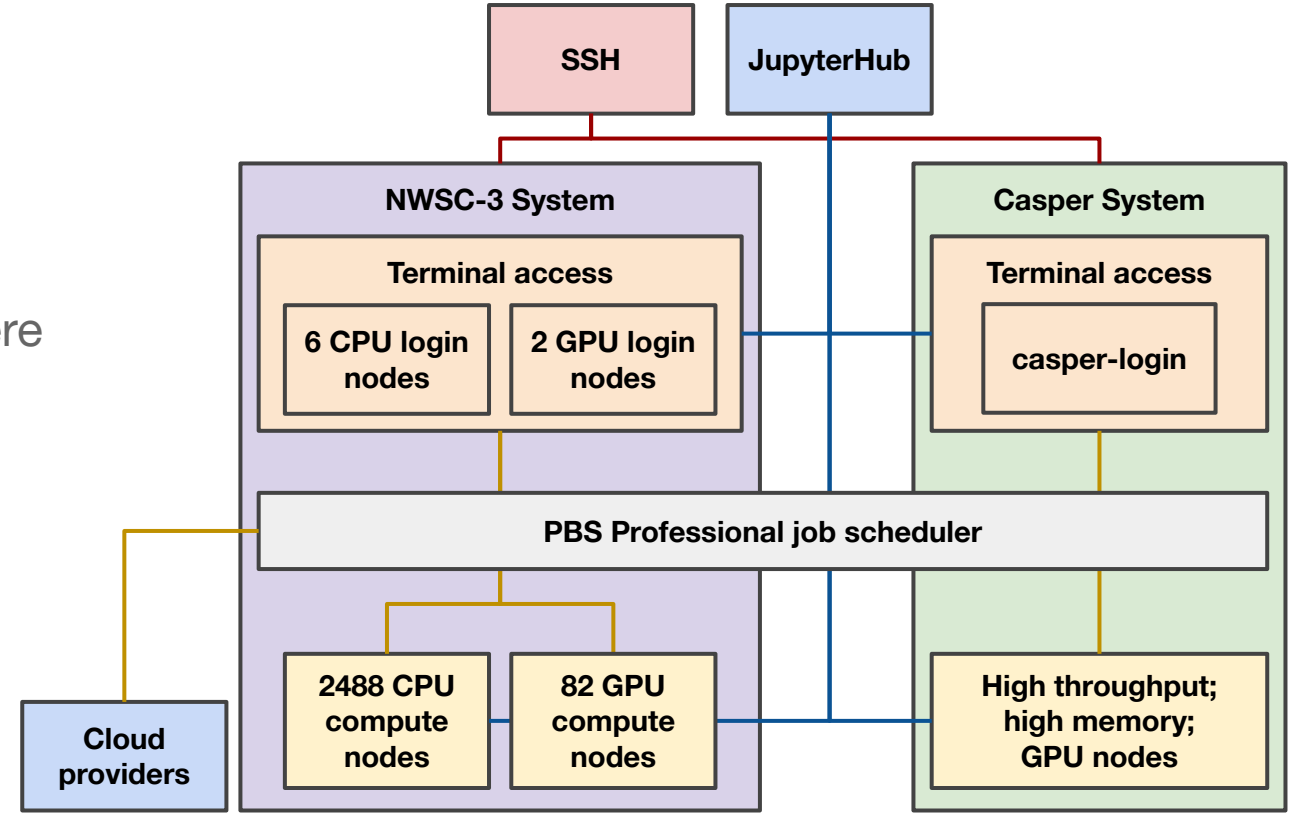
Application and User Environment Team

Team Members:

- **Brian Vanderwende**
- **Rory Kelly**
- Bill Anderson
- Irfan Elahi
- Jeff de La Beaujardiere
- John Dennis
- Marc Genty
- Mick Coady
- Tracey Baldwin
- Siddhartha Ghosh



Software to support traditional and new technologies

Maintain familiar environment with Lmod modules and increase usability and capability of modern interfaces like JupyterHub

Multiple compiler options with CPU and GPU support:

Cray Compiler, Intel oneAPI (Parallel Studio), NVIDIA HPC Compiler (formerly PGI), GNU Compiler Collection (GCC)

Multiple MPI options (subset with native GPU support):

Cray MPI, Intel MPI, MVAPICH2

*All MPICH-based - ABI compatible for **portable** MPI containers*

Large collection of GPU libraries to ease adoption

GPU software stack will be extensive at launch and will grow to match user and application needs

GPGPU Fortran, C/C++ coding and development

CUDA, OpenACC, OpenMP 5, MAGMA, GPU Direct MPI

TensorFlow, Keras, PyTorch, Horovod, & more...

Machine learning, deep learning and artificial intelligence

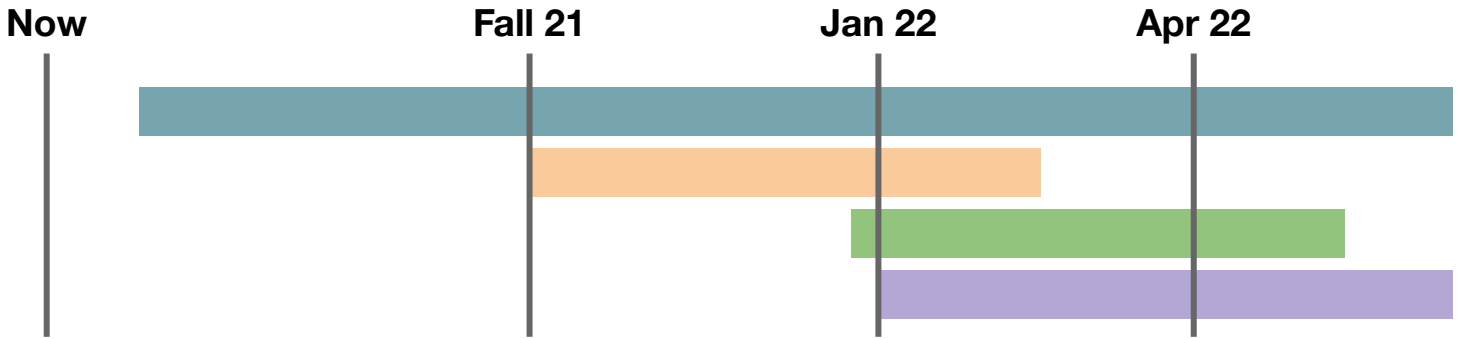
Many are available on Casper now; please let us know if you have a software need or want GPU consulting

Peer scheduling across and outside complex using PBS

PBS Pro job scheduling on NWSC-3 and Casper

- Queue visibility and submission across both systems; designing a “single-system” scheduling environment
- Built-in container support using Singularity/Docker
- Cloud integration - queue(s) for submissions to cloud vendors directly from log-in environment via PBS
- GUI and traditional CLI to PBS

Anticipated training timeline for users



Workshops on programming and using GPU resources

Training for existing users on migrating from Cheyenne to NWSC-3

Targeted early user training and application porting sessions

Training for all users on using NWSC-3 including optimal application settings and job configurations

Early users and primary applications

Now - GPU development on Casper
- Gather user group and application requirements

Fall 21 - Accelerated Scientific Discovery (ASD) call for proposals
- Targeted application work on NWSC-3 test machine

Jan 22 - Early/ASD users on NWSC-3

Apr 22 - NWSC-3 open to all users

2H 22 - Cheyenne is decommissioned

Applications Team Role

- Collect user requirements and provide recommendations to other technical teams regarding design and training
- Work with interested user and application groups to ensure readiness for the new system
    - Particular emphasis on prospective ASD and first year GPU projects, but open to all
- Evaluate software provided by HPE/Cray
- Learn from other institutions who are incorporating GPUs, containers, and cloud compute into their HPC
- Design applications tests for machine acceptance

Gathering Requirements

- **Software** - compilers, libraries, module structure, commonalities across systems
- **Storage** - concurrent usage, retention time, shared access, accessibility across systems, external transfer
- **Scheduler** - # nodes, memory needs, dependencies, workflow integration, special resources, frequency
- **Interface** - long running processes, continuous integration, GUI/remote desktop, other portals

User Group Outreach

Identified User Groups	
CAM-Chem	MuRAM
CESM	MUSICA
CM1	NEMO ocean model
DART	Pangeo
EcoSLIM	ParFlow.CLM
FastEddy	QES-Fire
GeoCAT	Regional Climate Impacts (RISC)
LES	SIMA
Machine Learning	TIEGCM
Solar Modeling	WACCM
MPAS-A (CPU)	WRF-ARW
MPAS-A (GPU)	WRF-Hydro

Contact Info

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Let us know if:

- We are missing your user group/application
- You want to be a subject matter expert for a group
- You have general feedback regarding aforementioned topics