

# AI+Science Hackathon 2024

Eric and Wendy Schmidt AI-Postdoctoral Fellowship  
A Schmidt Sciences Program  
Data Science Institute University of Chicago

May 6th – May 9th 2024



# Welcome to the AI+Science Hackathon!

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

## Unlock the Secrets of Molecules with AI

- ▶ 8 teams

## The Lives & Deaths of Stellar Binaries

- ▶ 6 teams



## Organizing Team

Aditya, Anthony, Chris, Colm, Georgios, Jordan, Ludwig, Mark, Ritesh, Simona

# Computational Environment

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

/project/dfreedman/hackathon/XXX



[github.com/uchicago-dsi/  
ai-sci-hackathon-2024](https://github.com/uchicago-dsi/ai-sci-hackathon-2024)

The screenshot shows a GitHub repository page for 'ai-sci-hackathon-2024'. The repository has 1 branch and 0 tags. The commit history lists 5 commits from 'InnocentBug' made 21 minutes ago. The commits include updates to slides, molecular\_project, stellar-paleontology, and README files, along with initial commits for .gitignore, example\_jax.py, example\_submission.sh, example\_tf.py, example\_torch.py, requirements.txt, requirements\_jax.txt, and setup.sh. Below the commit list, there is a section titled 'Getting Started with Midway3' which states: 'This guide is designed to help you quickly start using the Midway3 system and the hardware provided for this event.'

File	Commit Message	Time Ago
molecular_project	update slides PDF	21 minutes ago
slides	Adjust to the new repo	24 minutes ago
stellar-paleontology	Initial commit	1 hour ago
.gitignore	Initial commit	1 hour ago
README.md	Merge branch 'main' of github.com:uchicago-dsi/ai-sci-h...	23 minutes ago
example_jax.py	Initial commit	1 hour ago
example_submission.sh	Initial commit	1 hour ago
example_tf.py	Initial commit	1 hour ago
example_torch.py	Initial commit	1 hour ago
requirements.txt	Initial commit	1 hour ago
requirements_jax.txt	Initial commit	1 hour ago
setup.sh	Initial commit	1 hour ago

**Getting Started with Midway3**

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

# Teams Selection & Mentors

## Stars Mentors

Anthony, Georgios, Peter, & Colm

## Slack Space for Communication

- ▶ Join Slack Space
- ▶ Make a Group Channel

[https://join.slack.com/t/aisciencehack-qop3836/shared\\_invite/zt-2hx2lpvtf-coICNHwTFARxgFDYfwnvRw](https://join.slack.com/t/aisciencehack-qop3836/shared_invite/zt-2hx2lpvtf-coICNHwTFARxgFDYfwnvRw)



## Molecular Mentors

Aditya, Jordan, Chris, Adam, Ritesh, Stephan, Yihang, & Ludwig

## Spread Sheet for Teams

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

[https://docs.google.com/spreadsheets/d/1QbVzL1gxW0LiaMQ5dpUCMQXtT\\_bGgAvIDExyWpC9UM4/](https://docs.google.com/spreadsheets/d/1QbVzL1gxW0LiaMQ5dpUCMQXtT_bGgAvIDExyWpC9UM4/)



# Day 1: Excitement

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



## Day 2: Valley of Despair

- ▶ 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



# Day 3: Seeing the Light

- ▶ your models worked over night!
- ▶ you can actually see how you solve this!
- ▶ iterate on your models
- ▶ optimize your hyper parameters
- ▶ finalize your models

## Evening

- ▶ receive final evaluation data @ 3PM
- ▶ prepare your presentation



# Day 4: Bringing it over the Finish Line

- ▶ gather results for last night
- ▶ present us your success and hiccups
- ▶ you have 7 minutes per team
- ▶ 2 minutes for questions

## Deadline

Presentation must be submitted 9AM May 9th



# 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

### Unlock the Secrets of Molecules with AI

- ▶ Room Stuart 104

### The Lives & Deaths of Stellar Binaries

- ▶ Room JCL 298

## Thursday 9:30AM

### Unlock the Secrets of Molecules with AI

- ▶ Room JCL 298

### The Lives & Deaths of Stellar Binaries

- ▶ Room JCL 298