

# AI+Science Hackathon 2025

Eric and Wendy Schmidt AI-Postdoctoral Fellowship  
Data Science Institute University of Chicago  
supported by Schmidt Sciences, LLC

April 15th – April 29th 2025



# Welcome to the AI+Science Hackathon!

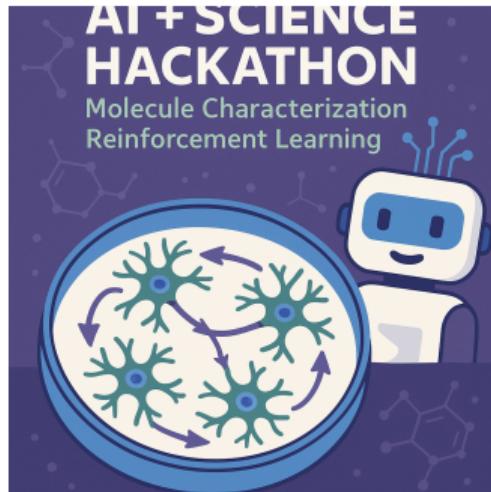
- ▶ exciting new ideas
- ▶ transfer models to new areas
- ▶ compete for a trophy
- ▶ 2 projects

## Characterizing New Materials using AI

- ▶ 5 teams

## Reinforcement Learning to Control Networks of Living Neurons

- ▶ 4 teams



## Organizing Team

Adam, Aditya, Alex, Anthony, Elena, Jordan, Ludwig, Marisa, Mark, Ritesh, Rui, Stephan, Victoria, William

# Computational Environment

- ▶ 2 project specific introductions
- ▶ resources on RCC Midway3
- ▶ 8 dedicated Nvidia A100 GPUs
  - ▶ ai4s-hackathon
- ▶ group storage

/project/ai4s-hackathon/XXX



github.com/uchicago-dsi/  
ai-sci-hackathon-2025

The screenshot shows a GitHub repository page for 'ai-sci-hackathon-2025'. The repository has 2 branches and 0 tags. The README file is the current view. The repository was created by 'ahudut11' on 06/04/23. It contains several files and folders related to the hackathon, such as '2024-files', 'material\_characterize\_project', 'rl\_and\_biological\_network\_project', 'gitignore', 'README.md', '1000.txt', 'example\_submission.sh', 'example\_torch.py', 'setup\_material\_characterize.sh', and 'setup\_rl\_and\_biological\_networks.sh'. The repository has 28 commits, 3 days ago. The repository has 0 stars, 4 watching, and 0 forks. There are sections for 'About', 'Activity', 'Custom properties', 'Releases', 'Packages', 'Contributors', and 'Languages'.

## Getting Started with Midway3

This guide is designed to help you quickly start using the Midway3 system and the hardware provided for this event.

## Accessing Midway3 on RCC

RCC provides a user guide for accessing the shared cluster systems, available [here](#). We have reserved a private partition of Midway3 for teams that require GPU resources for the challenge.

# Teams Selection & Mentors

## Characterizing New Materials

**Adam**, Jordan, Rui, Elena, Ludwig, Aditya

## Slack Space for Communication

- ▶ Join Slack Space
- ▶ Make a Group Channel

[https://join.slack.com/t/aiscienceuchi-pwb7058/shared\\_invite/zt-33dkfvdgm-QrNNZlG7Y0lt~2d\\_8uxnIw](https://join.slack.com/t/aiscienceuchi-pwb7058/shared_invite/zt-33dkfvdgm-QrNNZlG7Y0lt~2d_8uxnIw)



## Reinforcement Learning for Biological Networks

**Stephan**, Madeleine, Alex, Yihang, Kyle

## Getting to know your Team and Mentor

- ▶ Check out Your Team
- ▶ Check out the Mentors

# Excitement: Tuesday 15th to Thursday 17th

- ▶ get to know each other
- ▶ get to know your mentor
- ▶ brain storm model ideas
- ▶ pick a tech stack
- ▶ build a data pipeline

## Gain RCC access

Make sure, you successfully run a job on RCC before Thur. 17th. (Mentor)



# Valley of Despair: Friday 18th to Tuesday 22nd

- ▶ your first ideas didn't work
- ▶ the excitement is wearing off
- ▶ brain storm and select most promising idea
- ▶ iterate and build new models
- ▶ train new models over night



# Seeing the Light: Wednesday 23rd to Monday 28th

- ▶ your models start delivering results!
- ▶ you can actually see how you solve this!
- ▶ iterate on your models
- ▶ optimize your hyper parameters
- ▶ finalize your models

## Final Results: Monday 28th

- ▶ receive final evaluation data @ 3PM
- ▶ Or submit your final solution @ 3PM



# Day 4: Bringing it over the Finish Line

- ▶ gather results for last night
- ▶ present us your success and hiccups
- ▶ you have 10 minutes per team
- ▶ 2 minutes for questions

## Deadline

Presentation must be submitted 9AM April 29th



# Teams & Collaboration

- ▶ utilize slack!
- ▶ include your mentor in discussions
- ▶ In-Person collaboration opportunities

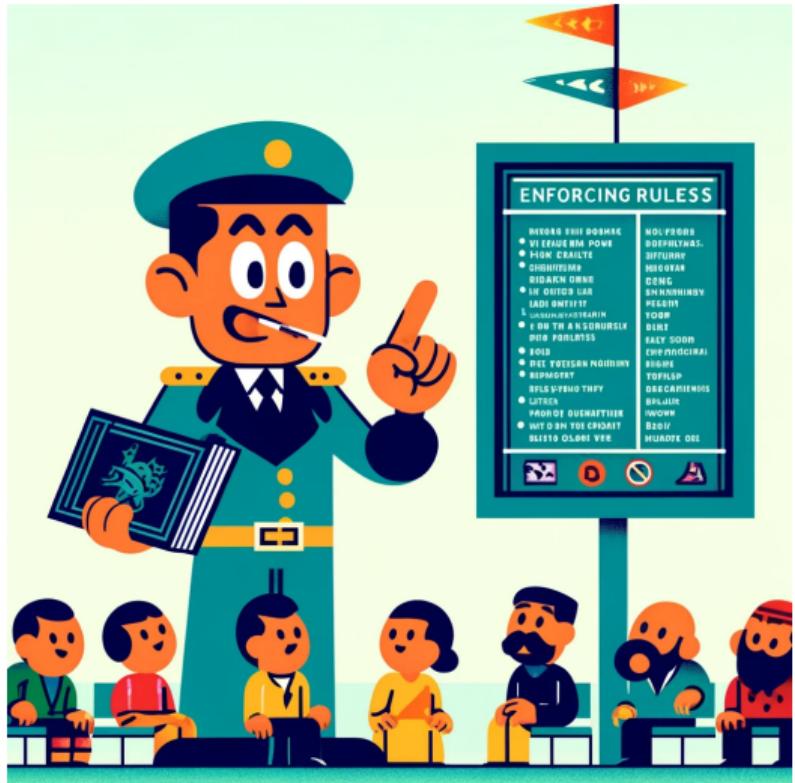
Day	Time	Room
Tue, April 15	1PM – 3PM	Searle 240A
Tue, April 15	1PM – 3PM	Searle 236
Thur, April 17	2PM – 4PM	JCL 151
Thur, April 17	2PM – 4PM	JCL 236
Tue, April 22	1PM – 3PM	Searle 240A
Tue, April 22	1PM – 3PM	Searle 236
Thur, April 24	2PM – 4PM	JCL 151
Thur, April 24	2PM – 4PM	JCL 236



# Rules for the Hackathon

## Play Fair!

- ▶ only use data provided in your challenge
- ▶ do not use other groups results
- ▶ use only the computation time you need
- ▶ do not use more presentation time as everyone else
- ▶ discuss publication with mentor and project mentor



Happy Hacking!

Today

**Characterizing New Materials using AI**

**Reinforcement Learning for Bio Networks**

► Room: JCL 390

► Room: JCL 298

Thursday April 29th: 10AM