
# CIML SI21 Main Sessions
# Logistics and Introductions

Mary Thomas

# Welcome to the FIRST CIML Summer Institute!

- Focus is on scalable machine learning.
- Great response:
  - Over 120 applicants; 90+ institutions; ~50% grads, 35% fac/staff; 28% MSI
  - 50+ invited; 40+ attending
- Event Website: https://na.eventscloud.com/website/22773/home/
- GitHub: https://github.com/ciml-org/ciml-summer-institute-2021
- Please be on time so we can stay on schedule.

# What is CIML?

- NSF CyberTraining Grant: *Developing a Best Practices Training Program in Cyberinfrastructure-Enabled Machine Learning Research (CIML)*
- Objectives:  Scalable Machine Learning
  - To create generalized machine learning training and project materials that run on large-scale NSF funded cyberinfrastructure resources such as XSEDE
  - Targeted towards researchers and educators who are using machine learning (ML) and big data analytics methods for their domain specific applications or instructional material
  - To develop a community of machine learning and data analytics CI Users (CIU) and Contributors (CIC) who actively contribute to the training material repository and incorporate the materials into their projects and courses.
  - Synthesize the training material into a domain independent CIML workflow system that can be used for creating applications that run on the NSF HPC ecosystem.

# Logistics

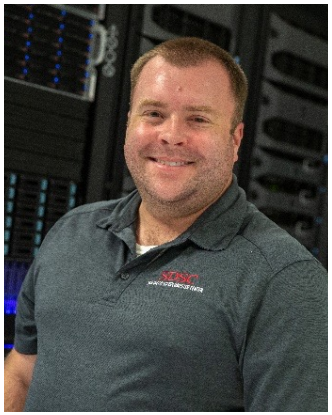
- Friday, June 18th was "Prep Day"
- We focussed on making sure you can connect to Expanse, run jobs, launch notebooks.
- We will use Slack for chatting/communicating
- We will use Zoom for
  - All presentations and group discussions
  - Breakout rooms for hands-on sessions
  - To avoid Zoom fatigue, we'll have lots of breaks
- When speakers have 5 mins left, we will make a clicker sound (demo)
- WebSite: https://na.eventscloud.com/website/22773/home/
- GitHub: https://github.com/ciml-org/ciml-summer-institute-2021

# Day 1 Agenda: Cyberinfrastructure & HPC (Tues, 06/22/21)

| TIME (PST) | TOPIC | PRESENTER |
|---|---|---|
| 8:00 AM - 9:00 AM | 2.1 Welcome, Orientation, & Introductions | Mary Thomas |
| 9:00 AM – 9:40 AM | 2.2 Introduction HPC/Cyberinfrastructure | Robert Sinkovits |
| 9:40 AM – 10:20 AM | 2.3 CPU Computing - Hardware, architecture, and software infrastructure | Mary Thomas |
| 10:20 AM – 11:00 AM | 2.4 GPU Computing - Hardware architecture and software infrastructure | Andreas Goetz |
| 11:00 AM – 11:45 AM | Break/Lunch | |
| 11:45 PM – 12:25 PM | 2.5 Data Management and File Systems | Manu Shantharam |
| 12:25 PM – 1:05 PM | 2.6 Introduction to Singularity: Containers for Scientific and High-Performance Computing | Marty Kandes |
| 1:05 PM – 1:35 PM | 2.7 Reproducibility in Science and Machine Learning | Peter Rose |

# 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.**
*Research Analyst*

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

**Manu Shanthanam, Ph.D.**
*Senior Computational Scientist*

**Robert Sinkovits, Ph.D.**
*Director of Scientific Computing Applications*

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

# Let’s get to know each other

1. Name
2. Institution/Company & Department
3. How do you like to spend your time when not at work?
4. What have you binged watched or read?

# Basic Information

- 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 XSEDE Allocation Request System
  - 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 @ https://portal.xsede.org/allocations/startup.

- Online repo and information:
  - https://github.com/sdsc-hpc-training-org/expanse-101
  - https://hpc-training.sdsc.edu/expanse-101/

# 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/

# We hope you all have a great workshop!