

Cyberinfrastructure-Enabled Machine Learning Summer Institute

CIML SI25 Prep Day

June 17, June 24–26, 2025

Logistics and Introductions

Mary Thomas

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:

<i>TIME (Pacific time)</i>	<i>TOPIC</i>	<i>PRESENTER</i>
9:00 AM - 9:15 AM	<u>1.1 Welcome & Orientation</u>	<u>Mary Thomas</u>
9:15 AM – 9:45 AM	<u>1.2 Accounts, Login, Environment, Running Jobs and Logging into Expanse User Portal</u>	<u>Mary Thomas</u>
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