MPS | DIRECTORATE FOR MATH AND PHYSICAL SCIENCES

NSF Workshop on the Future of AI

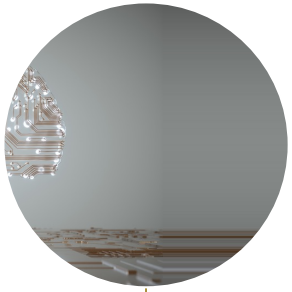
NSF WELCOME

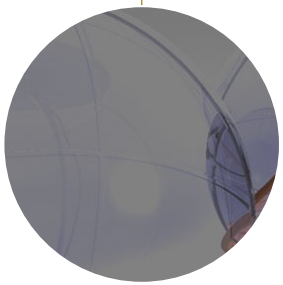
DAVID B. BERKOWITZ

ASSISTANT DIRECTOR

National Science Foundation
Directorate for Mathematical and Physical Science (MPS)

MPS AI Landscape



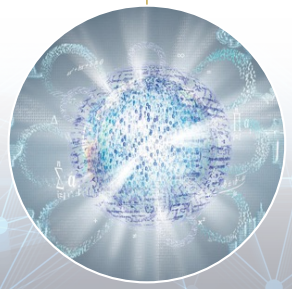


Solicitations &
Core Programs

Institutes
& Centers

Facilities

National AI
Research Institutes



HDR, CCI, MRSEC,
MIP, TRIPODS, ...

MPS and AI-Centric Individual/Small Collaborative

NSF-Wide:

- PD 24-8084: **CDS&E**: Computational and Data-Enabled Science and Engineering

Cross-Directorate/AI-Centric and AI-Driven Science Focused:

- NSF 24-554: **AIMing** : AI, Formal Methods, and Mathematical Reasoning
- NSF 24-569: **MFAI**: Mathematical Foundations of AI
- NSF 24-567: **MFS-SPEED**: Molecular Foundations for Sustainability: Sustainable Polymers Enabled by Emerging Data Analytics
- NSF 24-518: **CAIG**: Collaborations in AI and Geosciences
- NSF 23-614: **SCH**: Smart Health and Biomedical Research in the Era of AI and Advanced Data Science

Discipline-Specific With External Partners and Growing AI-Related Proposals:

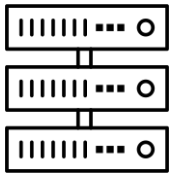
- NSF 23-530: **DMREF**: Designing Materials to Revolutionize & Engineer our Future/**MGI**: Materials Genome Initiative
- NSF 22-569: **AMPs**: Algorithms for Modern Power Systems
- NSF 24-607 **MFB**: Molecular Foundations for Biotechnology

MPS AI Initiatives:

- NSF 21-080: **ADAPT**: Advancing Discovery with AI-Powered Tools in the Mathematical and Physical Sciences

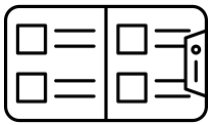
National AI Research Resource (NAIRR)

Vision: A widely-accessible, national research infrastructure that will advance the U.S. AI R&D environment, discovery, and innovation by empowering users through access to:



Secure, high-performance, privacy-preserving **computing**

High-quality **datasets**

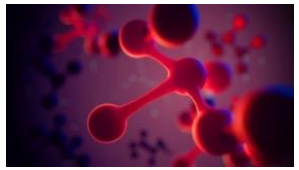


Catalogs of **testbeds** and **educational materials**

Training tools and **user support** mechanisms

NAIRR Pilot Users

AI Researchers



Domain Scientists Applying AI

Students and Educators

US-Based Institutions including:

- Academic institutions
- Not-for-profits
- Federal agencies or federally-funded R&D centers
- State, local, or tribal agencies
- Startups and small businesses with federal grants

National AI Institutes Led By MPS

Institute for Artificial Intelligence and Fundamental Interactions (IAIFI)
Hub: MIT
(PHY 2019786)

Molecule Maker Lab Institute (MMLI)
Hub: UIUC
(CHE 2019897)

NSF-Simons AI Institute for Cosmic Origins (CosmicAI)
Hub: UT-Austin
(AST-2421782)

NSF-Simons AI Institute for the Sky (SkAI)
Hub: Northwestern University
(AST-2421845)

National AI Institutes partnering with MPS

AI Institute for
Dynamical Systems

Hub: University of Washington
(ENG/CBET 2112085)
Partnering with DMS

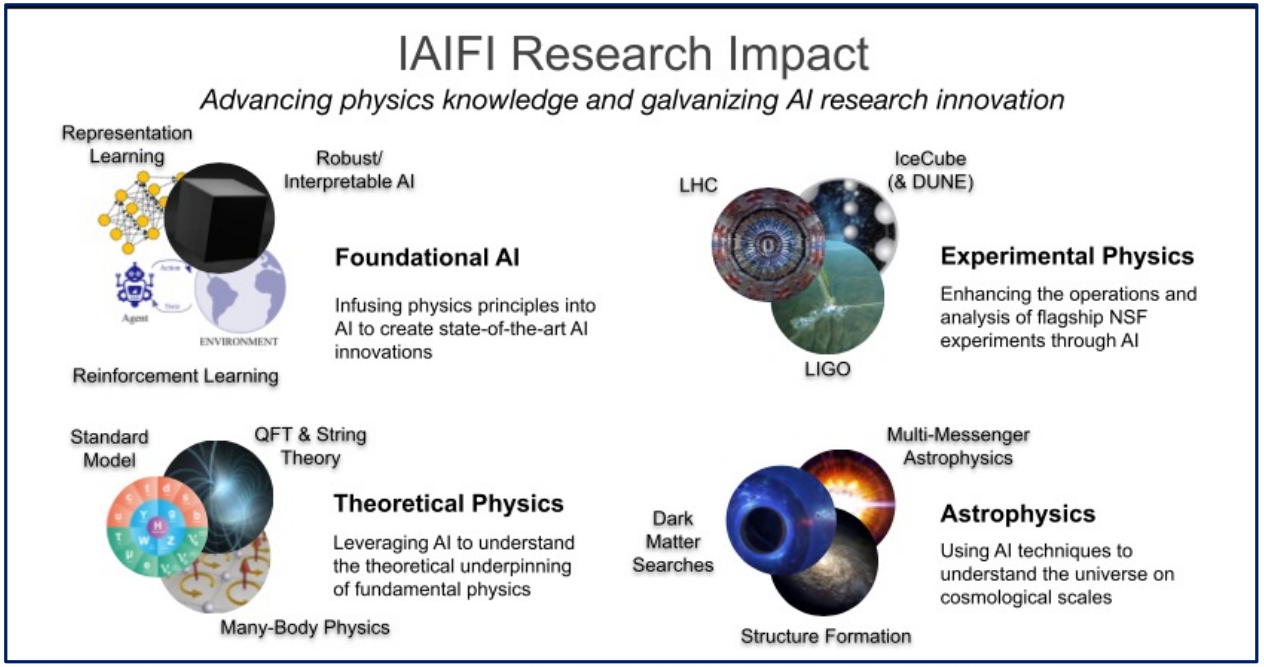
AI Institute for the
Foundations of Machine Learning
(IFML)
Hub: UT-Austin
(CISE/CCF 2019844)
Partnering with DMS

National AI Research Institutes

National AI Strategy	Sustained, Long-term Support for AI R&D Maintain And Grow U.S. Leadership In AI
Core Missions	Advance Fundamental Knowledge Of AI; Advance Use-inspired Work To Drive Innovation in Science and Engineering, Segments of the Economy, or Societal Needs. Grow The U.S. AI Workforce And Build Pathways For Students From Diverse Backgrounds.
27 NSF And USDA-NIFA Funded AI Research Institutes Funded As Of March 2025	Program Managed by NSF/CISE/IIS with Cross-agency and External Partners MPS-supported institutes managed by domain divisions

AI-centric Institutes/Centers in MPS

Software Institutes	Harnessing the Data Revolution Institutes	Additional complementary MPS Institutes and Centers with AI activity
MolSSI **CHE Software Institute**	a3d3 Accelerated AI Algorithms for Data-Driven Discovery **PHY HDR Institute**	CAMM CENTER FOR ADVANCED MATERIALS & MANUFACTURING **DMR MRSEC**
iris hep **PHY Software Institute**	NSF ID4 Institute for Data Driven Dynamical Design **DMR HDR Institute**	National Institute for Theory and Mathematics in Biology
	TRIPODS Transdisciplinary Research in Principles of Data Science **DMS-CCF-ECCS TRIPODS Institutes**	NSF-Simons Research Collaborations on the Mathematical and Scientific Foundations of Deep Learning
		C-CAS NSF CENTER FOR Computer Assisted Synthesis **CHE CCI**



- Deep Learning (AI) + Deep Thinking (Physics) = Deeper Understanding
- Collaboration of physics and AI researchers at MIT, Harvard, Northeastern, and Tufts.

INTRODUCTION TO THE MOLECULE MAKER LAB INSTITUTE
AN INNOVATION ECOSYSTEM

Huimin Zhao
UIUC,
Director

Martin Burke
UIUC

Scott
Denmark
UIUC

ENABLING TECHNOLOGIES

- AI / ML
- Dynamic Databases
- Automated Synthesizer
- iBioFAB

AI-enabled Synthesis Planning

Education & Workforce Development

AI-enabled Catalyst Development

AI-enabled Molecule Manufacturing

AI-enabled Molecule Discovery

Alphasynthesis & Closed DBTL Loop

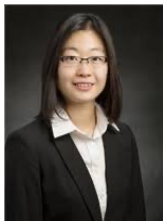
AI tools to address:
1. Cold start problem
2. Small data
3. Standard tools failing to give good models

RIT

Industrial Partnership

abbvie
REVOLUTION MEDICINES
LanzaTech
NVIDIA
AMGEN
IBM

Jiawei Han
UIUC



Ying Diao
UIUC

Rachel Switzky
UIUC

NSF/CHE Molecule Maker Laboratory Institute

SCIENCE HIGHLIGHT: OCTOBER 2022

CLOSED-LOOP OPTIMIZATION OF GENERAL REACTION CONDITIONS FOR HETEROARYL SUZUKI-MIYAURA COUPLING

MOLECULE MAKER LAB INSTITUTE

BACKGROUND/OBJECTIVE

General conditions for organic reactions are important but rare, and efforts to identify them usually consider a narrow region of chemical space. A large matrix of substrates crossed with a high-dimensional matrix of reaction conditions renders exhaustive experimentation impractical.

APPROACH

- Use of a simple closed-loop workflow, leveraging data-guided matric down-selection, uncertainty-minimizing machine learning, and robotic experimentation
- Application to heteroaryl Suzuki-Miyaura cross-coupling

RESULTS

- Identified conditions that double the average yield relative to a widely used benchmark developed using traditional approaches

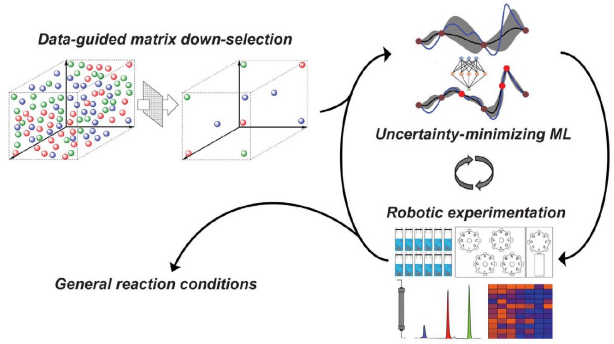


Figure 1. Workflow developed in this study for the discovery of general reaction conditions.

SIGNIFICANCE

This study provides a practical road map for solving multidimensional chemical optimization problems with large search spaces. The power of down-selection as an entry point into large multidimensional search search is revealed.

Angello, et al. 2022. DOI: 10.1126/science.adc8742

NSF-Simons AI Institute for Cosmic Origins (CosmicAI)

PI: Stella Offner
University of Texas

Lead Institutions

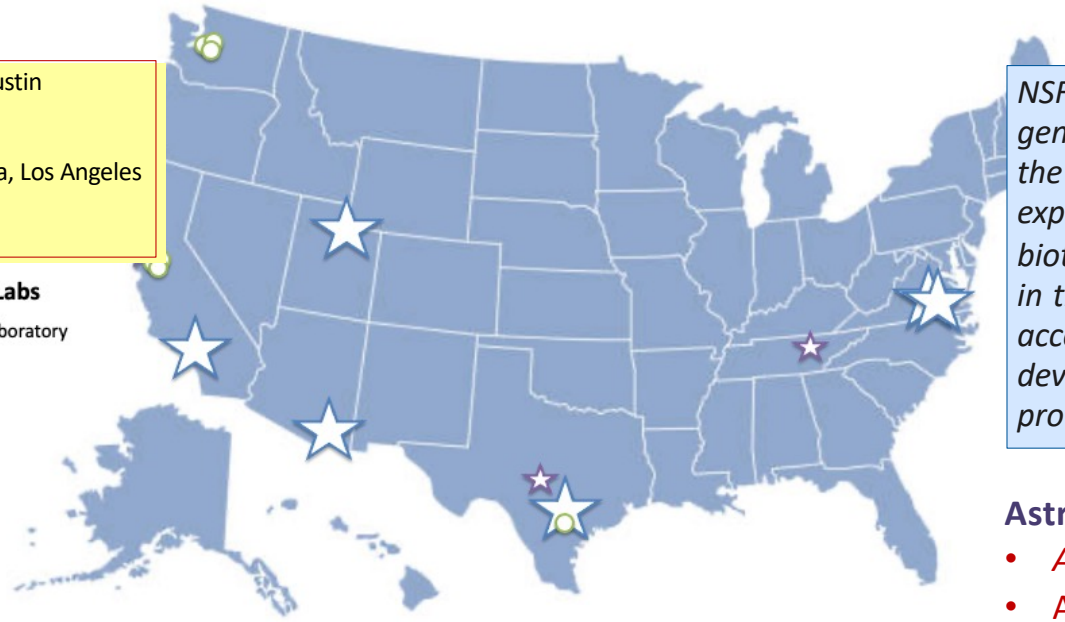
- University of Texas, Austin
- University of Virginia
- University of Utah
- University of California, Los Angeles
- NRAO
- NOIRLab

Academic Parters & Labs

- SLAC National Accelerator Laboratory
- University of Texas Arlington
- University of Tennessee

Industry Partners

- AI2
- Microsoft
- Intel
- NVIDIA
- Sony AI
- Amazon
- SparkCognition



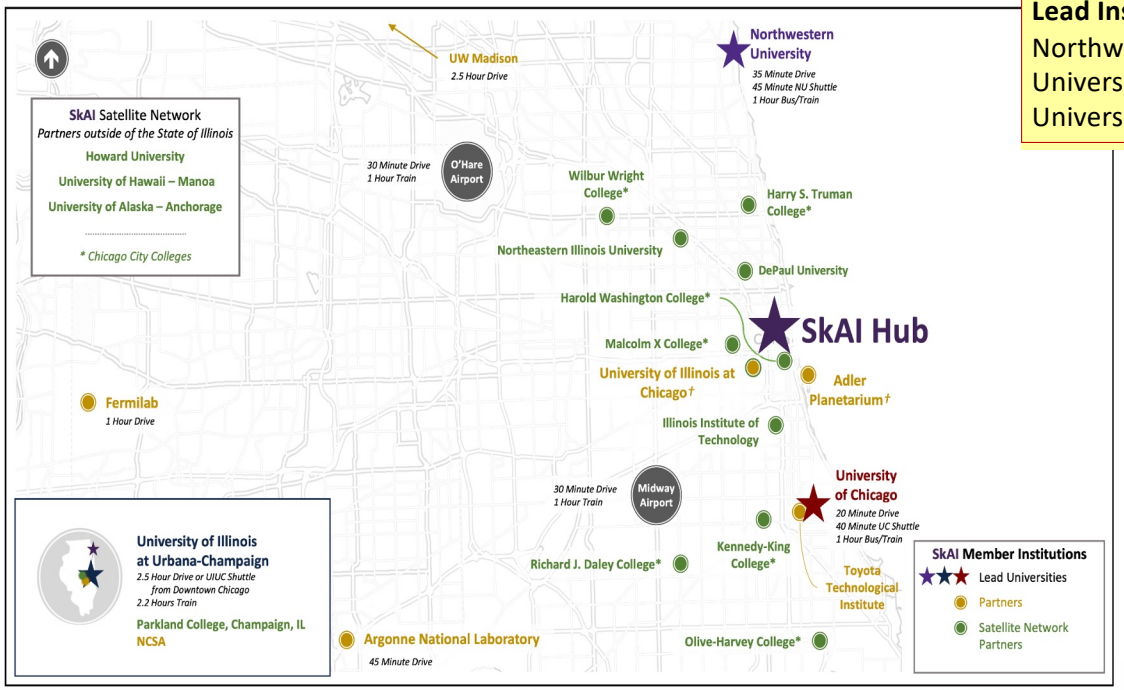
NSF-Simons CosmicAI aims to create next-generation AI tools to accelerate discoveries, tackle the analysis of large astronomical datasets, explore the nature of dark matter, and model pre-biotic molecules that are key to understanding life in the Universe. The institute plans to democratize access to astronomical data and analysis by developing a powerful AI-based assistant that provides accurate responses to scientific queries.

Astronomy research themes

- *AstroCopilot* and Data Platform
- Analysis of large radio datasets
- Dark matter
- Modeling prebiotic molecules

NSF-Simons AI Institute for the Sky (SkAI)

Funded by the U.S. National Science Foundation and the Simons Foundation



Lead Institutions:
Northwestern University
University of Chicago
University of Illinois at Urbana-Champaign

PI: Vicky Kalogera
Northwestern University

NSF-Simons SkAI will tackle exceptionally complex problems in astrophysics and astronomy across a broad range of cosmic scales, from the physics of exotic objects like neutron stars and black holes to the formation of galaxies and the role that dark matter and dark energy play across the entire universe.

Astronomy research themes

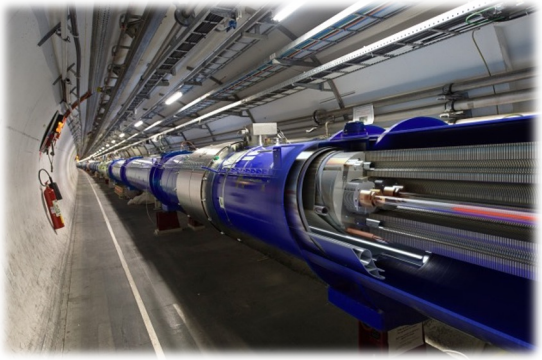
- Time domain astronomy
- Precision cosmology
- AI-Accelerated simulations
- Instrument design

MPS Large Facilities

- Generate enormous amounts of data
- Great potential for harnessing and synthesizing this data through AI
- MPS-led AI-centric Institutes are collaborating with MPS-facilities

Cornell High Energy Synchrotron Source (CHESS)

Large Hadron Collider (LHC)



National Optical-Infrared Astronomy Research Laboratory (NOIRLab) - e.g., Rubin Observatory

National Solar Observatory (NSO) - e.g., Daniel K. Inouye Solar Telescope

IceCube Neutrino Observatory

National Radio Astronomy Observatory (NRAO) - e.g., Atacama Large Millimeter /submillimeter Array (ALMA)

National High Magnetic Field Laboratory (MagLab)

Laser Interferometer Gravitational-Wave Observatory (LIGO)

NSF's 75th Anniversary

On May 10, 2025, the U.S. National Science Foundation commemorates its 75th anniversary.

NSF is planning a series of in person and virtual events across the U.S. throughout 2025.

Strengthen Research Infrastructure

- Will produce 10 million transients a day for 10 years to map the Milky Way
- "First Light" (first images with the science camera, fully functional) will happen ~ July 2025
- "Dedication" (ribbon cutting with NSF Director, DOE and Chilean dignitaries) will take place sometime in October to December of 2025

VERA C. RUBIN OBSERVATORY

U.S. National Science Foundation | U.S. DEPARTMENT OF ENERGY | Office of Science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