National and Regional Computing Resources

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Outline

• Computing Resources
• People Resources
• Training
• Educational Opportunities
Computing Resources
TACC Stampede2 Update of Stampede in production Fall 2017. With 4,200 KNL (Intel Xeon Phi 7250) compute nodes along with 1,736 Skylake (48 core, 192GB) compute nodes it is designed for large scale computing needs. 18 petaflops

SDSC Comet About 1950 Intel Haswell nodes (24 cores, 128GB RAM), SSD local scratch. It is intended for moderately scalable parallel applications with an emphasis on improving productivity for a broad spectrum of users. Additional nodes with NVIDIA K80/P100 GPUs; others have 1.5TB RAM (Expanse funding awarded July 2019)

XStream (Stanford), K80 GPU cluster with 65 nodes each with 20 cores (Ivybridge) and 8 K80s; 20% cycles to XSEDE

SuperMIC (LSU) Intel Ivybridge nodes with MIC coprocessors; 40% cycles to XSEDE

IU Jetstream Cloud Computing resource

PSC Bridges A connected set of interacting systems offering a flexible mix of gateways (web portals), Hadoop and Spark ecosystems, batch processing (large shared memory and GPU nodes) and interactivity. Regular and large memory resources (bridges-2 funding awarded July 2019)
20 Storage Building Blocks, implementing the parallel Pylon filesystem (~10PB) using PSC’s SLASH2 filesystem

4 MDS nodes
2 front-end nodes
2 boot nodes
8 management nodes

6 “core” Intel® OPA edge switches: fully interconnected, 2 links per switch

Intel® OPA cables

4 HPE Integrity Superdome X (12TB) compute nodes

42 HPE ProLiant DL580 (3TB) compute nodes

12 HPE ProLiant DL380 database nodes

6 HPE ProLiant DL360 web server nodes

20 “leaf” Intel® OPA edge switches

32 RSM nodes with NVIDIA next-generation GPUs

16 RSM nodes with NVIDIA K80 GPUs

800 HPE Apollo 2000 (128GB) compute nodes

Purpose-built Intel® Omni-Path topology for data-intensive HPC

http://psc.edu/bridges

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Jetstream can be used in several different virtual machine (VM) sizes which are charged in service units (SUs) based on how much of the total system resource is used. The table below outlines the VM sizes created for Jetstream.

<table>
<thead>
<tr>
<th>VM SIZE</th>
<th>VCPUS</th>
<th>RAM (GB)</th>
<th>LOCAL STORAGE (GB)</th>
<th>SU COST PER HOUR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tiny</td>
<td>1</td>
<td>2</td>
<td>8</td>
<td>1</td>
</tr>
<tr>
<td>Small</td>
<td>2</td>
<td>4</td>
<td>20</td>
<td>2</td>
</tr>
<tr>
<td>Medium</td>
<td>6</td>
<td>16</td>
<td>60</td>
<td>6</td>
</tr>
<tr>
<td>Large</td>
<td>10</td>
<td>30</td>
<td>120</td>
<td>10</td>
</tr>
<tr>
<td>XLarge</td>
<td>22</td>
<td>60</td>
<td>240</td>
<td>22</td>
</tr>
<tr>
<td>XX Large</td>
<td>44</td>
<td>120</td>
<td>480</td>
<td>44</td>
</tr>
</tbody>
</table>
Other Services

• Science Gateways
  • https://www.xsede.org/web/site/ecosystem/science-gateways/

• Storage at TACC (Ranch), PSC (Bridges Pylon), SDSC (Data Oasis), Indiana (Jetstream)
  • request with allocation of compute time
  • https://portal.xsede.org/storage
Creating an XSEDE portal account (XUP)

- Now requires DUO 2Factor authentication
- Fill in personal information
- Choose a registration key
- System will send you email with a confirmation number
- Use confirmation number together with passkey to verify your account
Your XSEDE portal account
Types of Allocations

- **Campus Champion**
  - Get your feet wet with XSEDE
  - See campus champion for access and limits
  - 2 day lead time

- **Start-Up**
  - Benchmark and gain experience with resources
  - Different limits per resource

- **Education**
  - Class and workshop support
  - Short term (1 week to 6 months)

- **Research**
  - No Limit
  - 10 page request, 4 month lead time

FREE

https://portal.xsede.org/allocations-overview
https://portal.xsede.org/allocation-policies
Research Allocation

- Use the new XRAS system to submit request
- https://portal.xsede.org/allocations/announcements for details
- Review occurs four times a year by XSEDE Resource Allocation Committee (XRAC)

<table>
<thead>
<tr>
<th>Submit Requests during</th>
<th>for the Allocation Starting</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dec 15 through Jan 15</td>
<td>Apr 1</td>
</tr>
<tr>
<td>Mar 15 through Apr 15</td>
<td>Jul 1</td>
</tr>
<tr>
<td>Jun 15 through Jul 15</td>
<td>Oct 1</td>
</tr>
<tr>
<td>Sep 15 through Oct 15</td>
<td>Jan 1</td>
</tr>
</tbody>
</table>

- Documents required: PI CV, Main Document and Code Performance and Scaling
- Look at sample requests provided!
Submit Allocation Requests: XRAS

• Go to XSEDE portal and login:
  • http://portal.xsede.org
• Go to “Submit/Review Request”
• For more details, see:
  • https://portal.xsede.org/allocations/policies
Single Sign On (SSO) Login Hub

- `ssh <XUPlogin>@login.xsede.org`
- `gsissh <machine-name>`
- Easy to setup host alias file
- [https://portal.xsede.org/web/xup/single-sign-on-hub](https://portal.xsede.org/web/xup/single-sign-on-hub)
Other National Computing Resources
• Open Science Grid
• Blue Waters (NCSA)
• Frontera (TACC)
• Summit/Titan (OakRidge LCF)
• Theta/Mira (etc at Argonne LCF)
• Cori (NERSC)
• Cheyenne (NCAR)
RMACC Computing Resources

http://rmacc.org/accessingsummit

RMACC-Summit funded by a MRI grant by CU Boulder and CSU -- 10% cycles for institutions in RMACC region, especially institutions without own compute resources

- General compute
  - Haswell 24 cores/node, 128GB RAM
- High memory
  - 48 cores/node 2TB
- GPU nodes
  - 24 cores, 2 K80s/node
- KNL Xeon Phi

- Now can access with XSEDE login credentials via SSOHub
RMACC-Summit Access

After you have XSEDE login:

• send request from your institutional email address to rc-help@colorado.edu

• Allocations
  • Can run without allocation for smaller needs
  • https://www.colorado.edu/rc/userservices/allocations

• For training
  • https://www.colorado.edu/rc/userservices/training
People  Resources
Campus Champions -- NSF funded program to connect People with CyberInfrastructure

- HPC
- Visualization
- Data Analysis
- Storage
- Training
- Education
- Subject Matter Experts
Campus Engagement Mission Statement

The Campus Engagement program promotes and facilitates the effective participation of a diverse national community of campuses in the application of advanced digital resources and services to accelerate scientific discovery and scholarly achievement.
Who are the champions?

- 625+ champions at 270+ institutions
- HPC Directors
- System Administrators
- User Support specialists
- Faculty evangelists
- Central IT staff
- Non-academic organization staff, e.g. USGS, Idaho National Labs
What do champions do?

• Facilitate computing- and data-intensive research and education
• Help their local researchers and educators to find and use the advanced digital services that best meet their needs
• Share CI challenges and solutions at all levels: workgroup, institutional, regional, national, and international
• Increase scalable, sustainable institutional uptake of advanced digital services from providers at all levels;
• Foster a broader, deeper, more agile, more sustainable and more diverse nationwide cyberinfrastructure ecosystem
• Cultivate inter-institutional interchange of resources, expertise and support
interactive map found at:
https://www.xsede.org/community-engagement/campus-champions/current
Ask.CI -- NEW

- [https://ask.cyberinfrastructure.org/](https://ask.cyberinfrastructure.org/)
- Q&A site for people who do research computing
- platform for
  - sharing frequently asked questions
  - comparing solutions
  - leveraging each other’s work pertaining to research computing
XSEDE – Extended Collaborative Support Services

https://www.xsede.org/for-users/ecss

- ECSS offers domain science expertise
- Request ECSS assistance via the XSEDE Allocation process

Mission is to improve productivity of the XSEDE user community through collaborations to optimize applications, improve work and data flows, increase effective use of the XSEDE digital infrastructure and broadly expand the XSEDE user base by engaging members of underrepresented communities and domain areas
RMACC HPC Center Staff and Web Sites

- https://www.colorado.edu/rc/
- www.chpc.utah.edu
- http://inside.mines.edu/HPC-Home
Training
XSEDE Training

https://www.xsede.org/for-users/training

• Online, webinars, and in person
• XSEDE HPC Monthly Workshop and Summer Boot Camps
• https://www.xsede.org/web/xup/online-training for listing of all online offerings
Other Training for Using HPC

• The carpentries
  • Software Carpentry – https://software-carpentry.org/
  • Data Carpentry – https://datacarpentry.org/
  • HPC Carpentry – being developed -- https://hpc-carpentry.github.io/hpc-intro/

• Blue Waters
  • https://www.citutor.org
  • https://bluewaters.ncsa.illinois.edu/education-overview
Educational Opportunities
• NSF Research Experiences for Undergraduates (REU)
  • https://www.nsf.gov/crssprgm/reu/reu_search.jsp
  • Number of opportunities with computational focus including one at Jetstream
• Blue waters Internship program: https://bluewaters.ncsa.illinois.edu/internships
• Blue waters Graduate Fellowships: https://bluewaters.ncsa.illinois.edu/fellowships
• Shordor http://www.shodor.org/
• Science Gateways - https://sciencegateways.org/engage/bootcamp
• Student campus champion program
• XSEDE EMPOWER Expert Mentoring Producing Opportunities for Work, Education, and Research - http://www.computationalscience.org/xsede-empower
• sighpc education - https://sighpceducation.acm.org – see training and education resources