Draft Minutes Advanced Scientific Computing Advisory Committee February 10, 2014 Teleconference

ASCAC members present:

Marsha Berger Vinton G. Cerf Vincent Chan Barbara M.P. Chapman Jacqueline Chen Jack J. Dongarra Roscoe C. Giles (Chair) Anthony Hey Gwendolyn L. Huntoon Juan Meza John Negele Vivek Sarkar Victoria White Dean N. Williams

ASCAC members absent:

Sharon C. Glotzer

Linda R. Petzold

Also participating:

James Belak, Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory Christine Chalk, ASCAC Designated Federal Officer, Office of Advanced Scientific Computing Research, Office of Science, USDOE

Barbara Helland, Office of Advanced Scientific Computing Research, Office of Science, USDOE Rishi Khan, Vice President, Research and Development, ET International, Inc.

Robert Lucas, Director, Computational Sciences Division, Information Sciences Institute, University of Southern California

Frederick O'Hara, ASCAC Recording Secretary

About 15 others monitored the discussion via telephone or online.

The meeting was called to order by the Chairman, **Roscoe Giles**, at 11:00 a.m. to consider the report on the top-10 challenges to the exascale. O'Hara called the roll and ascertained a quorum. The draft report is on the web at science.energy.gov/~/media/ascr/ascac/pdf/meetings/20140210/Top10reportFEB14.pdf It has findings, recommendations, and detailed analyses of 10 challenges. Concerns and suggestions about the recommendations were brought up at the previous teleconference on January 21, 2014.

Giles initiated a discussion of the findings and recommendations. The specific charge to the Committee was to identify the top-10 challenges, describe them, show how they relate to the exascale, and suggest approaches that may be made to each of them. During the previous teleconference, it was decided that these top-10 challenges were to be listed in an introductory paragraph at the beginning of the report. In addition, the concern was raised that findings that were not about the challenges but were important observations nonetheless seemed to outweigh the challenges. Currently, short discussions of the challenges appear in Section 2.1. This is a good way to present them, but they might better appear in the Executive Summary.

Robert Lucas, Chairman of the ASCAC subcommittee responsible for producing the "Top-10 Report," noted that no one had disagreed with the statements regarding observations. The community should use this report as an opportunity to advocate the development of exascale computing.

Cerf pointed out that everyone reads the Executive Summary, but not all the readers read the full report. Putting the important points in the Executive Summary is well advised. Hey agreed.

Rishi Kahn said that there is a need to simulate the environment that will be experienced at the exascale, particularly looking at heterogeneity between cores and at the resilience issue. Lucas pointed out that those topics are brought out in the chapter on energy and in the chapter before the findings and recommendations.

Giles noted that the current structure of the report puts the challenges first and then goes on to the findings and recommendations. He asked if the Committee wanted to proceed with this structure.

Berger noted that the charge is not quoted in the Executive Summary and said that it should appear there to make the Executive Summary a stand-alone document. Chapman agreed; the charge should be summarized at the beginning of the Executive Summary. Negele said that the Executive Summary's structure would then include the charge, the introduction, the top-10 exascale research challenges, and the findings and recommendations.

V. Chan said that a short paragraph on why and how the findings and recommendations were made is needed. Negele and Sarkar agreed. Negele suggested that a paragraph be inserted in the Introduction, saying that, in the course of conducting the study, the Subcommittee considered a number of related issues as context for the top-10 research challenges to further assist DOE in planning its future research direction. Giles suggested adding Negele's statement, as submitted in an e-mail, and recapitulating the key elements of the charge in the Introduction. There was general agreement to use that structure.

Giles initiated a discussion of the findings.

Negele asked where Item 13 (Codesign and Integration Framework) on page 59 came from and why it appears there. It appears after the last challenge and before the findings and recommendations. It is an implementation of Recommendation 1.2.4 and seems to come from a recommendation that it precedes. Lucas said that one cannot consider these issues in isolation. Negele noted that, on page 71, a text refers to the discussion in Section 13 of the report; that topic should be moved to a later section so the topic is mentioned in the recommendations and *then* is fleshed out later with this discussion of the implementation. Giles agreed with that recommendation as a suggested editorial change. Lucas said that making it an appendix would make it look less important, and the report should conclude with the findings and recommendations. Negele said that it does not really respond to the charge. It is a fleshing out of a recommendation; it could even be part of that recommendation. Berger said that putting it in an appendix makes it an afterthought. Huntoon interjected that one cannot edit anything by committee.

J. Chen agreed with Lucas that the codesign and integration framework section should have gone at the top. It needs to be in the list, not relegated to an appendix. Cerf said that the suggestion resonated with him; otherwise one is producing a bunch of loose ends. Giles said that the topic should at least be previewed in the Introduction. Cerf said that, if one has this organizing principle up front, people will understand the top-10 challenges better. Lucas replied that there is just one sentence in the Introduction now; that would certainly allow room for embellishment. Giles asked where the discussion of code design and integration should be placed, at the beginning or the end. Berger suggested explaining the principles of codesign and integration in the Introduction (putting a framework around the top-10 challenges) and then putting the full discussion at the end. There was general agreement to do this. Chapman suggested that it should be kept with the technical material and previewed in both the Executive Summary and the Introduction, Meza said that the first two pages of Section 13 could go into the Executive Summary, and the rest could go where it currently stands. Giles agreed with moving the history to the Introduction, including some illustrations. Lucas liked that idea; that order would help the reader. Sarkar stated that the Introduction should present a roadmap to the main body of the report. Lucas pointed out that the Executive Summary would be very big if all the challenges were described at some length.

Giles asked if everyone was satisfied with the findings. He read the first finding (that exascale computing is critical to executing the DOE mission) and suggested adding the word "reaffirm" to underscore that this assertion has been made in several previous reports.

Negele questioned the meaning and use of the word "findings." Giles said that this was a cultural usage; the charge does not specifically require "findings." The usage seemed to frame the report well. Sarkar agreed that some flexibility should be employed in structuring and titling the narrative.

Negele said that findings and recommendations are coupled. Lucas pointed out that the recommendations do follow the findings. Negele observed that they do not map one another very directly: there are five findings and three recommendations. The report recommends addressing all ten challenges, but there are fewer than ten recommendations. Lucas pointed out that all the challenges appear in one recommendation or another.

Giles noted that, in the individual chapters on each challenge, there are recommendations on how to address each challenge. Those recommendations are not recapitulated in the summary of recommendations section; the recommendations that appear in the summary are broader in nature.

White pointed out that the first recommendation is at a very different level than the others, which are much more specific. The first is a general statement like one for motherhood and apple pie. Lucas said that billions of dollars had been spent by programs on "milestones" (like the petascale) by people who forgot about that very detail, that they should be looking beyond the 5-year milestone. White stated that those sentiments belong in the overarching introduction. Lucas said that everything matters to someone. Giles added that the first recommendation stresses the need for continuity and a sustained effort rather than a series of short-term milestones. It would be good to point it to one of the findings. The exascale initiative has to be coherent and continuous. White said that it should say that the exascale initiative should be a continuous process rather than a series of fits and starts. Lucas agreed.

Giles said that a modification to Section 1.1.4 seems to be needed. The Government's continuous leadership and investment are required and should be achieved according to planned milestones that are set in the recommendations. He suggested a reordering of the recommendations:

- The top-10 first
- Exascale computing is going to put DOE mission and leadership at risk
- The United States has the technical foundation to create exascale systems
- An evolutionary approach will not be adequate
- Continuous U.S. Government leadership and investment will be needed

Cerf pointed out that the tenth challenge listed (scientific productivity) is actually the main goal here; scientific progress influences economic productivity and national security. All the other recommendations follow from the need for scientific productivity. White agreed that one should lead with the science. Cerf suggested stating in the Introduction that scientific productivity is the motivation driving this proposed initiative. V. Chan said that the point has to be made somewhere that scientific leadership is important. Currently, this assertion is made in Section 14.1.2; it needs to be made up front. Cerf volunteered to write a paragraph on this topic for insertion into the report.

Giles summarized (1) the reordered and expanded findings and (2) the recommendations. He suggested that the Committee was close to agreeing on these findings and recommendations. Hey agreed. Giles offered several options:

- Vote to accept the report subject to editorial changes that would be approved by the Chair, obviating the need for another meeting, or
- Vote to accept the findings and recommendations and put off the acceptance of the full report until a future meeting.

Hey suggested moving ahead with the entire report subject to editorial changes. Dongarra said that he would second this sentiment as a motion. V. Chan, Sarkar, Chapman, Berger, and Cerf said that they were comfortable with pursuing this motion. Berger expressed a desire to see the final report again after the editorial changes were made.

Giles opened the floor for further discussion of the recommendations.

Belak said that FastForward seems to be demonstrating the emergence of an open-development environment that is not reflected in the report. Lucas said that that topic was included in Chapter 13. Dongarra said that some of that topic is also treated in Chapter 6. Belak volunteered to check those sections and submit any needed alternative language.

Meza asked if Recommendation 3 were related to any finding. Negele said that one possibility would be to have no findings and just recommendations. The way it is set up now is asymmetrical. Certainly, one wants to recommend all of the things in the top-10 issues. Lucas pointed out that the guidance and scope of the report from DOE have gotten broader during the past 6 months. Giles noted that a couple of findings are general statements to the effect that the challenges can be met. There should be a statement that specifically says that all the challenges can be met.

Meza stated that recommendations should lead to findings. The two are not hand-in-hand here, yet.

Berger agreed with the essence of the report and stated that she would vote yes to the motion on the floor.

Giles asked if there were any other changes to the findings and recommendations. Negele asked if there were any potential investment by DOE that was being overlooked. Giles said that all of these are recommendations for the development of the exascale. There are a lot of other investments to be made that do not relate solely to the exascale. The sense to be gotten across is that all four of the areas of the recommendations should be invested in. All of the recommendations should contain connections back to the challenges.

V. Chan asked if the report should refer to "a leadership role." Lucas pointed out that the second sentence says that the DOE missions are driving this effort and agreed that the concept of leadership should be included. V. Chan suggested new text to be inserted in three places:

- In the first sentence in 14.2.4, "To guide the U.S. investments in exascale research, DOE should assume a leadership role in fostering innovative strategies to establish a new discipline"
- In the fourth line of the second paragraph, "technology challenges and application requirements. Other government agencies and HPC stakeholders might be invited as partners to the study. The resulting quantitative studies will provide"
- In the third line from the end, "... They should complement and benefit from on-going U.S. Government-sponsored research programs"

Giles called for a vote on the motion to accept the report subject to editorial changes and a final review by the entire Committee. Huntoon asked if there were a timeline for completing this report. Giles replied, yes: the April 1 meeting of the Secretary of Energy Advisory Board (SEAB). Giles called the question. The motion was accepted unanimously.

Giles asked if there were any other comments on the report.

Meza noted that one suggestion that had previously been made was to consolidate all ten of the top-10 chapters into one giant chapter entitled "Research Challenges." That would cause all the findings to be renumbered but not the chapters; alternatively, the Executive Summary could be unnumbered and the introductory chapter could be Chapter 0. Giles noted that there should be no significance attached to the order of presentation of the challenges; the charge letter did not call for a ranking of the challenges. That equanimity should be made clear in the Introduction.

Belak asked if there should be a gap analysis of all the numerous projects under the exascale umbrella. Giles replied that that would be a separate process. Belak asked if the Committee wanted to coordinate with the DOE exascale review process. Giles said no; it just wants to respond to the charge.

There being no further discussion, the meeting was adjourned at 12:31 p.m.

Respectfully submitted, Frederick M. O'Hara, Jr. Recording Secretary February 11, 2014