

Overview of GACRC Resources and the CSP compute nodes

Georgia Advanced Computing Resource Center (GACRC)

Enterprise Information Technology Services (EITS)

The University of Georgia

Outline

- What is GACRC?
- Overview of Sapelo2 hardware
- Overview of CSP compute nodes
- Overview of Sapelo2 software
- Transferring Files using Globus
- Open OnDemand
- Consulting and Support
- Documentation

What is GACRC?

- A high-performance computing (HPC) center at UGA
- A partnership between the Offices of the VP for Information Technology and for Research
- Provide to the UGA research and education community an advanced computing environment:
 - Computing hardware, storage, and networking infrastructure
 - Large collection of math libraries, scientific, and engineering applications
 - Consulting and training services
- Sapelo2 (main cluster, for research use)
- Teaching cluster (for instructional use, includes 2 A30 GPU nodes for Franklin College)
- Buy-in program (faculty contribute nodes to Sapelo2)

Wiki: <http://wiki.gacrc.uga.edu>

Web Site: <http://gacrc.uga.edu>

Computing clusters at Boyd Data Center



Accounts and Access

- UGA faculty (PIs) can register a lab and request accounts for group members.

Step 1: Lab registration by PI:

<https://uga.teamdynamix.com/TDClient/2060/Portal/Requests/ServiceDet?ID=25846>

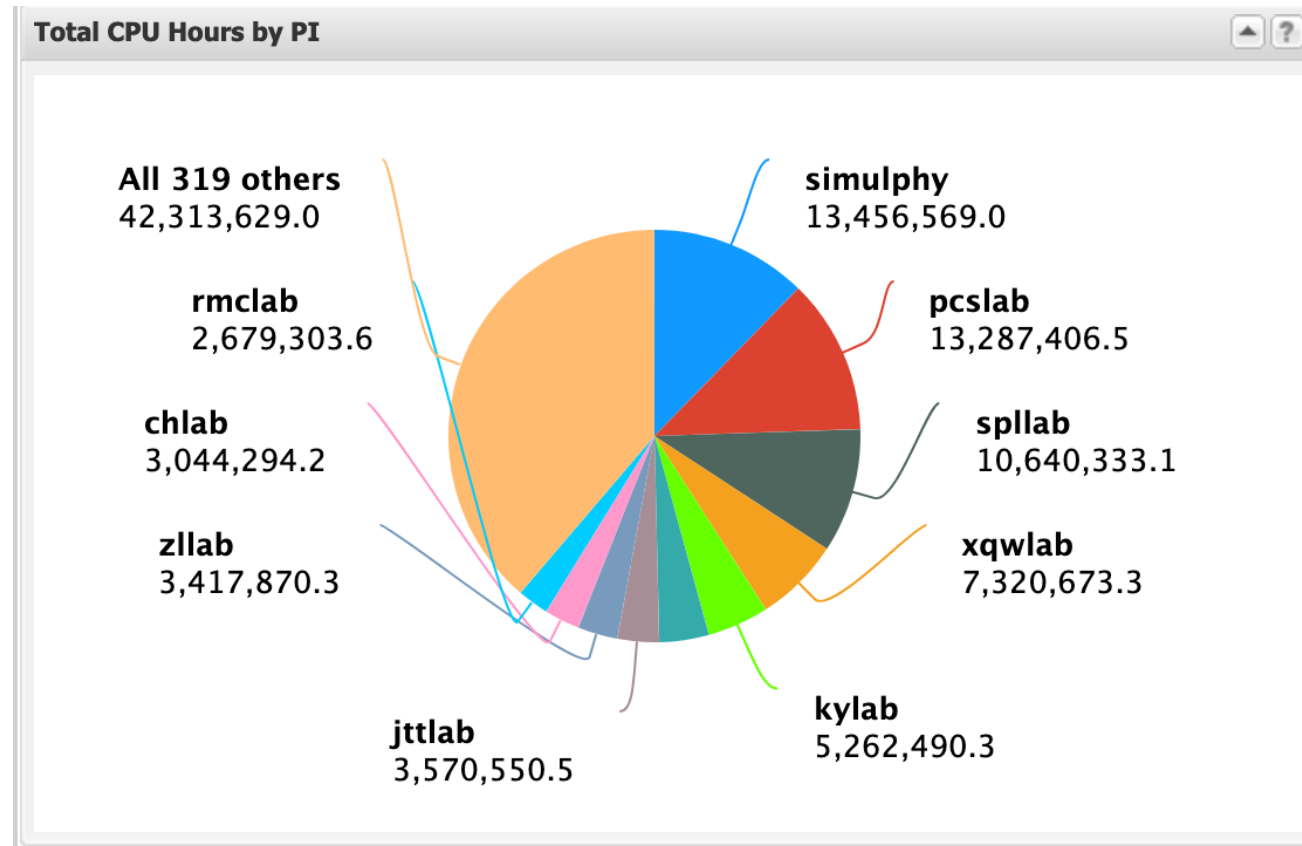
Step 2: PI requests user accounts:

<https://uga.teamdynamix.com/TDClient/2060/Portal/Requests/ServiceDet?ID=25839>

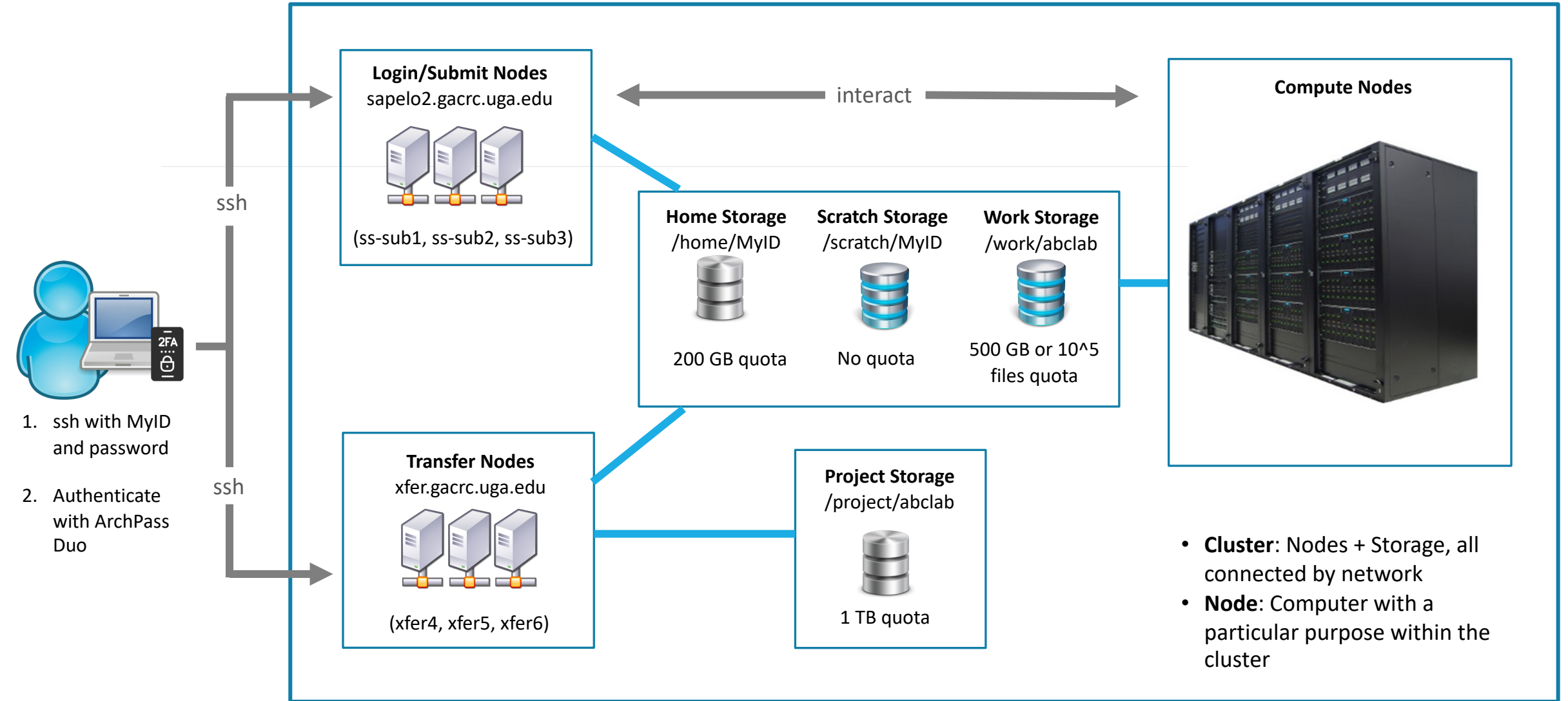
- User accounts provided using UGA MyID.
- Connection to the cluster via SSH on Linux/Mac OS X, PuTTY on Windows.
- Authenticate with UGA MyID password and Archpass Duo.
- From off campus, connect to the UGA VPN first.

<https://wiki.gacrc.uga.edu/wiki/Connecting>

Sapelo2 usage by group (7/31/23 to 7/31/24)



Sapelo2 Cluster Overview



1. ssh with MyID and password
2. Authenticate with ArchPass Duo

- **Cluster:** Nodes + Storage, all connected by network
- **Node:** Computer with a particular purpose within the cluster

Note: You need to connect to the **UGA network using VPN** when accessing from outside of the **UGA main campus**.
UGA VPN: https://eits.uga.edu/access_and_security/infosec/tools/vpn/

Sapelo2 – Computing Hardware

➤ Resources available to all users (summary on next slide)

- Regular memory nodes: 32 to 128 cores/node, 2GB to 6GB/core
- High memory nodes: 512GB, 1TB, 2TB, or 3TB/node
- GPU nodes: NVIDIA A100, P100 devices (**coming soon**: 12 quad H100; 12 quad L4 nodes)
- Number of CPU cores: ~ 33,400

➤ Buy-in nodes

- Various configurations, including GPU nodes.
- Number of CPU cores: ~ 10,300

➤ Total number of CPU cores: ~ 43,700

Processor Type	Cores/Node	RAM/node (GB)	# Nodes	GPU Cards/Node	
AMD EPYC Genoa	128	760	4	-	Regular Nodes
AMD EPYC Milan	128	512	120	-	
AMD EPYC Milan	64	256	4	-	
AMD EPYC Rome	64	128	120	-	
AMD EPYC Naples	32	128	52	-	
Intel Xeon Skylake	32	192	42	-	
AMD EPYC Genoa	48	3000	3	-	High-Memory Nodes
AMD EPYC Milan	128	1000	2	-	
AMD EPYC Milan	32	1000	12	-	
AMD EPYC Rome	32	2000	2	-	
AMD EPYC Naples	64	1000	2	-	
AMD EPYC Naples	32	512	18	-	
Intel Xeon Broadwell	28	1000	4	-	
AMD EPYC Milan	64	1000	14	4 NVIDIA A100	GPU Nodes
Intel Xeon Skylake	32	192	2	1 NVIDIA P100	

Sapelo2 – CSP Compute Nodes

➤ Pool of nodes

- ra1-8 : 52 cores, 256GB RAM, Intel Icelake, local drive with 890GB of space
- ra1-9 : 40 cores, 192GB RAM, Intel CascadeLake, local drive with 890GB of space
- ra1-10 : 36 cores, 256GB RAM, Intel CascadeLake, local drive with 440GB of space
- ra1-11 : 24 cores, 256GB RAM, Intel Skylake, local drive with 930GB of space
- ra1-12 : 36 cores, 256GB RAM, Intel Skylake, local drive with 930GB of space

➤ Partition name

- csp_p (maximum walltime limit of 30 days, can be extended)

➤ Available to all CSP members

Sapelo2 – Storage and Cluster Network

- Storage to support projects that use the computing cluster only.
- ZFS storage: home directory **/home** (200GB/user quota, no purge, backup)
- DDN Lustre storage device:
 - /scratch** (no quota, 30-day purge, no backup)
 - /work** (500GB and 500k file/group quota, no purge, no backup)
- ZFS JBOD: **/project** (1TB/group, no purge, backup)
- Local hard drive (SSD, NVMe) on compute nodes: **/lscratch** (~890GB)
- Internodal and compute node to Lustre network:
 - EDR Infiniband (100 Gb/s bandwidth)

Sapelo2 – Software

- 64-bit Linux OS (Rocky 8.8).
- Slurm queueing system to submit jobs to the compute nodes (e.g. sbatch, squeue, sacct).
- Over 1500 environment modules, conda environments, Singularity containers.
- Cannot run applications that need Windows OS.
- Cannot run Docker containers, convert to Singularity (Apptainer) containers.
- Very limited number of commercial software (e.g. MATLAB, Amber, Gaussian), some limited to a few groups that purchased licenses (e.g. SAS, Stata, Ansys, Schrodinger).

Software Environment

<https://wiki.gacrc.uga.edu/wiki/Software>

- Software loaded via **environment modules** (Lmod).
- Compilers (C/C++, Fortran): GCC, Intel , PGI
- MPI Libraries: OpenMPI, Intel MPI, MVAPICH
- Math Libraries: Intel MKL, GSL, OpenBLAS, LAPACK, FFTW, etc.
- GPU Tools: NVIDIA CUDA Toolkit, cuDNN, NVHPC
- High-Level Languages: Python, Perl, R, Julia, Java
- Plotting: gnuplot, xmgrace, matplotlib, ParaView, etc.
- Other Programming/Visualization Tools: MATLAB, Mathematica
- Machine Learning and Deep Learning Tools: scikit-learn, Tensorflow, Keras, PyTorch, etc.
- Applications for Bioinformatics, Chemistry, Physics, Engineering, etc.

Transferring Files

➤ UGA has a subscription for **Globus**, a high-performance data-transfer platform that allows you to perform and/or automate:

- Transfer data from your local machine to GACRC resources.
- Transfer data between file systems on Sapelo2.
- Data transfers between servers in your group or a server and your laptop.
- Sharing data with researchers at UGA and at other institutions.
- Automate data backup.

<https://wiki.gacrc.uga.edu/wiki/Globus>

https://kaltura.uga.edu/media/t/1_vlprwoc7/176125031

➤ Other file transfer programs are available: scp, FileZilla, WinSCP

https://wiki.gacrc.uga.edu/wiki/Transferring_Files

Open OnDemand

- Alternative way to access Sapelo2, **connecting from a browser.**

URL: <https://ondemand.gacrc.uga.edu>

- Provides a graphical desktop on the cluster

Graphical applications can be utilized on the cluster far more easily and smoothly than using X11 forwarding.

- Interactive applications (MATLAB, Rstudio, ParaView, Jupyter notebook, VSCode, etc)

- Sessions are not lost when network connection is interrupted or local computer is shutdown.

Can start a session from a browser on one computer, and connect to it from a browser on another computer.

<https://wiki.gacrc.uga.edu/wiki/OnDemand>

https://kaltura.uga.edu/media/t/1_u9d1xrpp/176125031

Consulting and Support

- Install and update software per user request.
- Troubleshoot programs, jobs, and workflows.
- Help users optimize their code.
- Help users implement or automate pipelines.
- Provide user training (Linux, Sapelo2 new user, virtual environment, etc.).
- Assistance with grant proposal preparation, where GACRC resources are used.

https://gacrc.uga.edu/about/how_we_help_researchers.php

Documentation and Contact

Wiki: <http://wiki.gacrc.uga.edu>

Web Site: <http://gacrc.uga.edu>

Help: <https://help.gacrc.uga.edu>

Videos: <https://kaltura.uga.edu/channel/GACRC/176125031>

Offices: GACRC staff are located in the Computing Services Building (formerly called Statistics Building), rooms 101 to 108.

Office Hours (in person and via Zoom)

Thank you!