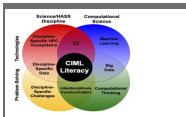
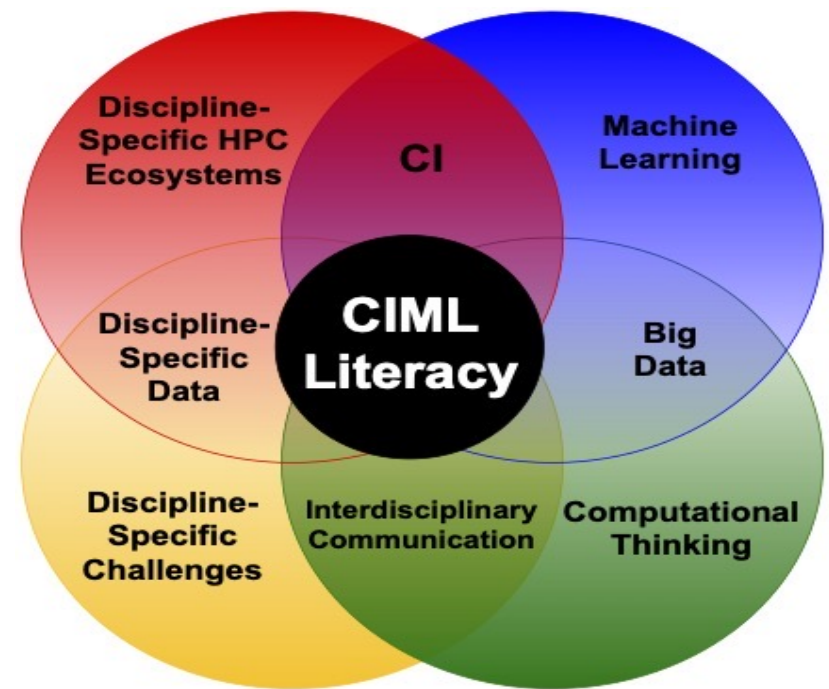


CIML Day2 Welcome and Logistics

June 27, 2022

Mary Thomas
(SDSC)

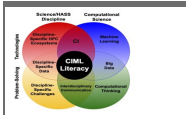


NSF Award 1928224

SDSC SAN DIEGO
SUPERCOMPUTER CENTER
UC San Diego

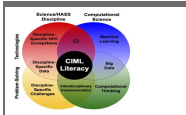
Welcome to the 2nd CIML Summer Institute!

- Today is “Prep Day”
- We’ll focus on making sure you can connect to Expanse, run jobs, launch notebooks so that next week goes smoothly
- 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*
- 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-2022>



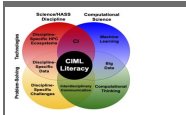
What is CIML?

- NSF CyberTraining Grant: *Developing a Best Practices Training Program in Cyberinfrastructure-Enabled Machine Learning Research (CIML)*
- Objectives: **Scalable Machine Learning**
 - To *facilitate* 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.
 - To create generalized machine learning training and project materials that run on large-scale NSF funded cyberinfrastructure resources such as XSEDE



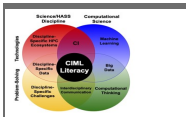
Logistics

- Wednesday, June 22nd was “Prep Day”
- We focussed on making sure you can connect to Expanse, run jobs, launch notebooks, access the Expanse Portal.
- 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
- Web Site: <https://na.eventscloud.com/website/35357/home/>
- GitHub: <https://github.com/ciml-org/ciml-summer-institute-2022>



Day 2 Agenda: HPC/Cyberinfrastructure Concepts (Mon, 06/27/21)

TIME (Pacific time)	TOPIC	PRESENTER
8:00 AM - 8:05 AM	2.1 Quick Welcome	Mary Thomas
8:05 AM - 9:05 AM	2.2 Introduction HPC/Cyberinfrastructure	Robert Sinkovits
9:05 AM - 10:05 AM	2.3 CPU Computing - Hardware, Architecture, Software, Running Jobs	Mary Thomas
10:05 AM - 11:35 AM	2.4 Data Management and File Systems	Marty Kandes
11:35 AM - 12:05 PM	Break/Lunch	
12:05 PM - 1:50 PM	2.5 GPU Computing - Hardware architecture and software infrastructure	Andy Goetz
12:05 PM - 1:50 PM	[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*



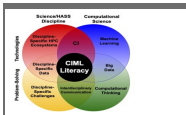
Paul Rodriguez, Ph.D.

Computational Data Scientist



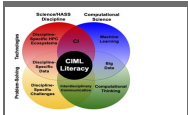
Robert Sinkovits, Ph.D.

*Director of Education and
Training*



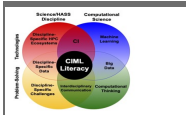
Let's get to know each other

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?



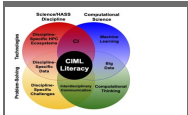
Basic Information

- 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/>

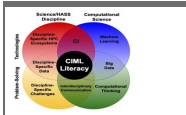


Resources

- 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



**We hope you
all have a great
workshop!**



Thank You!

If you have problems, please contact help@xsede.org

