

Leveraging HPC for Alzheimer's Research and Beyond

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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



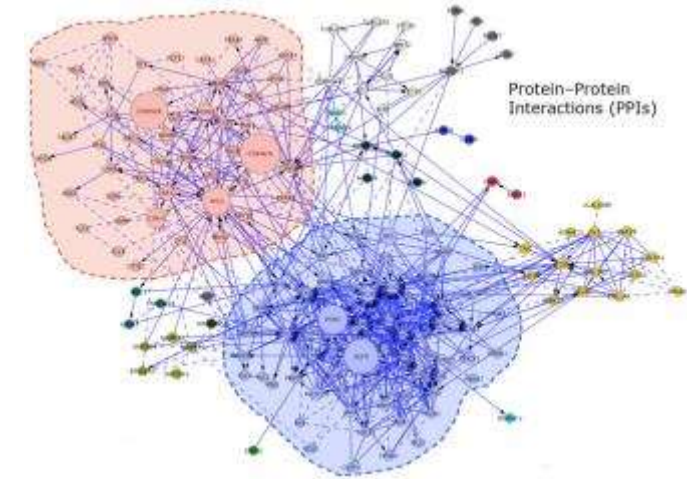
Thus, a powerful and reliable infrastructure is a key requirement!

- **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



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

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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Questions?

Thank you for your attention!

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