Symposium on the Impact of Generative AI in the Physical Sciences

MIT Schwarzman College of Computing
March 14–15, 2024

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Additional support
a3d3.ai

Sponsored by MIT Office of the Provost
Mapping out the future of Generative AI at MIT

July 2023

Call for proposals: Impact papers on generative AI

July 13, 2023

Sally Kornbluth, President | Cynthia Barnhart, Provost

Dear colleagues,

Given the rapid evolution and mounting societal impact of generative AI, we believe now is the time to foster a community-wide dialogue that is informed by rigorous research. In the spirit of the symposium scheduled for October 2023, we invite you to submit proposals that articulate effective roadmaps, policy recommendations, and calls for action across the broad domain of generative AI. Our goal is to disseminate findings widely to industry leaders, other academic institutions, policymakers, and the general public.

With the goal of marshaling MIT's expertise in this arena to inform public discourse on the development and application of generative AI, we are pleased to announce a call for proposals: We seek to fund the work of individual PIs or groups of faculty to develop impact papers that articulate effective roadmaps, policy recommendations, and calls for action across the broad domain of generative AI. Our goal will be to disseminate these papers widely to industry leaders, other academic institutions, policymakers, and the public.

Noticeably missing: science!

New call for proposals: Impact papers on generative AI

October 24, 2023

Sally Kornbluth, President | Cynthia Barnhart, Provost

Dear colleagues,

Over the summer, we wrote you to invite proposals to develop impact papers that articulate effective roadmaps, policy recommendations, and calls for action across the broad domain of generative AI.

The response was beyond anything we could have predicted – a total of 75 proposals, across a broad swath of topics. From the first round, 27 proposals were selected for funding.

But the groundswell of interest and the caliber of the ideas overall made clear that a second round was in order – so we write with excitement to announce that today.

We encourage you to submit a proposal, as an individual or as a group, provided you were not part of one of the proposals selected in the first round.

Multidisciplinary teams are particularly welcome, especially in those realms where generative AI intersects with education, with scientific discovery, or with design and creativity. We encourage school, college, and DLCI leadership to help identify and foster multidisciplinary
AI + Science: A growing movement

Particle physics
DeZoort et al [Nat.Rev.Phys. 2023]

Molecules & materials
Batzner et al [NeuIP; Nat.Comm. 2021]

Astrophysics

Proteins
Watson et al [RFDiffusion; Nature. 2023]

Climate & weather
Google (Neural GCM 2023)

Cosmology
Hahn et al (SimBIG; PNAS 2023)

Proof of concept → Adoption → Progress!
AI + Physics: A new frontier?

Many fields within AI4Science are pushing the frontiers of AI… what about physics?

Reliable inference with complex forward models

- Sampling under complex symmetries and exactness guarantees (e.g., in lattice QFT)
- Statistical anomaly detection
- Highly structured models/data-generating processes
- …

Extremely fast real-time inference

Physics can be a frontier for AI!

(From A3D3 website)
Generative AI / foundation models: *More of the same? A paradigm shift?*

**Augmenting existing capabilities?**

300 ns MD

AlphaFlow

**New ways of doing things?**

**Nanoparticles**

Amorphous carbon

Batteries

Multicomponent alloys

Cathode materials

Carborane

Ammonia/borane

Dissolution

Solvent mixtures

Hydrogen

Perovskites

MOFs

Ice & water

Polymerisation

Aqueous interfaces

Combustion

Molten salts

Dichalcogenides

Dislocation

Pt surface

Si interstitial

Zeolites

Heterogeneous catalysis

**Figure 1:** A foundation model for materials modelling.

Trained only on Materials Project data (Battatia et al), MACE-MP-0 is capable of molecular dynamics simulation across a wide variety of chemistries in the solid, liquid and gaseous phases.

**Collider physics**

Cosmology

Batatia et al, *A foundation model for atomistic materials chemistry*
Broad themes and questions

- What is the potential impact of generative AI in the physical sciences?
  - David Hogg (NYU/Flatiron): Physics-Motivated Approaches to Model Design: Observations and Data Analysis
  - Anna Scaiffe (Manchester): Foundation Models in Physics: Successes in Astrophysics
  - Thea Aarrestad (ETH Zurich): Physics-Motivated Approaches to Hardware Design
  - David Hogg (NYU/Flatiron), Pavel Izmailov (OpenAI), Matt Schwartz (Harvard): Panel: Potential impacts of generative AI in physics

- What are the synergies and differences from other fields?
  - Kevin Yang (Microsoft Research): Foundation Models beyond Physics: Successes in Molecular Biology
  - Simon Batzner (Google): Physics-Motivated Approaches to Model Design: Deep Learning
  - Song Han (MIT EECS): Big vs. Small Generative Models (Song Han)

- What are pathways for contributions from the physical sciences to influence generative AI?
  - Hidenori Tanaka (Harvard): Physics-Motivated Approaches to Model Design: Natural Science of AI

- What is needed from a community perspective to achieve these impacts
  - Dan Huttenlocher (MIT), Vijay Reddi (Harvard), Jesse Thaler (MIT/IAIFI): Panel: Community Perspectives on what is needed for gen AI to fulfill its promise in physics
NSF AI Institute for Artificial Intelligence and Fundamental Interactions

One of the inaugural NSF AI Institutes

(AIAIFI, 🧠: eye-φ)

= AI + Physics*

*Not just “fundamental interactions”!
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https://www.youtube.com/IAIFIInstituteforAIFundamentalInteractions

Public Colloquia

In-person at MIT + Zoom. Next up:
• March 22: Soledad Villar (JHU)
• April 12: Jennifer Ngadiuba (Fermilab)

Summer Workshop

Pre-registration now open
https://iaifi.org/summer-workshop.html
IAIFI Organizers

Phil Harris
Associate Professor, MIT/IAIFI/A3D3

Phiala Shanahan
Associate Professor, MIT/IAIFI

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IAIFI Fellow, MIT/Harvard/IAIFI

Gaia Grosso
IAIFI Fellow, MIT/Harvard/IAIFI

Marisa Lafleur
Project Manager, IAIFI
# Schedule: Day 1

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<th>Speaker</th>
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<th>Time</th>
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<tr>
<td>Anna Scaife</td>
<td>Foundation Models in Physics: Successes in Astrophysics</td>
<td>9:30–10:30 am</td>
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<tr>
<td><strong>Coffee Break</strong></td>
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<td>10:30–11:00 am</td>
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<tr>
<td>Simon Batzner</td>
<td>Physics-Motivated Approaches to Model Design: Deep Learning</td>
<td>11:00 am–12:00 pm</td>
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<tr>
<td><strong>Lunch Break</strong></td>
<td></td>
<td>12:00–1:30 pm</td>
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<tr>
<td>Kevin Yang</td>
<td>Foundation Models beyond Physics: Successes in Molecular Biology</td>
<td>1:30–2:30 pm</td>
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<tr>
<td><strong>Coffee Break</strong></td>
<td></td>
<td>2:30–3:00 pm</td>
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<tr>
<td>David Hogg</td>
<td>Physics-Motivated Approaches to Model Design: Observations</td>
<td>3:00–4:00 pm</td>
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<td></td>
<td>and Data Analysis</td>
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<tr>
<td>Dan Huttenlocher, Vijay Reddi, Jesse Thaler</td>
<td>Panel: Community Perspectives on what is needed for gen AI to fulfill its promise in physics</td>
<td>4:00–5:30 pm</td>
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## Schedule: Day 2

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<tr>
<td>Pavel Izmailov, Matt Schwartz, David Hogg</td>
<td>Panel: Potential impacts of generative AI in physics</td>
<td>9:00–10:30 am</td>
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</tr>
<tr>
<td>Hidenori Tanaka</td>
<td>Physics-Motivated Approaches to Model Design: Natural Science of Artificial Intelligence</td>
<td>3:00–4:00 pm</td>
</tr>
<tr>
<td>Jared Kaplan</td>
<td>Fireside Chat: Jared Kaplan, Anthropic (Virtual) Moderated by Jesse Thaler</td>
<td>4:00–5:15 pm</td>
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**Panel**

**Talks**

**Fireside chat**

**Coffee Break**

**Lunch Break**