ADVANCED SCIENTIFIC COMPUTING ADVISORY COMMITTEE
OFFICE OF SCIENCE

Rockville Hilton – 1750 Rockville Pike
Rockville, MD
Tuesday, August 23, 2011 – 9:00 am to 5:30 pm.

Agenda Tuesday, August 23, 2011

Time	Topic	Page	Speaker
9:00	Opening Remarks From the Committee Chair		Roscoe Giles, ASCAC
9:05	View From Washington		William Brinkman, Director of the Office of Science
9:50	View From Germantown		Daniel Hitchcock, ASCR
10:35	Break		
10:50	Exascale Co-Design Center for Materials in Extreme Environments (EXMATEX)		Timothy Germann, LANL
11:30	Update on CSGF Subcommittee		ASCAC
11:45	Committee Lunch		
1:00	Early Career – Sustainable Silicon – Energy-Efficient VLSI Interconnect for Extreme-Scale Computing		Patrick Chiang, Oregon State University
1:45	EU Data Initiative		Mario Campolargo, European Commission
2:30	Update on Data Policy Input from Science Advisory Committees		Laura Biven, Office of Science
3:00	Break		
3:15	Applied & Computational Mathematics: Challenges for the Design and Control of Dynamic Energy Systems		Michael McQuade, Senior Vice President of United Technologies Corporation
4:15	Developments in High Performance Computing in China		Dona Crawford, Lawrence Livermore National Laboratory
5:30	Adjourn for the Day		

Agenda Wednesday, August 24, 2011

Time	Topic	Page	Speaker
8:30	Update on Exascale Research		Bill Harrod, ASCR
9:15	Fundamental Problems of Wind Energy and the Potential to Address them Through High-Performance Computing		Henry Kelly and Chris Hart, EERE
10:00	Break		
10:15	Early Career – Separating Algorithm and Implementation via Programming Model Injection (SAIMI)		Michelle Strout, Colorado State University
11:00	Update on Networking COV		ASCAC
11:15	Update on ASCR Recovery Act Projects		Vince Dattoria, ASCR
11:45	ASCR Investments in Small Business Innovative Research		Walt Polansky, ASCR
12:15	Public Comment		
12:30	Adjourn Meeting		

Dr. Roscoe C. Giles, Chairman, was presiding.

OPENING REMARKS FROM THE COMMITTEE CHAIR

Dr. Giles thanked all the members and participants for coming and noted that he looked forward to an informative and productive meeting. He advised that there were various threads that the committee would be following up on regarding events in Washington and the office and he looked forward to the active engagement of the committee members in that discussion. He welcomed Dr. Barbara Chapman, a new member and noted there was another new member, Dr. Sharon C. Glotzer from the University of Michigan who was unable to attend due to a family emergency. Finally he took the opportunity of introducing Dr. William F. Brinkman, the Director of the Office of Science (OS) who would give a review from Washington.

Committee/Voting Members Present:
Dr. Roscoe C. Giles, Chair
Dr. Marsha Berger
Dr. Barbara Chapman
Dr. Jackie Chen
Dr. Jack J. Dongarra

Committee/Voting Members Absent:
Dr. Sharon C. Glotzer

Dr. Susan L. Graham
Dr. Anthony Hey
Dr. Thomas A. Manteuffel (by telephone)
Dr. John Negele (by telephone)
Dr. Linda Petzold
Dr. William M. Tang

Liasons/ex officios Present: **Liasons/ex officios Absent:**

Staff/Others Present:
Laura Biven
Dr. William F. Brinkman
Dr. Mario Campolargo
Dr. Patrick Chiang
Dr. Dona Crawford
Mr. Vincent Dattoria
Dr. Timothy Germann
Dr. William Harrod
Dr. Chris Hart
Dr. Daniel Hitchcock
Dr. Michael McQuade
Ms. Michelle Mills-Strout
Dr. Walter Polansky
Dr. Taieb Znati (on the telephone)

VIEW FROM WASHINGTON

Dr. Willam F. Brinkman, *Director, Office of Science*

- Noted that politics was having a dynamic effect of the ability of the OS (Office of Science) to accomplish objectives.
- Detailed three areas in the OS that were having a huge impact that he considered to be important developments being done from applied technology and of benefit to society.

High Powered Computing:

- He discussed the electronic role of new technological advances such as the iPhone and the iPad.
- He felt that these new advances in technology were influencing what was going on in the world such as the political awakening and the Arab Spring .

Biology:

- He discussed biology and the DOE's (Department of Energy) contribution to biology and site testing which was important in recent years in particular through the synchrotrons.

- As an example he discussed a new cancer treatment for melanoma. He described the molecule that would assist the cells divide rapidly. He stated it was a molecule that they were able to model in terms of structure with the synchrotron. He said that they then turned to the structure of drugs that would latch on to the molecule at an appropriate place and stop it from reproducing. He stated that it worked and the drug was doing extremely well.

- He noted that the value of using the capability they have with synchrotrons to do x-ray-crystallography on large proteins. He confirmed that work in that area had already received two Nobel prizes and this would probably continue to be the case.

Climate and Related Biology:

- He noted that this concerned their biology and environmental sciences research group. He stated that they were obtaining better models and more conclusive statements about what is actually happening in the climate.

- He stated that the challenging issue was to convince the world that what the science community is saying about climate is factual.

- Confirmed that those three areas were areas that the OS had been involved in for many years and they felt that they were now having a significant impact.

- Discussed high performance computing:

High Performance Computing

- He considered that computing would play a significant role and there was no better problem to use computers for than the challenges associated with climate. Stated that there was an increasing effort and the OS was making a large contribution to a better understanding of climate and climate modeling.

- He noted that in his opinion the materials scientists seemed to be the first to use high performance computing. He gave an example of how they used computers from a search point of view where they numerically simulated huge classes of materials for a specific property. He noted that that type of analysis was called genomic materials.

- He noted that there were other areas in science where high performance computing was used. He stated that what is known about astronomy and astrophysics and plasma physics is completely dependent on high performance computing today.

- He discussed the advances in microprocessors in chips that are put into phones. He noted the amount of computing power that was essential to be able to design and build such chips. He

considered the chips not just from the point of view of the design of the circuit but also from the point of view of making a mass. He noted the smallest dimensions are getting to being 10 percent of the wavelength of the light you would be using to write the lithography.

- He discussed Intel and Boeing and the truck industry in particular where in past years they were able to simulate long-haul trucks and show that you could improve the wind resistance by 12 percent by changing simple additions to the way the truck was built.

- He stated that the ubiquity of computing was quite remarkable.

- Noted that a year ago this coming fall they were still discussing 7 percent increases of the government curve that would finish out in 2016/17. Stated that this would mean that they would have had twice the money and then the OS would be at $10 billion instead of $4.8. Stated that the situation changed in January when the new Congress came in and the OMB (Office of Management and Budget) wrote a letter to all departments asking for them to come in with a 5 percent decrease in total expenditures and give suggestions on how to make a 10 percent decrease.

- Noted that it was not clear how it would affect the OS. Confirmed that President Obama had always been a strong supporter of science and still was. Stated that he believed the president would protect the OS as much as he could.

- Stated that the OS did not suffer financially in 2011 as much as other organizations. Said that they were told their budget was level but he interpreted the term level as being 1 percent down. Confirmed that the budget would be finalized once Congress returned now that the debt ceiling issue was resolved. Stated that it was a foregone conclusion that they would have some form of continuing resolution for a period of time. Noted that after the Senate would pass the budget then it would go into conference which would take time again.

- Confirmed that one of the highest priorities in the department was to think about exascale and to try to fund that to drive their computing capabilities to the next level. Stated that they had been working hard to ensure that money went into the program.

- Stated that Dr. Daniel A. Hitchcock had done an excellent job working with NNSA (National Nuclear Security Administration) to pull the two organizations together and to push for exascale in a positive way which he applauded. Stressed the importance of keeping that momentum going and getting plans together as much as possible within the financial constraints already discussed.

- Noted it was important to get their act together for the 10 to 20 petaflops level. Stated that they had two machines that were supposed to be coming in next year which he hoped would put them back in the lead for a period of time.

- Stated that regardless of the turmoil in Washington it was important for their voices to be heard. Noted that there were a lot of people on the Hill sympathetic to science and who wanted to assist and so he said it was important to encourage these people and ask for their

assistance to ensure that the OS budget did not fall subject to a damaging decrease being advocated by some people.

- Emphasized the importance of providing supporters on the Hill with examples of successes in the OS to help them, something that he found had worked well in the past. Repeated that the economic impact of the truck research brought up in a previous year was well received. Suggested that the implications of a new cancer treatment were another example about which to encourage discussion.

COMMITTEE DISCUSSION

Dr. Giles noted that they shared his concern about the budget levels and future uncertainty. He asked if Dr. Brinkman had a sense of any impact of that uncertainty on the office and its operations such as its ability to retain the best people and maintain a sense of optimism and excitement about the science. Dr. Brinkman responded that they still were retaining the best people at their national laboratories and the universities. He confirmed that the hiring process for the position currently being held by Dr. Hitchcock as Acting Associate Director was completed and that position would be filled, others were also discussed. He said that there were some problems with state universities with related to funding.

A committee member asked about IBM and their recent announcement that they were withdrawing from the NSF (National Science Foundation) Blue Water Project to build a petaflop system. He asked if that would have any impact on the exaflop process. Dr. Brinkman responded that he did not know but what he had been told to date was that IBM was committed to two machines for the OS and that commitment was solid. He added that he didn't know if it would have a big impact on high performance computing. He said that there was an ongoing debate about cloud computing and Amazon versus high performance computing and how those two approaches would evolve. He suggested the committee might be more informed on that debate than him. He thought that high performance computing was something that would continue to develop so he did not see that as a big setback, however, it might have been a setback for the NSF.

Dr. Marsha Berger noted that he had discussed issues he considered priorities but what about issues that he did not consider priorities, would they suffer? He was asked if he had a strategy. Dr. Brinkman responded that it was often a case of relative suffering. He mentioned three areas, nuclear physics, particle physics and plasma physics and confirmed that they were trying very hard to obtain funding necessary to make ITER (International Thermonuclear Experimental Reactor) go and it was a huge burden. He noted that it was $250 - $300 million a year for four years so it was a big burden on the budget.

He stated that fusion in the United States was not progressing as fast as it was in other countries which could be a result of a more fragmented science community and a tendency to have a more cynical outlook on it. He said that in high energy physics they were having a debate regarding what the direction of high energy physics in the United States should be. He said that the energy frontier was at the SLAC (Stanford Linear Accelerator Center) and that it was running very well. He noted that the

cancellation of the DUSEL (Deep Underground Science and Engineering Laboratory) Project at the NSF caused a major ripple in the completion of the neutrino experiments and they were re-examining the situation to decide how to move ahead. He added that completing those experiments was another billion dollar project.

In considering the third area of nuclear physics he confirmed funding was a major issue for them in that they wanted to build an upgrade to the Thomas Jefferson National Accelerator Facility (TJNAF) from a 6GEV to a 12GEV. He noted they were also trying to build a large project at Michigan State University which needed funding in the amount of $550 - $600 million.

Dr. Brinkman emphasized that the OS could not get confused but had to consider what was having an impact in the world and consider clearly as the OS wanted to support those three areas of physics but they also had to recognize priorities.

Dr. Giles asked if there were any updates or changes with regard to international collaborations. Dr. Brinkman responded that there was nothing new but that the big international collaboration was ITER. He noted that a lot of work had been done to get a strong management team in place at ITER and they now had an excellent Director-General in Osamu Motojima. He also noted that Japan, due to the earthquake and tsunami, the EU (European Union) and the United States all had serious financial problems. This was a serious issue for all.

VIEW FROM GERMANTOWN

Dr. Daniel Hitchcock, *Acting Associate Director, ASCR*

- Noted that the goal of ASCR (Advanced Scientific Computing Research) was to deliver world-leading computational and networking capabilities to extend the frontiers of science and technology.
- Noted that the scientific challenges as per the rollout in the FY12 budget were the same:
    - Deliver next-generation scientific applications using today's petascale computers and in addition plan for the future at the same time.
    - Discover, develop and deploy tomorrow's exascale computing and networking capabilities.
    - Develop in partnership with U.S. industry next generation computing hardware and tools for science.
    - Discover new applied mathematics and computer science for the ultra-low power, multicore-computing future.
    - Provide technological innovations for U.S. leadership in information technology to advance competitiveness.

- Provided FY2012 highlights:
  - Research in Uncertainty Quantification (UQ) for drawing predictive results from simulation.
  - Co-design centers to deliver next generation scientific applications by coupling application development with formulation of computer hardware architectures and system software.
  - Investments in U.S. industry to address critical challenges in hardware and technologies on the path to exascale.
  - Installation of a 10 petaflop low-power IBM Blue Gene/Q at the Argonne Leadership Computing Facility (ALCF) and a hybrid, multi-core prototype computer at the Oak Ridge Leadership Computing Facility (ORLCF)
- Discussed the ASCR budget overview and the proposal and noted that the House mark was $5 million above FY11 and $38 million below the request. Stated that he was unsure how that would be resolved in the Senate but that they would have to work with the funding provided as ASCR moved forward.
- Reviewed the language in the House Budget and emphasized the importance of this because the House Budget Report language has the force of law unless it was contradicted in the conference report. Stated that because of that, the language was important even though it was just the House. Stated that if the Senate did not say it did not agree and the Conference did not agree to that then the language had a great deal of impact. Noted that the House liked the OS and the NNSA working together on the development of systems.
- Read significant parts of the House Budget language that were considered relevant and important:
  - "The Committee continues to support science activities in the United States that improve and develop the world's fastest supercomputing systems."
  - "The Committee commends efforts to collaborate on exascale research across these two programs and encourages further coordination and collaboration."
  - "The Department is directed to provide to the Committee, not later than February 10, 2012, a report including its current target date for developing an operational exascale platform, interim milestones towards reaching that target, estimated total ranges of Department investment likely needed to it those targets, and a complete listing of exascale activities included in the budget request broken out by program and activity with comparisons to the current year's funding levels."
  - "The Committee is supportive of investment in the national laboratories to expedite the exascale initiative, but also recognizes that small technology companies frequently provide the breakthrough innovations that are needed to achieve the kind of low power, high-speed

systems needed for exascale computing, particularly as the leap to exascale may require unconventional technology solutions."

- Noted that the request from the House asking for a plan by February 10, 2012 was currently being addressed. Reviewed the language of the House Budget as he noted that it was the Congressional context under which ASCR was operating.

- Stated that there would be some discussion about exascale activities on August 24th in the presentation by Bill Harrod.

- Stated that in relation to the House Budget comments about considering small businesses as well as the big players they were taking steps to try to figure out how to get the ASCR software out into the hands of small business industries more effectively and how to make the ASCR more commercially available to companies.

- Stated that they were looking at programs in two ways, backward and forward. He noted backward in the respect that they would look at SciDAC (Scientific Discovery through Advanced Computing) and partners today and what their requirements currently were to make their codes operate better. Noted that they also needed to look forward to estimate what their needs would be in a decade because if that research was not done then what they would need in the future would not be in place. Advised that in looking at that they changed certain things in SciDAC moving forward. He reviewed the current programs and possible programs of the future such as Titan going to Oak Ridge National Laboratory (ORNL) and Mira going to Argonne National Laboratory (ANL).

- Stated that the SciDAC conference took place in Denver and there were 377 participants. Noted that they had had this type of meeting for a decade and the 2011 meeting would be the last. Advised that they decided that they would have PI (Principal Investigator) meetings which would be considered more working meetings enhancing collaboration work. Thanked all people involved in making SciDAC successful.

- Stated that they had a call for SciDAC institutes and received proposals for 37 institutes requesting $217 million a year and they had $13 million to spend. Said that after Letters of Intent (LOI) they were down to 27 full proposals that only would request $141 million a year. They reviewed 20 proposals and ended up selecting three and spending $10.5 million a year. Stated that they had no proposals in the data management and visualization space which they considered a critical part of SciDAC and as a result they were now in the process of going back out and looking for data management and visualization.

- Advised that for the SciDAC institutes for FY11 they supported FASTMath, QUEST and SUPER. Each of these areas was described

- Noted that they had negotiated in partnership with the other offices in the OS a series a strategic partnerships and they would do pair-wise funding opportunities. Noted that the FOA (Funding Opportunity Announcement) for Fusion was out and the rest were in the administrative process.

- Decided that they would do focused announcements with the other offices in areas where the combination of applied mathematics and their application people would let them do something that was strategic and would change the face of their science. Noted they have had intensive negotiations with all the associate directors to find the topic areas they think would be of significance. Provided some challenges that these types of partnerships would undertake and described them in detail. Noted that they had started the process early to enable prospective applicants enough time to submit well-considered proposals.

- Outlined the goals and objectives and emphasized the importance of the strategic aspect for the offices.

- Outlined what he meant by co-design where future design would mean that hardware, software and applications people would work on design together not in isolation. Stated that they wanted the centers to look at things across the spectrum of kinds of applications that the OS cared about and figure out how you might allocate the complexity from the mathematics, the computer science, the algorithm in the formation of the problem and the hardware to figure out the design choices.

- Advised that they funded three exascale co-design centers: the Exascale Co-Design Center for Materials in Extreme Environments (EXMatEx) under Director Timothy Germann; the Center for Exascale Simulation of Advanced Reactors (CESAR) under Director Robert Rosner; and the Combustion Exascale Co-Design Center (CECDC) under Director Jacqueline Chen.

- Described ASCR interactions with applied programs including:

    - BES/EERE Workshop – Predictive Simulation for Internal Combustion Engines (PreSICE) – March, 2011.

    - Office of Electricity Delivery and Energy Reliability (OE) Workshop: Computational Needs for the Next Generation Electric Grid April 18-20, 2011, Cornell University.

    - Presentation at ASCAC meeting on August 23rd by Michael McQuade on Applied & Computational Mathematics: Challenges for the Design and Control of Dynamic Energy Systems.

    - Presentation at ASCAC meeting on August 24th by Chris Hart on Fundamental Problems of Wind Energy and the Potential to Address Them through High-Performance Computing.

- Stated that they currently are having work done on data driven science. Noted there was a call and all the advisory committees considered how they would deal with data in their space. Advised and described issues as a result of some of the following issues: data from instruments that were still on 18-24 month doubling because detectors on CMOS feature size path; 100 gigabit per second per lambda networks; and disk read and write rates and the need for improved hardware infrastructure.

- Advised that in partnership with BES (Basic Energy Sciences) they were running a workshop on October 24 and 25, 2011 on the topic of what you would do with data from large facilities called Data and Communications in Basic Energy Sciences: Creating a Pathway for Scientific Discovery. He outlined the goals and objectives of this workshop. He noted that they were beginning a conversation with BES about their requirements and how their science works and the parameters. Noted that the size of the teams at LCLS (Linac Coherent Light Source) was increasing from single investigators to teams of 16 to 60 researchers.

- Outlined details on workshops held in July and August and upcoming workshops in October 2011.

- Discussed some ideas from the 1970s that researchers could look at again using more updated computing.

- Reviewed companies that were currently using software developed by ASCR inside their product. He noted some of the software as MPICH, Fastbit, OSCARS and perfSONAR. He noted that illustrating this was considered a powerful story by members of Congress.

- Discussed the NERSC-6 facility which was one of the first Cray systems. Noted they had five months of early user testing. They went into production about six months ahead of schedule and under budget. Illustrated the breakdown by percentage of early user hours by science area.

- Outlined the leadership computing facilities progress. Advised that ALCF had its on-site operation assessment in August and is on schedule to deliver the 10 petaflop BGQ (BlueGene/Q) starting next summer. For ORLCF they revised the plan of record to upgrade the machine in place.

- Noted that the Energy Sciences Network was lighting up in mid September, the first coast to coast 100 gigabit per lambda network. He explained that you send it over existing fiber without digging additional holes, plant ten times as much data over the existing fiber. He described the extent of the network in detail.

- Advised that LEDs are great for lighting but the performance tended to degrade over time. He advised that NERSC (National Energy Research Scientific Computing) users were able to simulate that and figure out why the efficiency drops from the current scales. He noted that as a result they had a way to figure out how to build new materials for LEDs to avoid the degrading.

Added that since LEDs gave more light per watt and less heat meant you did not have to get the heat out of the building.

- With INCITE (Innovative & Novel Computational Impact on Theory and Experiment) University College in London studied blood flows at extreme speeds using Intrepid and this was used in the study and treatment of aneurisms.

- Advised that ORNL had been doing work with Los Alamos National Laboratory (LANL) to determine how to use data from things on planes from lightning detection to improve hurricane prediction so their course could be figured out so early warnings could be issued about evacuation.

- Introduced new ASCR staff, Dr. Lenore M. Mullin who came from NSF. Advised that she was the new program manager with computer science and provided more details on her background.

- Provided details on all the new website addresses following the change in the OS website to be www.energy.gov Noted that the addresses were:

  - ASCR: www.science.energy.gov/ascr/
  - ASCR Workshops and Conferences: www.science.energy.gov/ascr/news-and-resources/workshops-and-conferences/
  - SciDAC: www.scidac.gov
  - INCITE: www.science.energy.gov/ascr/facilities/incite/
  - Exascale Software: www.exascale.org
  - DOE Grants and Contracts info: www.science.doe.gov/granst/

COMMITTEE DISCUSSION

Dr. Jack Dongarra asked about the SciDAC program within the OS. He said when he took a look at the grants that have been given for the institutes two of them were going to the NNSA labs as leads and one was going to a university. He said when he looked at the co-design centers and two of those were going to NNSA labs and one was going to the OS lab. He explained he was trying to understand what was happening, if they were phasing out SciDAC within the OS labs. He wanted to understand what the plan was for retaining the high quality staff that they had at the labs.

Dr. Hitchcock described partnerships and said that they responded largely to proposals and noted that they tried to fund the highest quality work. He noted that the OS labs had a lot of exposure because of the partnerships with the OS programs and strategic partners. He advised that there was a lot of computer science and applied mathematics work at the OS laboratories. He stated that this was the natural evolution of proposals as you would try to get the best value during times of restricted funding.

Dr. Dongarra noted that they had built up great team of people over the years doing multi-disciplinary research and the funding levels at the OS labs appeared to be down $2-$3 million at each of the labs. He asked what the plan was for retaining high-quality staff at the labs. Dr. Hitchcock noted that the plan was to support the best research they could wherever it is and at times laboratories went through periods where they would write bad proposals and they were not going to be funded. He said that his advice was that they had to prepare great proposals as the environment was becoming more and more competitive. Dr. Dongarra asked if they were switching the model for funding and gearing towards NSF. Dr. Hitchcock disagreed and said that was not the case, they had always tried to fund the best work.

Dr. Susan Graham asked about the congressional language and the request for a response. She noted that there was no time scale in the request in that they wanted a plan but they did not say how many years that plan should take. She asked about his strategy for dealing with that and asked to what extent would he try to factor in projections of what a likely budget would be in laying out the plan. Dr. Hitchcock responded that they were in intense discussions in the department regarding what assumptions they might be allowed to say in such a plan. He said that one of the reasons these plans take so long to prepare is that they have to go through the department, the chief financial officer and through OMB (Office of Management and Budget) and OSTP (Office of Science & Technology Policy) to get to Congress and that process had a timescale of its own that could not be accelerated. He explained that they would put cost ranges in there but he added what they would finally be allowed to say in the plan and whether it would be satisfactory to them is still a matter of discussion. He added that their nominal goal was to have it by the end of the decade.

Dr. William M. Tang noted he had a comment and a question. He noted that Dr. Hitchcock had mentioned in his presentation that SciDAC had served the U.S. program very well. He said he felt it was unfortunate that the SciDAC conferences would be ending. He noted that Lori Diachin advised that the last conference was well attended and they could not accommodate all the people who wanted to attend. He added that it was a showpiece for the U.S. impact in inter-disciplinary computational science. He noted that he understood funding constraints but he thought that it should be continued in some form. He asked about international collaborations and noted that when Dr. Hitchcock reviewed upcoming events that he should include international events also and that should be emphasized. He thought that it would help to make the case for Congress just how competitive an arena is was in which the U.S. excelled.

Dr. Tang went on to describe many different events that he thought important. He stated that he had just returned from Asia and noted that there were a number of interesting collaborations there and the committee would hear more about that from Dona Crawford later in the day. He emphasized that a strategy should be developed in the area of collaborations which might help alleviate some of the funding issues. Dr. Hitchcock agreed and noted that he would be talking at the EESI (European Exascale Software Initiative) in Barcelona and would be trying to determine the best course forward with the EU (European Union). He added that in the networking area they had had a lot of international collaborations. He added that they had to figure out the right thing to do that brings in the most benefit without increasing the risk profile. He added that the issue of collaborations was often complicated

because of a duality of thought in Congress. Many representatives wanted international collaborations and many wanted the research should be export-controlled to keep the intellectual property.

Dr. Tang noted Dr. Hitchcock's comment about the difficulty in organizing international collaborations but he added there were unique opportunities. He noted that the international scientific community was taking part in a very high level of research and development and he thought the U.S. should take advantage of any opportunities to take part in those opportunities with them and would be very helpful to the U.S. program.

Dr. Anthony Hey asked about the SciDAC institutes where Dr. Hitchcock mentioned he was going to look for a data visualization ware. He asked if he would elaborate on the processes and timescale. Dr. Hitchcock responded that the new funding opportunity would be out on the street before the end of the fiscal year so it could be available in a timely way to support users. He added that the end of the fiscal year would be September.

Dr. Giles asked about the SciDAC application partnerships and if they are between ASCR and a single other office or were there three-way and more complicated partnerships. Dr. Hitchcock responded yes, that they had turned out to be ASCR and one other office. He said it was this way because their scientific priorities were too different to put two offices together.

PUBLIC COMMENT

Ms. Dona Crawford, Lawrence Livermore National Laboratory

- Noted that Congress was getting interested in foreign HPC (High Performance Computing) capabilities. She read "the House through the National Defense Authorization Act approves statutory language originally proposed by HASC the (House Armed Services Committee) requiring a net assessment of foreign HPC capabilities".

- Said it would be coordinated and would be a large effort and they would tentatively be giving the community six months. Stated that they were interested in it particularly from a national security perspective which was why the National Defense Authorization Act had put the language forward but it would be coordinated with ASCR due to its involvement with exascale.

Paul Messina (sp?), Consultant for the National Library

- Noted he was asking about the partnerships within the OS. Asked if there was a plan for providing computer time. Noted he was concerned about the double jeopardy issue. Said that if you put in a proposal, it got funded but then one had to go through another process which would take as long as 11 months to get an inside award for example. Asked if he had a plan for providing the computer resources to successful proposals.

- Asked if there would be any requirement for the resulting software that would yield a breakthrough to be generalized enough so it could be of use to other people and advance the whole state of the art instead of just solving a simple problem.

Dr. Hitchcock responded that they had thought about the double jeopardy issue and noted that it also existed at every light source and other DOE facility, that one would get funding for the research and then you would have to get time at the light source. If they have picked the right partnerships they hopefully would get insight awards, and if they can't, perhaps they aren't the right partnerships. They have the ALCC (ASCR Leadership Computing Challenge) to assist in the early years to smooth this issue out. They haven't put specific language in in the FOAs about the software that comes out, each office has a different culture about this and ASCR should not get in-between them. Mr. Messina asked Dr. Hitchcock to consider making that part of the FOA. Dr. Hitchcock responded that it was ASCR's policy that any software developed under ASCR funding solely or in collaboration with NNSA should be released on an Open Source license. This was more difficult with application software, which they had substantially less control over.

BREAK

The Advanced Scientific Computing Advisory Committee recessed for a 15 minute break.

EXASCALE CO-DESIGN CENTER FOR MATERIALS IN EXTREME ENVIRONMENTS (EXMATEX)

Dr. Timothy Germann, *LANL (Los Alamos National Laboratory)*

Dr. Giles introduced Dr. Germann and noted that he was the PI for the new funded Exascale Do-Design Center for Materials in Extreme Environments.

- Noted that there had been a trend over the past 10 to 15 years to encourage an air gap between the application developers and the computer scientists.

- Described the difference between the two in that the application developers had a problem which they would need to solve and he described the process if they were posed with such a problem. Noted that they would pick a solution method and then solve it numerically.

- Compared that process with the computer science side where the people developing the hardware and the systems software would have a big picture of what the applications looked like which could be outdated or overly simplistic. Noted that based on that they would have a very good picture of how memory was laid out and what the software stack and runtime systems look like.

- Noted that the gap needed to be bridged because the problem had increased with increasingly complex machines delivered and put into operation. Stated that the application developers

would then be faced with the problem of figuring out how to use it. Emphasized that the paradigm had to change.

- Stated that the concept of co-design was to bring together the computer scientists, applied math and domain science folks together at an early state to work on the problems together. Emphasized the importance of this at this time because of the dramatic changes in hardware. Stated there was a revolution that was following the serial to vector machines and vector to parallel and now heterogeneous and hierarchical architecture with a massive increase in concurrency. Noted that algorithms and methods would also have to be rethought and revisited. Stated that flops would not be a limiting factor, that it would be more memory. Noted also that power was a constraint for large scale systems and resiliency was a challenge.

- Emphasized that the broad knowledge required a team to work on these problems. Touched on the early co-design teams such as Richardson and Metropolis from LANL in the 1950s with the development of the MANIAC 1, 2 and 3 systems.

- Described computational co-design at LANL in 2008 with hybrid computers. Noted Roadrunner was the first large-scale heterogeneous system, first petaflop system and that 96 percent of the computing power was in the accelerators. Listed some of the successful applications that came out of Roadrunner. Noted there was not enough time to influence hardware in a significant way.

- Noted that their application area was materials in extremes which would include a large area of extreme environments including corrosion. Stated that they were focusing specifically on mechanical extremes, dynamic loading and high pressure. Stated they were also concentrating on irradiation extremes. Noted and described a number of workshops on these areas in the last five years and laboratories that hosted them.

- Described that the traditional modeling approach was to develop and use models at a variety of length scales. Noted that they ranged from the electron structure scale, molecular dynamics, phase-field modeling and continuum methods. Noted that each of them had somewhat different aspects in them regarding their computational motif and all were developed over the past 10 or 15 years based on an MPI approach.

- Described certain constraints and showed scales accessible by molecular dynamics simulation. Noted that current trends would increase the length but not the time. Used Roadrunner as an example and illustrated his points on a graph.

- Noted issues that had to be confronted included computer architectures that were becoming more heterogeneous and hierarchical with flop/byte rations increasing. Stated that with that in mind the algorithms, programming models and tools must go in a similar direction. Noted that the SPMD bulk synchronous approaches (109-way) parallelism could no longer be used.

- Stated that their ExMatEx goal "to establish the interrelationship between hardware, middleware (software stack), programming models and algorithms required to enable a productive exascale environment for multiphysics simulations of materials in extreme mechanical and radiation environments". Described the task-based approach and the programming models and approaches to be used. Stated that the goal of the center was the interactions between the three areas reflected in the graphic.

- Described the more specific objectives, the first one being to inter-communicate the requirements and capabilities between the three communities and stated how this was to be done:

    - Through proxy applications that communicated application workload to the hardware architects and system software developers. They are used in models/simulators/emulators to assess performance, power and resiliency.

    - Exascale capabilities and limitations would be continuously incorporated into the proxy apps through an agile development loop.

    - Single-scale SPMD proxy apps would be used to assess node-level data structures, performance, memory and power management strategies.

    - System-level data movement, fault management and load balancing techniques would be evaluated via the asynchronous task-based MPMD scale-bridging proxy apps.

- Described the second objective as performing a trade-off analysis between competing requirements and capabilities in a highly coupled optimization loop:

    - A three-pronged approach combining node-to-system-level models and simulators, exascale emulation layer (GREMLIN) to introduce perturbations similar to those expected on future architectures and performance analysis on leadership-class machines.

    - Co-optimization of algorithms and architectures for price, performance, power (chiefly memory and data movement) and resilience (P3R).

- Described the third as the full utilization of exascale concurrency and locality:

    - The heterogeneous, hierarchical MPMD algorithms map naturally to anticipated heterogeneous, hierarchical architectures.

    - It escapes the traditional bulk synchronous SMD paradigm and improves data locality and reduces I/O burden. It is task-based.

- Described the fourth as the application friendly programming model side:

  - The goal is to take hardware capabilities to the application programmer while at the same time hiding the continuous flux and complexity for the underlying hardware through a layer of abstraction that would aid portability.

  - Use a task-based MPMD approach to leverage concurrency and heterogeneity at exascale while enabling novel data models, power management and fault tolerance strategies.

- Stated that the process was not like building a bridge where it would be known that you would need to do a, b and c and then put them altogether. Noted that a timeline could not be mapped out for a sequence of steps. Explained that what was needed was an adaptive process that would provide feedback on the most important areas. Went on to describe it as an agile development method with an adaptive method like a spiral development process. Stated that you first gathered the application requirements from the stakeholders and customers and continuously iterated and collected feedback on those communities. Stated that it was not a one-time what do you need and then go and develop it and meet with them again in five years, it was a continuous development. Stated that this type of development was more flexible and they could deal with changes particularly in the architecture and software design as they evolved and as it would fit in with the other co-design efforts.

- Described the agile development cycle as a development code and analyze sequence and the model is test-early, test-often. Noted that the goal was during the past year's planning efforts was largely a preparation effort, getting buy-in from the science and mission communities, the stakeholders such as the vendors and then feeding them to the initial set of proxy applications. Described all the stages of the cycle and continuing issues of the proxy applications as the development moved along.

- Reviewed staff under the executive advisory board, Exascale Co-Design Center for Materials in Extreme Environments, SC/ASCR , the Exascale C0-Design Consortium and the Advanced Algorithm and Co-Design "Code-Team" and the laboratories involved under the three main areas of computer science, applied math and computational materials science.

- Detailed an interconnected task areas diagram showing nine areas: CM, center management; PA, proxy applications; AD, algorithm development and uncertainty quantification; PM, programming models; RT, resource/task management; ST, scalable tool development; MS, performance models and simulators; TA, tradeoff analysis and simulation and VS, vendor and software (ecosystem) engagement. Stated that each area acted as its own agile development process. Noted that there was quarterly synchronization among all task areas.

- Discussed the approach and stated that they would develop an adaptive physics refinement. Described the coarse-scale model that propagates long and as needed dynamically spawns off fine-scale models. Confirmed again that it was a task-based approach that would naturally map to the heterogeneity, concurrency and resiliency issues.

- Described the details of an adaptive sampling technique demonstrated at LLNL. Noted it was a coarse-scale model and was a finite element model (FEM) and as needed it called a lower length-scale model (polycrystal plasticity) model to compute the response. Described the processes in more detail. Stated that it was discussed in a subsequent paper entitled, "A call to arms for task parallelism in multi-scale materials modeling."

- Stated they were using the paper as a starting point to get a two-scale proxy application which they could start using to explore the design considerations. Stated their focus was on coupling the macro (coarse-scale model) and meso (fine-scale model) scales with all unit physics being deterministic. Noted they would build off of the adaptive sampling success but would move to the use of temporally evolving mesoscale and spatial adaption. Described embedded scale-bridging algorithms in more detail.

- Described single-scale proxy applications as having a main focus at the node level where they would look at data structures, memory access, storage and access, formatting, power management and node-level performance issues. Described secondly the task-based MPMD scale-bridging proxy application which was more at a system level for system issues so it would be data movement, system level resilience, load balancing and performance scalability. Emphasized again that they were not static entities but were continually evolving.

- Described the hierarchical programming models which were two levels, the on-node parallelism of the vector instructions and multiple threads and at the system level, the more loosely-coupled collection of tasks. Noted that they were also developing domain-specific languages.

- Described a hierarchical set of tools, performance models, simulators and emulators. Described the ASPEN, the SST and the GREMLIN.

- Stated in summary that their four main focuses were: scale-bridging algorithms, programming models, proxy applications and co-design analysis and optimization.

- Noted that they had a kickoff meeting August 24th and 26th in Santa Fe, NM. Described the three sessions which would deal with stakeholder input, task area discussion and Y1 work plan development.

COMMITTEE DISCUSSION

Dr. Graham noted that the plan was well thought-out and was in no sense critical but she had concerns about the application developers. She said that application developers in experimenting with applications would learn things which would cause them to change the model. She was concerned that it would be difficult for the application developers to do. She asked if there would be a way that the developers could test the applications before deploying it. Dr. Germann responded that yes this was one of the pieces of the agile cycle and this was that they would need continuous assessment from the

committees which would include the application developers and users to see if they were going in the right direction.

Dr. Jackie Chen asked if he could comment about the vendor interaction model with the co-design center. Dr. Germann responded that that had been the more challenging. He said that the two laboratories LANL and LLNL had been on different sides of the vendor fence. He indicated that there were a whole set of vendors they wanted to work with and some had wanted to work directly with the co-design team. He said the vendor process would form one of the main discussions at the workshop.

Dr. Giles noted that the process he was talking about he would consider a development framework but he asked how much of the infrastructure and methodology in the context of co-design would need to persist into what they would think of as the deployment phase. Dr. Germann responded that there had been some issues in testing at one of the laboratories in which an applications developer was not working well using evolving architectures under the new system. He thought that showed testing the program models was useful.

Dr. Hey said he understood how they would explore different models of parallelism but he said he thought the essence of co-design was that you had the hardware architecture being influenced by the applications. He asked how he would make that happen. Dr. Germann responded that there was not a lot that could be influenced at the node level on the exaflop machines. He noted that at the system level there was more of an opportunity to influence that. He said that he thought what would come out of it from working with various proxy applications with different vendors and then the vendors using them in their internal simulators they thought would start to show the highest-opportunity areas that could give the most pay off. He thought it was not a single optimization process with one application it was the whole spectrum of applications.

Dr. Tang noted that his definition for vision for co-design was almost identical to the SciDAC principle. He also said the new element of co-design as he understood it was the connection to future hardware development. He thought that if you looked at all the top 500 list, the top 10, the migration was clearly very low memory per core and he thought that that was not going to change. He asked as they were going forward with the challenging activity of mixing the scales, microscale simulations and feeding them back into a larger macroscale code, how much experience was there in the application domain and were there examples that could be pointed to now or was it in a development stage. He asked what the timeline was for generating a concrete result. Dr. Germann stated that there had not been any much research over the past several years on multi-scale applications. He described research concerning algorithms at the laboratories.

Dr. Chen asked about the greatly reduced I/O anticipated at exascale. She asked what he planned to do for getting information out. She asked if he would be doing embedded or institute-type methods and if he would comment. Dr. Germann responded that for the global check point restart picture it was only for the core scale model that they would need to save. He noted for the most part it was the same for a lot of the analysis and visualization that they needed to do.

UPDATE ON CSGF SUBCOMMITTEE

Dr. Giles called on Dr. Marsha Berger to give an update the Computational Science Graduate Fellowship charge on behalf of Dr. Thomas A. Manteuffel who is the Chair for that subcommittee.

Dr. Marsha Berger, ASCAC, *Courant Institute, NYU*

- Noted that it was an interim report and she was giving it as Dr. Manteuffel, the Chair of the committee could not be there.
- Reviewed the members of the committee.
- Read the charge given to the subcommittee, "By this letter, I am charging the ASCAC to assemble a sub-committee to examine the effectiveness and impact of the CSGF, as compared to other educational activities, and the quality and breadth of the program over the past decade. The sub-committee should take into account the unique qualifications and skills of computational scientists and their role in the public and private sectors. It should also address the participation of women and under-represented minorities, the projected need for trained computational scientists in the DOE laboratories and to continued U.S. leadership in computational science."
- Noted that there were no other comparable educational activities. Said for example that the NSF had graduate fellowships but they did not have the important practicum requirement of the CSGF where the fellows spend a summer interning at the DOE labs. Stated that this was felt to be important and got the young scientists exposed to the laboratories. Noted also that the program of study was a unique aspect of the CSGF where the fellow would map out the different aspects of their program of study by the committee that oversees them.
- Listed areas including the following: list of winners and their outcomes, applicants and awards, the process of selection and budgets as well as many sub fields of information supporting those headings as part of a process of gathering facts and background material.
- Listed the reports that they had collected which would form part of their discussions.
- Listed some of the actions of the committee which has included e-mail discussions and a teleconference in early July.
- Stated that they had interviewed the DOE program managers, the Krell Management that oversaw the CSGF program and alumni. Noted that it was done by a subcommittee of the committee consisting of Dona Crawford, Jeff Hittinger and Dr. Tang. Advised that they interviewed the DOE program managers Barb Helland (SC) and Thuc Hoang from the NNSA and the Krell Management, alumni and existing fellows.

- Advised that their future plans included more e-mail discussions and teleconferences and producing the final report for the November meeting of ASCAC.

COMMITTEE DISCUSSION

Dr. Dongarra asked if the program was limited to U.S. citizens would there be any concern that they may be missing some of the best students as a result. Dr. Berger responded that they did discuss that and she said it would be premature to state any findings but she said she would be happy to take that back for further discussion. She stated that that was one of the requirements of the program.

Dr. Giles asked if the program was the right size. Dr. Berger noted that if he was talking about the need for future computational scientists and how to judge that then she said that the size of the program had varied over the years and they had data which showed a fluctuation in the budget and the number of students. She said that one of the things they were looking at was that it grew could they maintain the quality of the students. She stated that it appeared to show at the present time that the program was doing a good job and they would like to see that continue. She said that the question might be could it be exported to other areas following their successful model.

LUNCH

The Advanced Scientific Computing Advisory Committee recessed for one hour for lunch.

EARLY CAREER – SUSTAINABLE SILICON – ENERGY-EFFICIENT VLSI INTERCONNECT FOR EXTREME-SCALE COMPUTING

Dr. Patrick Chiang, *Assistant Professor*, *Oregon State University*

Dr. Giles welcomed Dr. Chiang from Oregon State University and noted that he was one of ASCR's early award winners and stated that he would be presenting to the ASCAC his work on sustainable silicon and VLSI interconnect.

- Advised that he would be talking about research and his group at Oregon State University. Advised his group was about 13 students and one post-doctoral fellow. Noted that there were a number of collaborators and funders. Thanked the DOE, Intel, LSI and nVIDIA.

- Explained what exascale meant and reviewed the graph which compared the IBM Roadrunner 2009 and projected improvements in 2018. Reviewed power, speed, space, memory and cost.

- Discussed the DARPA (Defense Advanced Research Projects Agency) 2008 exascale report and discussed the solving the problem related to power efficiency for super computers then one should also be able to apply that technology towards other applications. Discussed attributes such as: aggregate computational rate; aggregate memory capacity; aggregate bandwidth; volume; and power. Discussed calculations they had done.

- Noted that in the DARPA report they mentioned four major problems with current hardware technology. Listed them as:
    - Memory and storage and discussed capacity and latency.
    - Concurrency and locality and discussed parallelism and software/hardware
    - Resiliency challenge and discussed low VDD and process variability
    - Energy and power and discussed interconnect
- Discussed the interconnect energy wall and microprocessors. Stated that approximately 51 percent of microprocessor power was consumed by interconnect and that without changes in design that figure would rise to 80 percent within the next five years.
- Stated that according to the study the energy and power challenge was the most pervasive and had its roots in the inability of the group to project currently mature technologies that would deliver sufficiently powerful systems.
- Stated that according to the study it might be easier to solve the power problem than to reduce the problem of transporting data from one site to another.
- Discussed graphs and calculations concerning: power density; shortage of power; need for more off-chip bandwidth; interconnect energies; alternatives (3D stacking and silicon photonics); problem 1: on-chip wires; problem 2: off-chip I/O; low-power interconnects overview with On-chip I/O and Off-chip I/O; near-threshold operation; synctium: near-threshold parallel processor; (1) energy-efficient, On-chip links (detailing router power and out goal: low-power on-chip links); token flow control NoC (detailing conventional router, proposed TFC router, tokens for advance allocation and NoC power dominated by XBAR and LT); low-swing, Bitcell-based crossbar; measurement summary; next goal: 1-5fJ/mm; energy-scalable on-chip TxRx; dynamic operation; on-chip links – measurement results; measured energy/b/mm; inverter cross-over point; off-chip I/O scaling trends; (2) off-chip links: global clock distribution optimization (with Intel); chip #1: injection-locked receiver architecture; ILRO: extension of Adler's Equation; chip #2: near-threshold, 0.15mW/Gbps, 9GBps serial link receiver; measured deskew range and BER; comparison table.
- Discussed his take-away points as follows:
    - Lower energy silicon is possible and aggressive interconnect circuits show: off-chip: 5x improvements and On-Chip: 50x improvements.
    - Reliability at low-Vdd is issue and explore in-situ adaptation to self-heal autonomously.

- Magic bullets do not exist and lower energy leads to lower performance, dynamically adapt the entire system and it requires co-design interaction between software, architecture and underlying silicon.

COMMITTEE DISCUSSION

Dr. Giles said when he was talking about dynamic reconfiguration, what would the timescale for this be? Dr. Chiang responded that at the silicon level, it would be instantaneous. There would be sensors everywhere on the die for leakage, power, capacity. Dr. Giles said that was almost the second part of his question. He asked would they have a lot more sensor capability. Dr. Chiang said yes, only 10 percent of the real estate was being used in 10 years, so the issue would be power, not space.

Dr. Tang noted that it was exciting from a co-design standpoint because they were working to improve the soft spots and seeing where they could improve performance. He asked about his interaction with Intel and nVIDIA and asked when he would come up with new ideas and if something looked great what would he estimate roughly the time to impact, in terms of manifestation of an actual product that would be used in a system. Dr. Chiang said in 2009 they published an initial paper of the first link with Intel Surface Lab. He advised that the co-author on that was running the I/O technology of that particular group. He noted that once they published that paper with them and the follow-up journal paper Intel immediately would design a group of five engineers to look at the practicality of whether it was feasible. He noted that in terms of their collaboration with Intel he thought they had done a good job in translating R&D (Research and Development). With regard to his second question regarding relevancy he responded that Intel were forward-thinking in his opinion and had steered them towards relevant areas of research.

Dr. Barbara Chapman noted that she thought the co-design implications were exciting. She asked if he had interacted with people and the software stack to enable information to flow that would support the savings of energy. She asked if he had interacted with people in the software design or applications area. She asked how he would like to do that. Dr. Chiang responded that sometimes a hardware person would tend to not want to be in the software world. He said that if he wanted to be a good academic he had to find the right problem to solve. He said that yes, he was starting to have some interaction.

EU DATA INITIATIVE

Dr. Mario Campolargo, *European Commission*

Dr. Giles introduced Dr. Campolargo who is the principal scientific officer with the DG information society and had come to talk about data initiatives in the EU.

- Stated that he had been with the European Commission for a number of years and had been involved with a number of initiatives and in the context of which they had established relations with the United States, in particular the NSF and the DOE and others.

- Noted that he wanted to share information about some of their activities in the domain of what they call e-infrastructures that range from topics already discussed today, global connectivity to the use of high performance computing.

- Stated that both Europe and the United States are both well known for their investment in research and innovation. Stated that they had just launched a European initiative called Europe 2020 setting milestones and objectives for the EU in the 2020 timeframe and the initiative was characterized by three key words, smart, sustainable and inclusive in their society.

- Said that within Europe 2020 they had formed a number of flagship initiatives to develop and try to address from different and complementary points of view basic objectives. Advised they had launched two important initiatives called Digital Society "A Digital Agenda for Europe" and within the area of innovation, "Innovation Union". Noted that they were two of the seven flagships that form the backbone of initiatives that supported the Europe 2020 strategy. Explained that they were brought up as they fell within the context of research and innovation.

- Stated that for the strategy of the model Europe 2020 model it would be noted that research and innovation were key perspectives and elements.

- Noted that the digital agenda for Europe was to exploit the potential by creating a virtual circle of a digital economy, creating attractive content and services stimulating demand and in turn creating a demand for faster networks.

- Noted that Neelie Kroes, the vice-president of the EC, Digital Agenda also emphasized the importance of research and innovation was a key priority of the agenda.

- Noted that science had to be made to be more efficient. Stated that new research methods that had exploited advanced computational resources, data collections and scientific instruments had all changed the scientific discovery process. Noted that funding was an issue for all countries and that scientific research would assist everyone in making better use of resources.

- Emphasized the importance of teams working together with co-design and bringing expertise in multi-disciplinary fields.

- Noted the importance for educators and students for taking advantage of and making use of this modern attitude towards science based on information that can be obtained internationally.

- Stated that there were two questions and those were what could science do for us but also what could we do for science? Stated it was important to have this dual perspective when decisions were being made.

- Detailed some of the areas in Europe that were instituted to support science. Noted they were developing a high performance network called GEANT. Noted they are involved in research internationally with internet two or ESnet. Noted they are developing and playing a role in

research networks. Stated that they believed that expertise exists in all parts of the world and when they thought of biodiversity it would include the significant contributions from researchers in Brazil or the Philippines. Stated that they did not just invest in a high performance networks in Europe but they also established a policy for ensuring they assisted other regions to develop regional networks and to link them.

- Noted that the second aspect in which they invested was the ability to share the best resources and he advised that they had been motivated by communities like high energy physics. Noted they were trying to broaden their requirements to be applicable to other communities. Said their experts were also tackling aspects of cloud computing for science and this might also be used for government services.

- Noted another aspect they were investing in was future facilities in the domain of high performance computing. Said that they had an excellent set of high performance computing centers with a wide knowledge in the domain of applications. Noted that they had brought the investment of high performance computing together in PRACE.

- Stated that one o f the highest investments now being done in Europe was in the domain of scientific data, not just research but from a perspective of data that could be used by citizens to generate new services, applications or business.

- Advised the document, ICT infrastructures for e-Science, had been prepared and approved by the EC, submitted to the council and to the European parliament and it had received support from scientific communities. Noted it had three objectives: to ensure that Europe embraced more paradigm of e-science, to ensure that the e-infrastructure became a significant enabler for underpinning all European research and innovation and to ensure the EU, the member states and the scientific communities could work together.

- Described Horizon 2020, a European framework program that would bring them from 2014 to 2020. Stated how Horizon 2020 would be structured and this would be done in three ways: creating industrial leadership and competitiveness, tackling societal challenges and excellence in science base. Noted that it was around these three areas that Horizon 2020 program was structured. Stated that the current program in which the research took place was a framework that tackled ICT related but also non-ICT related aspects and was a framework currently worth 54 billion Euros over seven years. Noted the strong support that their scientific programs are receiving from the EC.

- Described some areas of cooperation between the United States and the EU. Noted he decided to concentrate on only several areas this meeting was an advisory committee. Proposed cooperation in the area of high performance computing and data infrastructures.

- Noted that under high performance computing area of exascale would be particularly important. Said that they had been collaborating with DOE initiatives in domain of the IESP (International Exascale Software Project) but had also launched their own initiatives in Europe.

- Noted that in Europe they did not just want to be a partner in the development of research projects and initiatives but they wanted to ensure that they could congregate their industry that they would be active in the domain of high performance computing and it would bring them to an industrial perspective.

- Described the second aspect for cooperation and that was a global framework to develop an open and interoperable data infrastructure and with this there were two aspects. Stated first that they believed that there could be joint participation in groups such as the G8 and O5 working group on data and second, to help research communities work together on interoperability, access policies and standards.

- Noted one activity they would have liked to launch was an establishment of data access and an interoperable taskforce so that at global level they needed to establish a taskforce to focus attention on data access and interoperability and this was one of the recommendations that they would have liked to discuss with their partners in other continents.

- Stated that he believed they should work together on exascale and innovative research. Stated that they believed there was a certain urgency but although both countries had their own roadmaps and activities there was now an opportunity to work together.

- Noted that he looked forward to the visits of some committee members in October in Barcelona at which time they could discuss exascale strategies and data infrastructure strategies in Brussels.

COMMITTEE DISCUSSION

Dr. Dongarra asked if he could be more specific about the funding levels for Horizon. Dr. Campolargo responded that Horizon would start in 2014 and that meant they would be seeing the first calls for the new projects by the end of 2013 and they would utilize the budget allocated for 2014. He noted that the process was that they had sketched their proposal to the parliament and to the council and in that context they had forwarded a proposal of 80 billion over the seven years. He stated that that was the proposal that would allow them to do those three vectors identified. He stated that by the end of the year they would have a better understanding about the figures they would be able to negotiate. He stated it was the decision of both the EC and the European parliament and if they were not aligned they would try to find a solution.

Dr. Tang asked about PRACE being active and working to distribute HPC resources to various partners. He asked about the allocation of HPC resources and in particular three new exascale projects being launched in Europe. He asked how they work through, what was his algorithm for working through, and

how did he distribute time from his HPC centers to specialized projects versus the overall community requests and then factoring in the G8 projects that have been funded. He said that they have to have some meetings with them to find out how to get access to actual cycles to do their work on some of the G8 projects. He asked for his comments.

Dr. Campolargo responded that the high performance centers were essentially national and the national sovereignty in that domain was very important in Europe. He noted that they started several years ago to try to launch some technical solutions that would allow the interconnection of those centers and that would work in a way that the governance of those centers would allow that and would be a single point of conduct and projects could submit and then receive the cycles from the most adequate type of super computer. He stated this would be working on the consumption side. He stated that the challenge when they launched PRACE was not to just have 'x' high performance computing centers in various countries working together in another fashion. He noted the challenge was that they have a pot of money and they have to get together and PRACE has to be able to have a say in the way the new machines are going to be developed and implemented and access to those machines. He stated that was the vein that was still working.

UPDATE ON DATA POLICY INPUT FROM SCIENCE ADVISORY COMMITTEES

Laura Biven, *Senior Science and Technology Advisor, Office of Office, Office of the Deputy Director for Science Programs*

- Thanked the committee for their report on the dissemination of the results of federally-funded research. Noted that it was one of six reports commissioned from the six advisory committees.
- Advised that she would like to say how they would use those reports and what the next steps would be. Noted that first she would advise what the motivation was to begin with. Advised that the motivation for the charge came from the COMPETES Act of 2010. Noted that from the Act the Office of Science would be called upon to participate in conversations at the inter-agency level on the accessibility to the results of federally-funded research. Advised that it called for setting up an NSTC (National Science Technology Council) sub-committee on the topic.
- Noted that they saw the need to obtain information from their programs before they could participate in those discussions. Stated that they gave a charge that was focused in terms of the scope because of time constraints. Noted the same charge was given to all six committees.
- Advised that the COMPETES Act 2010 called for the formation of two sub-committees and the second one would deal with public access to publications and that working group had met. Advised that there was also another working group on the accessibility of digital data which had not yet met.
- Advised that there were conversations going on at the inter-agency level on digital data on a broader level. Stated that it was motivated by the challenges they were facing in terms of the

volume and complexity of data being generated, the opportunities that were coming from new tools being developed and the sense that they could obtain more value out of the data being generated. Advised that there was a component there about the federal responsibility to steward that data.

- Advised that the OS was using the reports in a number of ways, to inform the conversations in inter-agency groups but they have also set up an internal OS working group on digital data and this group was looking at the reports.

- Stated that she could not at this time provide all details about the next steps but stated they were looking at both the policy side and the research activity side. Said that they were considering how to respond to the reports in the best way.

- Stated that there were common findings across all the reports and one of them was the sense that public accessibility to the results of federally-funded research would be costly both in terms of dollars and time. Noted that they understood that there would be a need to prioritize. Stated also that there was a sense that each community was unique and no one solution fits all.

- Stated that this was an update and advised that the reports had been extremely useful.

COMMITTEE DISCUSSION

Dr. Giles said that two ideas had come which were a common theme and these were that their committee as a whole had a lot of ideas regarding the subject. He also noted that they wanted to be careful that whatever policies emerged did not get too far ahead of the practices in technology. He thought that there were elements of the areas, technology and data that were evolving rapidly and one did not want to create a policy that was not aligned with what was possible. He stated there was concern that there might be a policy that overly constrained the technical possibilities. Ms. Biven stated that they understood that there was a lot of talent and expertise in the group and they intended to tap it. She also noted that they appreciated their concerns with regard to the second point.

Dr. Dongarra asked if they would have the opportunity to see a comparison of the all the reports. Ms. Biven advised yes and all but one were on their OS website. She stated they were listed under each program, but they were there. Dr. Dongarra asked if there was more of a summary. Ms. said that she could mention some of the common issues and one was of the cost issue for public accessibility and time. She said that the departments did not want to have an unfunded mandate or they would not be subject to too many requirements. Public accessibility was not usually science-driven. She said that looking at data both raw and analyzed data, the raw data was harder to make accessible to the public. She said that there was evidence showing that their user facilities were becoming data centers by default, and perhaps this could be dealt with in a more strategic way.

BREAK

The Advanced Scientific Computing Advisory Committee recessed for a 15 minute break.

APPLIED & COMPUTATIONAL MATHEMATICS: CHALLENGES FOR THE DESIGN AND CONTROL OF DYNAMIC ENERGY SYSTEMS

Dr. Michael McQuade, *Senor Vice President of United Technologies Corporation*

- Noted that United Technologies Corporation was involved in the area before the current leadership at the DOE. Provided a quote from Secretary Steven Chu from March 2009: "We need to do more transformational research at DOE including computer design tools for commercial and residential buildings that enable reductions in energy consumption of up to 80 percent with investments that will pay for themselves in less than 10 years."

- Advised that UTC was the largest provider of building infrastructure in the world so for example with elevators, air conditioning, security systems etc. Noted that with regard to the quote 10 years was not acceptable in today's market and stated that five years or less would be acceptable today.

- Stated that there were substantial areas for improvement in buildings for energy efficiency and he noted that there was reason to want to focus on the topic which was amenable to high performance computing and the relevant computational mathematical structure that went along with it.

- Advised that the thing he would like them to take away from the presentation was that buildings were important to reducing energy consumption and energy-efficient buildings could be done. Said that they could be done with a lot of time, effort, custom work and the challenges associated with accomplishing that at a single building level. Added that the challenge of making that deployable were challenges that would speak to fundamental issues in computational science, control science, dynamics and computational methodology.

- Stated that system integration was difficult with buildings where there were multiple components and that to make them energy efficient and to have them interact in ways that they did not before. In addition these were dynamical systems that interact with one another, and how they are tuned and change over time, so it was an uncertain atmosphere in terms of the aging of the building, the utilization path and the external environment.

- Advised that combining passive and active components was difficult with complicated multi-scale dynamics that could change significantly with weather, occupancy and use patterns.

- Stated that there were productive topics that were investable for research in mathematics and computational sciences. He noted several:

- The characterization of dynamics and uncertainty, quantification and robustness management in the way they would manage complex systems.
- It was a control problem, a complex, dynamic control problem and one that changes dramatically over time and how they would look at a generation of reduced order models and how they would look at the generation of control structures that could be managed and monitored in real time.
- Simulation enabled design and operations with the ability to use models for design, installation and commissioning, prognostics and diagnostics throughout the building lifecycle.

- Stated that buildings mattered and buildings were approximately 40 percent of the total energy consumed in the United States. Stated that if we were to reduce the energy consumption in buildings in the United States by 10 percent that would be equivalent to all the renewable resources that they have been deployed in the United States other than large scale hydro electric. Stated that it was about 70 percent of the electricity in the United States and about 50% of carbon emissions.

- Referred to a graph and stated if you added the building section and the building relevant section of the power industry what the model would tell you was that if buildings were going to do their part between 2005 and 2050 the energy consumption in the building had to reduce by about 70 percent, which was about half of what buildings consumed now.

- Referred to the graph concerning the amount that needed to be spent on average every year incrementally to what was spent in the building industry now to make buildings more energy efficient, to achieve that 70 percent goal by 2050. Noted that the three bars represented different payback periods. Reviewed each annual investment needed to reduce energy consumption in buildings, giving three examples.

- Detailed two low energy buildings, the LEED design in New Orleans, LA that achieved 20-50 percent energy reduction and the Deutsche Post in Bonn, Germany with a 50 percent reduction. Provided building characteristics for each and stated both were boutique-designed buildings. Detailed two buildings where energy reduction was not achieved.

- Described buildings that did not achieve their efficiency potential and the reasons. Noted three challenges that would prevent them from making buildings as efficient as possible. Stated that at the present time they did not have the deployable scalable tools to provide for the architecture and design community to allow them to fully explore buildings. Stated that we would build buildings but tended not to construct them as designed. Stated that the third issue was how buildings matured and were managed over time.

- Asked what was needed by the industry and what technology needed to deliver in the area of predictive computation. Stated the first was scalability and noted that they could design low-

energy buildings and they would take months and they were usually one-off. Said what was needed was to be able to do this in a matter of days on desktop hardware. Stated that secondly they needed to be able to commission buildings in a week which was an improvement of about 10X from the current position. Stated the third issue was the quality of the simulation modeling and predictive control. Said that currently they achieved approximately 30 percent accuracy in estimating energy flows but needed 5 percent accuracy with quantification of uncertainty and connection to commissioning and controls.

- Stated that there was much work going on in the DOE and the Department of Defense (DoD) but the work was in the middle of the TRL (Technology Readiness Level) range. Noted there were some good work and one example was the Energy Hub in Philadelphia. Noted that DoD could play a major role with about 300,000 buildings that they managed. Stated if they were managed in an intelligent way, helping to do energy optimization would be an opportunity.

- Advised that approximately a year ago there was a community meeting with people from national laboratories, industries, academic institutions to review the subject of investments in computation and mathematics for buildings. Noted that they had copies of the report available.

- Discussed integration-enabled high performance buildings and considered the challenges. Detailed in graphs all the systems that would be in buildings today. Noted that the challenge was in looking at optimizing those buildings and was the fact that to make buildings much higher performance than before you would have to have the systems interact in more complex ways. Noted that many building systems operated on completely different time frames, so differences of scale so the challenge was taking those systems and making them interact and coupling in ways that had not been done before. One system he discussed was lighting.

- Stated that they would need progress on underlying physics to understand how energy flowed in those buildings and particularly how that energy flowed in an environment where there would be significant uncertainty in the calculations and in the parameters that were used for the optimization.

- Discussed complexity in building systems where multiple dynamic systems would be operating under different timescales. Discussed computational barriers and industry metrics giving several examples.

- Discussed work done on uncertainty and optimization: progress and gaps and gave specific examples.

- Discussed computational science research needs under three areas, multi-scale dynamics and uncertainty, controls and modeling. Provided details under each area.

- Discussed a roadmap for the development of computer tools for design, optimization and control of energy efficient buildings. Stated that they had a need in early TRL levels, in the basic

science and math that would need to be constructed as they move forward to make the necessary difference in buildings that has been discussed.

- Recommended next steps and stated that it was a topic that would be amenable to a workshop that ASCR does. Noted that it would be their recommendation if ASCR was willing to commission that workshop in the fall of 2011 and bring together the academic, industrial, high performance and computation and math communities. Suggested that they determine the thematic areas, generate the metrics and identify the participants.

COMMITTEE DISCUSSION

Dr. Graham asked about one of his slides; hours to days on desktop hardware. She asked if he meant that the designer or the engineer needed access from a desktop or did he mean that the whole computation had to run on a desktop machine. Dr. McQuade said he did not know the answer to that. He said that whether they needed to run it on their machine and have access to it. It had to be on a cost scale that one would have at a desktop.

Dr. Graham asked about the control part, that the consequences of the kinds of designs that people were coming up with was that the control of the building as it was inhabited was getting more complex as well. She asked if the computational demands were very large or was it just the complexity of getting that control. Dr. McQuade said it was both. He said there was an opportunity to do the kind of controls that they did now much more computationally, effectively. He thought the bigger issue was the first one which was that the highly energy efficient buildings were substantially more complex so the coupling of systems would raise the computational demand higher and the step of connecting the early-stage modeling and understanding of how the building could and should perform in various configurations. Dr. Graham asked if they were treating each building independently so how important was it that buildings would be adjacent to one another. Dr. McQuade discussed how buildings interact with one another.

Dr. Hey asked whether the DOE had developed energy-plus which was integrated modules and was it widely used. Dr. McQuade stated that energy-plus was a very widely used and highly supported code. He noted that it had one major problem in that it was not fundamentally about managing dynamic uncertainty. He stated it was a static modeling code.

Dr. Marsha Berger discussed an energy efficient building she knew in which people did not want to work there due to limitations such as the number of monitors or the fact it was all open, no individual offices. She asked would that be an isolated case or a typical problem. Dr. McQuade stated that there were many energy-efficient buildings where things had been done incorrectly. He stated there was a period in the 70s where they made homes so sealed that they lost how you would manage air quality in a home. He said he would turn it into less an issue of whether he would be concerned about it than to say it would be exactly the kind of usage uncertainty and usage real-time management that would have to go into the way you would operate a building.

Dr. Giles asked about modern buildings today and asked what fraction of the expenditure was used on computing either for design or operation of the buildings. Dr. McQuade stated it was a very small part of the calculation although he noted that for the premier design shops one could spend 5 percent on computational resources and this was not an uncommon number.

DEVELOPMENTS IN HIGH PERFORMANCE COMPUTING IN CHINA

Dona Crawford, *Associate Director, Computation, Lawrence Livermore National Laboratory*

- Stated that she went to China to ascertain the current state of China's supercomputing capability and the application of high-performance computing to R&D and to explore China's drive to develop clean energy technologies.
- Reviewed the group of people that went on the trip. Confirmed that Dr. David Kahaner, who is the director of the Asian Technology Information Program (ATIP) assisted her in the planning of the trip.
- Advised that the trip ran from June 27th to July 1, 2011. Stated that there was not a lot of time to delve deeply into topics due to time constraints. Hoped that the trip could have been more comprehensive.
- Stated that they visited four computing centers and two computing institutes, several universities and energy companies. Added they also visited the Ministry of Science and Technology and the Chinese Academy.
- Noted that a symbol on a slide represented the 90th anniversary of the Communist Party in China. Stated that there was a lot of media coverage and news.
- Showed the sites of their visits on a map of China. Stated that she had put Changsha on the map because last November they announced the new national supercomputing center. Noted that the specs for the center were 30,000 square meters. Stated that it was going to be 6.7 times the size of her computing facility at LLNL.
- Stated that China had a staggering rate of growth in S&T infrastructure build-out including HPC and research facilities. Noted it was discussed in terms of five-year plans. Noted there was an aggressive campaign to recruit back to China so their staff was trained in the United States and Europe. Said the average age was the early 30s. Stated that they had an aggressive campaign for indigenous technology development. Advised their own technology was cheaper and a national security priority. Said that they were looking at board-based balanced HPC approach at hardware, software, applications and industrial use.
- Stated that in the United States they were pushing HPC out to American industries and they saw that a lot in China.

- Noted that as at June 2011 with the top 500 list there were 61 systems on the list. Stated that in June of 2001 there were no Chinese systems on the list. Listed the top six on the Chinese Top 100. Stated that it ranged from a peak of 4.7 petaflops to 2.6 petaflops and all the way down to a 100 teraflop machine.

- Detailed three domestic HPC Systems as follows:

  - #2 system Tianhe-1A uses Intel, nVIDIA, plus 2048 Chinese FeiTeng processors (open SPARC based) Chinese developed interconnect and Kylin OS, located in Tianjin.

  - #4 system Dawning Nebulae uses Intel, nVIDIA. Dawning 6000 (2011) not yet ranked will enlarge Nebulae and initially use 3000 Chinese Godson/Loongson processors (open MIPS based) in new center in Shenzhen.

  - Sunway system @ Shandong SC Center (Jinan City). Uses Chinese HW (Alpha-enhanced ShenWei processor, Infiniband-like interconnect); being tested (1.1 PFlop peak, 738 TFlop Linpack) [$100 M (1/3 MOST, 2/3 Shandong Prov govt)]; home of Inspur, host of HPC China 2011.

- Gave details of name of group in day one in Beijing with members of the Ministry of Science and Technology (MOST). Mentioned Mr. Chaochen Li who is the Director General of MOST and noted that he was coming to the Chinese Embassy as the minister's counselor for science and technology. Stated that he was very much interested in collaborations. Explained that MOST was the policy body and can make things happen as it has funds.

- Described the visit to the Chinese Academy of Science (CAS) . Compared it to the American National Academy of Sciences except that it had an affiliated university and had graduated 43,000 students over the past several years. Founded in 1949 and had institutes and field sites all over China. Known as the nation's supreme scientific advisory board. Noted that Yutong Li brought a Chinese Academy delegation to visit LLNL in July to visit NIF (National Ignition Facility) and talk about fusion energy.

- Visited the Institute of Computing Technology (ICT) of the CAS. Noted that Mr. Zhiwei Xu had a master's degree from Purdue University and his PhD from USC and he is the CTO of ICT where all the indigenous technology is developed.

- Provided details of ongoing technology for ICT:

  - Working on indigenous technology for Godson (Loongson) microprocessors; Dawning HPC servers; Blue-Whale file system and storage; and Vega Ling Cloud software.

  - Collaborating with the Europeans: EC 6th and 7th frameworks; OS, Many core architectures, Semantic Web; New: European Commission Future Emerging Technologies (FET) Flagships.

  - New Challenges; complexity in time, space, effort, energy, sensors dictate review of full HW/SW stack for 2015 (and beyond) computing systems.

- Detailed new challenges and tests with description and examples, that the ICT was looking into from an ICT presentation slide:
  - Ranking low-carbon households in big cities automatically.
  - Using IT assets via Universal Compute Account (UCA).
  - Increasing datacenters efficiency by orders of magnitude.
  - Facilitating mass creations of value net services.
  - Enabling science-based macro information policies.
- Visited the Institute of Process Engineering (IPE) and noted that they were interested in flow and transport of substances under physical or chemical conversion.
- Visited the Institute of Process Engineering (IPE) and noted that they have a #3 on China's Top 100 computers. Noted it was one of the least efficient in terms of Limpac machines. Stated it was a 2 CPU 12GPU board. Described some of the multi-scale simulations of complex, multi-phase systems and industrial applications. Described some of the experiment processes done there.
- Visited the Computer Network Information Center (CNIC) a Supercomputing Center, in Beijing. Stated that they have their big machine under the Lenovos and stated that under the 10th and 11th five-year plan they got five and then 150 teraflop machines.
- Described the CNGrid (Chinese-Nordic) and noted they have over 1400 users.
- Described the CAS Supercomputing Center. Stated they had the #5 computer which had over 200 users. Described the current system and future updates. Described the list of commercial software, Open Source Software and self developed software available to the users.
- Visited the College of Engineering (COE), Peking University. Noted that Peking University had about 30,000 students and was founded in 1898. Stated that all of the faculty except one was trained in the United States. Asked how many American students they had at their university and was told that American students were not academically qualified to come to their university.
- Visited Tsinghua University in Beijing which had a more receptive feel with regard to collaborations. Provided some statistics for their students showing a high amount of exchange. Noted it was established in 1911. Visited some of the energy departments and noted that they

had a small 10 MW pilot plant for nuclear energy and described other energy projects. Noted that it cost much less to set up power plants there compared to the United States.

- Visited Tianjin Supercomputing Center with the #1 computer on China's Top 100. Described the specs for the computer. Visited the GreenGen IGCC Power Plant and noted they began construction in 2009 and it should be completed by the end of 2011.

- Visited Shanghai and the GE China Research Center. Noted that GE was a multi-national company with research centers all around the world. Noted that 60 percent of the research is funded out of direct contract work in China, 30 percent from the CEO of GE and the balance of 10 percent from the U.S. government.

- Described the 12th five-year plan which is 2011 to 2015 and focused on consumption and growth, urbanization, low carbon emissions and solving the shortage of basic goods. Noted that with regard to urbanization currently 80 percent of the people lived in the rural areas and 20 percent in cities. Noted that their goal was to make it 50/50. Noted that to accomplish the four goals they had seven research areas.

- Visited the Shanghai Supercomputing Center which is also on the CNGrid. Noted that their computer is #4 on China's Top 100. Stated that they had the Doubling Scheme and were focused on scientific research, industrial applications, engineering and consulting. Described the R&D going on at the center.

- Visited Shenzhen and the Shenzhen Institute of Advanced Technology (SIAT). Noted that it was a fishing village but in the last ten years had grown to 14 million people. Noted that SIAT was founded in February 2006 with five employees and today it had 1200 employees. Stated their goal was to have 4500 employees by 2015. Described information about the institute and patents. Stated that their computer is #2 on China's Top 100. Noted that they are focused on industry and on data management.

- Described the issue of exaflops in China and discussed certain areas such as: lessons China had learned over the past few years; China's current knowledge and how they view technology, research and working with other countries; and their steps forward. Stated that the information was courtesy of ATIP.

- Stated that she still considered the leader in HPC but she thought the United States needed to vigorously maintain that leadership. Stated that the development of exascale was part of that. Said that she thought collaboration was important where possible and compete where necessary.

COMMITTEE DISCUSSION

Dr. Giles asked if there was any chance that indigenous Chinese technology would come to the United States for them to study. Ms. Crawford responded that she had asked if they could buy some of their hardware and could she get access to some of their "Open Source Software" and they replied yes. She added that she now had to look into the process.

Dr. Chen asked if she got a sense of what their big application areas would be for the large machines. Ms. Crawford responded that the biggest application was energy across the board and entertainment.

Dr. Tang noted that when he went to a meeting co-sponsored by NSF and the Chinese Academy there was an emphasis on visualization. He thought some of their work was impressive with 3D visualization of traffic patterns and he thought looking into those methodologies could be useful. He thought more collaboration should be encouraged.

Dr. Hey asked whether she had looked at the BGI in Shenzhen. She responded that they did go to BGI and noted that they had their own computing center because they had so much data. She said it used to be the Beijing Genomics Institute but because they are now in Shenzhen they go by BGI to avoid confusion. She said it was a short meeting with both sides presenting.

Dr. Dongarra asked about how much the investment was in terms of software and algorithms. She replied that there was no discussion of money. She noted that they were making large software investments, low-level software large application investments and large hardware investments.

ADJOURNMENT

The Advanced Scientific Computing Advisory Committee adjourned for the day at 5:30 p.m. The committee will reconvene tomorrow, Wednesday, August 24, 2011 at 8:30 a.m.

WEDNESDAY AUGUST 24, 2011

UPDATE ON EXASCALE RESEARCH

Dr. William Harrod, *ASCR*

- Stated that he would be discussing three recent workshops held. Stated that he would be touching on some current programs and would also discuss anticipated future programs they would like to fund. Stated that he would also touch on upcoming workshops
- Stated that there were four efforts underway now started over a year ago as follows:
    - Advanced Architectures and Critical Technologies for Exascale.
    - R&E prototypes

  - X-Stack Software Research, looking at systems software and the programming environment.
  - Scientific Data Management and Analysis at Extreme Scale – stated that this was one of the biggest problems, the volume of data and the data movement within the system.

- Mentioned the Co-Design Centers which he confirmed were discussed by Dr. Germann the day before. Included the issue as he felt that would play central role in the future exascale effort.
- Noted that in all discussions with teams undertaking architectural system software design he advised they would want to know the applications, what the driving applications would be.
- Stated previously there were three workshops as follows:
  - Programming Challenges Workshop held July 27-29, 2011. The workshop goal was to understand, prioritize and shape the future research agenda that addressed challenges for programming exascale systems.
  - Architectures 1, Exascale and Beyond Gaps in Research, Gaps in our Thinking held August 2-3, 2011 at Stanford University. The goal was to discuss and explore the lessons learned from exascale projects and develop reverse timeline for accepting the exascale system in 2020.
  - Architectures II, Exascale and Beyond Configuring, Reasoning, Scaling held August 8-11, 2011 at Sandia National Laboratories. The goal was to investigate how we design computers so future exascale computers enable DOE critical applications.
- Discussed the first workshop, Programming Challenges Workshop. Stated that the idea was to take a look at what changes would need to be made as the systems were changing and there was the issue raised of driving the voltage down which caused an explosion of concurrency. Stated that there would be a switch from bulk-synchronous computing to synchronous fine grain computing which would mean the models had to change.
- Provided some highlights from the workshops. Stated that all of the presentations are online but he would be touching on some of the interesting points. Added that they were working on final reports for all the workshops. Detailed some of the presenters:
  - Keshav Pingali (U Texas) does a lot of interesting work in large irregular data sets and graph theory and with parallelization of algorithms. Some of the issues he was discussing are automatic parallelization has basically failed and a further explanation was given. He also thought that success required multiple levels of programmers in the exascale environment.
  - Richard Lethin (Reservoir Lab) focused on code complexity as systems were becoming more complex.

  - Vivek Sarkar (Rice) discussed the constructs required to bridge the gap between the low-level interfaces to a higher level of extraction and a further explanation was given. Discussed issues of tasking and point to point communications.

  - Kathy Yelick (LBNL) discussed the issues of processors and memory locality. How would one write codes so you could move between two platforms and not have it tied to a particular architecture? Considered the approach was good because you would be abstracting the system and allowing the programmer to focus on their goal.

- Discussed the conclusions from the workshop but added that the reports were still outstanding. Stated some of the conclusions included: multiple levels of program and programmers; performance portability is a requirement; domain specific languages (DSL) constructs would hide code complexity; new mechanisms; and runtime support and control.

- Discussed the second workshop Architecture 1. Stated the idea behind it was that within the government a number of exascale reports were completed one to two years ago. Noted that research directions were proposed and teams followed up with that research. Stated that the question was what did they learn? Stated that people were funded to do something and it was considered important to take the time to ascertain what was learned. Advised that 40 people took part with vendors and laboratories also there. Stated that they attempted to do a reverse timeline which was a process where they would establish a delivery date of 2020 for an exascale computer and then work backwards identifying each step so that delivery date would happen. Commented that this was an excellent discussion.

- Detailed some highlights of the Architectures 1 Workshop:

  - Bill Dally (Stanford & nVIDIA) stated he was the premier computer architect in the United States today. He thought that historic scaling had stopped. He stated that it was not about flops but it is about data movement and people need to change the way they think. They discussed legacy codes. He thought there was a need for a research vehicle to do experimentation toward exascale computing.

  - Shekhar Borkar (Intel) provided a detailed research plan and discussed gaps in research.

  - Keren Bergman – noted she was an expert in optics. Discussed a need to focus on packaging issues and also the integration of photonics and CMOS.

  - Dave Resnick noted he was a former Cray employee and went to Micron and is now at Sandia Laboratories. Gave a talk on Micron's plans for a 3D stack memory.

- Discussed the Architectures I Workshop conclusions. Stated that energy efficiency was both a static and dynamic concern. Noted that programmability needed to be clarified and extended and that resilience would ultimately limit the system utilization.

- Discussed Architecture II and stated that they were rethinking how computers would be designed and would use abstract machine models or an abstract design of the architecture but also picking some parameters and simulating what it would be.

- Detailed some presentation highlights:

  - Rich Lethin (Reservoir Lab) had experience with abstract machine models and he concluded that it was a doable approach.

  - Marc Snir (UIUC) emphasized the issue of operation counting. Discussed issues of energy consumption due to communication and data locality. He feels the software stack itself needs to be engaged in this.

  - Dan Campbell (GTech) talked about his experiences. His involvement had been in an effort that was doing a high-level compiler that was reconfigurable for different processor types.

  - Arun Rodrigues (SNL) has done work with simulators and modeling tools and dealt with the idea of an abstract machine model and simulations.

- Discussed Architecture II Conclusions and stated that: abstract machines are critical to the future; the timeline for exascale research was extremely short; abstract machines needed to be backed by modeling, simulation and emulation; and there was a good mixing of ideas. Stated that the workshops were a good start.

- Discussed some future programs and noted that they had plans for some solicitations on programming models, languages, compilers and tools; X-stack; exascale architectures; and extreme scale solver algorithms.

- Detailed information on upcoming workshops and principal investigator meetings from October 2011 to April 2012.

COMMITTEE DISCUSSION

Dr. Graham asked about the discussion of the first workshop and noted that the summary seemed to be all about language and not about tools. She asked whether there was a discussion of tools. Dr. Harrod stated she was correct in this assessment. The solicitation they plan to release will have a heavy emphasis on tools. His guess is that they are ready to start talking about tools. She stated her suggestion was that he should start to think about it in concert with the language decisions that might be made. He responded that he didn't dispute that, they just hadn't taken the step yet.

Dr. Hey asked about Architecture I. He said besides the design of the nodes they also had a software track going on and he remembered a talk given by Rob Ross about an exascale software center and the co-design and applications. He said he did not understand how they all fit together. Dr. Harrod responded that the exascale software center is not being funded, and he wouldn't know what the plan

was for this until later. Dr. Hey sought clarification that the exascale software center presented in November wasn't funded. Dr. Hey stated that this was correct.

Dr. Chen asked about Bill Dally's comment about a research vehicle to tie together various elements of the exascale computing. She asked what he meant by that. Dr. Harrod responded and said he was guessing he was referencing where they were going to pull together a simulation environment where they could do co development.

Dr. Dongarra noted that the office had a long tradition of funding mathematical and systems software at a research level but also has had the ability to take the research and put it into production software. He asked what would be done in the exascale plan to ensure that the research that would be funded could transition to production-quality software. Dr. Harrod responded that they needed to make sure that they funded the production effort, however they couldn't answer completely since the final plan wasn't available. Dr. Dongarra asked if he would fund the research as well as the development of production software. Dr. Harrod responded that if they were investing in some software required for exascale, they had better fund the development of production work, otherwise they wouldn't be able to use that system.

Dr. Tang noted that he had heard some of Bill Dally's presentations. He asked if Bill Dally had given any examples of a new generation low memory type core codes that had been developed along those lines and to what extent the codes had been verified. He asked if he had given a specific example of employing these in the application domain. Dr. Harrod responded that he wasn't sure that Bill Dally looks at low memory per core. Dr. Tang again asked for some evidence of employment that verified Bill Dally's arguments. Dr. Harrod responded that he hadn't looked into it, and that Bill Dally was more focused on the design not on application.

Dr. Chapman asked about the experimental system indicated in the presentation scheduled for 2015. Had they any discussion of how developers would prepare for this? Dr. Harrod responded that these developers would be working with DOE co-design centers, and this would resolve this issue, bar the proprietary processers. If these parties were research groups, they would be more open.

Dr. Dongarra asked about the workshops, and how does one get invited to these? Dr. Harrod stated that the participants, by and large, were selected by the organizing committee. They want to keep the participant number low, and broadly cover the DOE space. Larger groups become a huge problem as far as he is concerned, and this is a hard problem.

Dr. Giles asked about the development of exascale and wondered if new technical innovations or ideas occurred if there was a mechanism that it would be possible to incorporate these new ideas into the planning and take advantage of them. Dr. Harrod said yes and stated they had just released the R5 for Critical Technology and that had received a lot of attention. If anyone thought they had a great idea that would be one avenue. He added there was a strong focus on small business. He said they were not easy problems.

FUNDAMENTAL PROBLEMS OF WIND ENERGY AND THE POTENTIAL TO ADDRESS THEM THROUGH HIGH-PERFORMANCE COMPUTING

Dr. Chris Hart, EERE (Energy Efficiency & Renewable Energy)

- Explained how the topic of offshore wind became a topic for discussion. Noted that in November 2010 he met with Secretary Chu's office discussing their plan for an offshore wind initiative at DOE and that discussion eventually led to the release of a national offshore wind strategy in February. Stated that one of the things that Secretary Chu asked was if there was an opportunity for bringing high performance computing assets into solving some of the challenges that offshore wind faced. The answer was yes and since that time they have explored several possibilities. Stated that this was some of the information that they would go through today.

- Noted the first two topics would be wind technology evolution and deployment and wind resource and potential contribution to the U.S. energy demand. Stated that the main discussion would revolve around future technology challenges in achieving high penetration and then the last point detailing the HPC needs and opportunities in wind energy.

- Discussed the changes in design of land and offshore turbines from the 1980s to 2000 and beyond. Noted that offshore turbines were supported by more expensive bases. Noted that offshore turbines got larger and one of the things that would happen because of that growth would be changes in material capabilities. Stated that another was as the blades got longer (164 meters in diameter) the blades tended to behave differently and this was not well understood. Stated that this was an example where increased computational capability could be brought to bear. Detailed some areas and issues concerning the blades that had to be better understood.

- Some of the issues that were discussed included wind resource assessment with regard to geographical location. Stated that 80 percent of the domestic load was within 150 miles of the coast and the Great Lakes. Discussed total wind resource potential for land-based wind and shallow and deep water. Detailed future technology challenges to achieving high penetration and how would it affect climate. Noted that there were several federal agencies engaged and participating.

- Showed a diagram with computational modeling scales and noted that it illustrated how HPC would be very helpful in calculating climate effects, mesoscale processes and micro-siting and array.

- Discussed four sub-sets, turbine modeling challenges, offshore wind system modeling, offshore system modeling and weather modeling. Detailed each area with several areas for each.

- Discussed improved physics for wind prediction. Stated that HPC had three ways of solving this problem, global high-resolution model, global variable-resolution model and nested regional climate model.

- Discussed atmospheric measurement and HPC code validation. New technologies included Doppler volumetric scanning remote sensing, computer-controlled coordinated scanning and computational and storage capacity to support sophisticated wind field retrieval algorithms.
- Discussed the complexity of multi-array wakes and focused on deployment and technology performance. Noted how turbines affected one another with regard to placement.
- Reviewed wind farm simulation capability and loads driven by turbulence.
- Detailed wind energy fundamental science issues requiring HPC. Noted HPC code development for predictive, rational design and operation supporting high penetration wind energy:
    - Wind & solar resource assessment as a strategic national energy resource.
    - Weather driven energy forecast models – coupled wind and solar.
    - Quantify potential effects of high penetration scenarios.
    - Characterize inflow and outflow resource.
    - Coupled physics models inflow/wind plant international/grid response.
    - Establish the design criteria for future turbine and plant innovation.
- Noted wind plant scientific questions requiring HPC:
    - Turbine scale dynamics.
    - Wind plant performance and array effects.
    - Mesoscale processes and weather monitoring.
    - Regional impacts.
- Advised that potential follow-on collaborations would include collaborative workshops, internal working groups and future joint FOA solicitations.

COMMITTEE DISCUSSION

Dr. Graham mentioned that he had given them some idea of where the U.S. currently stood with deployment compared to other countries. She asked if he could do the same thing for modeling. Dr. Hart responded that he thought the use of HPC was an opportunity for the U.S. to take the lead. Other staff members elaborated on its complexity. He stated this was not just a domestic opportunity, but a chance to bring together the international community. No one had the resources to attack this with HPC, so this was an opportunity.

A member followed up asking which scales are of critical importance for design issues, would these be boundary layer/phase change simulations, or were higher order details about where the wind is more important on a longer scale. The response was that this was a large multiscale problem, where larger scales greatly affect the smaller scales. The boundary conditions which control the flow, along with small scale flow, and historically they haven't been able to reflect this, and instead they have used approximations which still resonate in simulations. HPC would greatly assist with this. In addition, the vision is now for much large scale deployment and within this context they have no way of measuring the effect on the resource at present due to the deficiencies of current modeling. Dr. Berger also said that matching demand with supply was another area where HPC modeling would assist, moving to a stable grid on a far more grand scale.

Dr. Berger stated it was quite a grand challenge problem, the turbulent flow, the moving geometry and once you have been able to simulate one of them she stated that she assumed they would want to optimize the placement of the rest of them. She asked who was doing the modeling now. She asked if they were bringing in some expertise. A staff member elaborated and said that the machines were there and working but they wanted to take it to the next level using state of the art computation capability and they wanted to elevate that conversation. Dr. Berger said they had talked about workshops where they would bring in people from other domains. They responded that they started that back in 2007 and it had since involved other people from different areas of government.

Dr. Tang asked if they had a physics model on hand or were they waiting for the computational firepower to get them to the next level. He also asked if the physics model was sufficiently important with the HPC implementation to affect the quality of their validation verification and certainty quantification. Staff members responded that as they move to smaller scales with higher resolutions, the basic understanding is there, but how they represent this highly non linear process on a small scale was far less clear. Staff responded that the gaps in the physics were significant, because they accept current wind modeling errors as negligible on the large scale, but on the wind producing scale, these errors become very significant.

Dr. Petzold asked to what extent these arrays could be instrumented with sensors. Staff responded that conventional sensors are in situ, but when trying to capture the spatial variability of a field, they need to be able to sample the field, not simply locations. There have been some advances in remote sensing recently, but they are just beginning to get to the point where multiple remote sensing systems can be coordinated with retrieval algorithms over short periods of time. This represents an intriguing opportunity to simulate local flows better, as well as validating that simulation in the real world. Dr. Petzold asked to what extent they could implement active controllers. Staff responded by bringing up the wind farm active controls in response to boundary conditions to optimize things, which can go down to an individual turbine level.

BREAK

The Advanced Scientific Computing Advisory Committee recessed for a 10 minute break.

EARLY CAREER-SEPARATING ALGORITHM AND IMPLEMENTATION VIA PROGRAMMING MODEL INJECTION (SAIMI)

Michelle Mills Strout, *Colorado State University*

- Stated that she was going to be discussing program models and the problem from the perspective of a compiler was that scientific simulations needed to run faster. Noted that developers tend to modify their codes, fine tune them by hand for performance. Stated that after hand-tuning the algorithm and implementation details become tangled and that made the code difficult to force and maintain.

- Gave an example on a slide of matrix-matrix multiply and described in detail. Stated to get the performance that they wanted they were writing programs that would be difficult to maintain. Described the difficulties of writing fast code. Provided another example of hand-tuning (tiling). Discussed orthogonal loop scheduling using Chapel.

- Stated that in the SAIMI project they were focused on staying with the programming languages that the applications were written in and then using pragmas to inject implementation details into the programs. Stated they were focusing on three injectable programming models. Stated that to evaluate their approach they were showing how the approach could be used within the context of DOE applications.

- Provided details on how specifying implementation details orthogonally could be used with tools. Discussed certain headings: Source to Source compilation tool; algorithm specification an implementation details. Described SAIMI project focus with Mesa and IEGen.

- Described the key components in the SAIMI project including the Mesa transformation, sparse polyhedral Framework (SPF) and an evaluation within the context of applications relevant to DOE.

- Gave some examples of using Mesa and Lookup tables for expressions as an injectable programming model. Explained how rather doing a lookup table manually you could generate a code that created the lookup table itself. Discussed in further detail an approach used in Mesa.

- Discussed key SAIMI components and sparse matrix computations. Noted that the kinds of codes they were looking at were iterative codes, iterating either over a mesh or a sparse matrix. Explained and illustrated parallelizing iterative sparse matrix computations and showing full sparse tiled iteration space and a task graph. Explained in descriptive detail.

- Showed experimental results for blue ice and explained the graph results.

- Explained the sparse polyhedral framework: an injectable programming model and showed the specifying sparse computations and specifying transformations like full sparse tiling.

- Noted that they were evaluating the ideas within the context of applications relevant to the DOE. Detailed how they would be evaluating the research. Noted they would evaluate programmer control and performance. Stated the three applications they would be working with include: SAXS: small angle x-ray scattering; CGPOP: miniapp for parallel ocean program; and matrix powers kernel: (CACHE project related). Described each of these applications in detail.

- Noted the following conclusions:

  - Scientific computing needs detangling of simulation codes.

  - Complete rewrites are not feasible so gradual approaches need to be developed.

  - Pragmas already have buy-in and can be used to orthogonally specify implementation details with minimal tangling.

  - The concept of SAIMI should direct future programming model development.

- Reviewed the SAIMI crew and special research areas.

COMMITTEE DISCUSSION

Dr. Chapman asked about the mini applications and noted that it was difficult to evaluate ideas with something that was realistic. She asked her how much better she thought they were than the benchmarks that had been traditionally used in the field. Ms. Mills Strout noted that they had started comparing the performance results of this mini app to things like the NAS Parallel Benchmarks and the scaling properties of NAS CG was very different than the full application.

Dr. Giles asked an abstract question. He asked if someone woke up and said all of a sudden that the most important thing to worry about was energy and communications instead of operations and programmers had some model about how implementation affected that, would some of these ideas, orthogonality and ways of approaching the interface to the higher level program still be applicable. Ms. Mills Strout responded that yes, this would still applicable; the main reason they had been rescheduling the irregular computations was that data locality has been the main goal for a long time in that research area.

UPDATE ON NETWORKING COV

Dr. Giles ascertained that there was no one on the phone and advised he would provide the update.

- Stated that originally the networking Committee of Visitors report was requested for the meeting.

- Advised that the Chair for that committee encountered a late-developing conflict of interest. Advised that a proposal call came out later than originally intended from the office and her institution submitted under that proposal in the networking area. Explained for that reason she had to recuse herself.

- Advised that they searched for a new Chair for that committee and that Chair is in place and he is Dr. Taieb Znati of the University of Pittsburgh and he is in the process of forming the committee including Ms. Victoria White and advised that they expected that the report would be on track for the next meeting. Confirmed that the OS is patient in receiving this report.

UPDATE ON ASCR RECOVERY ACT PROJECTS

Mr. Vincent Dattoria, *ASCR*

- Stated that these projects were associated with ASCR and were up to $154 million:
    - A six-core upgrade to Oak Ridge LCF machine to take the OLCF to 2 petaflops peak and which is completed. ($19.9 million)
    - Advanced networking initiative which has the components for the 100Gbps testbed and the demonstration prototype and research they had funded. ($66.8 million)
    - Advanced computer architectures, the P7 board has been delivered and has been integrated and noted if people needed to schedule time on it there is capability up on the website. ($5.2 million).
    - Magellan – the ability to evaluate clouds as it relates to mid-range high performance computing. ($32.8 million).
    - The SciDAC-e with three components: Energy Frontier Centers, the applied math research on electric grids and the post docs. ($29.2 million)
- Discussed SciDAC-e and gave some points on progress since August 2010:
    - 14 projects that they awarded in FY2010 and the interim reports were coming, due in August an there would be reviews with ASCR and BES PMs (Program Managers).
    - The applied math projects are ongoing.
    - The post docs are almost all hired and he noted that the list included 9 PDs hired at NERSC, 7PDs at OLCF and 11PDs at ALCF.
- Noted that the next thing for the two offices, ASCR and BES was to get together and reconcile their reviews on the interim reports for the EFRCs (Energy Frontier Research Centers).

- Discussed the research, "Reduced Measurement-space Dynamic State Estimation for Power Systems" completed at the University of North Carolina at Chapel Hill. Described the objectives, impact and accomplishments. Noted that there was an IEEE (Institute of Electrical & Electronic Engineers) that comes out in June that discusses this research more in depth.

- Discussed the Magellan Cloud Computing Testbed. Stated that there was a lot of outreach going on now for the project. Detailed some of the science being supported by the Magellan project include: the NP – STAR project analysis jobs, the researchers ran DNA comparisons for the German E-Coli outbreak and ANL ran a number of smaller jobs that used up to 80 percent of the cluster. Discussed how 100 Gbps testing was done in work with science communities to demonstrate 100 Gbps technologies.

- Discussed the ANI project and stated that they had contracts in place. Started they had a contract for $47 million with Internet2. Discussed the national prototype network and the national dark fiber facility. Described the deployment progress.

- Discussed the ANI testbed access is based on the merits of the research being proposed. Advised of the link for the submission process: Https://sites.google.com/a/lbl.gov/ani-testbed/

- Noted that for the proposal submission process there were two cycles a year for soliciting research open to anyone, researchers funded by DOE, other federal agencies or industry. Advised that now they had 17 active research projects spread across industry, labs and universities. Said that the next round was in October 2011. Showed the website for the existing research that was going on presently in the testbed. Noted that of the four recent selections for projects two are from industry. Reviewed some of the details of the ongoing projects.

COMMITTEE DISCUSSION

Dr. Hey asked what was the software stack being used by Magellan cloud testbed. A member of the team replied that the Magellan project was designed to experiment with multiple different software stacks, focused on how they would work for operators. They started off with the Eucalyptus stack, and migrated from that, trying various different operating systems, as well as various clusters.

Dr. Hey asked how it compared to something like Amazon web services. A member of the team replied that Amazon was a function of the Eucalyptus and operates with one stack. Magellan had higher end networking, and various other features that Amazon doesn't have. Dr. Hey asked what the cost comparison would be here. A member indicated some slides from a report on this cost comparison were available, and they would put links to the report on their website.

Dr. Giles asked about the ANI. He noted it was very quick and asked how it affected the lifecycle of that project. Mr. Dattoria stated that the project ended at the attempt to demonstrate the 100G across the end points, so between the Magellan and the other activities they were trying to do, the demonstration part of the project would end once they could actually demonstrate, or they would fail to demonstrate

the 100G throughput from the end points. He noted that there would be a bit more residual activity on the project for the research, on the testbed, the research that they selected through a peer process, the merit review as well as the research funded under the ANI project. He noted once those research projects were over then the project part would be complete. He advised the timeline would be roughly a year.

ASCR INVESTMENTS IN SMALL BUSINESS INNOVATIVE RESEARCH

Dr. Walt Polansky, *ASCR*

- Noted that he would be discussing the SBIR (Small Business Innovation Research) and STTR (Small Business Technology Transfer Research) programs and the relationship with ASCR, past, present and future.
- Noted the SBIR/STTR program had its beginning in 1982 and the P.L. (Public Law) 97-219 had four major goals. Focused on two of the goals which are: to use small business to meet federal R&D needs and to increase private sector commercialization innovations.
- Noted that initially the OS used the SBIR/STTR program funds to supplement its own program. Advised now they were rethinking that.
- Advised that the legislation called for a three phase program based on competitive solicitation, proposals subject to standard peer-review practice and budgets established were set aside from the extramural R&D appropriation. Reviewed the percentages that were set aside as per a graph.
- Noted that to take part in the SBIR/STTR game agencies had to have an extramural R&D budget of $100 million or more. Stated that how awards were made was under the jurisdiction of the Small Business Administration which was chartered to collect the data. Reviewed the amounts allocated to different federal agencies with $154 million going to the DOE and of that $105 million going to the OS (ASCR for $10 million).
- Reviewed the history of ASCR with the SBIR/STTR and stated in the early years that their engagement was to emphasize the research component of SBIR, sometimes spinning off something commercially. Reviewed the position, proposals submitted and those that received funding for years FY1996, FY2007 and FY2011. Explained how the number receiving funding improved.
- Provided information on the FY2011 ASCR Phase I Portfolio showing the range of topics.
- Discussed how they would use SBIR as a lever to get ASCR results into a broader community. Described the program's trajectory. Noted that the program was operating under a series of continuing resolutions which would expire September 30, 2011. Noted that there are current House and Senate bills. Provided a chart and focused on the topic, Venture Capital (VC)

Participation. Stated that both the House and Senate thought it was useful to have VC firms engaged directly in SBIR activities. Said that it showed the House and Senate were interested in pushing continued commercialization.

- Noted the SBIR program was managed by the OS and that the office studied the commercialization challenges by program office. Looked at the programs in terms of commercial opportunity, customer base, nonfinancial success factors and reasons for lack of private investment. Discussed the chart in detail. Noted that the OS contributed 65 percent of the funds for the department's SBIR/STTR program yet the opportunities for commercial engagement appeared slim.

- Noted the discrepancy between their investment and commercial engagement opportunities and to study this area there was a series of workshops (ASCR Workshop for Industry Software Developers). Reviewed the key findings.

- Stated that their SBIR office, program office made a major change in how the solicitations were released. Reviewed the changes including the separation of Phase I and 2 for FY2012. Discussed some areas including ASCR topics, letters of intent and proposals.

- Outlined their strategy for SBIR/STTR where they would take a systemic look at ASCR results across the board and then determine the best candidates for leveraging into the industrial base through SBIR and STTR. Noted they would look at current and future solicitation topics, engage ASCR research and facility communities, establish and maintain dialogue with industry and collaborate with the Applied Technology Program Offices on future joint solicitation topics (Wind Energy and Smart Grids).

COMMITTEE DISCUSSION

Dr. Giles asked in the longer run would there be any issue in SBIR relative to the Open Source kind of policy. He asked if there was any issue there. Dr. Polansky responded that at the current time the discussions were at the early stage at highest levels and that there was recognition of their policy and there did not appear to be a problem. He noted few of the industries that they were talking to were using open source software, it was either homegrown or they were purchasing it.

PUBLIC COMMENT

Dona Crawford, LLNL

- Stated that she would like to publicly register a concern regarding exascale.

- Stated that she thought they were in a precarious situation, funding was extremely tight and global competition was intense and the challenges to get to exascale were difficult.

- Noted that the challenges had been recognized and research activity had been started.
- Said that her concern was that they were not well coordinated and given the situation and the challenges faced it was important that they pulled together across the science communities and that the exascale community move towards producing an integrated plan which would pull together individual pieces and the players.
- Stated that she was concerned about there being a lack of focus on the end goal which is DOE mission success. Stated that they needed to tie their plan towards nuclear weapons deliverables and science deliverables, not just producing an exascale system. Stated that the exascale was an enabler to DOE mission success.
- Stated that she would like to see the community seriously consider what she had said and try to come together and produce an integrated plan.

COMMITTEE DISCUSSION

Dr. Hey said he was going to give similar comments as Dona Crawford. Stated that he only learned at the meeting that there was a plan presented in the November meeting but he said he just learned that it was not funded, meaning the exascale software center. He stated he was confused there being FOAs and workshops and co-design but he was confused about some core competencies of DOE/ASCR and if the software ended up being deployable and widely used. He stated that he did not see an analogous thing for the exascale project at the moment. He thought it would be helpful if there was an overall outline of when calls were coming and how they would be coordinated. He thought that might be helpful. He thought they needed a clear plan to see where they were going.

Dr. Hitchcock noted that they had to deliver a plan to Congress by February 10, 2012, a federally-approved plan that would get through the approval process into the department of OMB to Congress and that plan would be an outline of their program. He said however there was intense discussion within the NNSA and within the department as to what they might be allowed to say in the plan and what numbers they could put into the plan given the budget considerations. He confirmed that it was difficult to give budget numbers before the president publicly discussed and released the budget.

Dr. Giles noted the importance of keeping the program and leadership moving given global competition even though there were budget constraints.

Dr. Linda Petzold noted they had a world-class math program yet it was her sense that the vast science community had no idea to what extent exascale was probably going to change the mission of that program. She thought that there were a lot of smart people in the science community and asked about what plans they might have for educating the community. Dr. Hitchcock replied that they had an applied math PI meeting coming up and there would be a lot of discussion at the applied math PI meeting as to what the context would be and it was primarily not exascale that would be changing but many core and

energy-awareness that was changing things plus the fact that they had a long history of counting operations in numerical analysis that was less relevant than it might have been two years ago.

ADJOURNMENT

The Advanced Scientific Computing Advisory Committee adjourned for the day at 12:30 p.m.