Leveraging HPC for Alzheimer’s Research and Beyond

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Agenda

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- Computing Challenges
  - Spotlight on Alzheimer’s Research
  - Other Research Areas that Benefit from HPC
- Solution with Altair PBS Professional
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- Next Steps
About the NSCEE

• **Full-service** supercomputing facility

• **Mission** for excellence in education and research in supercomputing and its applications

• **Provides** supercomputing training and services to academic and research institutions, government and private industry

• **Supports** energy, the environment, medical informatics and health care

• **Serves** researchers at the University of Nevada Las Vegas and other statewide, nationwide and global research
In Q4 2014, UNLV moved its NSCEE facilities to Switch facility in Las Vegas.

Hosted on Cherry Creek system – large Intel system for scientific and economic R&D:
- 26,000 compute cores
- Intel Xeon E5-2697v2 12C 2.700GHz, Intel Truscale, Intel Xeon Phi 7120P
- Dedicated Research Network (DMZ) with 100Gb/s potential

Switch SUPERNAP and Intel Partner with UNLV to Boost Scientific Research and Economic Development

Intel’s “Cherry Creek” supercomputer brings world-class computing power to UNLV; Switch SUPERNAP to lead high-tech industry partnerships.
NSCEE Computing Challenges

• Numerous and complex workloads
  • Hundreds of projects worldwide
  • Highly compute-intensive research
• Massive data needs
  • Users must access massive data remotely to do their work
• Time-sensitive projects
  • Many NSCEE projects have critical governmental and environmental significance, so timely and reliable performance is a key requirement

Thus, a powerful and reliable infrastructure is a key requirement!
Spotlight: Alzheimer’s Research

• The need for innovation
  • Alzheimer’s Disease continue to cause tremendous familial, social, and economic burdens to modern society
  • Despite substantial progress, existing treatment approaches are limited – so new therapeutic approaches are desperately needed

• The NSCEE project
  • NSCEE works with researchers to compare genomes of Alzheimer’s patient with normal patients
  • **Challenge**: Researchers wanted to enhance the statistical power of previous analyses by including more than 10,000 additional patients (and thus genomic data sets) in the study – meaning a massive leap in computational requirements
Alzheimer’s Project Results

- Reduced overall runtimes for processing workload
  - PBS Professional in conjunction with Rocks and an improved system with shared memory compute node, reduced processing time by more than 50%
  - Alzheimer's project researchers can process a genome in about 3 hours instead of the 8+ hours it previously took
- Fast, easy implementation
- Powerful, flexible customization capabilities -- can be easily extended by adding site-specific processing plugins/hooks
- Improved system manageability and extensibility:
  - Lightweight solution
  - Very easy to manage
  - Not dependent on any specific operating system

“PBS Professional has simplified the administration of our compute clusters immensely. What used to cause problems with our old workload management software is now simple.

In addition, Altair is an outstanding supplier and partner -- their responsiveness and support have made a huge difference and really differentiate them from our previous supplier.”

--Ron Young, Research support analyst at NSCEE
Other NSCEE Research that Benefits from HPC…

Quantum Dynamics of Chemical Reactions
• HPC dramatically improves ability to understand how atoms and molecules interact and the chemical reactions that occur in different environments
• Researchers use complex theoretical calculations to explore how molecules behave at absolute zero temperatures and other conditions

Fracking
• Hydraulic fracturing often takes place >1 mile below groundwater supplies
• Mechanical engineers use sophisticated numerical models to more accurately predict prime locations for extraction and assess possible contamination associated with the process

Magnetically Dominated Jets in Gamma-Ray Burst
• Gamma-ray bursts are the most luminous, and violent, explosions in the universe -- they signify the deaths, collisions or swallowing up of stars
• Astrophysicists’ computational research advances our understanding of the physical mechanisms behind GRBs and other high-energy astrophysical phenomena

UNLV’s National Supercomputing Center
High Performance Computing and Communications in Nevada
HPC Scheduling Solution: Altair PBS Professional

• Market-leading workload manager
  • Proven for 20+ years at thousands of sites
  • Fast, easy implementation
  • Powerful, flexible customization capabilities
  • Simplified management
  • PBS Works suite won “Best HPC Software” in 2014

• Reliable vendor
  • 30-year track record of customer satisfaction
  • Global presence with 40+ offices in 22 countries
  • “Altair is an outstanding supplier and partner -- their responsiveness and support have made a huge difference.”
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• Fracking:
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Questions?

Thank you for your attention!

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