Symposium on the Impact of Generative AI in the Physical Sciences





MIT Schwarzman College of Computing March 14–15, 2024

Sponsored by MIT Office of the Provost

Additional support <u>a3d3.ai</u>



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Mapping out the future of Generative AI at MIT

July 2023

Call for proposals: Impact papers on generative Al

July 13, 2023

Sally Kornbluth, President | Cynthia Barnhart, Provost

Dear colleagues,

Given the rapid evolution and mounting societal impact of generative AI, we believ has an opportunity to promote the technology's responsible and publicly beneficia inform the public conversation, and foster wise, farsighted policy. As articulated a inauguration, we must help society "come to grips with the tectonic forces of artif intelligence, containing its risks and harnessing its power for good."

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

Noticeably missing: science!

This symposium: Gen AI + physical sciences

October 2023

New call for proposals: Impact papers on generative Al

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 Al 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

Molecules & materials



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

Batzner et al [NequIP; Nat.Comm. 2021]

Proteins

Ian C. Haydon/UW Institute for Protein Design

Watson et al [RFDiffusion; Nature. 2023]



Astrophysics



Cosmology





Climate & weather



Google (Neural GCM 2023)

Hahn et al (SimBIG; PNAS 2023)

Proof of concept \longrightarrow Adoption \longrightarrow Progress!



Al + 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

• • • •

Framing: Kyle Cranmer

Extremely fast real-time inference



Physics can be a frontier for Al!



Generative AI / foundation models: More of the same? A paradigm shift?

Augmenting existing capabilities?



Jing et al, *AlphaFlow*

Collider physics

Cosmology





New ways of doing things?





Broad themes and questions

• What is the potential impact of generative AI in the physical sciences?

- Anna Scaiffe (Manchester): Foundation Models in Physics: Successes in Astrophysics
- Thea Aarrestad (ETH Zurich): Physics-Motivated Approaches to Hardware Design
- 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

what is needed for gen AI to fulfill its promise in physics

• David Hogg (NYU/Flatiron): Physics-Motivated Approaches to Model Design: Observations and Data Analysis

• David Hogg (NYU/Flatiron), Pavel Izmailov (OpenAI), Matt Schwartz (Harvard): Panel: Potential impacts of

• Dan Huttenlocher (MIT), Vijay Reddi (Harvard), Jesse Thaler (MIT/IAIFI): Panel: Community Perspectives on



NSF AI Institute for Artificial Intelligence and Fundamental Interactions One of the inaugural NSF AI Institutes (IAIFI, \P : eye- ϕ)









Harvard

= AI + Physics*



Northeastern

*Not just "fundamental interactions"!





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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



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Marisa Lafleur Project Manager, IAIFI



Schedule: Day 1

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



Schedule: *Day 2*



Title	Time
I: Potential impacts of generative AI in physics	9:00–10:30 am
	10:30–11:00 am
Big vs. Small Generative Models	11:00am–12:00 pm
	12:00–1:30 pm
cs-Motivated Approaches to Hardware Design	1:30-2:30 pm
	2:30-3:00 pm
vated Approaches to Model Design: Natural Science of Artificial Intelligence	3:00-4:00 pm
side Chat: Jared Kaplan, Anthropic (Virtual) Moderated by Jesse Thaler	4:00–5:15 pm

