Exascale Update SC14 - ASCAC

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Mission: Extreme Scale Science Next Generation of Scientific Innovation

- DOE's mission is to push the frontiers of science and technology to:
 - Enable scientific discovery
 - Provide state-of-the-art scientific tools
 - Plan, implement, and operate user facilities
- The next generation of advancements will require Extreme Scale Computing
 - 1,000X capabilities of today's Petaflop computers with a similar size and power footprint
- Extreme Scale Computing, however, cannot be achieved by a "business-as-usual" evolutionary approach



• Extreme Scale Computing will require major novel advances in computing technology – Exascale Computing

Exascale Computing Will Underpin Future Scientific Innovations



Exascale Applications Respond to DOE Missions in Discovery, Design, and National Prosperity

Scientific Discovery

- Mesoscale materials and chemical sciences
- Improved climate models with reduced uncertainty
- Plasma physics for fusion energy systems

Engineering Design

- Nuclear power reactors
- Advanced energy technologies
- Resilient power grid

National Prosperity

- Energy Technologies
- Advanced manufacturing
- Health Care
- Transportation









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Exascale Challenges and Issues

• Four primary challenges must be overcome

- Parallelism / concurrency
- Reliability / resiliency
- Energy efficiency
- Memory / Storage

Productivity issues

- Managing system complexity
- Portability
- Generality

System design issues

- Scalability
- Efficiency
- Time to solution
- Dependability (security and reliability) must be integrated at all levels of the design





Exascale Strategy

- Exploit co-design process, driven by the full application workflow
- Develop exascale software stacks
- Partner with and fund vendors to transition research to product space
- Collaborate with other government agencies and other countries, as appropriate



Exascale Project Schedule



Science

Fast Forward and Design Forward Programs

Fast Forward Program

- Jointly funded by SC & NNSA
- Phase 1: Two year contracts, started July 1, 2012, Phase 2: Two year contracts, starting Fall 2014

Project Goals & Objectives

- Initiate partnerships with multiple companies to accelerate the R&D of critical node technologies and designs needed for extreme-scale computing.
- Fund technologies targeted for productization in the 5–10 year timeframe.

Design Forward Program

- Jointly funded by SC & NNSA
- Phase 1: Two year contracts, started Fall 2013, Phase 2: Two year contracts. Starting Fall 2014

Project Goals & Objectives

- Initiate partnerships with multiple companies to accelerate the R&D of interconnect architectures and conceptual designs for future extreme-scale computers.
- Fund technologies targeted for productization in the 5–10 year timeframe.



FastForward 2 Projects

- **AMD** will conduct research for an integrated exascale node architecture. Particular areas of emphasis include near-threshold-voltage logic and other low-power computing technologies. AMD will investigate a new standardized memory interface
- **Cray Inc.** will explore alternative processor design points, including ARM microprocessor designs.
- Intel will use this award to continue to advance research in energy efficient node and system architectures, including software targeted at developing extreme-scale systems.
- **NVIDIA** will build on its work in FastForward 1, with a strong focus on energy efficiency, programmability, and resilience.
- **IBM** will investigate next-generation standardized memory interface.



First steps on a Path Towards Exascale: Three Exascale Co-Design Centers

Exascale Co-Design Center for Materials in Extreme Environments (ExMatEx)

- Director: Timothy Germann (LANL)
- <u>http://www.exmatex.org</u>

Center for Exascale Simulation of Advanced Reactors (CESAR)

- Director: Andrew Siegel (ANL)
- https://cesar.mcs.anl.gov

Center for Exascale Simulation of Combustion in Turbulance (ExaCT)

- Director: Jacqueline Chen (SNL)
- <u>http://exactcodesign.org</u>





ASCR Exascale Co-Design Status

Notable Successes

- Informed & influenced vendors node designs by providing "proxy apps", codes derived from actual applications, that go beyond the traditional math kernels
- Re-examined current algorithms and made changes so that they take advantage of anticipated exascale architectures
- Explored programming models and environments that are suitable for the data layout of the applications

Lessons Learned

- Interdisciplinary teams discover key issues that could not have been discovered within the boundary of any one disciplinary - and find solutions that are "codesigned"
- Bandwidth for interactions: personnel in Co-Design Centers in high-demand, as the Centers provide the only "application use case" for testing research results from computer science, applied math, and hardware architectures
- Horizontal integration: need to create opportunities for the Centers to leverage each other



Exascale Programming Models X-Stack Goals

- New Programming Models: approaches to managing parallelism and data movement through innovations in interfaces
- **Dynamic Runtime Systems:** adapt to changing application goals and system conditions
- Locality-aware and Energy-efficient Strategies: manage locality and minimize energy consumption
- Interoperability: facilitate interoperability across different HPC languages and interfaces, as well as cross-cutting execution models







Exascale Programming Models Observations & Lessons Learned

- Computations and communications will be irregular due to heterogeneous processors characteristics, deep memory hierarchies, and much higher rate of faults than current platforms.
- Exascale system will have deep memory hierarchy: generating optimized code will be very challenging.
- Using DSLs, application code size can be reduced by 100x, and the code generated and optimized has about 3x faster execution time.
- Unprecedented parallelism, asynchrony, and irregular computations and communications are well matched to task/thread-oriented dataflow programming models.



Status

Meetings with

- Secretary of Energy
- SEAB
- OMB
- OSTP
- Congressional Meetings
- Other agencies

Project Design Planning

- Develop preliminary version of project design document, involving lab researchers and DOE/NNSA program managers.
- Held "Red Team" review of document
- Held external review of document (federal employees from other agencies)
- Updated project design document

Initiated New Programs

 FastForward 2 and DesignForward 2, Resilience, Analytical Modeling for Extreme-Scale Computing Environments, Scientific Data Management, Analysis and Visualization at Extreme Scale



Preliminary Conceptual Design for the Exascale Computing Initiative Document

- This document presents a preliminary strategy and contains limited descriptions of project management details.
- A preliminary list of proposed projects is provided

Table of Contents

Executive Summary

- **1** Introduction
- 2 Project Background
- **3** Justification of Mission Need
- **4** Barriers to Achieving Exascale Computing
- 5 Technical Approach
- 6 Project Management
- 7 Integrated Baseline
- 8 External Stakeholders Appendix 1



Technical Approach Project Components

1. Exascale Research, Development and Deployment (ExaRD):

- **Exascale Co-Design Centers and Beyond Exascale**, exploratory research to codesign hardware and software architecture
- **Software Technology Research and Development**, aimed at specific hardware and software technologies;
- Vendor Research and Development, aimed at developing exascale node and system architectures;

2. Exascale Application Development (ExaAD):

 Readiness to Use Capable Exascale Systems, initiating the development of a suite of exascale applications software packages that will be operational in 2023 to ensure maximal scientific and engineering impact of the exascale systems

3. Exascale Platform Deployment (ExaPD):

• Coordinated Acquisition Strategy for exascale platforms, including long-lead site preparations and system platforms



Risk	lmpact (H/M/L)	Likelihood (H/M/L)	Mitigation
Insufficient funding within either NNSA or SC	Н	М	Prioritize elements within the ECI and, if necessary, de-scope ECI and/or spread the acquisition costs over a longer time period
Full system is unreliable	Н	М	Invest in robust, multilayered approaches to manage or resolve faults
Failure to achieve critical integration of DOE-developed software into vendor software	Н	М	Early development of XBUS and integration with funded vendors software environments
Software environments do not satisfy DOE application needs	Н	М	Determine the workload requirements of critical applications as early as possible
Key algorithms that do not scale may not have timely, suitable alternatives	Н	L	Early investments in exploratory algorithms research
Exascale computer architecture departs significantly from expected designs, after significant R&D in software, tools, and algorithms were invested based on the expected designs	Н	М	A clearly defined communication channel with vendors and effective communication so that the ECI participants are well- informed regarding evolving architectures and new directions



Software Technology Projects Appendix 1

- **<u>1</u>** Application Foundations
- 1.1 Co-Design (CD)
- 1.2 Applied Mathematics (AM)
- **1.3 Data Analytics and Visualization (DV)**
- 2 User Experiences (UE)
- 2.1 Productivity (PR)
- 2.2 Collaborative Environment (CE)
- 2.3 Resilience (RE)
- 2.4 Application Integrity
- 2.5 Cybersecurity (CS)
- 3 Software Stack (SS)
- 4 Performance Execution (PE)
- 5 Data Management (DM)
- 6 Hardware Architecture (HA)
- 7 System Engineering and Integration



Delivering on the Exascale Promise

Exascale computing systems are essential for the scientific fields that will transform the 21st Century global economy

- Energy
- Biotechnology
- Nanotechnology
- Materials science

Goal: Lead computational sciences and HPC to continue to develop and deploy HPC hardware and software systems through exascale platforms

DOE ASCAC subcommittee identifies top 10 technology advancements

- Critical to making productive, economically viable exascale systems
- Innovations beyond anticipated conventional practices and their incremental extensions



Technical Approaches

The Top Ten Exascale Challenges, with Technical Approaches

- 1. Energy efficiency
- 2. Interconnect technology
- 3. Memory Technology
- 4. Scalable System Software
- 5. Programming systems
- 6. Data management
- 7. Exascale Algorithms
- 8. Algorithms for discovery, design, and decision
- 9. Resilience and correctness
- 10. Scientific productivity









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