Bruce Loftis
bruce.loftis@colorado.edu

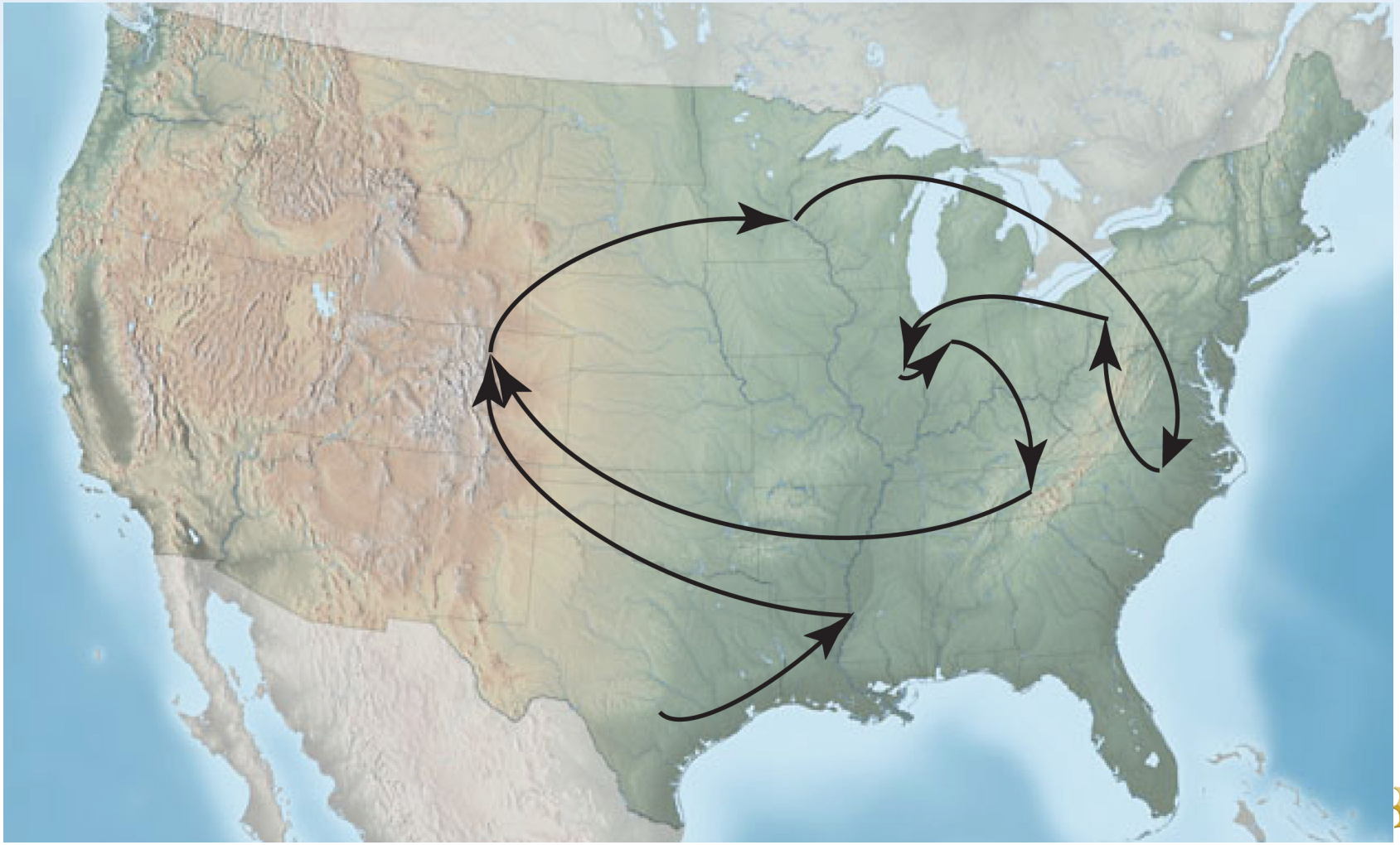
XSEDE

Extreme Science and Engineering
Discovery Environment

Agenda

- **A Little XSEDE-*ish* History**
- **Current Computational Resources**
- **Machines, Support, Software, Science Gateways**
- **Allocations**
  - How Can I Play ??
- **Other XSEDE Activities**
- **Blue Waters**
  - Not really part of XSEDE, but a cousin-of-sorts

A Professional Odyssey



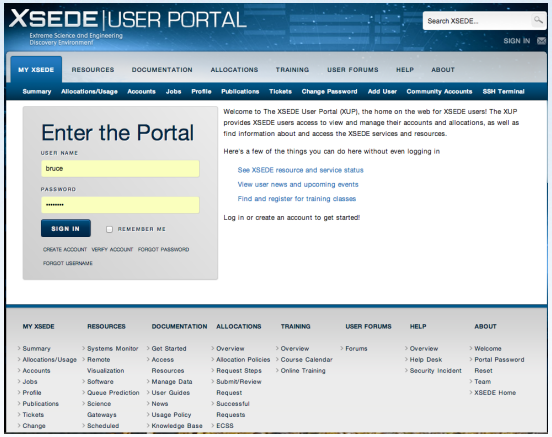
HPC Funded by the National Science Foundation

- **1985 – HPC Centers Program**
  - NCSA, SDSC, PSC, Cornell, JvNC
- **1996 – PACI Program**
  - Partnership for Advanced Computational Infrastructure
  - NCSA and SDSC
- **2001 – TeraGrid**
- **2011 – XSEDE**
  - 16 partners (and counting)
- **Resources are free – proposals are peer-reviewed**

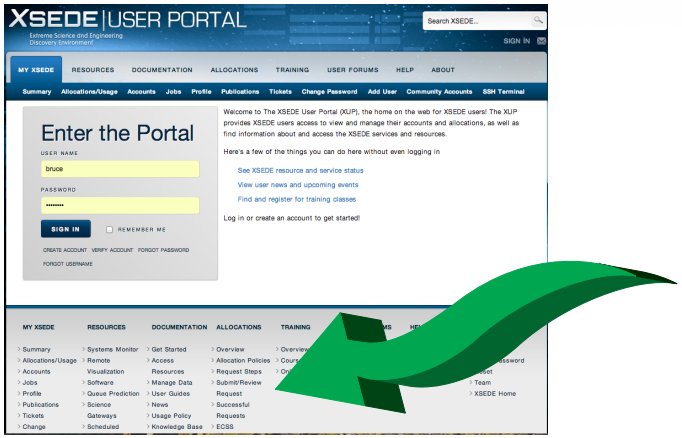
What Is XSEDE ??

- ***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**
  - computing, visualization, storage, data collections, software and tools, web services, advanced support services, …

Getting Started



- **XSEDE Portal**
  - *https://portal.xsede.org*
- **Apply for an XSEDE Allocation**
  - Startup
  - Proposal
  - Education
- **Accept User Responsibility Agreement**



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

Accessing XSEDE Resources

- **Single Sign-On using XSEDE Portal credentials**
- ***ssh* to most XSEDE resources**
- **Use X.509 certificates –** *gsissh* and GridFTP
- **RSA SecurID gizmo for access to NICS at U of Tennessee**

File Transfers

- **For Small Files**
  - *scp* or *sftp* from the command line

- **For Large Files (>1 GB)**
  - XSEDE User Portal File Manager
    - Needs Java – not Chrome
  - GridFTP: *uberftp* or *globus-url-copy* with X.509 certificate
  - Globus Online
  - Unicore

Allocated Resources

- **XSEDE**
  - Startup
    - Up to 100,000 cpu-hours (Service Units or SU) on some systems
    - Just an abstract required
  - Peer-Reviewed Proposal
  - Education – Classroom
  - Extended Collaborative Support
  - Storage

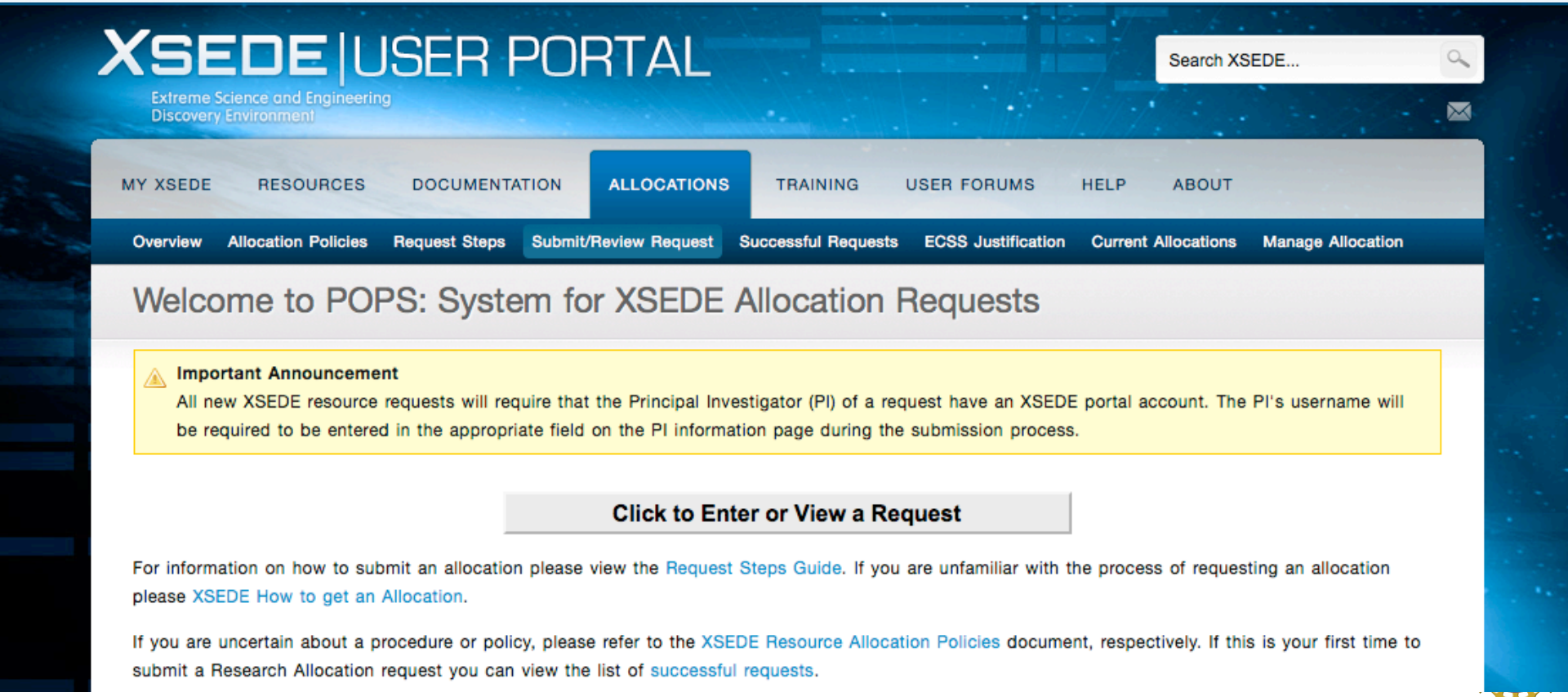
- **Local at Each XSEDE Service Provider**
  - Director's Discretionary

XSEDE Computing Resources

Stampede	Texas Advanced Computing Center	Large Dell cluster with Xeon Phi – capability computing
Keeneland	NICS and GaTech	GPU's
Maverick	TACC	Interactive visualization and data analytics
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	
Wrangler and Comet	Systems at TACC and SDSC	Jan 2015

Getting an Allocation

- **Log into XSEDE Portal** – *portal.xsede.org*



Prepare a Successful XRAC Proposal

- **Proposal Outline** *(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 rare exception)
- 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)

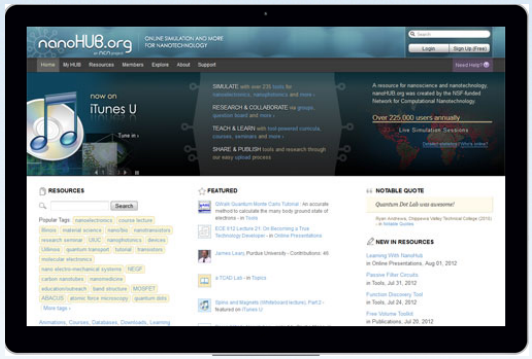
Preference During Review

- Lotsa NSF funding

Interesting Allo-Facts

- **~700** – Research requests per year
- **~900** – Startup and other requests per year
- **~4.0B** – Service Units (SUs) requested per year
- **~1.8B** – SUs awarded per year

Science Gateways



- ***www.xsede.org/gateways-listing***
- **nanoHUB** and **HUBzero**
  - Online simulation for nanotechnology and …
- **National Virtual Observatory**
  - Access to sky surveys

US National Virtual Observatory

- **PolarGrid**
  - Study glacial melting with polar ice sheet data
- **Social Informatics Data Grid**
  - Analysis tools
- **GridChem**
  - Access to large-scale chemistry codes

Science Gateways

- **Can Leverage Other Investments**
  - Increase access to instruments and technologies
  - To simulate and to analyze data
  - To 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, …
  - *Researchers can focus on challenging science problems rather than challenging infrastructure problems*

More than ~30 Gateways Use XSEDE Resources

NCN

Common Instrument Middleware Architecture

GRID CHEM

CHEMBIOGRID

Earth System Grid

SCEC Earthworks

Renci Science Portal

Neutron Sciences

CCSM Community Climate System Modeling Portal

NEEScentral

NVO National Virtual Observatory — US National Virtual Observatory

nanoHUB.org an ncn project — ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

GEON PORTAL

LEADPORTAL LINKED ENVIRONMENTS FOR ATMOSPHERIC DISCOVERY

TeraDRE TeraGrid Distributed Rendering Environment

NBCR NATIONAL BIOMEDICAL COMPUTATION RESOURCE — Conduct, catalyze and enable multiscale biomedical research

C4E4 CyberInfrastructure for End-toEnd Environmental Exploration

NSF

XSEDE

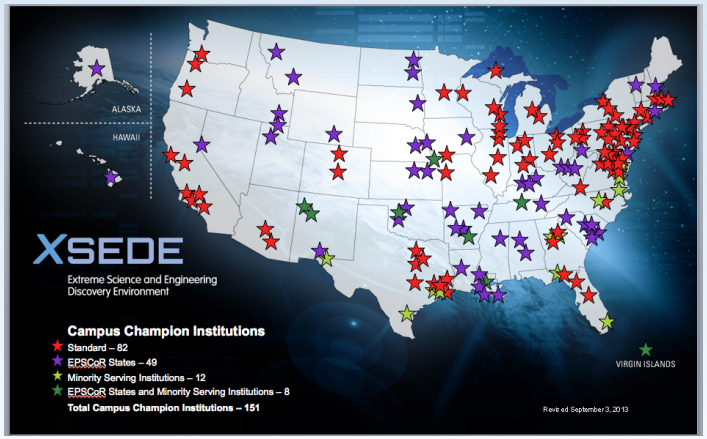
Advanced User Support

- **Extended Collaborative Support Services (ECSS)**
  - 20 Computational Scientists available
  - Port applications to new resources
  - Help with portal and gateway development
  - Implement algorithmic enhancements
  - Implement parallel math libraries
  - Improve scalability of codes to higher processor counts
  - Optimize codes to efficiently use specific resources
  - Assist with visualization, workflows, data analysis, file transfer, …

Training – Expand HPC Skills

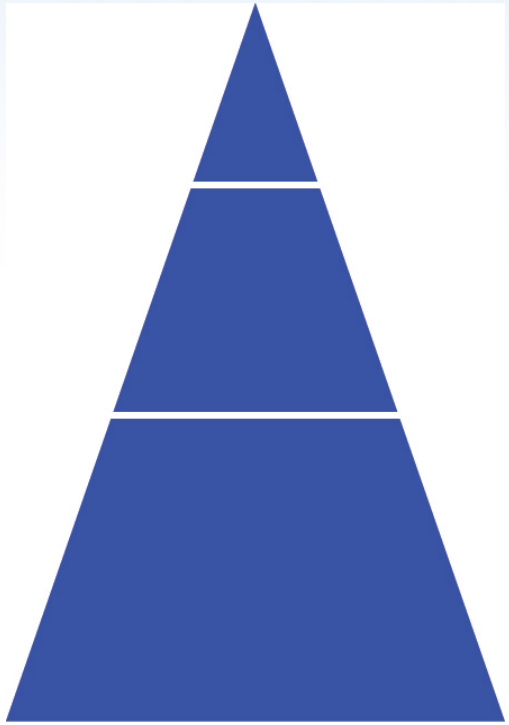
- **CI-Tutor** (asynchronous)
  - *www.citutor.org*
  - *www.citutor.org/browse.php*
  - MPI, OpenMP, Debugging, Visualization, …
- **Cornell Virtual Workshop** (asynchronous)
  - *www.cac.cornell.edu/vw*
  - Parallel computing, scripting, visualization, GPU and MIC, performance, data analysis, languages, …
- **Virtual School for Computational Science & Engineering** (synchronous)
  - *www.vscse.org*

Campus Champions



- **Local source for XSEDE information**
- **Provide guidance for selecting XSEDE resources**
- **Provide quick startup accounts on XSEDE systems**
- **Help with XRAC proposals**

Blue Waters



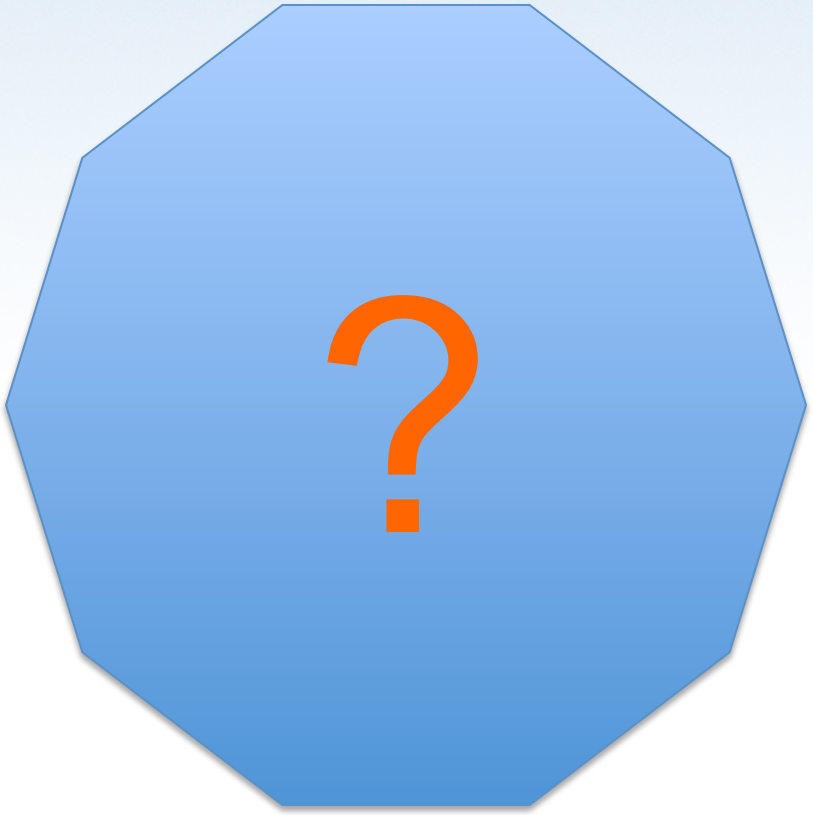
Highest Sustained Performance

National HPC Systems

Campus Systems

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**
  - 2 allocation cycles per year



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