ASCAC MEETING

UPDATE ON ASCAC SUBCOMMITTEE DOCUMENTING ASCR IMPACTS

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CHARGE LETTER: HIGH-LEVEL OBJECTIVES

- Steve Binkley charged the ASCAC with producing a report that assesses and documents the historical accomplishments of the Advanced Scientific Computing (ASCR) program and its predecessors over the past four decades.
  - Highlight outstanding examples of major scientific accomplishments that have shaped the fields of ASCR research
  - Identify the lessons learned from these examples to motivate ASCR investment strategies in the future
  - Illuminate the guiding strategies and approaches that will be key to ensuring future U.S. leadership in the full range of disciplines stewarded by ASCR
  - Inform the future investment strategy of the Office of Science
- The report should provide technical details as needed for context but should be primarily concerned with the essence of each story as it relates to the larger progress of science
- Report is due December 31, 2018

SUBCOMMITTEE MEMBERS

- Buddy Bland, ORNL
- Jackie Chen, SNL
- Phil Colella, LBNL
- Jack Dongarra, University of Tennessee and ORNL
- Thom Dunning, PNNL
- Wendy Huntoon, KINBER
- Bill Johnston, LBNL (ret.)
- Paul Messina, ANL, Chair
- Jim Pool, Caltech (ret.)
- Dan Reed, University of Utah
- John Sarrao, LANL

SAMPLE MATERIAL GATHERED SO FAR
COMPUTATIONAL SCIENCE (1)

- NERSC input
  - An Accelerating Universe - Saul Perlmutter, Nobel Prize in Physics 2011
  - Oscillating Neutrinos - The SNO team, Nobel Prize in Physics 2015
  - Multiscale Chemical Modeling - Martin Karplus, Nobel Prize in Chemistry 2013
  - Understanding the Function of Biomolecules - Joachim Frank, Nobel Prize in Chemistry 2017
  - The Birth of Precision Cosmology - George Smoot, Nobel Prize in Physics 20
  - Our Changing Climate - The 2007 Nobel Peace Prize
  - …
- OLCF: Revealing the Quantum World of Materials (1995)

SAMPLE MATERIAL GATHERED SO FAR
COMPUTATIONAL SCIENCE (2)

- NWChem: A Modern High Performance Quantum Chemistry Application
- Summary of ASCR contributions to research in other SC research offices (22 pages)
- Eight of the ten “significant advancements in computational science (Breakthroughs 2008 report)
- Input from SC Offices, e.g., Nuclear Physics Office
  - SciDAC: *NUCLEI, UNEDEF*
  - ECP: *LQCD, Nucl Astro*
- In preparation: document on the impact of SciDAC on BER, BES, FES, HEP, and NP as well as ASCR (see next two slides)

BACKGROUND OF SCIDAC

- Context
  - Major change in computer architectures in 1990s—parallel computers
  - Software technologies needed to use parallel computers in development
  - New mathematical algorithms required for parallel computers
  - Scientific codes not poised to take advantage of new computing systems
- Scientific Discovery through Advanced Computing
  - Fund teams of computational scientists, computer scientists and applied mathematicians to create new generation of codes
  - Fund development of software technologies needed by scientific applications to enable efficient and effective use use of parallel computers
  - Fund development of new algorithms need to optimize performance of scientific applications on parallel computers

STRUCTURE OF REPORT

- Background and Context
- General Observations
  - COV Report 2014: “SciDAC remains the gold standard nationally and internationally for fostering interaction between disciplinary scientists and HPC.” (ASCR COV 2014)
- Impact of SciDAC
  - Science and Engineering Codes: Scientific Advancements
  - Software Technologies for Parallel Computing Systems
  - Mathematical Algorithms for Parallel Computing Systems

SAMPLE MATERIAL GATHERED SO FAR
APPLIED MATHEMATICS

- Turning a Computer into a Numerical Microscope for Science (AMR story)
- What is the accuracy of our numerical simulations? (ADIFOR story)
- Auxiliary-space Maxwell Solver (AMS)

SAMPLE MATERIAL GATHERED SO FAR
MATHEMATICAL SOFTWARE

- DOE Libraries narrative (12 page overview of math software and related libraries, by Jack Dongarra)
- xxxPACKs (input from Margaret Wright)
- Discrete/combinatorial mathematics (input from Margaret Wright)
- Discrete math story (Bruce Hendrickson)
- PETSc (comprehensive description of the project, uses, impact)

SAMPLE MATERIAL GATHERED SO FAR
COMPUTER SCIENCE (1)

- 22 Computer science breakthroughs selected circa 2009, including
  - TCP Autotuning Highlights: 10x increase in TCP throughput on high bandwidth, high latency paths
  - Hybrid networks and virtual circuit services (OSCARS)
  - Bro Intrusion Detection System
  - Object Storage based Parallel File System Technology
  - FastBit: New algorithms for searching very large scientific datasets
  - Kepler: Facilitating dynamic monitoring and code-coupling of scientific large-scale simulations
  - Trilinos
  - Production-quality petascale visual data analysis software infrastructure
- The viz story: ASCR support for scientific discovery and the development of innovative visualization and analysis methods to address the challenge of understanding massive data

SAMPLE MATERIAL GATHERED SO FAR
COMPUTER SCIENCE (2)

- Computer Science 7 years of breakthroughs compendium
  - Programming models
    - MPI
    - PGAS languages
    - Global arrays library
  - Performance modeling
  - Architecture benchmarking
  - Performance tools
  - Lightweight OS
  - Analyzing, storing, accessing and moving large data sets
  - Parallel high-level I/O libraries
  - Grids and virtual organizations
  - Also includes material on scientific libraries and networking R&D

SAMPLE MATERIAL GATHERED SO FAR
COMPUTER ARCHITECTURE

- Ultracomputer history
- Cedar Architecture and its software
- Birth of the Hypercube
- Parallel computing timeline
- Input from Justin Rattner
- Input from Al Gara
- Input from Jim Sexton, Paul Coteus and others in preparation

SAMPLE MATERIAL GATHERED SO FAR
FACILITIES

- ASCR Facilities draft outline
- Argonne history of computing
- OLCF 25 Years of Leadership in High Performance Computing (draft)
- Timelines of ALCF, OLCF, NERSC (under preparation)
- 40 Years of Networking at the Speed of Science
  - The emergence of data-intensive science: ATLAS and CMS at the LHC
  - Extending ESnet to Europe with the same multiple hundred gigabit, reliable architecture, core as in the US to support Office of Science collaborations
  - Pioneering the next generation site connectivity: 400 Gb/s to support Super-Facilities
- The Importance of Research and Development in Networking
  - Tools supporting very large data transfers: ScienceDMZ and PerfSONAR
  - OSCARS: On-demand, guaranteed bandwidth (R&D 100)

SAMPLE MATERIAL GATHERED SO FAR
IMPACT ON INDUSTRY

- Selection of project write-ups
  - Improving Aircraft Engine Combustor Simulations (Pratt & Whitney)
  - GE researchers perform simulations in pursuit of more efficient jet engines and wind turbines
  - Taming Turbulence and Achieving Stability to Generate Fusion Energy
  - Better Combustion for Power Generation
  - Improving Everyday Products (Procter & Gamble)
  - Building a smart truck
  - HPC-driven Fuel Well Discovery
  - ESnet Taps Ciena for 400G Research and Education Network
- Examples of HPC Leadership: Understanding Behaviors in the Extreme Environment of Natural Gas Turbine Generators (Hyperion Research article)
- Computer and network industries impacts

SAMPLE MATERIAL GATHERED SO FAR
IMPACT ON WORKFORCE

- CSGF (have brief description, will request more)
- Training courses with access to state of art computers
  - Parallel programming short courses in the 1980s and 1990s
  - ATPESC
- ECP apps team participants who were traditionally funded by other than ASCR
- ECP new hires to labs

SAMPLE MATERIAL GATHERED SO FAR
IMPACT ON EDUCATION

- University curricula influenced by ASCR activities and people
- Specific courses designed by university faculty in collaboration with ASCR-funded national lab staff, e.g., Harvard School of Engineering and Applied Sciences course “Extreme Computing: Project-based High Performance Distributed and Parallel Systems”
- University courses that use lectures from ATPESC archives as part of the course.
  - For the last several years all ATPESC lectures are available online, approximately 80 each year.

SAMPLE MATERIAL GATHERED SO FAR
OTHER ACHIEVEMENTS AND CONTRIBUTIONS

- Awards and prizes
  - Nobel Prizes
  - Gordon Bell prizes and finalists
  - SIAM/ACM Prize in Computational Science and Engineering,
  - R&D100
  - DOE E.O. Lawrence Award
  - Best paper awards
- Support of standards committees
  - DOE Advanced Computing Committee Language Working Group c. 1977
  - National Lab staff participation in many formal and *de facto* standards committees

SAMPLE MATERIAL GATHERED SO FAR

LESSONS LEARNED FROM DIFFERENT MODES OF FUNDING AND RECOMMENDATIONS FOR THE FUTURE

- Have input from several people, gathering more
- Too soon to summarize

SAMPLE MATERIAL GATHERED SO FAR
APPENDIX A. COMPELLING STORIES

- NWChem: A Modern High Performance Quantum Chemistry Application
- ADIFOR story
- Rusty Lusk story: from automated theorem proving to UNEDEF
- Bruce Hendrickson story on discrete mathematics
- Examples of HPC Leadership: Understanding Behaviors in the Extreme Environment of Natural Gas Turbine Generators

INCOMING

- Impact of SciDAC program in BES, BER, FES, HEP, NP as well as ASCR
- ASCR-NNSA collaborations
- Insights from Dan Hitchcock and John Cavallini
- Computer vendor viewpoints and collaborations

YOUR INPUT IS SOLICITED – THERE IS STILL TIME TO USE IT

- Please suggest accomplishments to highlight, people to contact
- Your input on future directions
- Especially answers to these questions:
  - **What are the key aspects of the ASCR's investment strategy that have had the greatest impacts?**
  - **Looking to the future, and building on the ASCAC reports, what research areas and funding strategies to pursue those areas could further strengthen ASCR in serving the DOE missions?**
- Contact any subcommittee member to provide your input

NEXT STEPS

- Subcommittee meeting afternoon of Sept. 18th and morning of 19th
- Will examine all input gathered, decide whether to include in report and where, categorize as preliminary notes, rough draft, advanced draft

- In the remaining months, the daunting task of doing justice to all the input and producing an impactful report

SUMMARY

- ASCR's contributions to applied mathematics, computer science, computational science, computer architectures, computing facilities, networking – in short the scientific computing ecosystem – is astounding!
- Doing justice to its rich history will be challenging

THANK YOU!