

Introduction to SeaWulf HPC for CSE416 students

Dave Carlson September 24nd, 2024



What's an HPC cluster, anyway?

A High Performance Computing

(HPC) cluster contains multiple physically distinct computers ("nodes") that are connected over a network

A shared, parallel file system allows efficient access to the same data across all nodes



SeaWulf is ...

- An HPC cluster dedicated to research applications for Stony Brook faculty, staff, and students
- **Available hardware:**
- ✤ 5 login nodes = the entry points to the cluster
- *362 **CPU compute nodes** = where the work is done
 - □ 28 96 CPUS each
 - □ 128 GB 1 TB RAM each
- ✤ 8 GPU nodes each with 4 Nvidia Tesla K80 GPUs
- ✤ 1 GPU node with 2 Tesla P100 GPUs
- ✤ 1 GPU node with 2 Tesla V100 GPUs
- ✤ 1 1 GPU nodes with 4 Tesla A100 GPUs
- Two large memory nodes each with 3 TB of RAM



How do I connect to SeaWulf?

Mac & Linux users via the terminal:

ssh -X netid@login.seawulf.stonybrook.edu
ssh -X netid@milan.seawulf.stonybrook.edu

Windows use



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2-factor authentication with DUO

 Upon login, you will be prompted to receive and respond to a push notification, sms, or phone call:





Multiple failures to respond can lead to temporary lockout of your account

* DUO 2FA can be bypassed if connected to SBU's VPN (GlobalProtect)

Which login nodes should I access?

login.seawulf.stonybrook.edu provides access to:

- □ 28-core nodes
- □ All GPU nodes except A100

milan.seawulf.stonybrook.edu &

xeonmax.seawulf.stonybrook.edu provides access to:

- □ 40-core nodes
- □ 96-core nodes (AMD Milan)
- □ hbm-96-core nodes (Intel Sapphire Rapids)
- □ A100 GPU nodes







Point your browser to:

https://sn-ood.seawulf.stonybrook.edu/



See our OOD FAQ here:

https://it.stonybrook.edu/help/kb/accessi ng-seawulf-with-open-ondemand



Important paths to remember

/gpfs/home/netid = your home directory (20 GB)



- /gpfs/scratch/netid = your scratch directory (20 TB for housing temporary and intermediate files)
- /gpfs/projects/CSE416 = your project directory (5 TB shared space accessible to all class members)

How do I transfer files onto SeaWulf?

Mac & Linux users should use scp (secure copy) to move files to and from SeaWulf

To transfer files from your computer to SeaWulf

- 1. Open terminal
- 2. scp /path/to/my/file <u>netid@login.seawulf.stonybrook.edu</u>:/path/to/destination/

To transfer files from SeaWulf to your computer

- 1. Open terminal
- 2. scp <u>netid@login.seawulf.stonybrook.edu</u>:/path/to/my/file /path/to/destination

When possible, xfer archives (e.g. tarballs) or directories because:

1. It's faster to transfer one large file than many small files

2. Unless connected to the SBU VPN, you may receive 1 DUO prompt for every scp command you run!

How do I transfer files onto SeaWulf?

Windows users:



Using the module system to access software

Useful module commands:

module avail

module load

module list

module unload

module purge

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uda10.0/fft/10.0.130 cudi	a10.1/nsight/10.1.243	cuda80/profiler/8.0.61	cuda90/toolkit/9.0.176 cud	a92/blas/9.2.88 default-environ	ment netpert/2.7.0
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cml/gcc-int64/mp/64/5.3.1	fftw2/openmpi/	acc/64/double/2.1.5	intel/compiler/64/2020/20.0	.0 maltools/1.5.6	at/5.3
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Using the module system to access software



now available!

How do I do work on SeaWulf?

Computationally intensive jobs should *not* be done on the login node!

- ✤ To run a job, you must submit a batch script to the Slurm Workload Manager
- A batch script is a collection of bash commands issued to the scheduler, which which distributes your job across one or more compute nodes
- The user requests specific resources (nodes, cpus, job time, etc.), while the scheduler places the job into the queue until the resources are available

Example Slurm Job Script

All jobs submitted through a job scheduling system using scripts



How do I execute my Slurm script?

Jobs are submitted via the Slurm Workload Manager using the "sbatch" command

[decarlson@login1 iqtree]\$ [decarlson@login1 iqtree]\$ [decarlson@login1 iqtree]\$ [decarlson@login1 iqtree]\$ [decarlson@login1 iqtree]\$ [decarlson@login1 iqtree]\$ module load slurm/17.11.12 [decarlson@login1 iqtree]\$ sbatch gnu_parallel_example.slurm Submitted batch job 356633 [decarlson@login1 iqtree]\$

This is your job ID.

Useful Slurm commands

sbatch <script> = submit a job

scancel <job id> = cancel a job



squeue = get job status

sinfo = get info on node/queue status and utilization

(see the following for a full list of Slurm commands) https://slurm.schedmd.com/archive/slurm-21.08.8/man_index.html

What queue should I submit to?

How many nodes do you need?

How many cores per node?

How much time do you need?

- Only jobs using MPI should request more than 1 node!
- Use a "shared" queue if you don't need all the resources on a node
- There is often a tradeoff between resource usage and wait time!
- Don't wait until the last minute to submit jobs when you have a deadline!

Queues accessed from milan1 and milan2:

Queue	CPU Architecture	Vector/Matrix Extension	CPU Cores per Node	GPUs per Node	Node Memory ¹	Default Runtime	Max Runtime	Max Nodes	Min Nodes	Max Simultaneous Jobs per User	Multiple Users per Node
debug-40core	Intel Skylake	AVX512	40	0	192 GB	1 hour	1 hour	8	n/a	n/a	No
short-40core	Intel Skylake	AVX512	40	0	192 GB	1 hour	4 hours	8	n/a	4	No
short-40core- shared	Intel Skylake	AVX512	40	0	192 GB	1 hour	4 hours	4	n/a	n/a	Yes
medium-40core	Intel Skylake	AVX512	40	0	192 GB	4 hours	12 hours	16	6	1	No
long-40core	Intel Skylake	AVX512	40	0	192 GB	8 hours	48 hours	6	n/a	3	No
long-40core- shared	Intel Skylake	AVX512	40	0	192 GB	8 hours	24 hours	3	n/a	n/a	Yes
extended-40core	Intel Skylake	AVX512	40	0	192 GB	8 hours	7 days	2	n/a	3	No
extended-40core- shared	Intel Skylake	AVX512	40	0	192 GB	8 hours	3.5 days	1	n/a	n/a	Yes

See our FAQ page on SeaWulf's queues

Parallel processing on the cluster

□ Parallelization *within a single compute node*

✤ Lots of ways of doing this

- Some tasks easily parallelized with scripting (e.g, "Embarrassingly Parallel" tasks)
- Language-specific options (e.g., Python's Multiprocessing library)
- ✤ OpenMP for multithreaded C/C++/Fortran tasks

□ Parallelization across *multiple nodes*

- ✤ No communication Slurm Array
- Communication between processes needed Requires the use of MPI

Parallel processing on a single node with GNU Parallel

- Perfect for "embarrassingly parallel" situations
- Available as a module: gnu-parallel/6.0



- Can easily take in a series of inputs (e.g., files or values) and run a command on each input simultaneously
- Lots of tutorials and resources available on the web!

https://www.gnu.org/software/parallel/parallel_tutorial.html (thorough!!) https://www.msi.umn.edu/support/faq/how-can-i-use-gnu-parallel-run-lot-commands-parallel (many practical examples)

Parallel processing with GNU Parallel

#!/usr/bin/env bash

#SBATCH --nodes=1
#SBATCH --time=05:00
#SBATCH --partition=short-40core
#SBATCH --job-name=parallel_job
#SBATCH --output=squared_numbers.txt

load required modules

module load anaconda/3
module load gnu-parallel/6.0

parallelize the calculation across each input, running 40 processes at a time

parallel --jobs 40 python number_square.py {} ::: {1..100}

Optional flags to control behavior This command will The input values to be run on each parallelize over input

{} =
 placeholder
for each input

Parallel processing on a single node with Python's multiprocessing library



import numpy as np
import multiprocessing as mp

define a function for the calculation
def square_me(num):
 result = int(np.square(num))
 return(result)

spawn a pool of parallel workers

p = mp.Pool(processes=40)

using a pool of 40 parallel workers, loop over the values of 1 through 100 and apply the math function to each
for num in range(1,101):

```
results = p.apply_async(square_me, [num])
print(f'The square of {num} is {results.get()}')
```

close the pool of workers
p.close()



Brief introduction to parallelization options for python:

https://www.anyscale.com/blog/parallelizing-pythoncode

Multithreading on a single node with OpenMP

- Framework for parallelization (multithreading) in a sharedmemory (single node) context for C, C++, and Fortran
- Typically involves creating multiple threads within a single process instead of spawning multiple processes
- Useful when communication between parallel tasks is required
- Implemented in most modern compilers (GCC, Intel, LLVM, etc.)
- Resource usage controlled at runtime by environment



Multithreading on a single node with OpenMP

Estimating pi with C and OpenMP

<pre>#include <stdio.h></stdio.h></pre>	#!/usr/bin/env bash
<pre>#include <time.h></time.h></pre>	
<pre>#include <omp.h></omp.h></pre>	
<pre>#include <stdint.h></stdint.h></pre>	#SBATCH Job-name=openmp_p1
#define NPTS 100000000	#SBATCHoutput=openmp_pi.log #SBATCHnodes=1
void main() {	<pre>#SBATCHtime=05:00</pre>
uint64_t i;	"#SBATCH -p short-40core
double a,b,c,pi,dt,mflops;	
struct timespec tstart,tend;	# load a acc module Load a compiler
<pre>clock_gettime(CLOCK_REALTIME,&tstart);</pre>	
a = 0.5;	, module load gcc/12.1.0 module
b = 0.75;	
c = 0.25;	# Environment variable to set how many threads we'll be using
pi = 0;	
<pre>#pragma omp parallel for reduction(+:pi)</pre>	Specify # of
<pre>for (i = 1; i <= NPTS; ++i)</pre>	export OMP_NOM_THREADS=40
pi += a/((i-b)*(i-c));	threads
<pre>clock_gettime(CLOCK_REALTIME,&tend);</pre>	# compile the code
<pre>dt = (tend.tv_sec+tend.tv_nsec/1e9)-(tstart.tv_sec+tstart.tv_nsec/1e9);</pre>	acc /anfs/projects/samples/pj/openmp pj c -o openmp pj -fopenmr
<pre>mflops = NPTS*5.0/(dt*1e6);</pre>	gee / gpro/ projecto/ samples/ pr/ opermp_price of opermp_pr
<pre>printf("NPTS = %ld, pi = %f, threads = %d\n",NPTS,pi,omp_get_max_threads());</pre>	Compile w/ _fonenmp
printf("time = %t, estimated MFLops = %t\n",dt,mtLops);	# execute the code
}	./openmp_pi

Can I use multiple nodes for a single job?

Yes! (...well...maybe)

Message Passing Interface (MPI) facilitates communication between processes within or among nodes

Multiple "flavors" of MPI are available on SeaWulf

- Mvapich*, Intel* mpich, OpenMPI

*=officially supported



Open MPI



Can I use multiple nodes for a single job?

To use MPI:

*

- Write code with MPI functions
- ✤ Compile with MPI wrapper

Language	GCC command	Mvapich wrapper
с	gcc	mpicc
C++	g++	mpicxx
Fortran	gfortran	mpif90

Specify resource requirements in your Slurm script

ngle job?



MVAPICH



Example MPI Job Submission Script

#!/usr/bin/env bash

#SBATCH --job-name=mpi_pi **Specify resource** #SBATCH --output=mpi_pi.log #SBATCH --nodes=4 usage (nodes and MPI **#SBATCH** --ntasks-per-node=28 #SBATCH --time=05:00 #SBATCH -p short-28core Load an MPI # load a gcc module module load mvapich2/gcc12.1/2.3.7 module # set env variables which may help performance export MV2_HOMOGENEOUS_CLUSTER=1 export MV2_ENABLE_AFFINITY=0 #export HWLOC_COMPONENTS=-gl **Compile with** # compile the code with the mpi compiler wrapper MPI mpicc /gpfs/projects/samples/pi/mpi_pi.c -o mpi_pi # execute the code with MPI **Execute with MPI** mpirun ./mpi_pi

Estimating pi with C and MPI

Parallelization FAQS:

Part 1: embarrassingly parallel tasks

Part 2: OpenMP & MPI

MPI Hello World

"Hello from process 1 on node 1" "Hello from process 2 on node 1" "Hello from process 3 on node 1" "Hello from process 4 on node 1"

#!/bin/bash

#SBATCH --job-name=gcc_mpi_hello #SBATCH --output=gcc_mpi_hello.log #SBATCH --ntasks-per-node=4 #SBATCH --nodes=2 #SBATCH --time=05:00 #SBATCH -p short-40core

module load mvapich2/gcc12.1/2.3.7

mpirun ./gcc_mpi_hello

-8-18-36 10.50.00 REPORT PLACES 0.00000000 - HERE AND mpirun 10.50.00 A 16 16 10 10 01 President 1-00-00-1 10-00 000 10-10-20 HOLE ALL 10.8218

> "Hello from process 1 on node 2" "Hello from process 2 on node 2" "Hello from process 3 on node 2" "Hello from process 4 on node 2"

Need to troubleshoot? Use an interactive job!

Example:

[decarlson@dg-mem ~]\$ srun -N 1 -p short-40core --pty bash srun: job 293816 queued and waiting for resources srun: job 293816 has been allocated resources [decarlson@dn029 ~]\$

"srun": allocate a compute node in the short-40core queue

"--pty bash" run the bash shell on the compute node

Once a node is available, you can issue commands on the command line

Good for troubleshooting,

Inefficient once your code is working

Need more help or information?

Check out our FAQ: https://it.stonybrook.edu/services/high-performance-computing

Announcements

- August 24, 2626 Intel Panelal studio 2020 vension 20.0.2 has been mutable on SeaW.W.F. In order to ensure stability and improve the user experience, 20.0.2 has been rest as the default vension of the Intel complex, IMD, and MMI when the intel-stade module is loaded. Older vensions of the Intel modules are still evaluate on my bio loaded individually.
- July 20, 2028 Emergency electrical maintenance will be performed on the circuits feeding the 24-core guesses on Thursday 7/23/2020. This outage is not sepactive to impact the 28-core or 80-core guesses, nor the logit nodes. In anticipation of this maintenance, the 24-core guesses will be disabled istarting at 5 00 PM on Wednesday 7/22/2020. We currently anticipate the 24-core guesses will be back up by the end of business on 1/23/2020, pendig timely completion of the emergency electrical maintenance.
- July 02, 2020 Due to preventive maintainance on the Campus Data Center's generator and schedulad maintenance on SeaWulf's Compute Nodes, the SeaWulf duster's job queues will be disabled tarting at 3 00 PM on Nonday July 13th. During this maintenance window, all SeaWulf Nodes will be unavailable and login nodes will be off-line. We will be updating the operating system and security packages in order to provide a more robust computational environment. The work is expected to be completed by the end of business on Taesday July 14th.
- May 21, 2020 Swithill users may now receive email updates about their Slum jobs using the "--mail-type" and "--mail-user" SEATCH directives. For more information regarding this new functionality, please see the following FAQ page:

https://it.stonybrook.edu/help/kb/exemple-slumn-job-script

- Nanch 30, 2020 Gur (76C Support Taken will now be offering online office hours via a resump Zoom meeting. Support staff will be available from Zom Apm avery Wednesday starting this Wednesday, April 31, until the send of the sensater. You can also by joining the meeting at anytime and ...I available, one of support staff may be able to poin the meeting to assist you. Citch bere to join office hours.
- March 30, 2028 We will be performing scheduled maintenance Wednesdey. April 53th starting at 3:00 AM on the SeaWulf duster. During this maintenance window, all SeaWulf obsease will be down and login nodes will be off-line. We will be earling up Dus as a two-factor authoritication method and splitsting the operating system and security packages in order to provide a more robust computational anxingment. The maintenance is expected to be completed by the end of business on Wednesdey.
- February 17, 2020 We will be performing scheduled maintanance this Friday, February 21st starting at 9000 AM on the SestWall duster. During this maintanance window, all SastWall queues will be down and login nodes will be off-fine. We will be updating the operating system and security perforges in order to provide a more robust computational environment. The maintanance is expected to be completed by the and of business on Friday.

We apologize for the inconvenience and thank you for your patience while we complete these updates.

February 06, 2020 The IACE is sponsoring a SextraUnited training workshop on Mandey, Merch 2 and Taussiay, Merch 3 from 1 - Hom INte IACE Seminar Room. This workshop is aimed at researchers (gred students, profesors, postdock, and undergreds are all welcomel) who are interested in using right Performance Computing resources for thair research but have finited experience in this area.

The workshop is free but requires registration. Plasse see the IACS events calendar for more information. You may also register for the workshop here.

- December 05, 2019 The shared module is now depreciated on Seaw/II. All modules can now be loaded directly after logging in to Seaw/II. It does no harm to load or unload the shared module: It will just no longer have an effect on the search path for modulaties. This means there is no need to remove it from any profits you have. But it is no longer have needed or grange forward.
- November 21, 8019 The SeaWolf Guster will be going down for upgrades on Monday November 25th at the Gose of business. During this upgrade window, the remander of the SeaWolf nodes on Torque will be switched over to the Slurm scheduler. The upgrades are expected to be completed by the close of business on Tuesday November 25th.

The below section in our FAQ may be useful in assisting with switching workflows from the Torque scheduler to Slurm:

https://it.storybrook.edu/help/kb/using-the-slum-workload-manager

Qs	
ting Started	
How do I request a SeaWulf account?	
How do I get a project on SeaWulf?	
How do I log into SeaWulf?	
How do Lenroll in DUO Security?	
Getting Started Guide	
RM Jobs	
Can you give me an example of a slurm job script?	
How can I check the status of a SLURM job?	
How can I delete a SLURM job?	
How can I submit a Slurm job?	
How do Laiter my PBS scripts for use with Slurm?	
	As Started How do I request a SeaWulf account? How do I get a project on SeaWulf? How do I log into SeaWulf? How do I log into SeaWulf? Getting Started Guide RM Jobs Can you give me an example of a slurm job script? How can I check the status of a SLURM job? How can I delete a SLURM job? How can I submit a Slurm job

Submit a ticket: <u>https://iacs.supportsystem.com</u>

