Cyberinfrastructure-Enabled Machine Learning
Summer Institute

CIML SI25 Prep Day
June 17, June 24–26, 2025

Logistics and Introductions

Mary Thomas

SDSC SAN DIEGO SUPERCOMPUTER CENTER

UC San Diego

Welcome to the FIFTH CIML Summer Institute!

- Today is "Prep Day"
- We'll focus on making sure you can connect to Expanse, run jobs, etc, so that next week goes smoothly
- We will use Slack for chatting/communicating
  - maintains a persistent record of the meeting
- We will use Zoom today, next week is in-person:
- Please be on time so we can stay on schedule
- WebSite: https://na.eventscloud.com/website/83697/home-ciml/
- GitHub: https://github.com/ciml-org/ciml-summer-institute-2025
- Please be on time so we can stay on schedule.

Preparation Day – June 17, 2025

Prep Day Agenda:

TIME (Pacific time)	TOPIC	PRESENTER
9:00 AM - 9:15 AM	*1.1 Welcome & Orientation*	*Mary Thomas*
9:15 AM – 9:45 AM	*1.2 Accounts, Login, Environment, Running Jobs and Logging into Expanse User Portal*	*Mary Thomas*
9:45 AM – 10:30 AM	*Q&A, Wrap-up*	*All*

CIML Instructors

Andreas Goetz, Ph.D.
Director of Computational Chemistry Laboratory

Marty Kandes, Ph.D.
Computational and Data Science Research Specialist

Mai Nguyen, Ph.D.
Lead for Data Analytics

Paul Rodriguez, Ph.D.
Computational Data Scientist

Robert Sinkovits, Ph.D.
Director of Education and Training

Mary Thomas, Ph.D.
Computational Data Scientists, HPC Trainer

Basic Information

- Today is Day 1: Welcome-Orientation Day:
    - https://github.com/ciml-org/ciml-summer-institute-2025/tree/main/1.1_welcome_and_orientation
- Check out the 0_Prep doc – contains important information:
    - https://github.com/ciml-org/ciml-summer-institute-2025/tree/main/0_preparation
- Expanse User Guide:
    - https://www.sdsc.edu/support/user_guides/expanse.html
- You need to have an Expanse account in order to access the system. There are a few ways to do this:
    - You have been assigned a training accounts: they expire, save your data.
    - Request an Expanse trial account, send email to consult@sdsc.edu
    - Reach out to a PI with an active allocation can add you to their allocation.
    - Submit a proposal through the ACCESS allocation request system. https://allocations.access-ci.org
- Online Expanse training repo and information:
    - https://github.com/sdsc-hpc-training-org/expanse-101
    - https://hpc-training.sdsc.edu/expanse-101/

Other Resources

- GitHub Repo for this webinar: clone code examples for this tutorial – clone example code:
  - https://github.com/ciml-org/ciml-summer-institute-2025
- SDSC Training Resources
  - https://www.sdsc.edu/support/user_guides/expanse.html
  - https://education.sdsc.edu/training/interactive/
  - https://www.sdsc.edu/events/index.html
  - https://github.com/sdsc-hpc-training-org/hpctr-examples
- ACCESS Training Resources
  - https://support.access-ci.org/events

Thank You