High-Performance Computing (Resources and Capabilities)

https://github.com/wsphd/csun-hpc/

"High-Performance Computing (Resources and Capabilities)
California State University, Northirdge (CSUN)

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CSUN Faculty Retreat - Odyssey Restaurant

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(Note: This page is also available in alternate formats - .pdf, .odt, and .docx)

Introduction/Background/Motivation

- Some n i N needs are ≤ contemporary desktop/laptop and software
  - But double-check new methodologies and growth (and by extension, movement) of data
- Some n j N needs are > contemporary desktop/laptop and software
  - Essentially, "compute-intensive, data-intensive, or network-intensive"
  - Use primarily FOSS (Linux, Open Source, etc.) to complement COTS (Windows, SPSS, etc.)
- Private, "on-premises" servers (contact: Zack Hillbruner, *CSUN IT*)
  - Usually purchased by an individual faculty member or Dept. (often with a grant or project)
  - Usually located in the on-campus CSUN MDF
  - CSUN IT usually racks and networks the system; Users manage the system and applications
- Public Cloud (AWS, GCP, MS-Azure, OCI, Digital Ocean, etc.)
  - Use "free-tier" (still need to provide a credit card)
  - Purchase credits with a credit card
  - Scholars can ask for resources for substantive reseearch
- Or?
  - NSF-funded, multi-year, inter-institution, STEAM/SocialSTEM, R3s/CCC's too
  - CSUN IT Technology Resources for Research

General Advanced Computing/Data Management

- There are plenty of (non-HPC) advanced computing issues too (research and instruction).
- Ecosystem Transition: Compute

- o Beyond CPUs, there GPUs, FPGAs, DPUs, and others
- o COTS languages (e.g., SPSS, Stata, MPlus, Matlab, NVivo) -> FOSS languages (e.g., R, Python, Julia)
- o Single-threaded execution -> Parallel execution
- o COTS spreadsheets (e.g., Excel) -> FOSS spreadsheets(e.g., LibreOffice).
- o Operating Systems (e.g., Windows/MacOs) *plus* Linux, Excel -> LibreOffice, etc.
- o Beyond replication -> Reproducibility (not just 'A' journals)
- Ecosystem Transition: Data
  - o "Big Data"
  - o Research results can include output data (and perhaps even source data) too
  - o Desktop sizes (e.g., GiB, TiB) -> Beyond-Desktop sizes (e.g., PiB, ExiB)
  - o Human-readable file formats with no meta-data (e.g., CSV) -> Digital file formats with meta-data (e.g., Parquet)
  - o Row-oriented databases (e.g., MariaSQL, PostgreSQL, SQLite, etc.) -> Column-oriented databases (e.g., DuckDB, MonetDB, TileDB)
  - o Monolith APIs (e.g., REST) -> Robust APIs (e.g., GraphQL)
  - o Single-file access (e.g., HTTPS) -> Multi-file 'buckets' (e.g., AWS/S3, GCS, Azure/Blog)
- Ecosystem Transition: Network
  - o "High Throughput"
  - o Big Data needs to be moved over fast, reliable networks
  - o CSUN 'Science DMZ'
  - o Los Angeles Public Library (LAPL) Northridge branch and Mid-Valley branch (>2x file transfer, symmetric)
- Example: Technology Trends
  - o Campus Labs *plus* Home Labs, Open Science, Open Research, Open Data, Open anything...
- I'm happy to discuss these issues too but it's not the primary focus of this material.

Faculty/Disciplines

- CSUN is a big place--there are many faculty doing interesting things with HPC
- Ravi Absol (Chemistry)
  - o NRP
  - o Molecular Dynamics
  - o undergraduate student (Anita) - uses AMBER software (with many GPUs, including NVIDIA A100s)
  - o one protein combinatorics imulation took 3 months on a laptop -- now takes ~ 3 weeks
- Bingbing Li (Manufacturing Systems Engineering and Management)
  - o NRP
  - o Smart Manufacturing (e.g., Industrial AI, Multimodal Data Fusion for Autonomous System, Digital Twins, XR and Metaverse for Manufacturing)
- Xiyi Hang (Electrical and Computer Engineering)
  - o NRP

- o Bioinfomatics/Bio-medical applications (e.g., Gene expression, data mining)
- Xunfei Jiang (Computer Science)
  - o on-premises HPC and OSG/NRP
  - o Cloud and Infrastructure design and management
  - o Workforce development (full stack)
- Dr. Nicholas Kioussis (Physics)
  - o CalTech Quantum Computing (and others)
  - o Materials Science
- Wayne Smith (Management)
  - o ACCESS and NRP
  - o Federal Communications Commission (FCC) Universal Licensing System (ULS) data
  - o Github - R code
  - o Data output - multi-file data output
- Other future CSUN projects
  - o CTVA - UNREAL 3D imaging (e.g., digital twins, gaming, 3D mapping)
  - o Digital Humanities
- Representative CSU projects
  - o SDSU
  - o CSUSB - High Performance Computing
  - o Sonoma State
  - o CalPolyHumboldt
- CSU help
  - o Dr. Dung Vu (CSUSB)
  - o Kyle Krick (SDSU)

JupyterHub

- [Multi-user, interactive notebooks (including R, Python, Julia, etc.)]https://jupyter.org/hub
- CSU Technology Infrastructure for Exploration ("TIDE")
  - o *governance*: funded by NSF, provisioned by Cloudbank, managed/supported by UC Berkeley
  - o *hardware*: basic access
  - o *software*: R/RStudio, Python, Shiny, Linux terminal, generic notebooks
  - o *log in*: Select "California State University, Northridge" and then log in is via CILOGON (just log in as usual)
  - o Start here: [CAL-ICOR]https://csun.cloudbank.2i2c.cloud/
- CSU Technology Infrastructure for Exploration ("TIDE")
  - o *governance*: funded by NSF, provisioned by NRP, managed/supported by SDSU
  - o *hardware*: can have access to multiple GPUs, multiple cores, lots of RAM, some (shareable) storage
  - o *software*: R/RStudio, Tensorflow, Datascience, generic notebooks, discipline-specific notebooks
  - o *log in*: log in is via CILOGON (just select "California State University, Northridge" and log in as usual)

- o Start here: [CSUN TIDE]https://tide.sdsu.edu/
- CSUN myCSUNSoftware (aka "Apporto")
  - o n/a (but other GUI and CLI software runs here)
  - o Faculty will need to ask for it over time
  - o Start here: [myCSUNSoftware]https://www.csun.edu/it/software-services/software/all-software/mycsunsoftware

Jetstream2/ACCESS

- Managed by Indiana University
- 100's of GiB of RAM, 10's of PB of disk, 10's of GPUs, fast networks
  - o Best for new learners, data science projects (R, Python, Julia, etc.), large simulations, gateway to other systems, including several supercomputers around the country
- Need an "ACCESS ID"
  - o Like an ORCID ID but for Research Computing
  - o Have CV or Resume for upload (don't worry, your request will be approved)
- Be willing to learn:
  - o How to ask (nicely and well, for more (incrementally) resources, and read a simple dashboard
  - o the Command line and Linux
  - o Webshell
  - o SSH for logging int (and some learning curve for generating SSH keys and passphrases)
  - o SCP for file transfer (after the SSH process is done)
- (Live demo...if possible)
- Start here:
  - o [Jetstream ACCESS page]https://jetstream-cloud.org/get-started/index.html

Nautilus/NRP

- Managed by University of California, San Diego
- 100's of GiB of RAM, 10's of PB of disk, 100's of GPUs/FPGAs/TPUs/DPUs, very fast networks
  - o Best for leading-edge science and engineering, especially w/ funded labs and staff
- Be willing to learn:
  - o Must be comfortable with the Command Line, Open Source, and Linux
  - o Kubernetes (open source client-server), you use the "kubectl" binary
  - o You control just about everyting with ASCII ".yaml" files
- (Static demo -- sample .yaml configuration file with GPUs)

```
apiVersion: apps/v1
kind: Deployment
metadata:
  name: deployment-amber-gpu-ws
  labels:
```

```
      k8s-app: deployment-amber-gpu-ws
spec:
  replicas: 1
  selector:
    matchLabels:
      k8s-app: deployment-amber-gpu-ws
  template:
    metadata:
      labels:
        k8s-app: deployment-amber-gpu-ws
    spec:
      containers:
      - name: mypod-gpu
        image: gitlab-registry.nrp-nautilus.io/prp/jupyter-stack/tensorflow
        resources:
          limits:
            memory: 512Gi
            cpu: 1500m
            nvidia.com/gpu: 1
          requests:
            memory: 512i
            cpu: 1500m
        volumeMounts:
        - name: mydata
          mountPath: /mnt/myscratch
        command: ["sh", "-c", "sleep infinity"]
      volumes:
      - name: mydata
        emptyDir: {}
          sizeLimit: 10Ti
      nodeSelector:
        nautilus.io/disktype: nvme
```

- Start here:
  - Send Wayne an email - ws@csun.edu

Additional Resources

- Sometimes, researchers just need an unmanaged or managed (by students, supervised by faculty) resource to host public-facing files and applications
  - [Oregon State University Open Source Lab (OSL)](#)
- Recently, CSUN was added to the Cloudbank/2i2C JupyterHub resource (this complements CSUN Apporto and SDSU/CSUSB TIDE)
  - [Cal-ICOR JupyterHub Pilot](#)
- Increasingly, Libretexts is moving beyond "texts" and becoming a complete LMS solution, including a JupyterHub resource
  - General System - [LibreTexts](#)
  - Specific Application - [JupyterHub](#)
- Some researchers want to experiment with real Quantum resources
  - [D-Wave LEAP Quantum Launchpad/D-Wave Learn Program (D-Wave)](#)
- Many researchers require an AI system that *is* open, transparent, and reproducible (built *top-down*)

- o [NSF National Artificial Intelligence Research Resource Pilot (NAIIR)](#)
- Some researchers desire an AI system that *is* open, transparent, and reproducible (built *bottom-up*)
  - o [Non-Profit Personal AI Lab (Kwaai)](#)

Conferences/Fellowships

- There are plenty of zero-cost and low-cost U.S. domestic events for learning about HPC resources at the *Application*-level.

Name	Venue	Cost	Timeframe
[Practice & Experience in Advanced Research Computing (PEARC)](#)	varies	mid $	late July
[Science Gateways (SGX3)](#)	varies	$0 (NSF)	varies
[Confab (DOE)](#)	varies	low $	early April
[Institute for Mathematical and Statistical Innovation (IMSI)](#)	varies	$0 (NSF)	varies
[US-RSE Conference (US-RSE)](#)	varies	$0 (Sloan)	early October
[IEEE e-science](#)	varies	mid $	mid September

- There are plenty of zero-cost and low-cost U.S. domestic events for learning about HPC resources at the *Infrastructure*-level.

Name	Venue	Cost	Timeframe
[Research Computing at Smaller Institutions (RCSI)](#)	Swarthmore, PA	$0 (NSF)	early June
[National Research Platform (NRP)](#)	UCSD, CA	$600	late January
[Supercomputing (SC)](#)	St. Louis, Denver, Atlanta	low $	mid November
[Corporation for Networking and Research (CENIC)](#)	varies	low $	late March
[Southern California Linux Expo (SCaLE)](#)	Pasadena, CA	low $	early March

- And the list of *International* events for learning about HPR resources is growing quickly.

Name	Venue	Cost	Timeframe
[CINI HPC Summer School (CINI)](#)	Naples, Italy	N/A	mid June
[International Conference on Scalable Scientific Data Management (SSDBM)](#)	varies	N/A	late June

- The following are some of the Fellowships available:

- ICICLE: Intelligent CI with Computational Learning in the Environment (ICICLE)

National Workshops

- There are plenty of *in-person* events for learning about HPR resources.

Name	Venue	Cost	Timeframe
Minority-Serving Cyberinfrastructure Capabilities (MS-CC)	varies	$0 (NSF)	late May
Open Science Grig (OSG)	U of Wisconsin-Madion, WI	$0 (NSF)	late June
HPC and Data Science Summer Institute (SDSC)	UCSD, CA	$350	late July - early August
NERSC International HPC Summer School (NERSC)	varies	$0 (DOE)	early July
KNIT (FABRIC)	varies	$0 (NSF)	mid March
INTERSECT Research Software training (INTERSECT)	Princeton/Alabama	$0 (NSF)	mid July
SHINE Workshop (SHINE)	Iowa City	$0 fees	mid August

- There are plenty of *virtual* events for learning about HPR resources.

Name	Venue	Cost	Timeframe
OU Supercomputing Center for Education & Research (OU)	virtual, synchronous	$0 (NSF)	late June
HPC Pathways (NCSA)	virtual, asynchronous	$0	on-going
Cornell Roadmaps	virtual	$0	asynchronous, on-going
HPC Carpentry	in-person and virtual, synchronous	$0	varies
Ecosystem for Research Networking (ERN) Summit	virtual, synchronous only	$0	late April
Oklahoma University ACI-REF Virtual Residency (Henry Neeman)	virtual	$0	recurring
(comprehensive, searchable list of resources	N/A	$0	varies

Upskilling - Professional Associations/Societies

- Faculty - These HPC resources should be of use to *Faculty* over time.

- o [R OpenSci (ROpenSci)](#)
- o [PyOpenSci (pyOpenSci)](#)
- o [JuliaCon (annual Summer conference abstracts, proceedings)](#)
- o [Framework for Open and Reproducible Research Training (FORRT)](#)
- o [Open Accelerated Computing (OpenACC) (C/C++ optimizations for research, annual Summer conference)](#)
- o [NumFOCUS (NumFOCUS) (open resource software practices](#)
- o [Consortium for the Advancement of Scientific Software (CASS) (DoE sponsored)](#)
- o [Center for Open-Source Research Software Stewardship and Advancement (CORSA)](#)
- o [LF AI & Data (AI Innovation)](#)
- o [US Research Software Sustainability Institute (URSSI)](#)
- o [Open Molecular Software Foundation (OMSF)](#)
- o [ZENODO (open data/scholarship/publication repository - managed by CERN and OpenAIRE)](#)
- o [Software Carpentries (software engineering)](#)
- o (and check your discipline's pre-conference workshops and related conference themes for HPC events)
- Staff - These HPC resources should be of use to *Staff* over time.
  - o [US Research Software Engineering Association (US-RSE)](#)
  - o [Campus Research Computing Consortium (CaRCC)](#)
  - o [Campus Champions](#)
  - o [OpenOnDemand](#)
  - o [Internet2 Research Engagement](#)
  - o [Internet2 NET+](#)
  - o [EduCause Research Computing and Data Community Group](#)
- Administration - These HPC resources should be of use to *Administration* over time.
  - o [Coalition for Academic Scientific Computing (CASC)](#)
  - o [Research Software Alliance (ReSA)](#)
- Sundry - These HPC resources related to *networking* should be of use to various individuals over time.
  - o [ES NET (DOE)](#)
  - o [Globus](#)
  - o [The Quilt](#)
  - o [Fabric](#)
- Sundry - These miscellaneous open source research-related resources should be of use to various individuals over time.
  - o [Research Data Alliance (RDA)](#)
  - o [Center for Open Science - Open Software Foundation (OSF)](#)
  - o [Digital Management Plan Tool (DMPTOOL)](#)
  - o [UC Open Source Program Offices)](#)
  - o [Professional Development for Instructors Interested in Student Participation in Humanitarian Free and Open Source Software (POSSE)](#)
  - o [HPC Social (HPC community development)](#)
- Sundry - These resources related to *domestic* open science/reproducibility should be of use to various individuals over time.

- - Science Philanthropy Alliance
    - Crossref (Crossref
- Sundry - These resources related to *international* open science/reproducibility should be of use to various individuals over time.
    - Coalition for Advancing Research Assessment (CoARA)
    - UNESCO Open Science (UNESCO)
    - Global Research Council (GRC)
    - Society of Software Research Engineering (SocRSE) (provides £1,000 for conference travel too)
    - Science for Life Laboratory (SciLifeLab)
    - Turing Way (Turing Way)
    - Digital Research Alliance of Canada
    - International Conference on Scalable Scientific Data Management
    - Reach the World (K-12 supercomputing)
- Sundry - These charitable organizations provide regular funding for HPC-related and scientific software.
    - Chan/Zuckberberg Initiative (Essential Open Source Software for Science (Cycle 6))
    - Kavli Foundation (general science)
    - Wellcome Trust (generally, health-related research software
    - Simons Foundation (generally, math and physical sciences software)
    - Sloan Foundation (generally, emerging technology of any type)
    - Code for Science and Society (generally, open source software)
- Sundry - Parody.
    - Journal of Astrological Big Data Ecology (like the old "Journal of Irreproducible Results")