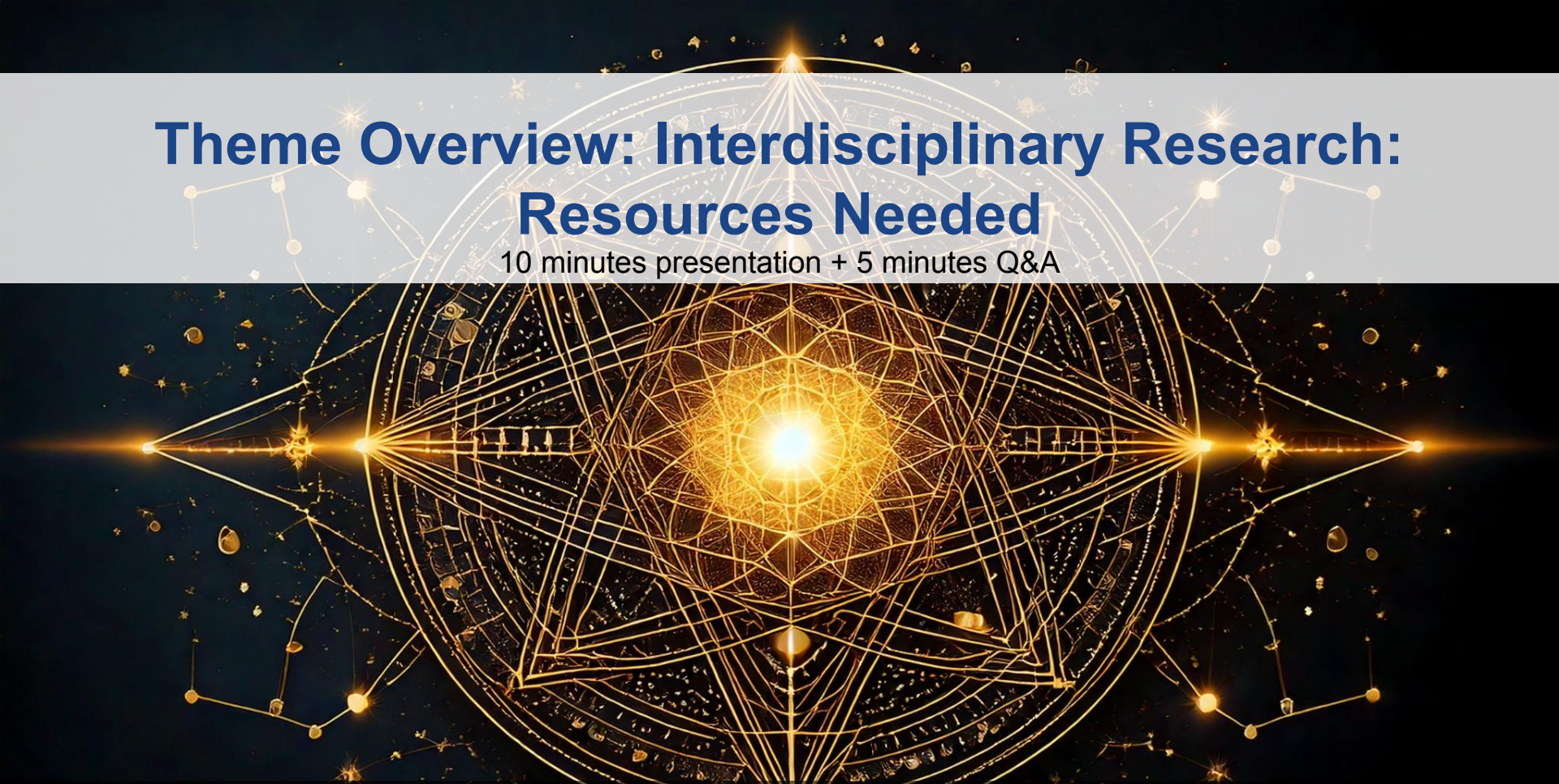
Questions to Consider

- What other challenges do you see in advancing AI+MPS research?
- What strategies are needed to help bring domain researchers together for AI+MPS research?
- What would be the most impactful interdisciplinary research directions to explore with AI?
- How can MPS advance a “Science of AI” strategy (and should we)?
- What opportunities are there to influence industry, policy, and funding entities regarding interdisciplinary research and the future of AI?

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

Theme Overview: Interdisciplinary Research: Resources Needed

10 minutes presentation + 5 minutes Q&A



Andrew Ferguson, University of Chicago

Theme Charge

- Many of the common barriers above could be addressed through **common resource development** that would help advance the broad use of AI tools in MPS.
- This theme outlines **needs of the MPS community** in order to advance AI.

Computing Resources

- **Access and Sharing:** Increased access and sharing of high-performance computing resources, such as moderate-scale GPUs, open-source data, and tool repositories will help offset the growing costs of AI tools
- **Allocations:** Equipment/computing allocations as part of grants or large, university-wide shared instrumentation grants would be most helpful and practical
- **Efficient Computing:** Domain sciences can help to develop algorithms that make AI run more efficiently on current hardware
- **Scalability:** While there are a lot of new algorithms for efficient training on small-scale systems, there is less work on practical implementation and inference on large-scale systems, where leadership-class computing is required.

Infrastructure

- **Centralized Data:** Moving towards centralized data that is not held by individual universities would help democratize AI tools
- **Structured Data:** Curated and freely accessible databases of high quality, structured data (for an example see the Open reaction database) are needed
- **Data Maintenance:** It will be important to assign/employ dedicated researchers to build and maintain these datasets and to offer appropriate incentives
- **Institutional Resources:** There are a number of opportunities to change how AI use is viewed and incentivized by universities, including better infrastructure for experimental integration and more coherent institutional strategies

Grant Funding System

- **Science of AI:** Additional funding towards developing a “Science of AI” would be beneficial and advance efforts towards reproducible and interpretable AI models
- **Funding Models:** There needs to be broader understanding that capability development takes time; funding models beyond the typical 3-year case needs to become more standard for this type of work.
- **Funding Allocations:** Grants are rarely structured to accommodate AI API services, despite these being functionally equivalent to traditional computing resource expenditures

Metrics, Benchmarks, and Best Practices

- **Community-Wide Standards:** We need community-wide agreement (and adoption of) data standards, benchmarks, policies and definitions.
- **Best Practices:** Establishing best practices for how AI tools should be trained and AI findings reported on would help standardize data practices to enhance reproducibility
- **Frameworks:** For evaluating AI-enabled research, we need frameworks that balance efficiency with preserving the human elements that make scientific discovery meaningful
- **Economic and Environmental Considerations:** Future MPS work will benefit from clearer guidelines and metrics on how AI and compute resources can be used most economically and environmentally

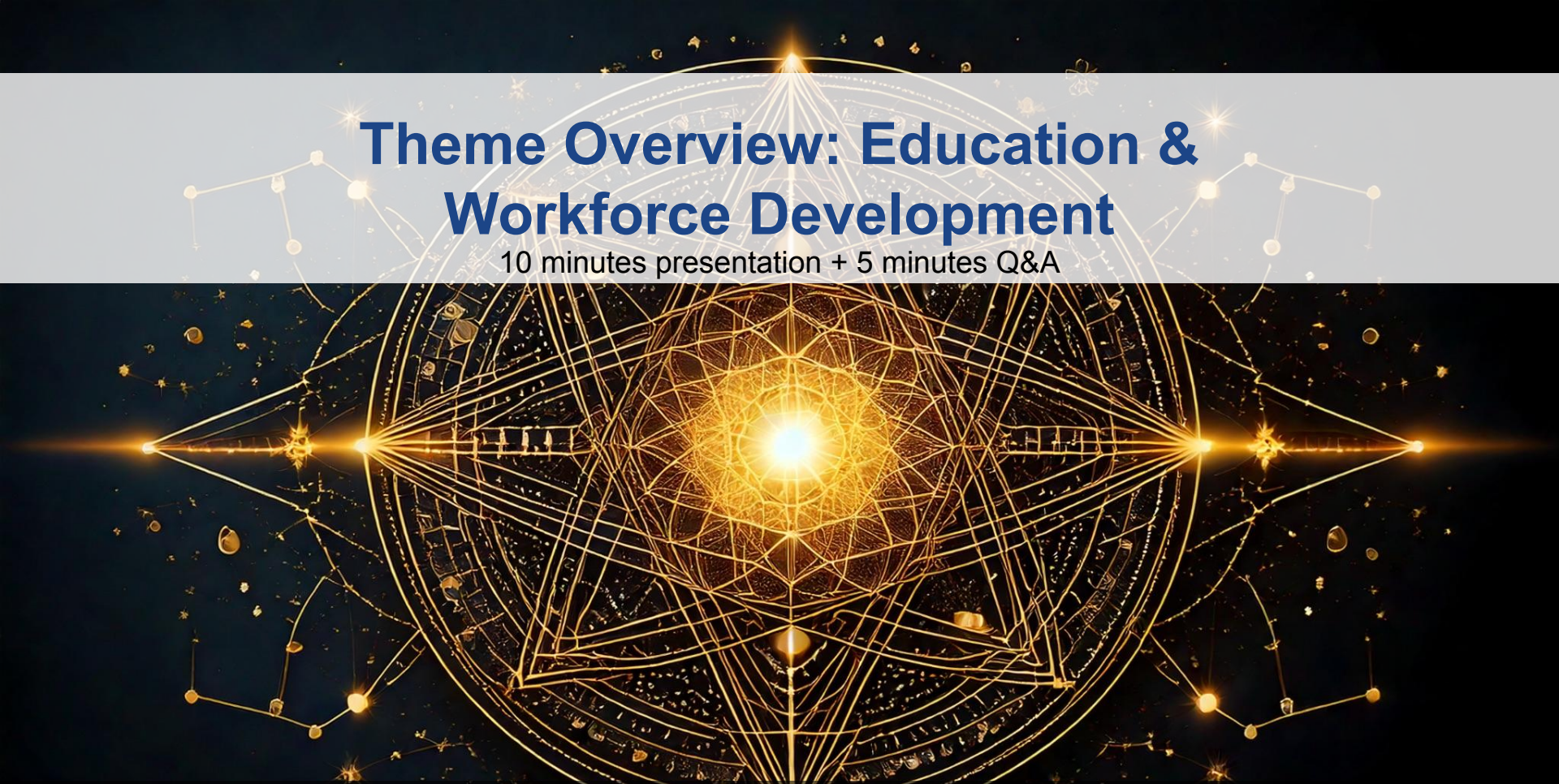
Questions to Consider

- What other resources need to be considered in order to advance AI+MPS?
- What strategies would best facilitate MPS-wide access to resources and development of best practices?
- What is needed from institutions and funding agencies to obtain the resources needed?
- How can we reward, support, and compete for the human resources critical to support physical resources and ensure AI+MPS success (e.g., systems administrators, research scientists, computational technicians)?
- How can the community organize and share best practices, scoreboards, competitions to catalyze innovation (cf. CASP)?

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

Theme Overview: Education & Workforce Development

10 minutes presentation + 5 minutes Q&A



Yuan-Sen Ting, The Ohio State University

Theme Charge

- A key factor shaping the future of AI+MPS will be **how we prepare the workforce**, with training needed for **researchers across all career stages**.

- This theme outlines specific **recommendations for funding agencies and universities** to strengthen training programs.

Common Problems

- **Negative Biases:** A lack of AI/statistical background among domain experts leads to false assumptions, especially for senior faculty who may view these tools with skepticism.

- **Banality in Techniques:** There is general concern that researchers working in the domains lack sufficient skills to advance AI efforts, often **confusing basic/classical machine learning** with modern-day AI techniques.

- **Steep Learning Curve:** Researchers face challenges when attempting to integrate **cutting-edge AI** into their research workflows and methodologies.

- **Retention Problem:** The researchers who are equipped with AI skillsets often choose to **pursue careers in industry** instead of academia.

Undergraduate Level

- **Curriculum:** Probability, statistics, data science, programming, and computational science should be compulsory components to complement standard education.

- **Teaching and Evaluation:** Ensure that students use AI as a research tool and not as a substitute for their own learning.

- **Resources:** Undergraduates should have **access to public domain AI tools** and datasets, with instruction on how to critically analyze and implement them.

- A key challenge is that **most MPS educators are currently underqualified** to introduce students to AI.

Graduate School Level

- **Curriculum:** The traditional semester-based structure of education may need to evolve to accommodate rapidly changing AI technologies.

- **Training:** Develop the **capacity to identify** which problems are suitable for AI tools and to **critically evaluate** AI results for potential issues.

- **Identifying Talents: Higher publication counts might be obsolete.** Students who demonstrate mastery across multiple domains through coursework may prove more adaptable.

- Career Pipelines: **PhD programs designed for AI+Science**, complemented by fellowships, internships, and industry partnerships.

Faculty Level

- **Continual Post-Training:** Comprehensive **upskilling of tenured professors** may become necessary over the next decade to keep pace with AI integration.

- **Faculty Hiring:** Universities should prioritize **hiring AI pioneers in the MPS** field rather than simply recruiting MPS researchers who use AI tools.

- **Reviewer Training:** Journals in MPS disciplines should invest in enhanced training for editors and referees to recognize meaningful AI research contributions.

- **Open Discussion:** Encourage **good-faith, open-minded debate** throughout educational contexts about the **fundamental purpose, foundations, and philosophy of science** in the AI era.

K12 and General Public

- Educational Outreach: Develop engaging activities and curriculum resources to introduce AI concepts to **K-12** students in age-appropriate ways.

- **Public Motivation:** Transform the "race for AI" narrative into a catalyst for scientific literacy and education, similar to how the space race inspired STEM interest.

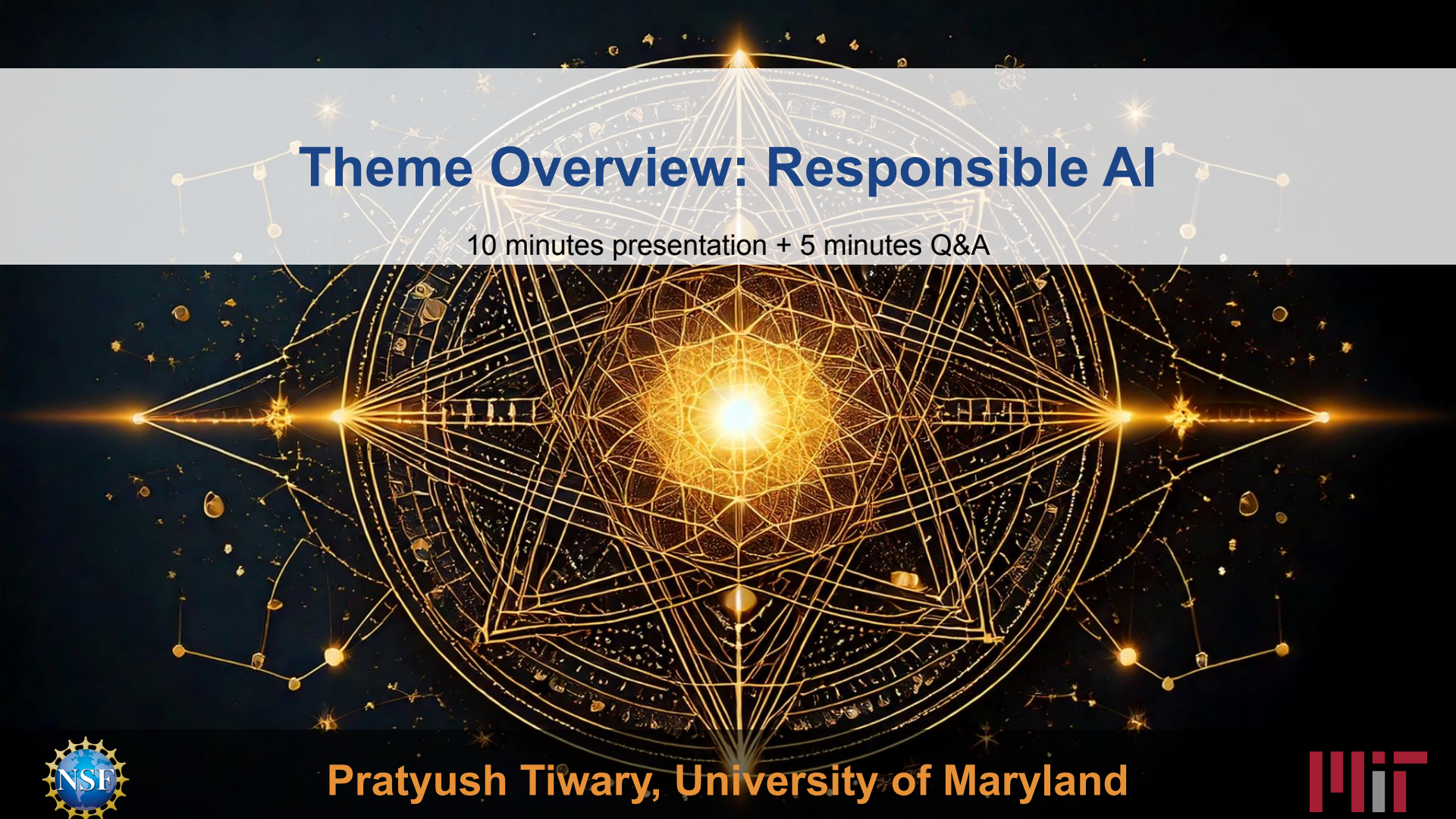
Questions to Consider

- What should **academic departments** be doing to address AI+Science?
- What updates need to be made to **PhD programs** to facilitate AI+Science?
- How can we strengthen the **career pipeline in AI+Science**?
- What can be done to enable AI+Science progress at the **faculty level**?
- How can **funding entities** help to facilitate education and workforce development?

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

Theme Overview: Responsible AI

10 minutes presentation + 5 minutes Q&A



Pratyush Tiwary, University of Maryland

Theme Charge

- Across the MPS disciplines, it is important to consider how to **integrate AI responsibly.**
- These considerations can range from **societal implications** to scientific **integrity** and have a significant impact on the **reliability of AI tools** as well as the **trust** instilled in these new methods.
- This theme identifies **key considerations for AI implementation** by the MPS community.

Interpretability, robustness, and uncertainty quantification

- **Transparent Comparisons:** Often, there is a lack of transparent comparisons with existing methodologies, making it unclear if an AI tool is the “best” way to solve a given problem, over a more classical tool
- **Interpretable Insights:** Researchers want AI methods that are less “black box” and that provide interpretable insights which can be tied to physical processes. (But then, what is interpretability?)
- **Robust Uncertainty and Out-of-distribution generalization Estimation:** In all applications that involve inference of some physical model parameters, uncertainty estimates on these parameters are critical. However generative AI approaches that are often used to make simulations and assess uncertainties are only as good as the model that makes them, the datasets used, and can suffer from errors (hallucinations etc) with little quantifications of out-of-distribution (OOD) generalization, which might be critical for AI in MPS

Distrust of AI

- **Case Studies:** To enhance adoption of AI in domain sciences, success stories need to be highlighted through real-world case studies.
- **Reproducibility:** Hallucinations remain a problem and reproducibility can be impossible even within the same group, both of which remain barriers to establishing trust
- **Scientific Rigor**: Common concerns are violations of fundamental laws and lack of rigor; there seems to be a compromise between speed and reliability
- **Expectations and Hype:** AI methods can be **significantly** exaggerated in their performance and there is very little trust for them; there needs to be care from the community and federal agencies to ensure that “good science” is being followed in order to mitigate potential falls off the “hype” curve
- **Communicating AI Potential:** AI could be considered the most positive and build-oriented development in a lifetime, so the community should imagine what can go right and push for that

Ethical Considerations

- **AI and Society:** The societal conversation involves topics like AI ethics, AI safety, AI alignment, AI trustworthiness, etc, and the MPS community should discuss how to connect their work to these concerns
- **Resource Use:** Science can develop algorithms to improve the data and computational efficiency of AI/ML, which will help democratize the use of AI and battle the immense energy costs.
- **Data Privacy:** Data privacy considerations, especially in fields like medical research, should not be overlooked.

Academic/Scientific Integrity

- **Peer Review:** It is important to examine the quality of scientific reviews; academic integrity is harder to enforce in the fast moving AI related areas
- **Expertise:** It is necessary to reconsider what gives meaning to scientific work:
  - What will we do when the trusted source of knowledge becomes ChatGPT rather than papers? How will this affect how we choose problems and evaluate the work of others?
  - As we move away from interpretable models towards black-box predictions, how do we establish domain assurance, validate results, and maintain scientific rigor? What does “rigor” look like?
  - What constitutes the essence of scientific discovery when AI systems can handle increasing portions of the research process?
  - What does it mean to “do science” when the boundary between human and AI contributions becomes increasingly blurred? How do we preserve the uniqueness of human inquiry and creativity while leveraging AI capabilities?
  - At what point does extensive AI assistance transform the nature of authorship and scientific contribution?
- **Academic Pipeline:** The scientific community should remain vigilant about the potential for AI to disproportionately attract researchers and students toward subfields more readily compatible with AI methodologies

Questions to Consider

- Should we have common minimum “guardrails” for AI in MPS, and if so, what should they be?
- How can science contribute to concerns of AI interpretability, trustworthiness and misuse?
- Are we willing to sacrifice interpretability for the sake of predictive power?
- What considerations of responsible AI are often overlooked and how can the MPS community address them?
- What can institutions and funding entities do to support and incentivize scientific integrity and responsible resource use?
- What are the top priorities for MPS researchers to consider in terms of responsible AI going forward?

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

Coming Up Next…

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