Department of Energy
Washington, DC 20585

NOV 13 2008

Professor Rick Stevens
Computing and Life Sciences
Argonne National Laboratory
9700 South Cass Avenue
Building 221
Argonne, Illinois 60439

Dear Professor Stevens:

I write to ask if you will co-organize and conduct an international workshop to examine the scientific opportunities in advanced modeling and simulation at the exascale in the biological sciences. You will be joined by co-organizer Professor Mark Ellisman of the University of California San Diego.

A key goal for the workshop is to present the biological community with the opportunity to shape the appropriate role for scientific computing at the exascale in the quest to advance the scientific frontiers in fundamental biological and ecology research and to examine the role of extreme scale computing in applied biological research such as bioenergy, bioremediation and the understanding of the global carbon cycle.

This workshop will build on the series of the ASCR sponsored town hall meetings held in the spring of 2007, examining the potential of exascale computing for applications in energy and the environment, the BER workshops addressing scientific opportunities in research in the global carbon cycle, GTL knowledgebase, and bioenergy held in 2008 and 2007, the workshop sponsored by NSF in 2006 looking at the opportunities in biology at the petascale and the recent national academy studies on The *Impact Of High-End Computing On Illustrative Fields* (evolution), *The Role Of Theory In Advancing Biology* and *The Frontiers At The Interface Between Computing And Biology*.

The report from your workshop is expected to be a document that should not exceed 100 pages and should be completed by the end of August 2009 if at all possible. The workshop will be a collaborative effort between BER and ASCR and we encourage you to involve the appropriate members of the community to create a balanced yet forward looking discussion and report. We would also welcome any other recommendations on program content, emphasis, or balance. This effort, we realize, is a large undertaking. However, we believe that biological research is poised to be dramatically influenced and accelerated by the likely advances in computing over the next decade and the benefits of fully exploiting future computing systems to advance our understanding will accrue not only to science but to society at large and thus justifies the effort.

A desired outcome of these meetings is to develop a short list of "global challenge" computational problems. Solving these problems should have the potential to transform

our understanding of science and its impacts and to improve our ability to apply knowledge in applications important to science, engineering, industry, and society. We anticipate that a final workshop report will address these global challenge computational problems.

This list of topics to consider include: *atomistic level biomolecular modeling, protein complexes, cell and organelles level modeling, protein folding, protein and pathway engineering, computational genomics and genome scale high-throughput data analysis, computational evolution, community and population level simulation, ecosystems modeling, artificial life and evolutionary computation, computational neuroscience and organ and tissue level simulation for complex organisms and computational approaches to imaging for biological systems.*

An effort should be made to identify the general scope of the funding required to achieve success.

As co-chair of this endeavor, you will play a critical role in ensuring the success of the workshop. It is a major responsibility: with your help, and that of your colleagues, you will enable ASCR and BER to identify key problems of national interest, document both the science and the computational case rigorously, and contribute to a focused DOE program for the next fifty years.

Dr. Susan Gregurick and Dr. Daniel Drell of the Office of Biological and Environmental Research and Mrs. Christine Chalk of the Office of Advanced Scientific Computing Research are the program managers responsible for this workshop. Susan, Dan and Christine will be contacting you shortly to discuss the schedule, deliverables, logistics and administrative needs.

If, at any time, you have questions about current plans, priorities and strategies, please fell free to contact us. Many thanks for your willingness to lead what we hope will be a landmark workshop in the field.

Sincerely,

Anna Palmisano
Associate Director of Science
for Biological and Environmental Research

Michael Strayer
Associate Director of Science
for Advanced Scientific Computing Research