

# *What Else Should I Know ???*

*or*

# *What Else Should I Consider as My Problems Become Larger ???*

A (vaguely organized) collection of  
other interesting and maybe useful  
information

*July 2014*

# *What Else ???*

- XSEDE resources are available**
- New / next / other technologies**
- Science Gateways**
- Workflows**
- Tools, libraries, other resources**
- High-Throughput Computing**
- ...**

# *What Is XSEDE ??*



- ❑ [www.xsede.org](http://www.xsede.org)
- ❑ **Extreme Science and Engineering Discovery Environment**
  - (No one *ever* remembers this name)
- ❑ **Funded by the National Science Foundation**
  - ~\$120M over 5 years
  - Not for hardware
  - Renewal anticipated
- ❑ **Rah-Rah:** *Most powerful integrated advanced digital resources and services in the world*
- ❑ **Makes computational resources available to researchers in academia, government, non-profits, for-profits**
  - Includes: computing, visualization, storage, data collections, software and tools, advanced support services, ...

# *XSEDE Computing Resources*

Stampede	Texas Advanced Computing Center	Large Dell cluster with Xeon Phi – capability computing
Keeneland	NICS and GaTech	GPU's
Lonestar	TACC	Visualization and GPU programming
Gordon	San Diego Supercomputing Center	Data intensive applications
Trestles	SDSC	High-throughput, science gateways, small core counts
Blacklight	Pittsburgh Supercomputing Center	SGI – large shared memory
	Open Science Grid	High-throughput computing
Quarry	Indiana U	Support for web services
	Storage and Extended Support	
Jan 2015	Systems at TACC and SDSC	

# Getting Started

## ❑ XSEDE Portal

- <https://portal.xsede.org>

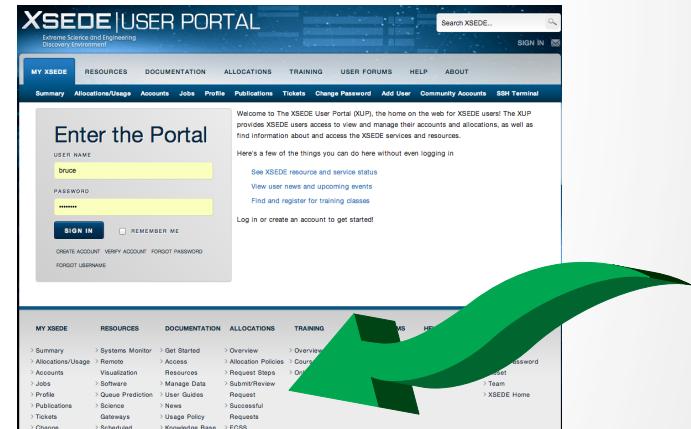
## ❑ Apply for an XSEDE Allocation

- Startup
- Proposal
- Education

## ❑ Accept User Responsibility Agreement

## ❑ Campus Champion Can Help

- Janice and Jeff



# **XSEDE User Portal**

## **□ Single Source for Everything in XSEDE-land**

- Information about accounts and allocations
- User Guides for each resource
- Machine status – resource monitor – file systems
- Interfaces for data management, data collections, . . .
- Science Gateways
- Remote visualization
- Access to Help Desk – submit tickets
- Training opportunities
- Knowledge Base
- User Forum
- *<https://mobile.xsede.org>*
- Describe modules to manage environment
- Student opportunities
- News

# *Prepare a Successful XRAC Proposal*

## **Proposed Research** (*in 15 pages*)

- Research Objectives
- Computational Methodology
- Computational Plan
- Performance and Scaling
- Justification for Service Units Requested
- External Funding
- Other Available Resources

# *XSEDE Allocations*

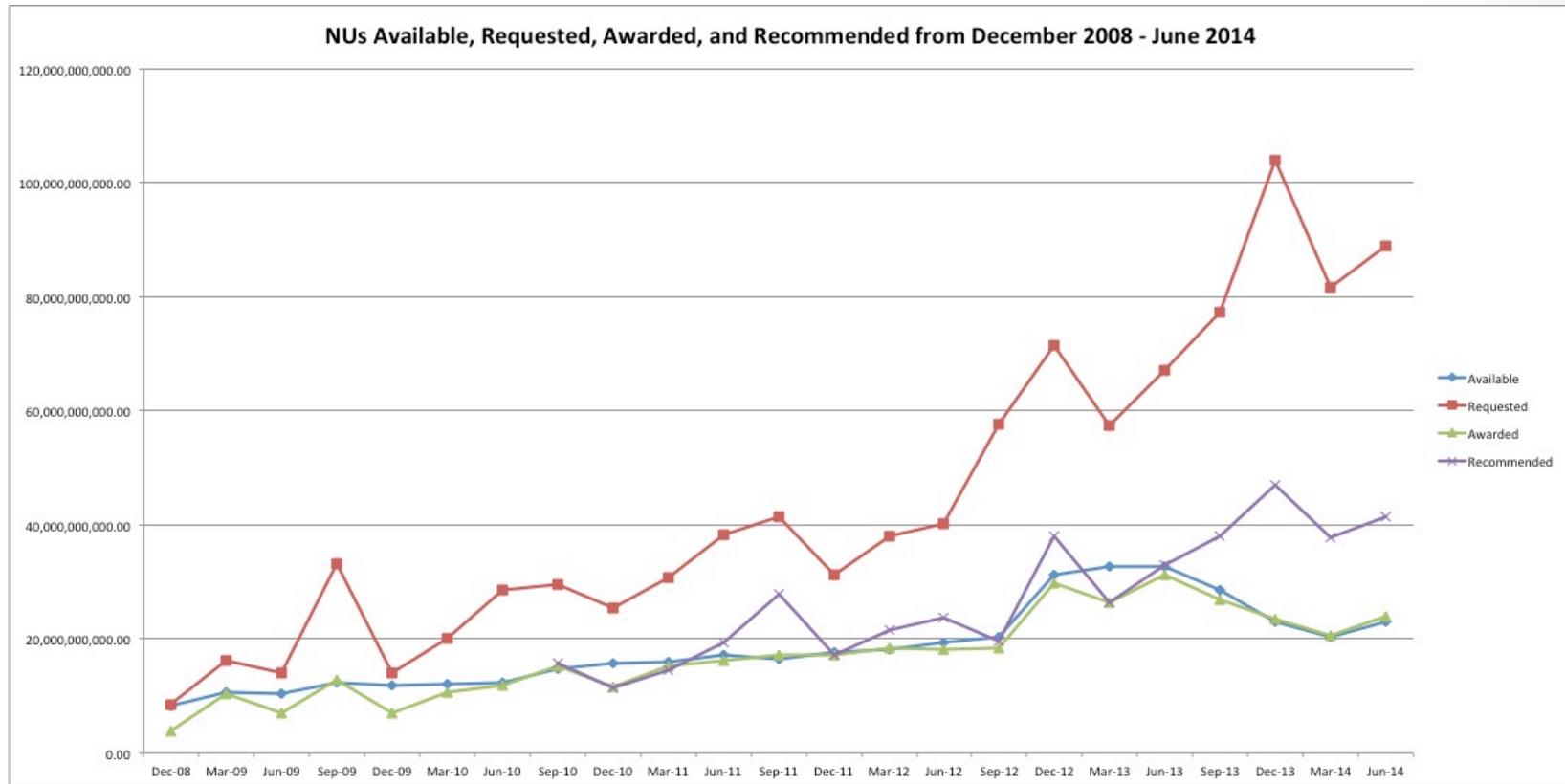
## ❑ Who Is Eligible to Submit Proposals ??

- Researchers at American universities (faculty, postdocs)
- Not students (with some exceptions)
- American researchers at foreign universities (probably)
- Not Not-American researchers at foreign universities (can be co-PI)
- Researchers at US Government labs
- Researchers at non-profit companies (not common)
- Researchers at US industry (not sure how this works)

## ❑ Preference During Review

- Lotsa NSF funding

# XSEDE Allocations



# *Interesting XSEDE Allocation Facts*

- ~700 – Research requests per year
- ~900 – Startup and other requests per year
- ~4B – Service Units (SUs) requested per year
- ~2B – SUs awarded per year

# *New (mostly not really new but other) Technologies*

## **GPGPU, Xeon Phi, FPGA**

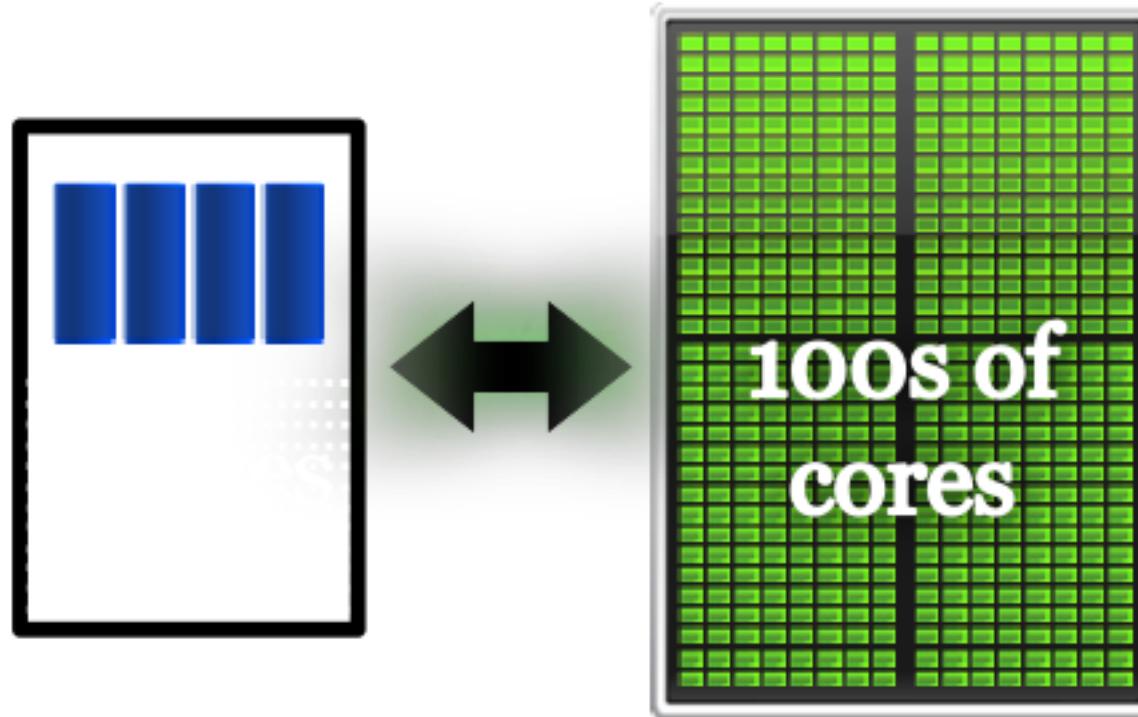
## **Nanotechnology**

- Nanometer – one billionth of a meter
- Materials have unusual and useful properties at nanoscale – strength, lighter weight, control of light spectrum, greater chemical reactivity, ...

## **Quantum Computing**

- Standard bits have a state of 0 or 1
- Qubits can be any quantum superposition of 4 states
- Long time off – but D-Wave ([www.dwavesys.com](http://www.dwavesys.com)) will sell you a computer now

# *Heterogeneous Computing with GPUs*

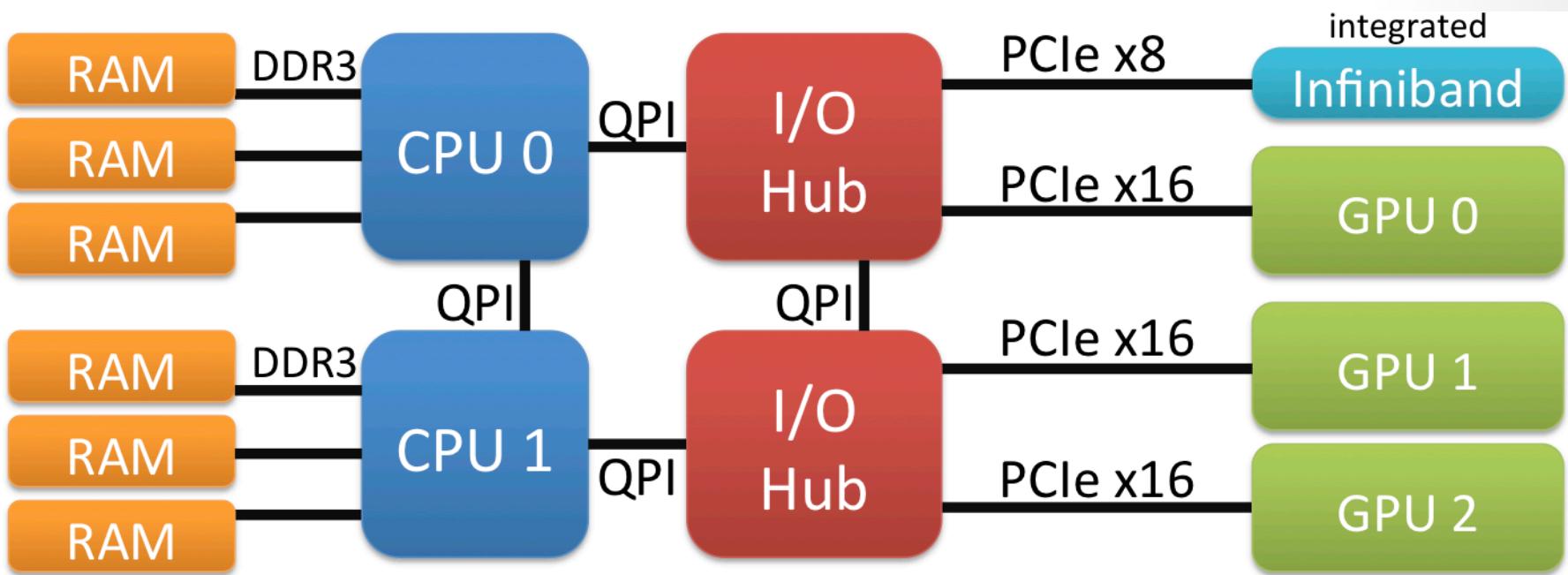


the UNIVERSITY of  
TENNESSEE



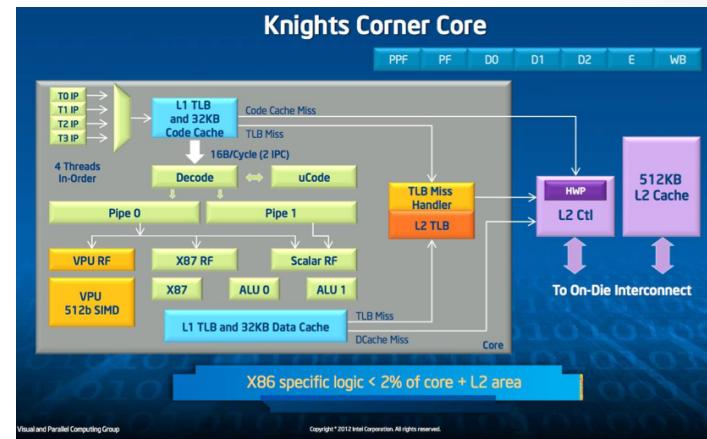
# *Keeneland Node Architecture*

## Hewlett Packard ProLiant SL390s G7



# Xeon Phi

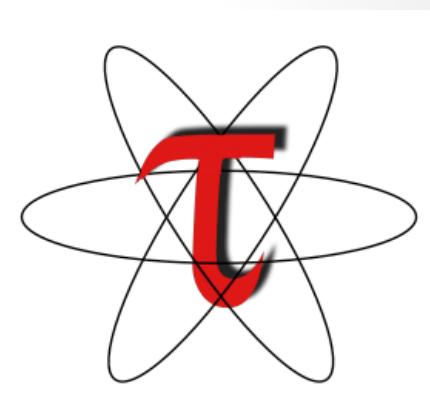
- ❑ Intel Many Integrated Core (MIC) or Xeon Phi
- ❑ Co-processor not an accelerator
- ❑ Vector arithmetic
- ❑ Leverages x86 architecture and programming models
- ❑ Lower power
- ❑ MPI, OpenMP, CILK+, OpenACC, Heterogeneous computing, Native Phi, ...
- ❑ Stampede at TACC



# *Tools and Other Resources*

## ❑ Debugger

- Totalview, DDT, ... printf



## ❑ Performance Analysis Tools

- Tau – Tuning and Analysis Utilities
- PAPI – Performance API



## ❑ Libraries

- ScaLAPACK - library of high-performance linear algebra routines for parallel systems – for dense and banded systems
- PETSc - Library of solvers and tools for sparse PDE systems

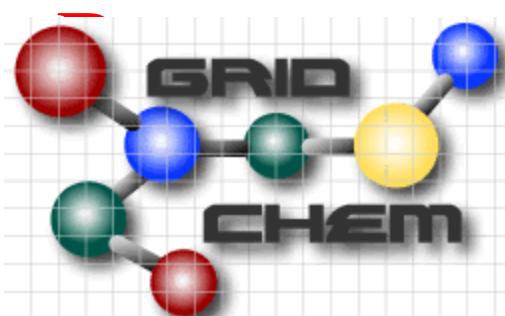


## ❑ HDF5

- Manage very large and complex data collections



# *More than ~30 Gateways Using XSEDE*



A 3D rendering of a complex organic molecule with many carbon and hydrogen atoms.



NATIONAL BIOMEDICAL COMPUTATION RESOURCE



# *Science Gateways Can Leverage Other Investments*

- ❑ [www.xsede.org/gateways-listing](http://www.xsede.org/gateways-listing)
- ❑ Increase access to instruments and technologies and software and data
- ❑ Encourage workforce development in underserved and other populations
- ❑ Increase public awareness of the value of investment in large facilities
- ❑ Slice bread – pack the kids' lunch, ...
- ❑ Scientists can focus on challenging science problems rather than challenging infrastructure problems

# *Scientific Workflows*

## ❑ Typical Workflow

- Retrieve data
- Pre-processing
- Simulation
- Validate results
- Data translation for next step
- More simulation
- Post-processing
- Move results home
- Archive in another zipcode
- Share with others
- Make movies
- Repeat when things break
- ...

## ❑ Kepler, Pegasus, DAGMan, ...

- ❑ Condor was originally designed to harvest cycles from idle workstations at night
- ❑ Now HTCondor can use all manner of computing resources
- ❑ Used for single-processor jobs
  - Monte Carlo
  - Parameter-sweeps
- ❑ Runs on idle machines – but gets out of the way when a higher priority jobs appears
- ❑ Open Science Grid and 30,000 processors at Purdue

# *Online HPC Tutorials and Other Content*

## □ Ci-Tutor — <http://ci-tutor.org/>

- MPI - Intro and Advanced
- OpenMP
- Parallel Numerical Libraries
- Debugging Serial and Parallel Codes
- Performance Tools – Strace, Gprof, Perfsuite, Tau
- Parallel I/O – Lustre
- Scientific Visualization



## □ Cornell Virtual Workshop

Cornell Virtual Workshop

- Introductions to Linux, C, Fortran, Python, R
- GPGPUs, CUDA, Xeon Phi, MPI, OpenMP, Vectorization
- Visualization, Paraview, VisIt
- Relational Databases, Hadoop, MapReduce

## □ Virtual School of Computational Science and Engineering

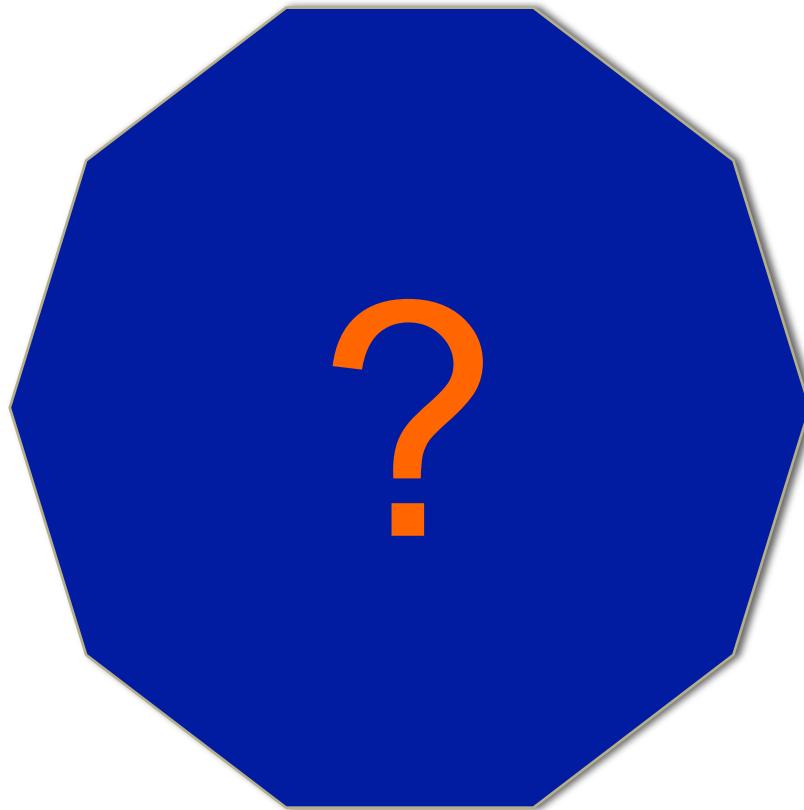
- <http://www.vscse.org/>



# *Blue Waters*

- Cost => Many \$\$\$**
- Located at NCSA**
- Designed for sustained petascale performance on 100,000+ cores for a broad class of problems**
- Cray**
  - 22,640 AMD XE6 compute nodes => 362,240 cores *plus*
  - 4224 XK compute nodes @ 8 cores + 1 NVIDIA Kepler GPU
  - 7.1 + 6.2 Pflops peak performance
  - 1.4 PBytes + 135 TBytes memory
  - I/O system: 26 Pbytes and >1 TB/sec bandwidth
- Anticipate 10-15 allocations per cycle**





*bruce.loftis@colorado.edu*