Computing at Argonne and ALCF Update

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Division Director (interim)
Argonne Leadership Computing Facility
Argonne’s computing ecosystem

Research / Departmental

Campus Computing/LCRC

Distributed/Cloud Computing

Storage / Data Intensive

Visualization / Collaboration

Global Research Networks

Leadership Computing
Argonne Magellan Cloud Hardware - Final

**Compute Servers**
504 Compute Servers  
Nehalem Dual quad-core 2.66GHz  
24GB RAM, 500GB Disk  
QDR Infiniband  
Totals  
4032 Cores, 40TF Peak  
12TB Memory, 250TB Disk

**Active Storage Servers**
200 Compute/Storage Nodes  
40TB FLASH/SSD Storage  
9.6TB Memory, 1.6PB Disk  
QDR Infiniband

**GPU Servers**
133 GPU Servers  
8.5TB Memory, 133TB Disk  
266 Nvidia 2070 GPU cards  
QDR Infiniband

**Big Memory Servers**
~10 Compute Servers  
~10TB Memory, ~10TB Disk  
QDR Infiniband

File Servers (8) (/home) 160TB

Mgt Servers (12)

Gateway Servers (16)

ESNet 10Gb/s

ANI 100 Gb/s  
Spring 2011
PADS  Petascale Analysis and Data Server

NSF MRI supported shared instrumentation
Beagle (coming soon)

NIH Supported
150 Teraflops – 18,000 cores
Cray XE6
For Biomedical Computing
Installation November 2010
ALCF-2: How We Got Here...

- **2009**: BG/Q Mira
- **2010**: Today 5/17/2010
- **2011**: T&D Delivery Complete
- **2012**: 10PF Delivery Complete
- **2013**: CD-4 DME Complete Steady State

**CD-0 Mission Need**

**CD-1/2a Acquisition & Baseline**

**Charge Questions**
- Is the ALCF approach to identify the preferred alternative for the follow-on upgrade reasonable and will the proposed alternative address the scientific requirements for Leadership Computing as planned?
- Is the ALCF management appropriately structured and empowered to ensure success delivering the proposed upgrade while continuing to deliver leadership resources to its users?
- Are the cost and schedule estimates reasonable and within scope for the proposed ALCF upgrade?
- Is the project ready for CD-1/CD-2 approval?

**Contract Package Complete**

**CD-2b/3 SOW/Contract Start Construction**
ALCF Early Science Program

- **Next-generation IBM Blue Gene machine *Mira***
  - 10 petaFLOPS, 750k cores, 750 TB memory
- **Engineer scientific codes for Mira**
- **Burst of large-scale science calculations**
  - 2 billion core-hours
### 16 ESP Projects

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7 National Lab Pls
9 University Pls
Early Science Program Projects

- **Climate-Weather Modeling Studies Using a Prototype Global Cloud-System Resolving Model**
  Science: Climate PI: Venkatramani Balaji

- **Materials Design and Discovery: Catalysis and Energy Storage**
  Science: Materials/Chemistry PI: Larry A. Curtiss

- **Direct Numerical Simulation of Autoignition in a Jet in a Cross-Flow**
  Science: Combustion PI: Christos Frouzakis

- **High Accuracy Predictions of the Bulk Properties of Water**
  Science: Chemistry PI: Mark Gordon

- **Cosmic Structure Probes of the Dark Universe**
  Science: Astro/Cosmology PI: Salman Habib

- **Accurate Numerical Simulations Of Chemical Phenomena Involved in Energy Production and Storage with MADNESS and MPQC**
  Science: Chemistry PI: Robert Harrison

- **Petascale, Adaptive CFD**
  Science: Aerodynamics PI: Kenneth Jansen

- **Using Multi-scale Dynamic Rupture Models to Improve Ground Motion Estimates**
  Science: Geophysics PI: Thomas Jordan

- **High-Speed Combustion and Detonation (HSCD)**
  Science: Combustion PI: Alexei Khokhlov

- **Petascale Simulations of Turbulent Nuclear Combustion**
  Science: Astro/Cosmology PI: Don Lamb

- **Lattice Quantum Chromodynamics**
  Science: Nuclear Structure PI: Paul Mackenzie

- **Petascale Direct Numerical Simulations of Turbulent Channel Flow**
  Science: Energy PI: Robert Moser

- **Ab-initio Reaction Calculations for Carbon-12**
  Science: Nuclear Structure PI: Steven C Pieper

- **NAMD - The Engine for Large-Scale Classical MD Simulations of Biomolecular Systems Based on a Polarizable Force Field**
  Science: Bio Protein PI: Benoit Roux

- **Global Simulation of Plasma Microturbulence at the Petascale & Beyond**
  Science: Fusion PI: William Tang

- **Multiscale Molecular Simulations at the Petascale**
  Science: Biology PI: Gregory Voth
Thank-you