

# Computing at Argonne and ALCF Update

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# Argonne's computing ecosystem

Research / Departmental



Campus Computing/LCRC



Distributed/Cloud Computing



Visualization / Collaboration



Storage / Data Intensive



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



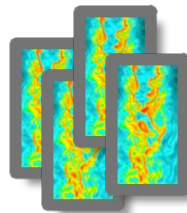
## Active Storage Servers

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



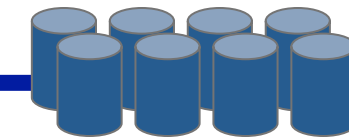
## GPU Servers

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



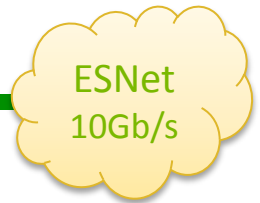
File Servers (8) (/home) 160TB



Mgt Servers (12)



Gateway Servers (16)



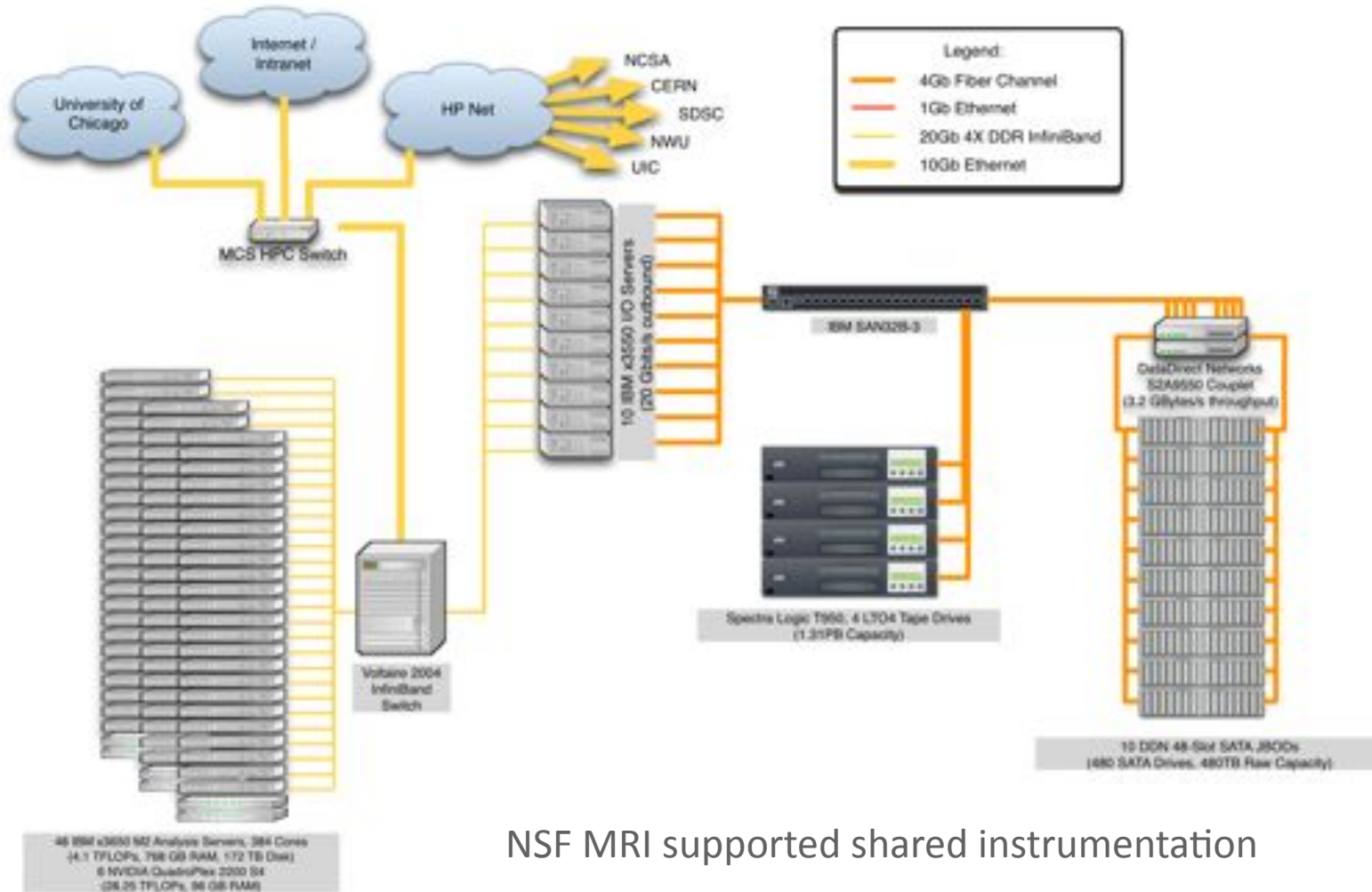
ESNet  
10Gb/s



ANI  
100 Gb/s  
Spring 2011



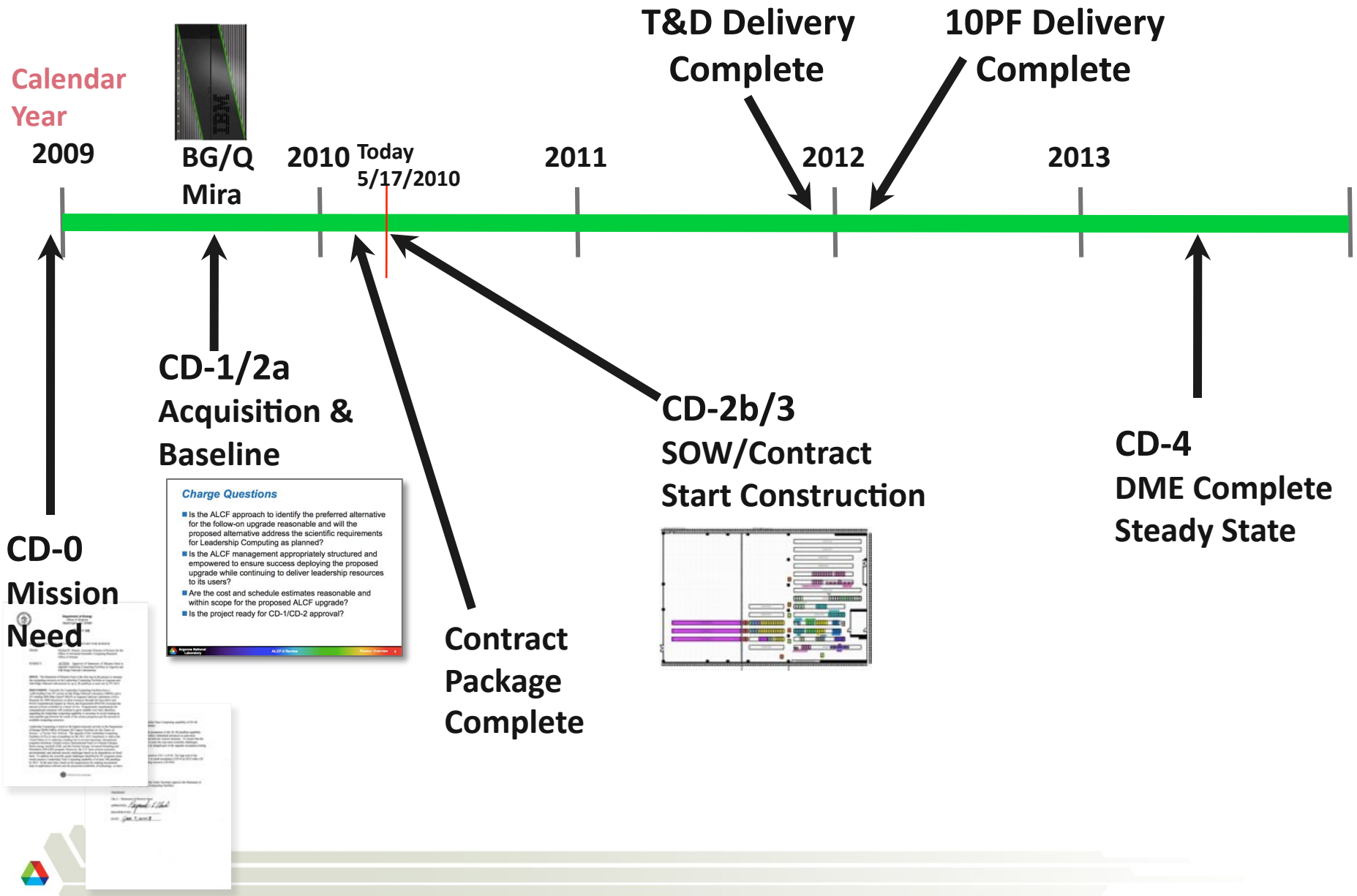
# PADS Petascale Analysis and Data Server







# ALCF-2: How We Got Here...



# MIRA



**BGQ Compute**  
10 PF  
768 TB RAM  
768 K cores  
48 racks



**BGQ IO**  
384 PCI slots  
6 TB RAM  
6 K cores



## Data Storage

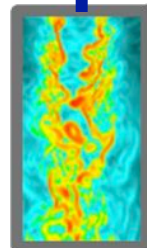
240 GB/s write BW (aggregate)  
28 PB capacity

## Future Storage Expansion

~478 GB/s write BW (aggregate for both phases)  
~74 PB aggregate capacity both phases



**Login Nodes**  
16 servers



**Viz**  
350 TF  
4 TB RAM  
2 K cores  
75 K GPU cores

**GridFTP Servers**  
12 servers



## Future Tape Expansion

500 PB

# Test & Development



**BGQ Compute**  
416 TF  
32 TB RAM  
32 K cores  
2 racks



**BGQ IO**  
16 PCI slots  
256 GB RAM  
256 cores



**Viz**  
13 TF  
144 GB RAM  
72 cores  
3 K GPU cores

**Data Storage**  
2.4 PB  
20 GB/s write BW (aggregate)



**Login Nodes**  
8 servers

# ALCF-2 10PF



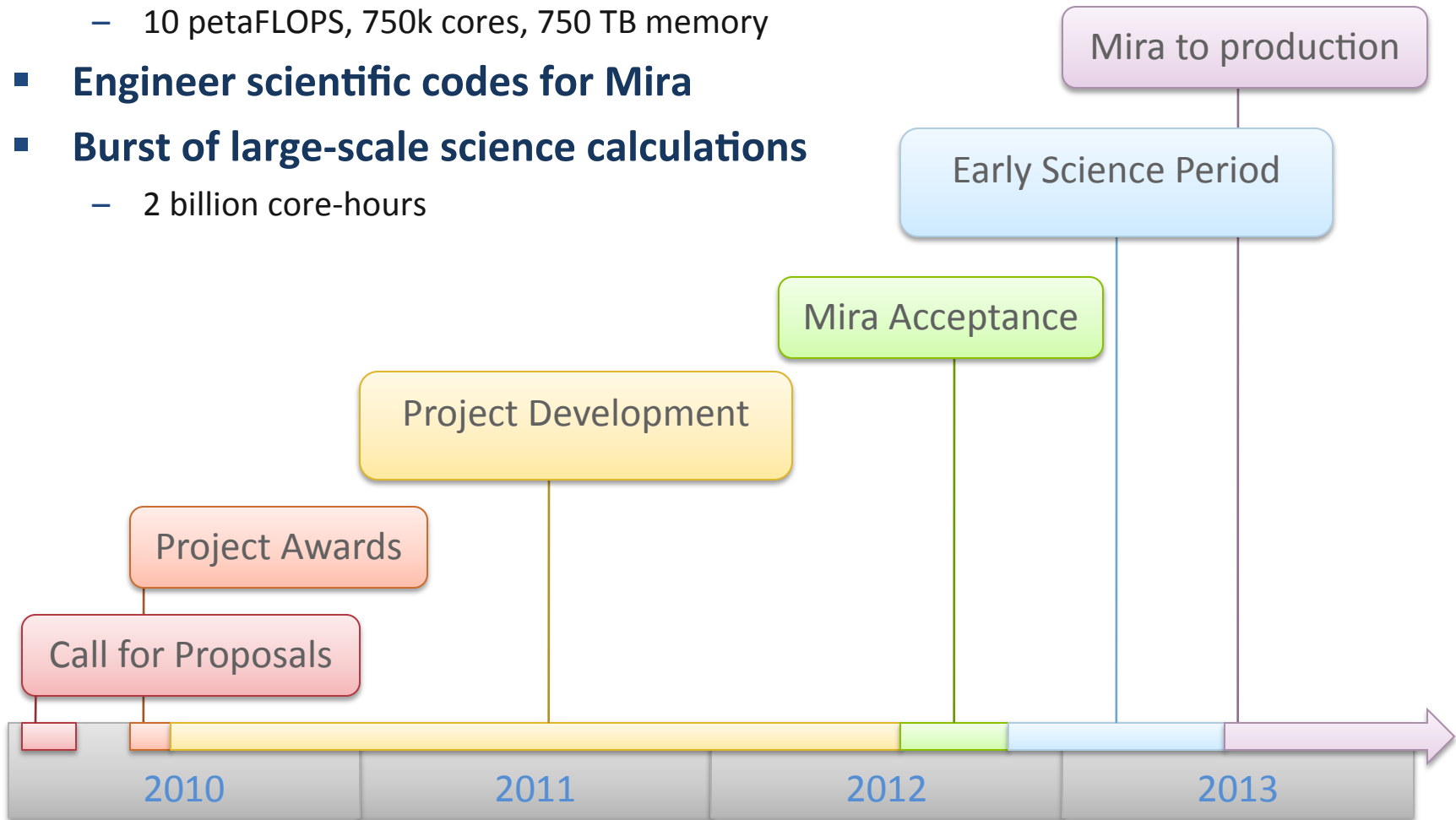
**WAN**  
100 Gb/s

- BG/Q Links (2x2GB/s)
- IB QDR (4GB/s)
- Ethernet (10Gb/s)



# 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

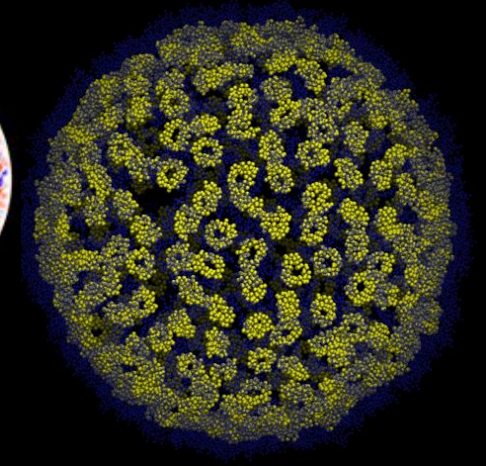
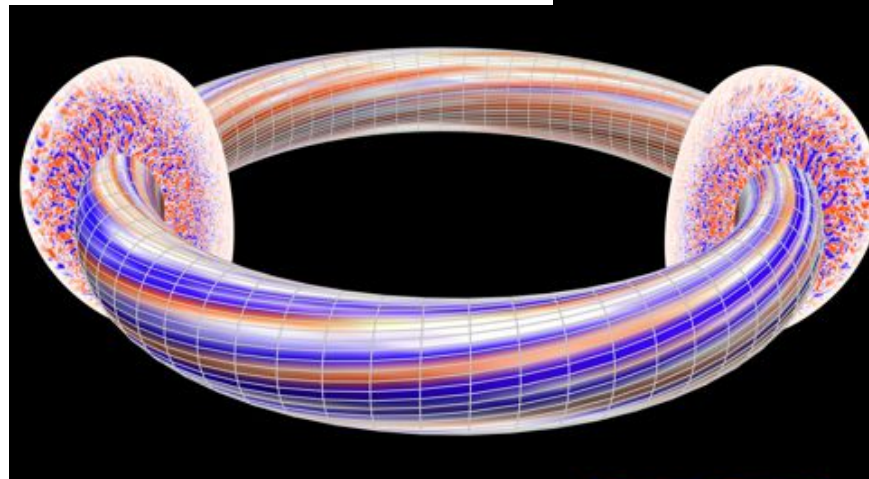
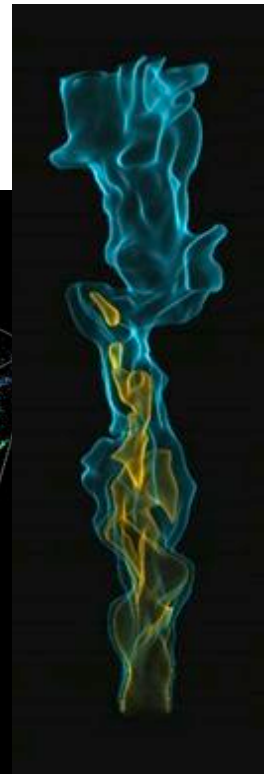
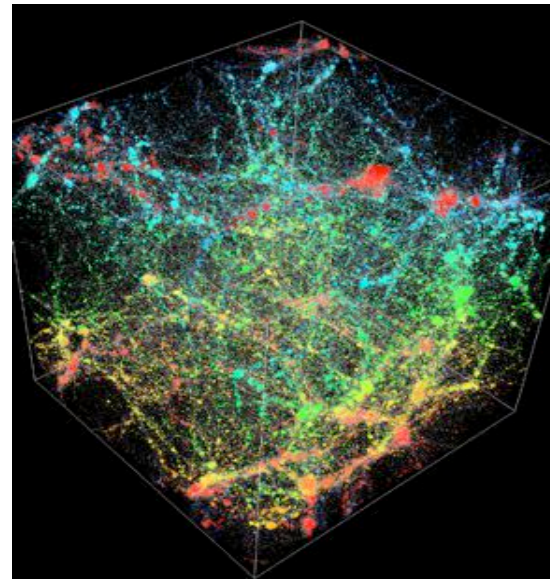




# 16 ESP Projects

Science Areas	Algorithms/Methods
Astrophysics	Structured Grids
Biology	Unstructured Grids
CFD/Aerodynamics	FFT
Chemistry	Dense Linear Algebra
Climate	Sparse Linear Algebra
Combustion	Particles/N-Body
Cosmology	Monte Carlo
Energy	
Fusion Plasma	
Geophysics	
Materials	
Nuclear Structure	

7 National Lab PIs  
9 University PIs



# 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 Voith



**Thank-you**

