MAGIC Meeting Minutes
September 7, 2016

Attendees

Dan Gunter	LBL
Shantenu Jha	Rutgers
Carolyn Lauzon	ASCR/DOE
David Martin	Argonne
Grant Miller	NCO
J.P. Navarro	OSG
Ryan Prout	ORNL
Arcot Rajasekar	RENCI
Alan Sill	U. T

Action Items

Proceedings

This MAGIC meeting was coordinated by Grant Miller of the NCO. Carolyn Lauzon of DOE/ASCR gave a presentation on developing requirements for DOE/ASCR High End Computing.

ASCR High End Computing Requirements Gathering: Carolyn Lauzon, DOE/ASCR

DOE/ASCR is currently in the process of identifying requirements for High End Computing. It addresses requirements for the ASCR facilities:

- Argonne Leadership Computing Facility, currently 10 PF to be upgraded to 180 PF in 2018-2019.
- Oak Ridge Leadership Computing Facility. Currently 27 PF to be upgraded to 150 PF in 2017-2018
- National Energy Research Scientific Computing (NERSC), currently 2.6 PF to be upgraded to over 30 PF in 2016
- ESnet

This study is addressing what HPC systems and ecosystem will best advance science in 2020-2025. DOE/ASCR is holding Exascale requirements reviews for the DOE/Office of Science. A Request For Information (RFI) is additionally soliciting information from the DOE national labs and, led by NIH, from NIH, NSF, and DOE for the broader community.

The study identifies key computational science objectives that push exascale and describe the HPC ecosystem needed to meet science goals. The process communicates to DOE SC scientists the known characteristics of upcoming compute systems and asks the scientists for feedback on the proposed architectures. Meetings with the science communities have included:

- June 2015: High Energy Physics for compute intensive modeling and simulation and data focused analysis and workflows
- November 2015: Basic Energy Sciences: Quantum materials, heavy element chemistry, exotic states, emergence, catalysis, photosynthesis, combustion, materials and chemical discovery, soft matter, biochemistry and other areas

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- January 2016, Fusion Energy Sciences, Turbulence and transport, MHD and energetic particles, RF heating, whole device modeling, validation and verification, materials science, and discovery plasma science
- April/March 2016: Biological and Environmental Research: Climate and biology areas
- June 2016: Nuclear Physics: Astrophysics, cold QCD, hot QCD, nuclear structure, data/experiment
- September 2016 (pending): ASCR

The reviews identified a need for rapid data movement between a compute facility and experimental facility. Fusion Energy Sciences discussed the possibilities for using computation for experiments. New use models are developing for HEP and ATLAS event generation. Biological and Environmental research is breaking current models for computation. There is a developing integration of data intensive research and experiments including:

- Real-time remote access to resources ssuch as databases
- Real-time data analysis
- Machine learning
- Data visualization tools
- I/O bandwidth challenges

Increasingly resource issues must be addressed for libraries, parallel primitives, methods for managing memory hierarchies, and portability. New partnerships need to be developed and a capable workforce must be assured.

The RFI has elicited responses form DOE laboratories (135 responses), Academics (94), industry (8), and others. The information from the RFIs identifies needs to support:

- Cybersecurity
- Self supported nano-assembly
- Galaxy formation and extreme gravitational fields
- Optimizing the Power Grid
- Hypeersonic flow for flight vehicles
- High resolution atmospheric and climate models
- N-by-N comparison of all patients in the U.S.
- Epidemic simulations

For the complete briefing please see the MAGIC Website, September meeting minutes at:
https://www.nitrd.gov/nitrdgroups/index.php?title=MAGIC_Meetings_2016

Potential MAGIC Tasking from LSN for FY2017

MAGIC members discussed potential tasks they would like to focus on for FY17. -MAGIC. These potential tasks include a continuation of the topics addressed last year:

- Convene the OSG, CERN, OGF… communities to discuss their different approaches and what has worked/what has not worked.
- Identify how commercial resources (e.g., cloud environments) can be used/integrated into science environments
- Bring the NSF funded cloud environments into the MAGIC discussions to represent academic community interests
- University community researchers and providers to identify current capabilities and desired future capabilities.

- SDN developers to identify how their developing technology might impact virtual environments and distributed resources/distributed processing

Additional tasks suggested by the MAGIC members include:
- Data movement and data management. Middleware is expediting movement of data across collaborating groups and among science disciplines. An example is cooperation among NSF data hubs for moving data to/from supercomputer centers. CASC is participating in this effort.
- Evolving Identity Management (IdM)
- Improving the reliability of middleware and grid environments. Software and networking are critical components for improving reliability.

Next MAGIC Meeting
October 5, 2016, 2:00-4:00 Eastern, NSF Room TBD