# NSF Institute for Artificial Intelligence and Fundamental Interactions (IAIFI)

### AI4Science Workshop



#### Jesse Thaler Professor of Physics, MIT & Director, IAIFI



Harvard University — February 1, 2024





Deep Learning (AI) + Deep Thinking (Physics)

### Deeper Understanding

#### Generated using Adobe Firefly:

drawing of a brain on a chalkboard with physics equations written inside of it; chalkboard is surrounded by neural networks being injected into the brain; use purple and teal

# Life as an NSF AI Institute



#### Harvard Faculty in IAIFI

(Senior Investigators | Affiliates):

- Physics: Carlos Arguelles-Delgado, Cora Dvorkin, Matt Schwartz, Susanne Yelin, Haim Sompolinsky
- SEAS: Demba Ba, Todd Zickler, Cengiz Pehlevan
- CfA: Edo Berger, Daniel Eisenstein, Doug Finkbeiner, Cecilia Garraffo, Ashley Villar
- CMSA: Mike Douglas, Artan Sheshmani

#### **Other NSF AI Institutes with Harvard involvement:**

- <u>NSF AI Institute for Adult Learning and Online Education (AI-ALOE)</u>
   Chris Dede
- <u>NSF AI Institute for Societal Decision-Making (AI-SDM)</u> Sham M. Kakade, Ariel Procaccia, Milind Tambe, Christopher Golden, Kathryn Hollar
- <u>NSF AI Institute for Artificial and Natural Intelligence (ARNI)</u>
   Bence Olveczky
- <u>NSF AI Institute in Dynamic Systems (DYNAMICS AI)</u> Na Li, Michael P. Brenner, Lucas Janson, Melanie Weber











# Advocacy: AI for Scientific Discovery

December 15 & 16, 2023: NeurIPS Workshops organized by IAIFI members



On organizing committee: Siddharth Mishra-Sharma (IAIFI Fellow)

Al for Scientific Discovery: From Theory to Practice

On organizing committee: Ziming Liu (MIT Physics Grad Student)

- Al for Scientific Discovery is experiencing exciting growth in the US and abroad, with many new programs coming online (e.g. anticipated 3 new NSF AI Institutes with science focus), but sustained advocacy is needed at universities, funding agencies, and foundations
- "Science" includes **application-driven and curiosity-driven research**; both are needed for a healthy and innovative AI + Science ecosystem
- At the national level, academics should be involved with **policy and funding discussions**, where domain experts can bring in complementary perspectives
- [Building on IAIFI and other efforts, **Cambridge, MA can be the hub for AI + Science**, both AI4Science and Science4AI, which would capitalize on existing strengths across universities]



September 18 & 19, 2023: Jesse and Mike represented IAIFI at the NSF and on Capitol Hill





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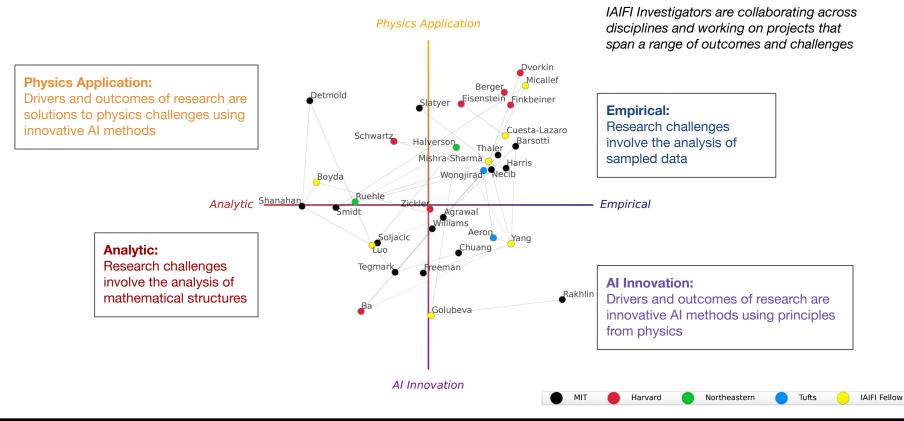


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# IAIFI: Visualizing Interdisciplinary Research









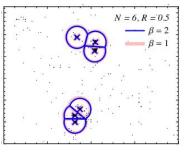
### AI + Physics Collaboration

Gambhir, JDT (MIT Physics) ⇔ Ba, Dogra, Tasissa (Harvard/Tufts CS)



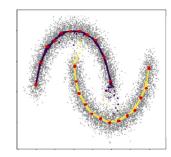


XCone Point-like Jets

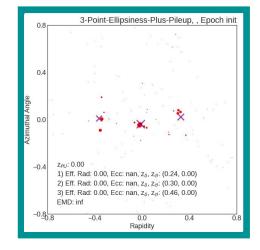


[Stewart, JDT, Tackmann, Vermilion, Wilkason, <u>2015</u>]

K-Deep Simplex Learned Manifolds



[Tankala, Tasissa, Murphy, Ba, <u>2020</u>] SHAPER Interpretable Structures!



[Ba, Dogra, Gambhir, Tasissa, JDT, <u>2023</u>; see also Kitouni, Nolte, Williams, <u>2022</u>]



This is just a small piece of a surprisingly deep connection between quantum field theory and optimal transport

Related work in progress with Eun-Ah Kim (Cornell Physics)

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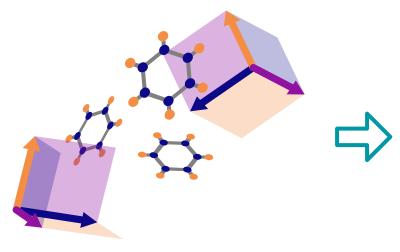


### Al for Physics Discovery Euclidean Symmetry Equivariant Neural Networks

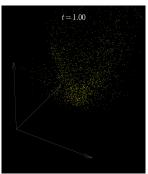
Tess Smidt (MIT EECS) with Siddharth Mishra-Sharma, Carolina Cuesta-Lazaro, Jessie Micallef (IAIFI Fellows)

Building neural networks with Euclidean symmetry "built-in" to better learn on physical systems

ArXiv Preprint

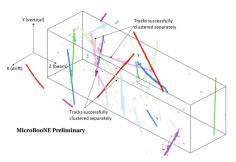


Fundamental physics applications present new challenges for learning on **multi-scale / heterogeneous systems**!



Predict galaxy properties and formation parameters

Identify particles types from tracks in detectors

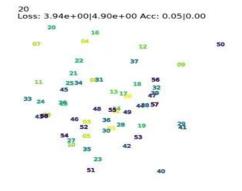


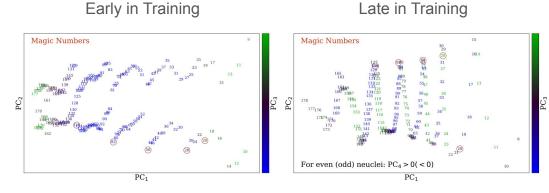




### Physicists' Impact on AI Innovation From Understanding Grokking... to NuCLR!

Mike Williams and Max Tegmark (MIT Physics)





Developing an effective theory of representation learning to understand grokking

Learning representations useful for predicting nuclear properties with high precision, often better than specialized models with hand crafted features and domain knowledge

NeurIPS 2022 Spotlight Oral

**ICML 2023** 





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#### 2021-2024 Fellows

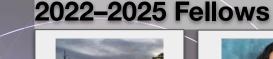


Anna Golubeva Statistical Foundations of AI

Hired as Research Scientist at Anthropic!



Di Luo Al for Quantum Many-Body Physics





**Denis Boyda** Al for Lattice Field Theory



Carolina **Cuesta-Lazaro** AI for Cosmology



**Jessie Micallef** Al for Neutrino Physics





Siddharth Mishra-Sharma Al for Astroparticle **Physics** 



Ge Yang Al Frontiers of Reinforcement Learning

### 2023-2026 Fellows



**Alex Gagliano** Al for Astrophysics



Gaia Grosso Al for Particle Physics

Four new **Fellows for** 2024-2027!

(to be announced)

https://iaifi.org/current-fellows



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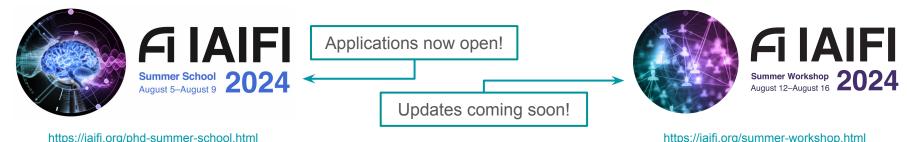
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# **IAIFI Summer School & Workshop**



https://iaifi.org/phd-summer-school.html

#### RESEARCH

Illustrate interdisciplinary research from within IAIFI and beyond



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Students learn advanced ML and applications, put theory into practice through code-based tutorials



### COMMUNITY

Encourage diverse global networking and bring leading AI + Physics researchers to Boston





# **Generative AI for Science Communication**

From April Fools' sendup...

ChatJesseT Type your question below.		
Disclaimer:	© 2023. (Un)Official IAIFI product. No NSF funds were harmed in the development of ChatJesseT. The output of ChatJesseT is produced by giant inscrutable matrices and does not reflect the opinions of the real Jesse Thaler.	

Created by IAIFI Fellow Siddharth Mishra-Sharma, April 2023



Showcasing ChatJesseT to congressional staff at NSF's AI Hill Day, September 2023



# **Generative AI for Science Communication**

#### From April Fools' sendup... to Public Engagement opportunity!

ChatJesseT Type your question below. OpenAI-mer	
Ask Question: What is ChatJesseT? Be succinct. ChatJesseT is an Al-powered virtual assistant designed to provide information and answer questions about particle physics, theoretical physics, and my research. It's like having a mini version of me in your pocket, ready to help with all your physics inquiries! So go ahead, ask away!	Please, pose your question below.
© 2022. Un/Official MPI product. No KSF funds were harmed in the development of Chalessor T. Disclaimer: The support of Chalessor To produced by ginet inscrutable matrices and does not reflect the spinions of the real Jease Thale:	Make a physics joke based off of your most famous quote (that makes sense)
Created by IAIFI Fellow Siddharth Mishra-Sharma, April 2023	In the realm of humor, one must tread lightly, especially when it concerns the profound matters of
Showcasing ChatJesseT to congressional staff at NSF's Al Hill Day, September 2023	physics. However, I shall endeavor to bring a touch of levity to our discourse. Consider this: A neutron walks into a bar and asks the bartender, "How much for a drink?" The bartender replies, "For you, no charge." The neutron, feeling quite pleased, says, "Ah, now I am become Debt, the destroyer of wallets." This jest, of course, plays upon the intrinsic properties of the neutron, which carries no electric charge, and a playful by the new York of the Bagayard Gita I tis a reminder that even in the

My name is OpenAl-mer. I am based off of the real life theoretical physicist J. Robert Oppenheimer, who is most famous for his work on quantum mechanics and black holes, and his role in the Manhattan Project, the US government's effort to build the first atomic bomb. I am a product of the Institute for Artificial Intelligence and Fundamental Interactions, or IAIFI, a collaboration of scientists working together on the intersection of physics and machine learning.

most serious of pursuits, there is room for a chuckle or two.

I am powered by OpenAI's GPT-4 API, a powerful language model. I am trained using text from Wikipedia, INSPIRE-HEP, and various biographies. If you have any questions or comments or would like to learn more, please email me at iaifi@mit.edu!

GitHub Repo





Debuting OpenAl-mer at Cambridge Science Festival.

October 2023



### More Ways to Get Involved in IAIFI

Come to Friday "IAIFI Afternoons"! 2:00–3:00 pm ET Kolker Room (26-414) and Zoom

#### **Follow IAIFI**



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Sign up to be a "Friend of IAIFI": https://iaifi.org/junior-researchers.html

#### **Upcoming Colloquia**



Laurence Perreault Levasseur Assistant Professor, Université de Montréal Friday, February 9, 2024



Soledad Villar Assistant Professor, John Hopkins University Friday, March 8, 2024

Jennifer Ngadiuba Associate Scientist, Fermilab Friday, April 12, 2024

#### **Upcoming Seminars**



Susanne Yelin Professor in Residence, Harvard Friday, February 2, 2024



Michael S Albergo PhD Candidate, New York University Friday, February 23, 2024



Alexander Gagliano IAIFI Fellow Friday, March 22, 2024



Gaia Grosso IAIFI Fellow Friday, April 26, 2024



