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# SDSC HPC User Training

## January 22, 2021

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Mary Thomas

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<https://www.sdsc.edu/~mthomas/>

Last updated: 1/22/21 @ 9:30am

# Agenda

- Welcome
  - Introduction to Program
  - Introduce Mentors
- HPC User Training Orientation
- HPC Overview
- Registration for Expanse Account



# HPC Training Mentors

- Mary Thomas <[mpthomas@ucsd.edu](mailto:mpthomas@ucsd.edu)
- Marty Kandes, Martin, [mkandes@sdsc.edu](mailto:mkandes@sdsc.edu)
- Jeff Sale, [jsale@sdsc.edu](mailto:jsale@sdsc.edu),
- Bob Sinkovits, [sinkovit@sdsc.edu](mailto:sinkovit@sdsc.edu)
- Mahi Tatineni, [mahidhar@sdsc.edu](mailto:mahidhar@sdsc.edu)
- Wong, Cindy, [cwong@sdsc.edu](mailto:cwong@sdsc.edu)>
- Susan Rathbun, [susan@sdsc.edu](mailto:susan@sdsc.edu)
- Others TBD

# Early parallel computers based on commodity hardware

## **Stone Soupercomputer (2003):**

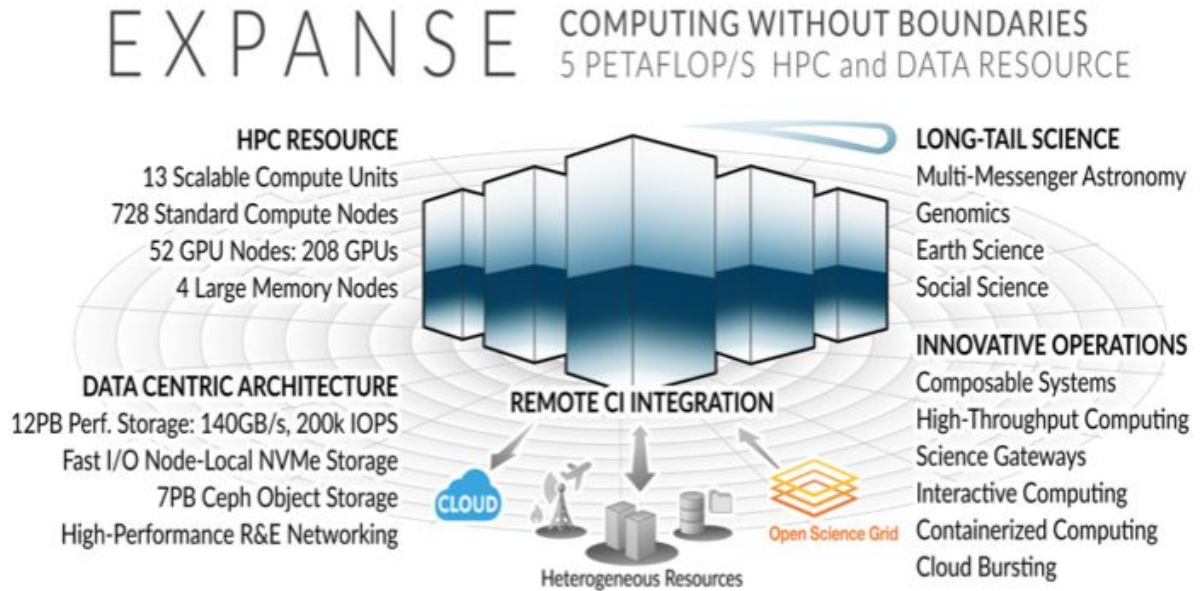
Cheapest cost/flop=\$0, ~20 MFlops

<https://web.archive.org/web/20031121211117/http://stonesoup.esd.ornl.gov>



# What is High Performance Computing?

- *Aggregating computing power*
- *Delivers much higher performance than desktop computer or workstation*
- *Solve large problems in science, engineering, or business.*



For more details see the Expance user guide @ [https://www.sdsc.edu/support/user\\_guides/expance.html](https://www.sdsc.edu/support/user_guides/expance.html)  
and the "Introduction to Expance" webinar @ [https://www.sdsc.edu/event\\_items/202006\\_Introduction\\_to\\_Expance.html](https://www.sdsc.edu/event_items/202006_Introduction_to_Expance.html)

# HPC User Training

- SDSC supports training of its user community in all aspects of High-performance computing (HPC).
- The [HPC User Training](#) activity is designed to promote workforce development in technologies needed to work in HPC.
- Training is provided free to all users, including:
  - UCSD students (both graduate and undergraduate),
  - Post-docs
  - Researchers, faculty, staff, and collaborators on SDSC systems.
- To encourage student participation, some projects and activities are supported/mentored by the Supercomputing Club.

# HPC Training: Scope

The scope of the training effort includes several skill development activities, including:

- Study HPC architectures (CPU, GPU), software, and admin skills.
- Learn the basics of parallel programming, including MPI using C, Fortran, and possibly other languages.
- Running HPC applications in the areas of performance characterization of the cluster, bioinformatics, numerical methods, password security, and other applications.
- Cloud Computing
- Visualization and analysis of big data sets.
- Intro to Machine Learning

# HPC User Training 2021

Registration & Information Page:  
<https://na.eventscloud.com/website/21055/home/>

- Series of 2 hour sessions:
  - SDSC Staff: Fridays from 1:00pm to 3:00pm
  - Session #1: 01/22/21 to 3/12/21 (8)
  - Session #2: 4/2/21 to 5/7/21 (6)
- Workload:
  - Regular attendance
  - Successfully complete assignments
  - 1-4 hrs/week
- *Evaluation metrics* will include:
  - Completion of tasks
  - Credit for experience (working/internships, classes taken)
- Participants who successfully complete the HPC Training program will:
  - Receive an SDSC Certificate of Completion in HPC Training.
  - Awarded account allocations on E X P A N S E for 1 year
- In addition, UCSD students who successfully complete the HPC
  - Receive an UCSD Co-curricular Record of credit in HPC Training.
  - Become eligible to apply to be on the SCC Core team.
  - Note: the final SCC team will be chosen from this group.



# HPC User Training 2021: Schedule

Week	Date	Session #1: January 22, 2021 - March 12, 2021
1	1/22/2021	Program orientation, history, plan, registration process & accounts HPC overview & <i>Expanse</i> Architecture
2	1/29/2021	Parallel Queues & batch scripting; intro to applications (hello world, 2Djacobian)
3	2/5/2021	GPU Architectures, CUDA
4	2/12/2021	GPU Computing with CUDA Python
5	2/19/2021	CPU Computing: Introduction to OpenMP/Threads
6	2/26/2021	CPU Computing: Introduction to MPI
7	3/5/2021	CPU Profiling, monitoring: gprof, mpiP/comms, uProf
8	3/12/2021	GPU Profiling, monitoring: comms, NSight
		<b>Session #2: April 2, 2021 - May 7, 2021</b>
9	4/2/2021	Containers for CPU and GPU computing
10	4/9/2021	Cloud Computing: AWS
11	4/16/2021	Cloud Computing: Azure
12	4/23/2021	Machine Learning: Tensor Flow
13	4/30/2021	SCC21 Applications: HPL, HPCG
14	5/7/2021	Accessing and Visualizing large data sets on HPC systems Using Jupyter Notebooks (pandas, to see Lustre data sets, Matplotlib, Bokeh, SeaBorn)

<https://na.eventscloud.com/website/21055/home/>

# SDSC HPC Students Program

# HPC Student Activities

- Support the Supercomputing Club
- SDSC Internships (CCR)
- HPC Training (CCR)
- Building/Supporting HPC Internship knowledge database
- Raspberry PI Cluster build:
  - Spring'21
  - SDSC Supplies hardware, location, network, etc.
  - Supercomputing Club students build-out/admin

## @Supercomputing:

- Student cluster competition (SCC) teams
  - SCC20: selected
  - SCC21: planning
- Student volunteers:
  - 4 selected for SC19
- All expenses paid by SDSC and Club sponsors!

Support the Supercomputing Club!



**SC21**

St. Louis,  
MO | science  
& beyond.

# Supercomputing and the Student Cluster Competition

<http://www.studentclustercompetition.us/>

<https://sc20.supercomputing.org/>

# SCC History/Background

- Began in 2007 to provide HPC experience to undergraduate and high school students.
- Students design and build small clusters, learn scientific computing, run applications.
- Compete in a non-stop, 48-hour challenge to complete a real-world scientific workload:
  - Operate and maintain the cluster
  - Run and test science applications
  - Reproducibility Challenge: students attempt to reproduce a science paper
  - Power outage challenge - restart system without warning



# SCC: How to Compete

<http://www.studentclustercompetition.us/>

- Entering is competitive: we must write a formal application
- Max of 6 undergraduate students can be on the official team, at SC
  - All travel and expenses will be paid for (SCC, SDSC)
- Participation requires a *significant* level of commitment and hard work:
  - Learn HPC, applications, cluster hardware
  - Work during Fall to build competition cluster
  - Be able to travel to the meeting

<https://sc21.supercomputing.org/>

# SCC Team Preparation Process: 3 Steps

- Step 1: HPC Training
- Step 2: Application submission
- Step 3: If selected, start learning the programs

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# Team Superscalar Celebration!!!

## 4th overall/ 19 teams

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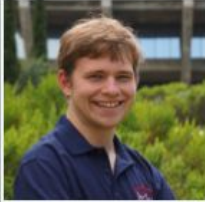
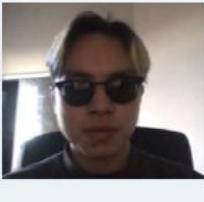
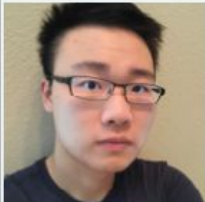
Student Cluster Competition 2020

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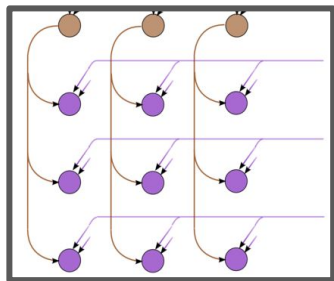
San Diego Supercomputer Center  
The University of California at San Diego



## About the Team

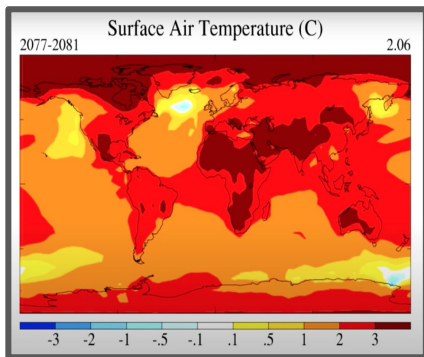
	<p><b>Jacob Xiaochen Li</b> Computer Science, Math</p> <p><b>Skills:</b> Cloud Administration, PID Control, RL.</p> <p><b>Role:</b> Team Leader, Team Lead for Reproducibility Challenge (MemXCT)</p>		<p><b>Arunav Gupta</b> Data Science and Math</p> <p><b>Skills :</b> Machine Learning, Cloud Computing, Statistics</p> <p><b>Role :</b> Team Lead for HPCG Benchmark, 2nd Lead for MemXCT</p>
	<p><b>Zihao Kong</b> Computer Engineering</p> <p><b>Skills:</b> RTL design, FPGA, Embedded programming, CUDA programming, Cloud computing</p> <p><b>Role:</b> Team Lead for Gromacs</p>		<p><b>Max Apodaca</b> Computer Engineering</p> <p><b>Skills :</b> Cloud Computing, Containerization, Checkpoint/Restore</p> <p><b>Role :</b> Team Lead for IO500, CycleCloud Templates</p>
	<p><b>Hongyi Pan</b> Cognitive Science</p> <p><b>Skills :</b> Machine learning, Natural Language Processing</p> <p><b>Role :</b> Team Lead for CESM</p>		<p><b>Hongyu Zou</b> Computer Science</p> <p><b>Skills :</b> Systems, Databases, and Networks</p> <p><b>Role :</b> Team Lead for HPL</p>

# Applications

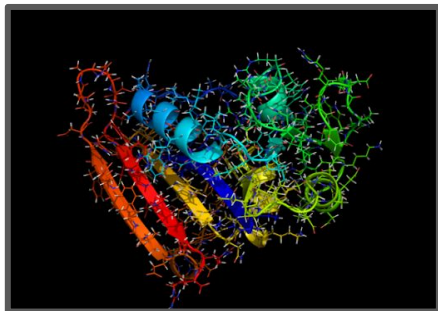


High Performance Linpack

IO<sup>500</sup>



CESM



GROMACS



MemXCT



## View of main Grafana dashboard

- Part of group of 13/19 teams
- Benchmarks:
  - HPCG (3rd): 4.056/15/8 TF/s
  - IO500 (6th): 16/144 "io500 pts"
  - HPL (11th): 53.9/300 TF/s

First teams at SDSC, HPCSD, and

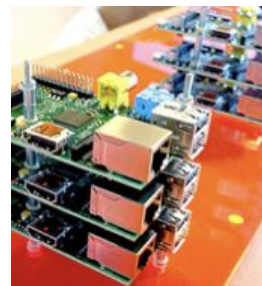
- Applications: (4)
  - MemXCT: completed, submitted paper
  - Mystery App (miniVite): completed
  - GROMACS: completed 60-70% (2 / 3 tasks)
  - CESM: completed 70% (3 / 5 tasks)

Learned about budgets, cloud costs and managing the costs



# Activity: Raspberry PI Cluster

- Spring Quarter 2021
- Goal is to build a 16 node PI Cluster:
  - 16 PI-4 (4 GB) devices
  - Large display monitor
  - MPI, visualization, WFI, TCP/IP
- Club Project (ACM):
  - members will build, admin
- Cluster dedicated to student projects:
  - Simulations
  - Running jobs will be displayed in lobby



# HPC Students Sponsors



HALICIOĞLU DATA SCIENCE INSTITUTE



# Tasks for Week 1:

- Register for the Training: <https://na.eventscloud.com/website/21055/home/>
- Clone the GitHub repo:
- Obtain your Expanse account
  - <https://portal.xsede.org> → create portal account
  - Submit XSEDE PortalID to Form: <https://tinyurl.com/hpc-user-training-signup>
    - Use xsede portal username
- Once your account is created, make sure you can logon
- Complete Homework for Week1 (see README file):
  - <https://github.com/sdsc-hpc-training-org/hpc-training-2021>