Advanced Scientific Computing Advisory Committee Teleconference October 5, 2010

ASCAC members participating:

Roscoe Giles (Chair) Tony Hey Ron Bailey Tom Manteuffel Marsha Berger John Negele Jackie Chen Linda Petzold Susan Graham Vivek Sarkar Other participants: Michael Burke, IBM T. J. Watson Research Center Ray Bair, Argonne National Laboratory Christine Chalk, Office of Advanced Scientific Computing Research, Office of Science, USDOE, and ASCAC Designated Federal Officer Dona Crawford, Lawrence Livermore National Laboratory and Subcommittee member Robert Rosner, University of Chicago and Chair of the Exascale Subcommittee Robert Lindsay, Office of Advanced Scientific Computing Research, Office of Science, USDOE Frederick O'Hara, ASCAC Recording Secretary Andrew Siegel, Argonne National Laboratory and Subcommittee member Rachel Smith, Oak Ridge Institute for Science and Education Fred Streitz, Director, Institute for Scientific Computing Research, Lawrence Livermore National Laboratory and Subcommittee member Andrew White, Los Alamos National Laboratory and Subcommittee member

A quorum being present, the Chair, Roscoe Giles, called the meeting to order at 1:07 p.m. to consider the exascale report from the Exascale Subcommittee and to consider whether the Committee should accept the report now, with revisions, or at the November meeting. This report was due after the August meeting. He suggested calling on Rosner to summarize the report and then polling the Committee for reactions. The procedure was agreed to by the Committee.

Robert Rosner introduced the other Subcommittee members on the line. The Subcommittee came to the structure and content of the report after recognition that the road ahead is complex, expensive, and in need of very strong justification. The report has six sections, an Introduction at the beginning, a Summary at the end, and the meat in between. Chapter 2 examines the question, why exascale? It summarizes the motivation for going ahead. Complexity was exemplified by the areas needing advanced computing (astrophysics, airframes and jet turbines, biological and medical systems, combustion, fusion, nuclear power, climate and weather, and materials). The chapter goes on to define what complexity means in each of these disciplines. The change from VAXes to petascale machines has made huge changes in the aerospace industry, which will benefit greatly from the exascale. Research is always at the forefront in using advances in computing, and industry lags one or two generations behind. Chapter 3 answers the question whether computation has delivered on its promises for six of the exemplar areas. In each case, it delivered. Chapter 4 describes the applications that might be transformed by going to the exascale. Chapter 5 describes the obstacles and challenges that are present and what will need to be done in hardware, codesign, applied mathematics, algorithms, computer science, and education. The caveat is made that the program would need to be well-funded. Underfunding will doom the program.

Jackie Chen pointed out that, for a historical perspective, the aerogas turbine example is great, but it is worrisome to project that technology into the future because it is not in the DOE mission. For political

reasons, it might be better to combine aerospace with gas turbines. Rosner said that he would not have a problem with that.

Roscoe Giles wanted to see the audience addressed and an impact made upon it. What high-performance computing has delivered in the past is stated at a level of detail appropriate for an expert in the field. A nonspecialist might get lost in such a plethora of detail.

Ron Bailey stated that the important people reading this report will not spend a lot of time on it. They should not be allowed to get bogged down. They should get the message that the exascale is the *only* way to get these data and that costs and schedules cannot be met without the exascale. Given the benefits to the aerospace industry, perhaps the National Aeronautics and Space Administration (NASA) should help out.

Susan Graham stated that it is a mistake to worry about this being in DOE's purview. There will only be one exascale project. It is important for the nation. It is not a special-purpose device. The Introduction to the report needs to say that the exascale will address the most pressing national problems (climate change, biomedicine, sources of energy, etc.). Inside sections are for the scientific community. The outside chapters need to address the policy community.

Linda Petzold said that the Introduction does not make a strong argument. The inner chapters do. The Introduction needs to be rewritten to be made more forceful and to increase readability. John Negele said that a hard-hitting Executive Summary would do the trick. Tony Hey added an Executive Summary *and* a rewrite of the Introduction. Vivek Sarkar concurred and added that U.S. competitiveness, education, and societal benefits should be stressed.

Roscoe Giles said that there are ways of pulling strong arguments forward into the Introduction and Executive Summary and also backward to Chapter 5. There should be a common language across the document.

Linda Petzold noted that the riskiness issue was lost in the report.

Susan Graham pointed out that the different science areas are in alphabetical order, putting astrophysics first, weakening the report. The scientific topics should be strategically ordered. Robert Rosner said that the Subcommittee had discussed that issue. It is very difficult. Everyone has his or her own order. From a purely political point of view, aerospace should be put first. Giles said that the ordering should help tell the story. Astrophysics is remote and does not do that. The story should show that knowledge will lead to impact.

Tony Hey summed up: the report can be fixed by an Executive Summary and by reordering the topics. It is necessary to show that the exascale is a national priority. He suggested giving guidance on the Executive Summary and Introduction and to accept the report.

Tony Hey left the meeting. Marsha Berger and Tom Manteuffel joined the discussion.

John Negele pointed out that national security should be mentioned as a driver, but a caveat should be provided on why it is not described in detail. Robert Rosner replied, no problem.

Roscoe Giles suggested that the application areas should be noted as exemplars, not an exhaustive list. The workshops should be mentioned in the Introduction and referred to in each of the examples. The status letter to Dr. Brinkman in August referred to "findings and recommendations." That should be done in the report, too (e.g., codesign, DOE pursuit of the initiative, and strategies for achieving the exascale). Rosner agreed that that could be done.

John Negele pointed out that many topics brought up in the workshops could not be included in the report but could be mentioned in passing (e.g., quantum chromodynamics and the calculation of nuclear reactions). Rosner agreed. The topics selected reflected the competencies of the Subcommittee members.

Roscoe Giles summed up: The content is supported; there is a need to tighten up some elements; an Executive Summary needs to be added; and the Introduction and Summary need to be rewritten for impact. Susan Graham agreed that there seemed to be agreement in principle by the Committee on all of these issues.

Tom Manteuffel pointed out that the Committee needed to be able to send in comments.

Roscoe Giles observed that Committee does not seem to be able to accept the report as it is. The Committee could conditionally approve an improved version, or the Subcommittee could revise it and hope to have it approved by the Committee at the November meeting. Christine Chalk stated that the budget process (which is in the midst of a continuing resolution) makes October 5 and November 9 not very different. Giles suggested having the Committee read the draft report thoroughly; having the Committee members make comments, and having the Subcommittee perform another iteration. It would be better to have the vote at the next meeting. The Committee members would need the draft report 10 days before the November (9–10) meeting. Graham agreed and asked if it were feasible. She suggested that the Subcommittee release sections of the report to the Committee as they were finished. Rosner agreed that that was a good idea. Manteuffel suggested that Giles set a timeline for the Committee members so the Committee will have a finished product in November. Negele also wanted to ensure that there is not another delay in November. Rosner offered to send out the final draft to the Committee members by October 15. Giles said that all Committee changes should be to Rosner at his University of Chicago e-mail address by October 8.

Negele offered a warm thanks to Rosner for his superb work on this report and to his Subcommittee.

Roscoe Giles opened the phone to public comment. There being none, the meeting was adjourned at 2 p.m.

Respectfully submitted, Frederick M. O'Hara, Jr. Recording Secretary October 5, 2010