Best Practices For Building an HPC/CI Training Program for the Next Generation NSF Workforce

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- Mary Thomas
- SDSC HPC Training Lead
Best Practices For Building an HPC/CI Training Program for the Next Generation NSF Workforce

The San Diego Supercomputer Center's HPC/CI Training program is designed to train the next generation of the NSF workforce community. Our program focuses on training our user communities in emerging technologies and relevant topics, including advanced cyberinfrastructure, high-performance computing, data management, reproducible computing, and scientific applications such as ML and deep learning. Our training team consists of SDSC/UCSD faculty and staff, collaborators, and vendors. We offer various types of training events, including webinars, tutorials, workshops, and institutes, which range from one hour to several days and cater to different communities, including K-12 students, undergraduates, graduates, and working professionals. All events and materials are archived for data provenance and converted into online, accessible training materials. We ensure that all training materials follow the FAIR (Findable, Accessible, Interoperable, and Reusable) practices and are freely available online through GitHub and our interactive video web pages. It is important to note that our training team collaborates with the UCSD EDI offices to ensure that our outreach follows established practices and meets diversity goals. Since the launch of this program, we have successfully hosted more than 110 events and made an impact on over 13,000 participants. In this presentation, we will describe our training program approach and development, highlight its current impact, and discuss our future plans.
Outline

• Introduction
• Defining HPC/CI
• Training Program Design
• Current SDSC HPC/CI Training Program
• Synergistic Activities Broaden Impact
• HPC Students Program
• Broadening Impact
• Conclusions & Future Plans
The San Diego Supercomputer Center

A leader in high-performance and data-intensive computing and cyberinfrastructure

https://www.sdsc.edu/

SDSC provides resources, services and expertise to the local, regional, and national research community, including industry and academia. It supports hundreds of multidisciplinary programs spanning a wide variety of domains.

https://timeline.sdsc.edu/
SDSC by the Numbers

250++ Employees

~3,000 Training & Event Participants/year

~10,000 Active Unix Accounts on HPC systems

1M++ users on Science gateways

1M++ Students took our Big Data courses

4 HPC Systems
~200,000 x86 cores
~1,500 GPUs

AI/ML Supercomputing Habana/Intel hardware
SDSC Expertise

Universal Scale Storage
Open for business from 200TB to 10’s of PB

Globally Federated Cyberinfrastructure
100++ institutions on 5 continents

We design, deploy, and operate end-to-end solutions for our partners from academia, government, industry & non-profits
Advanced Computing Systems:
Needed for large scale HPC applications

Expanse Supercomputer Overview

For more details see the Expanse user guide @ https://www.sdsc.edu/support/user_guides/expanse.html
and the “Introduction to Expanse” webinar @ https://www.sdsc.edu/event_items/202008_Introduction_to_Expanse.html
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Early parallel computers based on commodity hardware

Stone Soupercomputer (2003):
Cheapest cost/flop=$0, ~20 Mflops

HPC/CI Is Everywhere: You use it daily!

- The “Internet”
- Reaches 65% of the world (5.6 billion)
- 93% access via mobile technologies
- Data consumed globally in 2021: 79 zettabytes* (2021), projected to be 180 zettabytes by 2025

*Zettabyte=1,000,000,000,000,000,000,000 [10^21] bytes


HPC/CI Is Everywhere: billions of users performing billions of transactions sending billions of data packets

Number of people using social media platforms, 2005 to 2019

Estimates correspond to monthly active users (MAUs). Facebook, for example, measures MAUs as users that have logged in during the past 30 days. See source for more details.

Source: https://ourworldindata.org/exports/users-by-social-media-platform_v17_850x600.svg

Number of people using social media platforms, 2005 to 2019

Source: Statista and TNS (2019)

HPC/CI Is Everywhere: Where do we house all this data?

- Locate it where it is easy/cheap to keep cool (e.g. Iceland)
- Current Idea: build skyscraper sized data storage facilities
- Need to keep it “localized” for efficient access
HPC/CI Is Everywhere: How do we send all this data?

- Gigabit+ networks
What is High Performance Computing (HPC) and Cyberinfrastructure (CI)?

- **HPC**: Aggregating computing power
- **CI**: Connecting resources with distribute emerging technologies
- **Deliver much higher performance than desktop computer or workstation**
- **Solve large problems in science, engineering, or business.**

For more details see the Expanse user guide @ https://www.sdsc.edu/support/user_guides/expanse.html and the “Introduction to Expanse” webinar @ https://www.sdsc.edu/event_items/202006_introduction_to_expanse.html

SDSC SAN DIEGO SUPERCOMPUTER CENTER
UC San Diego
What is a Supercomputer Cluster?

A very large set of compute nodes ($10^5 - 10^{6+}$) that work together...

- **ORNL Frontier**: 100+ racks; 9000 AMD EPYC nodes, > $10^6$ cores; > 32 PB
  
  → **1.5 exaflops**
  
  ($10^{18}$ floating-point operations per second)

- **SDSC Expanse**: 13+ racks; 728 AMD EPYC nodes, ~ $10^5$ cores; 52 GPU nodes; > 12 PB
  
  → **5.2 petaflops**
  
  ($10^{15}$ floating-point operations per second)
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Training Program: The Challenge

• 2018 search of “what HPC training is available” nationwide?
• In-depth search yielded a large of number of events at several large HPC centers
• But very few events led to training materials (videos, presentations, etc.)

→ Serious lack of training material provenance

→ Decision to reorganize HPC training events, and ensure that training material available persistently.
Training Program Redesign: Clarify nature of training modalities

- **Webinars**: somewhat passive video presentations
  - Record & archive; large groups (zoom limits)
- **Tutorials & workshops**:  
  - A little more interactive, can be a few hours to a few days.
  - Record & archive; limited to large groups
- **Annual Summer institutes** (multiday, multiple topics)  
  - Highly interactive, small groups
  - Record & archive
- **HPC User Training**: 12-14 weeks of 2 hours sessions  
  - Highly interactive, small groups
  - Record & archive
- **Self-guided training**: base on webinars, tutorials, etc.
Training Program Redesign: Organization of Training Materials

- Archive all training materials and repurpose/reuse
- Define keywords/tags to describe/search events:
  - Title, abstract, date, presenter, related training materials, related training pages, GitHub repos, pdfs, YouTube, ….
- Integrate training terms into the SDSC Web content management system (Cascade)
- Create dynamic event pages for upcoming events
- Develop training catalog that lists past events
- Pull event data from content management system (Cascade) and use to build other pages
- Develop Tools as needed for accessing materials
Training Program Redesign: Identify/Expand Training Communities

- Users of SDSC HPC/CI systems and projects:
  - Systems: Expanse, Voyager (AI), TSCC (condo)
  - National programs: XSEDE/ACCESS

- HPC Students Program:
  - Undergrad, grad;
  - focus on UCSD, but keep open for all schools
  - Research Experience for High School (REHS)

- Identify ways to improve EDI of our programs

- NSF WFD: faculty, researchers, postdocs, gov, industry
  - Leveraging funding from CyberTraining awards
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Refactor SDSC Home Pages to Reflect Diverse Training Programs

K-12 (REHS) Coordinated by Ange Mason ~12-15 years

Multiple programs from Coursera to HPC Training

SDSC seeks to empower today's science and engineering communities and help develop the next generation of scientists, technologists and engineers. To these ends, SDSC offers professional development to provide them with knowledge and pedagogy to effectively engage and prepare their students for technology tools in whatever they pursue.

SDSC also offers hands-on training in computational thinking, high-performance computing and big data exploration to students and researchers at nearly every level of sophistication. SDSC "Training," for research professionals focuses on building their skills to use high-performance computing, data-intensive computing, and data analytics within their own research disciplines – from neuroscience and genomics to the humanities, arts and social sciences.

SDSC provides professional development in parallel computing, data science and computing applications through multiple channels and partnerships. Researchers, industry professionals, and college students participate in a wide range of workshops, institutes, and degree/certificate programs.

K-12 Programs

SDSC leverages its expertise and innovation to inspire the next generation of scientists, technologists and engineers, and to empower the educators who guide them. The K-12 outreach program broadly advances STEM participation through hands-on workshops, internships, and academic mentorship opportunities.

College through Career

SDSC offers hands-on training in computational thinking, high-performance computing and big data analytics to students and researchers at every level of sophistication. SDSC "Training" for research professionals focuses on building their skills to use high-performance computing, data-intensive computing, and data analytics within their own research disciplines – from neuroscience and genomics to the humanities, arts and social sciences.

TRAINING PROGRAMS

Advanced Computing

CIML Summer Institute

SDSC's Cyberinfrastructure-Enabled Machine Learning (CML) project teaches researchers and students the best practices for effectively running machine learning and data science applications on advanced cyberinfrastructure and high-performance computers.

Convergence Research (CORE) Institute

This training program provides graduate students and early and mid-career researchers and professionals with a foundational experience to position them for impact throughout their careers on the most challenging societal issues of our time.
Advanced Computing Training Program

- All events are in the CMS system
  → Event data provenance

- Dynamically build pages using CMS database:
  - Upcoming events
  - Training event catalog
  - Interactive video pages

- New tools to support training
- Moving towards searchable content
  - Metadata

https://www.sdsc.edu/education_and_training/training_hpc.html
HPC Training pages provide information for future and past events

- Training event data stored in web site database
  - Used to list upcoming events
  - Customize for HPC systems
  - Training repos accessed > 1000+ / cloned over 500+ times during reporting period
- Event information archived and dynamically available.
- Training Catalog
  - 49 archived events
  - Links to associated training materials
  - Interactive search via keywords/Tags: year, topics, type, system, level of difficulty, etc.
Interactive videos continue to be a rich source of training content

- Hosting 60+ current and archived events
  - Very popular: 4105 unique visitors; Up from 724 in 2021
  - Every training event with recordings is converted
  - During reporting period, converted 37+ Events, > 180 hours of recordings

- Features:
  - Synchronized, searchable table of contents and transcripts; keyword queries
  - Embedded annotations
  - Links to associated tutorials & GitHub repos

- Pages created dynamically:
  - Can now search by year and title keywords
  - Working on developing metadata tag system
Expanse User Portal

- Features: file browser & management; Pinned Apps; Job templates, submission, management
- Interactive applications: Notebooks, Jupyter Lab, Matlab, Rstudio
- Authentication: ACCESS (Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support) credentials
- Used for most training events
- Based on Open On Demand

https://portal.expanse.sdsc.edu
Satellite Reverse Proxy Service: Galyleo Client

- Continues to be used daily on Expanse, TSCC, and Comet
- Users launch secure (HTTPS) Jupyter Notebooks:
  - Simple command line client (galyleo)
  - Also use behind Expanse portal job submission
  - Supports system and custom containers, and Conda environments
Building WFD community through synergistic and connected activities

- Hosting training, workshops, and events:
  - Workshops on preparing for Expanse (CPU/GPU): Data science, & machine learning Institutes; Neurosciences Gateway; HSI-STEM workshops

- Deploying tools to make it easier to learn about and use HPC/CI

- Continuing engagements with partners:
  - AMD User Forum; OpenACC Hack-a-thon; HPC@MSI to support minority serving institutions; HPC Student sponsorships

- HPC Students
  - Campus impact: CSE collaboration; Supercomputing Club part IEEE chapter;
  - SC22 Student Cluster Competition team winning HPL benchmark

- Broadening impact:
  - Awarded two CyberTraining Grants; contributing to other grants & projects
  - Survey & DEI metrics; meet Campus and NSF standards

Targeting the NSF Workforce Development (WFD) Community
HPC/CI Training Program: Topics

- Parallel Programming Concepts HPC architectures (CPU, GPU), software, Linux, admin skills.
- Running HPC applications in the areas of bioinformatics, numerical methods, password security, and other applications.
- Cloud Computing
- Visualization and analysis of big data sets.
- Learn the basics of parallel programming, including MPI using C, Fortran, and possibly other languages.
- Performance characterization of the cluster
- Current Trends: Anything AI/ML; Singularity; Kubernetes; Jupyter Notebooks; cloud computing; accelerators
Training activities focus on productive use of SDSC HPC Systems & new concepts

<table>
<thead>
<tr>
<th>Date</th>
<th>Topic</th>
<th>Type</th>
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<tbody>
<tr>
<td>12/14/21</td>
<td>Expansive Webinar - Running Jupyter Notebooks on Expanse</td>
<td>W</td>
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<tr>
<td>01/14/22</td>
<td>[Week 1] Advanced HPC/CI User Training: Session 1 - Parallel Programming Concepts</td>
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<td>1/20/22</td>
<td>Expanse Webinar - Parallel Computing Concepts</td>
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<td>1/28/22</td>
<td>[Week 3] HPC/CI Training Series: Job Submission - Queues and Basics</td>
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<td>2/11/22</td>
<td>[Week 5] HPC/CI Training Series:</td>
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<tr>
<td>2/17/22</td>
<td>Expanse Webinar - Accessing and Using Expanse Resources</td>
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<td>2/18/22</td>
<td>[Week 6] HPC/CI Training Series: GPU Computing with CUDA Python (TBD to confirm with Andy on this topic)</td>
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<td>3/2/22</td>
<td>Voyager Training session</td>
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<td>3/17/22</td>
<td>Expanse Webinar - Singularity - Exploring Scalability</td>
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<td>4/1/22</td>
<td>[Week 9] Advanced HPC/CI User Training: Job Submission - Queues and Basics</td>
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<td>Expanse Webinar - Enduring Security - Secure Computing</td>
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<td>5/4/22</td>
<td>Kubernetes Tutorial</td>
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<td>5/3/22</td>
<td>NVIDIA GPU Hackathon - Prep Day</td>
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<td>05/10 - 05/12</td>
<td>NVIDIA GPU Hackathon (5 days)</td>
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<td>05/19/22</td>
<td>Expansive Webinar - Intro to Neural Networks and Deep Learning on Expanse</td>
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<td>6/16/22</td>
<td>Expansive Webinar - Reproducibility</td>
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<td>6/22/22</td>
<td>CIML Prep Day</td>
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<td>06/12 - 06/29</td>
<td>CIML 2022 Summer Institute (#applicants)</td>
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<tr>
<td>7/27/22</td>
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<td>08/01 - 08/05</td>
<td>SDSC HPC/DS Summer Institute (#applicants)</td>
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<td>09/22/22</td>
<td>Expansive Webinar - Parallel Concepts</td>
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<td>10/13/22</td>
<td>TSCC Interactive Computing Training</td>
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<td>10/13/22</td>
<td>AMD HPC User Forum Fall Meeting - 2022</td>
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<td>10/20/22</td>
<td>Expansive Webinar - Kubernetes</td>
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<td>11/8/22</td>
<td>Jupyter Notebook workshop for HSI STEM faculties and their collaborators</td>
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<tr>
<td>11/15/22</td>
<td>AMD HPC User Forum Meeting @ SC22</td>
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Training activities focus on productive use of SDSC Systems and new concepts

• Participation Summary:
  • 10/2018 – 12/2023
  • 110 scheduled events
  • 207 training days
  • Cum Registration ~ 12,907
  • Cum Actual ~ 6,664
  • Participation: ~54%
    • Mostly virtual

• Training Effort/Contact hours:
  • ~ 822 training hours
  • ~ 47,340 cum participant hours
Tracking impact: outreach and diversity efforts

- Current efforts to expand/enhance/ensure/diversity in our activities:
  - Work with UCSD EDI for input/guidance
  - Track diversity for event registrations; reach out to more organizations
  - Track all event registrations & participation
  - Reach out to more organizations & institutions
  - Survey participants before, during, after

- Expanse MSI program: allocation awards

- Focussed events: Summer Institutes, NSG workshop; SCC teams

- University of California orgs: designated as HSIs
Training Program Outreach Goal: Impacting Underrepresented STEM Communities

- Focussed events: Summer Institutes, NSG workshop; Student Cluster Competition team
- Training Metric Successes:
  - Participation: Somewhat reflects UCSD; some improvement in some cases
  - Graduates@50%
  - Improved participation by gender
- CIML’23: 67% MSI Appl’s

<table>
<thead>
<tr>
<th>Gender</th>
<th>Count</th>
<th>2022</th>
<th>2021</th>
</tr>
</thead>
<tbody>
<tr>
<td>Man</td>
<td>234</td>
<td>67.8%</td>
<td>68.6%</td>
</tr>
<tr>
<td>Woman</td>
<td>94</td>
<td>27.2%</td>
<td>20.1%</td>
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<tr>
<td>Do not wish to provide</td>
<td>14</td>
<td>4.1%</td>
<td>4.3%</td>
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<tr>
<td>Nonbinary</td>
<td>3</td>
<td>0.9%</td>
<td></td>
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</tbody>
</table>

Participation by Gender: some improvement
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Synergistic programs broaden impact

- **Broadening impact:**
  - Awarded two CyberTraining Grants; contributing to other grants
  - Monitor metrics, meet Campus and NSF standards

- **Continuing engagement between SDSC and partners:**
  - AMD User Forum; GPU Hack-a-thon; HPC@MSI to support minority serving institutions; HPC Student sponsorships

- **Deploying tools** to make it easier to learn about and use Expanse

- **HPC Students**
  - Campus impact: CSE collaboration; Supercomputing Club part IEEE chapter; SC23 Student Cluster Competition team winning HPL benchmark

- **Partners include:**
  - Dell, AMD, NVIDIA, Supermicro, Liqid, OpenACC, HPE
  - CloudBank, Univ. of Washington, NRP Project, CalIT2
  - Engage Partners in Training:
Cyberinfrastructure-Enabled Machine Learning Project

- CIML Summer Institute
  - introduces machine learning (ML) researchers, developers and educators to HPC and the techniques needed to run their models at scale

- Annual ML Summer Institutes:
  - 2021, 2022: virtual
  - 2023, in person

- NSF Award #2017767:

Cyberinfrastructure Professional (CIP) Fellows Program (CIP)

Program will Train (CI) professionals to

- Have interdisciplinary skills that bridge the science, engineering, and computing specialties;
- Support and facilitate research projects, fostering a long-term CIP community;
- Identify sustainable CIP career paths;
- Program includes: advanced computing, workforce development topics;
- CIPs will be embedded into institutional departments;
- NSF, award number 2230127, CyberTraining: Training and Developing a Research Computing and Data (RCD) CI Professionals Community.

Program Overview

A critical role within scientific research teams is the cyberinfrastructure (CI) professional who has interdisciplinary skills that bridge the science, engineering, and computing specialties. Readily finding such personnel, with the necessary experience needed to navigate CI ecosystems has become a bottleneck for many projects. The Cyberinfrastructure Professional (CIP) Fellows Program is designed to address this need by training and mentoring a team of interdisciplinary Researcher-Facing (CARF) CI Professionals with individualized training program in advanced computing and workforce development topics, embedding them into institutional departments, teaching them how to support and facilitate research projects, fostering a long-term CIP community, and defining sustainable career paths specifically for these kinds of professionals.

Eligible candidates include those who have domain science and/or computing backgrounds and want to advance their skills in CI, HPC, data science, and have an interest in facilitating scientific research teams who need to use CI resources and services. Potential candidates include: CI research support staff, software engineers, and system administrators, data curators, computational research scientists and engineers, and CI facilitators (people who work directly with researchers to help them to make effective use of Cyberinfrastructure (CI). The creation of these new CIP-Fellow positions supports the goal of creating long-term career development paths and opening doors to new opportunities for CI Professionals.

The CIP-Fellows program is seeking candidates who have the appropriate science and/or computing background and the motivation to work with research teams. [see below]
ICICLE REHS Project: Creation of Remote Knowledge Graphs

- Students worked on the Intelligent Cyberinfrastructure with Computational Learning in the Environment (ICICLE) project
- Created command line and Jupyter Notebooks to create/populate/modify knowledge graphs
- Software contributions to the production SW components catalog
AMD HPC User Forum: an Active and International Community

• AMD Support/Sponsorship continues
• 3 years old and growing strong:
  • 75+ Institutions; 17 countries; 125 members
  • 9+ events (over 1000 regs/750 attendees).
  • Strong technical meetings: e.g. Fall’22 Program: AMD Instinct (Day 1); Adaptive & Embedded Compute + AI (Day2); EPYC + Q&A (Day3)
• Organization: SDSC continues to lead
  • Executive Team: President: Mary Thomas (SDSC); Vice President: Melyssa Fratkin (TACC); Chief Communications Officer: Susan Rathbun (SDSC)
  • AMD Liason: Guy Ludden (C. Fronczak)
  • Programming & Events: Bob Sinkovits (SDSC), Lev Gorenstein (Purdue)
  • Special Interest Groups (SIG): Mahi Tatineni, All Sills (Texas Tech)
  • Planning for 2023: meetings, syncs, new SIGs

See: https://www.amdhpcuserforum.org
The HPC student program

A program for educating and training the next generation of HPC professionals and researchers

• Motivate students to pursue HPC careers
• Serve as a bridge between students and HPC-related research and researchers at SDSC.
• Work with UCSD undergraduates, graduates; expand to other groups as time and budget permits.
• Advances UCSD EDI goals
HPC Students continues to connect SDSC activities to students at UCSD and elsewhere

- Sponsor UCSD Supercomputing Club: merged with IEEE campus chapter
  - 2023 kickoff meeting: >65 attendees; planning 5+ significant projects
- Annual HPC User Training 2022 (14-weeks) focused on UCSD students; open to research/EDU communities:
  - 90+ Registrants; 50+ Expanse accounts; 19 active.
- Research Experience for High School Students (REHS) brings students to SDSC to work on HPC projects.
  - REHS’22 contributed software to ICICLE Project
HPC Students: Participation at Technical Meetings

- Student Cluster Competition:
  - Competition team of 6 undergrads.
  - Appx 15 undergrads + a few graduate students are part of “home” team → extends impact
  - Undergrads: independent study credit through CSE department
  - Team composition: 33% from underrepresented communities
  - Appx 15 mentors from SDSC, UCSD, and partners
  - SCC competition history:
    - SCC23: planning
    - SCC22: in person; AMD EPYC+INSTINCT; placed 3rd in US and won the HPL benchmark;
    - SCC21: virtual competition, placed 4th overall;

- Student Volunteers at SC (& PEARC): SDSC sponsors students at these meetings.
- 2023: Supercomputing club hosted its own student cluster competition.
HPC Student Activities

- SDSC Internships (paid, CCR)
- HPC Training (CCR)
- Supercomputing Club
- Club Projects:
  - Raspberry PI Cluster build:
    - SDSC Supplies hardware, location, network, etc.
  - Supercomputing Club students build-out/admin

@Supercomputing:
- Student cluster competition (SCC) teams
  - Selected for: SCC20 & 21
  - SCC22: planning
- Student volunteers:
  - 1 selected for SC21
  - 4 selected for SC19
- All expenses paid by SDSC and sponsors!

https://www.sdsc.edu/education_and_training/hpc_students.html
K-12 Education Programs

- ABLE
- ForMIDABLE speakers
- MAP Symposium changes
- REHS
- Summer Workshops.
- K-8 summer camps?
- PI-Wars
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Conclusions & Future Plans

• Training program changes have resulted in an active program with room to grow and adapt to emerging technologies

• 2023 HPC Training:
  • 12 Webinars scheduled for 2023 + Training events: SDSC DSI’23, CIML’23, GPU Bootcamp (July’23), others
  • Add/develop tutorials, bootcamps, workshops as requested
  • Refactoring to reduce staff time, train CIP-Fellows program and SCC23 effort

• Training material catalogue webpage:
  • https://www.sdsc.edu/education_and_training/training_catalog.html
  • Prototype searchable custom pages using metadata/taxonomy
  • HPC Training gateway

• HPC Students:
  • Club’s 2023 kickoff meeting scheduled for January 19, 2023, 5-7pm
  • SCC23 preparation and planning
SDSC HPC Training Team

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Sponsors/Vendors
• AMD
• DDN
• CloudBank
• LIQID
• NVIDIA
• Supermicro
• Intel
• Oracle
Thank You
Key Links

- SDSC HPC Training Program:
  - [https://www.sdsc.edu/education_and_training/training_hpc.html](https://www.sdsc.edu/education_and_training/training_hpc.html)

- SDSC HPC Students Program:
  - [https://www.sdsc.edu/education_and_training/hpc_students.html](https://www.sdsc.edu/education_and_training/hpc_students.html)

- SDSC’s HPC/CI Training Series
  - [https://www.sdsc.edu/event_items/202201_HPC-CI-Training-Series.html](https://www.sdsc.edu/event_items/202201_HPC-CI-Training-Series.html)

- SDSC HPC Students Site:
  - [https://hpc-students.sdsc.edu](https://hpc-students.sdsc.edu)
  - SCC activities: [https://hpc-students.sdsc.edu/scc](https://hpc-students.sdsc.edu/scc)