Lonestar 5:

Customizing the Cray XC40 Software Environment

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Overview

- Introduction to TACC and LS5
- Motivation for XC40 software customizations
- Live demonstration
- Discussion of customizations made



Who We Are

- Texas Advanced Computing Center (TACC)
- Based at University of Texas in Austin
- 160 full-time technology & support staff
- 15K sq. ft. data center with 10 MW capacity
- >10 production and experimental systems
- >10K users in 2100 unique research projects

Our Focus Today: Lonestar 5

- Cray XC40
 - 5th in series; Production started in January 2016
 - 1252 Intel HSW/IVB nodes w/ Aries interconnect
 - 30K cores @ 1.25 PFLOPs
 5 PB & 20 PB Scratch & Work Lustre filesystems





Our Challenge:

- New system rollout replacing Lonestar 4
- How do we:
 - Transition 3500 LS4 users?
 - Support existing and future workflows?
 - Minimize disruption and need for retraining?



We Need Lonestar 5 to Provide

- Familiarity:
 - Recognizable to those who use other TACC resources
- Consistency:
 - Same Full Linux environment everywhere
- Flexibility:
 - Adaptive platforms that respond and evolve to meet user needs
 - ...All while maintaining performance at scale



LS5 Modification Summary

- Customized network
 configuration
- Tailored workload management
- Shell startup behavior
- Hierarchical software stack

- Adaptive virtual esLogin nodes
- MPI distribution
 wrappers
- RPM development
 environment

Live Demonstration of **Lonestar 5 XC40 Environment**

Customized Network Configuration

- Direct Slurm traffic from esLogins to Slurm database node
- No need for internal login node or esWrapper module
- Ability to access compute nodes via ssh





Tailored Workload Management

- Run Slurm in "native" mode
- Custom Slurm plugins to qualify user jobs
- PAM Slurm module
- Extended Prolog and Epilog features



Virtual esLogin Nodes

- Solution for specialized workflows
- Quick deployment of a reproducible, agile configuration
- Capable of supporting International Traffic in Arms Regulations (ITAR) data



MPI Distribution Wrappers

- Access to Cray MPICH distribution
- Provides same expected performance found in Cray environment
- Includes scripts for mpicc, mpicxx, and mpif90 for Intel and GCC compilers
- Provide standardized job launcher (ibrun)



Shell Startup Behavior

- Provides consistent, full Linux environment on esLogin and compute nodes
- Allows two independent Cray and TACC startup environments



Hierarchical Software Stack

- Lmod: A new Environment Module system
- Location-based dependencies
- Automatic dependency resolution
- Multiple enhancements (e.g. reset, swap, collections)



RPM Build Environment

- Sandboxed change-rooted environment
- Uses a copy of compute node image
- Develop RPMs without impacting production status
- Capable of multiple, reproducible, and consistent instances



Conclusion

- We're coming up on 5 months in production (tomorrow)
- We judge that the transition was smooth for our users
- Lonestar 5 offers a variation of the Cray environment and a highly customized vendor-independent, open science TACC environment
- More to be done: we are constantly learning, adapting and improving

Thank you for your time and attention!

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