

CIML SI21 Prep Day Logistics and Introductions Mary Thomas



# Welcome to the FOURTH 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 for:
  - all presentations and group discussions
  - Breakout rooms for hands-on sessions
  - To avoid Zoom fatigue, we'll have lots of breaks
- Please be on time so we can stay on schedule
- WebSite: https://na.eventscloud.com/website/22773/home/
- GitHub: https://github.com/ciml-org/ciml-summer-institute-2024
- Please be on time so we can stay on schedule.



### **Basic Information**

- Check out the 0\_Prep doc contains important information:
  - <a href="https://github.com/ciml-org/ciml-summer-institute-2024/tree/main/0">https://github.com/ciml-org/ciml-summer-institute-2024/tree/main/0</a> 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:
  - Submit a proposal through the <u>XSEDE Allocation Request System</u>
  - PI on an active allocation can add you to their allocation (if you are collaborators working on the same project).
  - Request a trial account, instructions @ <a href="https://portal.xsede.org/allocations/startup">https://portal.xsede.org/allocations/startup</a>.
  - Training accounts expire, save your data.
- Online repo and information:
  - https://github.com/sdsc-hpc-training-org/expanse-101
  - https://hpc-training.sdsc.edu/expanse-101/



### **Prep Day Agenda**

## Tuesday, June 18 Preparation Day (virtual)

9:00 am - 9:15 am	1.1. Welcome & Orientation  Mary Thomas, Computational Data Scientist & Director of the CIML  Summer Institute  Cindy Wong, Events Specialist
9:15 am – 9:45 am	1.2 Accounts, Login, Environment, Running Jobs and Logging into Expanse User Portal Mary Thomas, Computational Data Scientist & Director of the CIML Summer Institute
9:45 am – 10:30 am	Q&A & Wrap-up



#### **CIML Instructors**



Andreas Goetz, Ph.D.

Director of Computational

Chemistry Laboratory



Mai Nguyen, Ph.D. Lead for Data Analytics



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



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



**Peter Rose, Ph.D.** *Director of Structural Bioinformatics Laboratory* 



Paul Rodriguez, Ph.D.
Computational Data Scientist



Robert Sinkovits, Ph.D.

Director of Education and

Training

### Thank You



#### Resources

- Expanse User Guide
  - https://www.sdsc.edu/support/user\_guides/expanse.html
- GitHub Repo for this webinar: clone code examples for this tutorial – clone example code:
  - https://github.com/sdsc-hpc-training-org/expanse-101
- SDSC Training Resources
  - https://www.sdsc.edu/education and training/training
  - https://github.com/sdsc-hpc-training/webinars
- XSEDE Training Resources
  - https://www.xsede.org/for-users/training
  - https://cvw.cac.cornell.edu/expanse/

