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SIAM CSE 2009 Forward-Looking Panel

Julianne Chung and Carol Woodward

This report summarizes a panel discussion that was held during the SIAM Conference on Computational Science and Engineering. The conference took place on March 2-6, 2009 at the Miami Hilton Downtown in Miami, Florida. Chair of the session was Carol Woodward, Lawrence Livermore National Laboratory, and panel members included:

David L. Brown, Lawrence Livermore National Laboratory

Donald Estep, Colorodo State University

Omar Ghattas, University of Texas at Austin

Hans Peter Langtangen, Simula Research Laboratory and University of Olso, Norway

Objectives: Lead researchers from the SIAM CSE community were invited to discuss their visions of the future of the CSE field and indicate their views on opportunities for future development. The goals of the session were to give attendees some perspective of the field and to alert people to emerging hot topics and trends in CSE. Panelists addressed topics such as funding potential, new applications, and requirements of applications in terms of mathematical models, approaches, and methods. The organization of the session included a brief discussion from each panelist, followed by time for questions and open discussions with attendees. The session lasted one hour and was well-attended by conference participants.

Summary Overview: Three key topics were discussed during the SIAM CSE 2009 forward-looking panel: future challenges in CSE research, funding interests, and educational concerns. The first section of this report focuses on the panelists' remarks on the importance of effective interdisciplinary research in CSE. They drew our attention to a few applications, mathematical advancements and computational challenges on the horizon of cutting edge research. Then, later sections of this report summarize their comments on the role of funding agencies and universities in promoting interdisciplinary CSE research.

1 Future Challenges in CSE Research

Computational science and engineering is a multidisciplinary field, requiring a mix of mathematics, computer science and scientific application. Applications are the drivers of CSE, but fundamental mathematics and computer science research is essential to ensuring sufficient progress in the field of CSE. In this section, we summarize the panelists' views on new applications that will require CSE methods, the mathematics and computer science advancements that will make significant inroads in critical problems, and potential barriers that we as an interdisciplinary community will need to overcome.

1.1 Applications

The panelists identified some scientific applications that they believe are fertile research grounds for CSE impact and, thus, are rich in funding opportunities. We remark that these are the views of the panelists and may not be an exhaustive representation of all potential applications.

Energy and environment, two topics that have received increased attention from the new Obama administration, will be significant applications for CSE research in the coming years. With growing interest in new energy sources, energy efficiency, and energy storage, the Office of Basic Energy Sciences in the U.S. Department of Energy's Office of Science has recently established a $100 million Energy Frontier Research Centers (EFRC's) initiative, under which new energy centers running at $2-5 million dollars per year will focus on developing new solutions and technology for future energy. Undoubtedly, these centers will need help and expertise from computational scientists. Another hot topic for computational science and engineering is climate modeling, especially as we a push to go to 1 km global resolutions (as a post-exascale goal). Currently ice sheet modeling, such as in Greenland and Antarctica, has been left out of climate models. However, incorporating ice dynamics modeling can significantly affect the models and will be a grand challenge for the future. Other upcoming climate applications include real-time severe weather prediction, storm surge modeling, and carbon sequestration.

Although some application areas have long traditions in mathematical theory and modeling, empirical fields such as geology and medicine have little to no mathematical background. Thus, these applications are new to the field of CSE and are rich in opportunities for problem solving and for funding. The main challenge in these multi-physics applications is the complicated combination or interplay of chemical, biological, and physical processes. Solving problems in science and engineering requires us to simplify models and use mathematics to understand these simpler systems. Then, these models serve as building blocks to create a meaningful solution, an understanding of some process, or a means to predict outcomes.

With advanced algorithms and increased capabilities of computers, large scale computations and experiments can be used to answer open questions in science. However, for effective integration of basic science with applications, we should consider what we want from our application codes. Outputs from computational simulations should match outputs from physical experiments. Similar to the requirements for experimental data, we should provide error bars and confidence intervals for results obtained from computation. Early realization of this need for quantification of uncertainty for computational experiments can help in the initial design of the codes and algorithms.

1.2 Mathematics

Building new models and simulation codes requires early collaboration among applied mathematicians, computer scientists, and application scientists. Although mathematicians typically enter in the later stages of a project to help with algorithms and implementations, the demonstrated ability of smart mathematical algorithms to significantly impact the performance of scientific codes has shown the need for early collaboration. Here we report on some of the mathematical models, approaches and underlying methods that the panelists expect to be of great importance in future mathematical contributions to CSE research. We have divided their comments into four main classifications: data-modeling and algorithms, uncertainty quantification, inverse problems, and predictive methods.

There will be a strong need for methods and theory for data-model fusion and related activities like data assimilation in simulation. Seeing more statistics and probabilistic modeling researchers at this CSE meeting is a positive step toward that direction, but we need to develop new methods, theory, and numerical analysis for combining stochastic and deterministic methods into a whole. Rather than just getting one solution, we should focus on using models in computation for things like sensitivity analysis, inverse problems, outcome prediction, and optimization. The mathematical models are important for capturing physical phenomena, but we also need effective algorithms for fully complex problems. The issue here is that real problems arising from multi-physics, multi-scale applications are typically nonlinear and inherit significant complexities from the underlying models. In addition to simplifying the problem to focus on the most important features, we need scalable algorithms and adaptive approaches to deal with these complicated problems.

Every member of the panel remarked on the importance of uncertainty quantification as a central problem facing computational science today. Methods for error analysis and uncertainty quantification require propagation of uncertainty in the model parameters through the forward model to provide confidence measures on the output computations. The major challenge is that the model parameters often lie in a very high-dimensional space, resulting in large, difficult statistical inverse problems. Developing the necessary tools for uncertainty quantification is a topic that has and will continue to receive increased attention from the community.

Another area where we will see mathematical progress is in solving inverse problems to aid in decision making. A first principles approach leads to extremely complex models with many parameters, and solutions of inverse problems are needed to identify these parameters. Important research areas for future CSE impact are methods for optimal design and inverse problems, when the forward model simulation is a black box. For many problems, we are almost done understanding the forward problem and just starting to understand how to solve the inverse problem.

The ultimate goal, or the "pot at the end of the rainbow", is to influence decision making. The appropriate model will be crucial to decision-making algorithms, and it should be low risk and useful. For example, in geology, simulation is a tool to explore and better understand the dynamics of a process or system. However, it is a completely open problem right now as to whether these models can be used for prediction, that is, to predict the future. Decision making algorithms will require some sophisticated optimization techniques, but will be critical in industrial applications.

1.3 Computer Science

Computer architecture challenges will be as great as what we faced 15 years ago when we moved to the parallel environment. At the time, the future of parallel computing was uncertain, and it was just as important to develop methods for the single processor as the parallel one. The main questions we now face are "how do we effectively use the new machines?" and "what are the implications for future development of applications?"

The advancement of high-end computer architectures immediately impacts lower end machines. That is, in 1-2 decades, we are likely to see mid-range machines and multicore laptops that look like today's current high-end machines. We must consider some of the practical considerations from exascale computing. Current trends in computer architecture, such as multi-core, memory wall, and various hardware accelerators, pose great challenges. Furthermore, as high-end computer architectures move toward multicore, load balancing and parallel adaptivity will be important topics to consider. We should address these challenges using the old fashioned way; that is, by rolling up our sleeves and making sure we have enough support and help, e.g. from hundreds of PhD students with multidisciplinary backgrounds. We tend to think that all we need are bigger machines, but hardware is just the tip of the iceberg. Machines are essential, but we need much, much more.

Developing software and robust codes for efficient execution on newer multicore architectures is another issue and challenge for the future. For example, consider the possibility that MATLAB will need to run on 100 cores per chip in 2020. One panelist commented that this community spends too much time writing software, and our tools are too primitive. However, there are challenges to producing and maintaining good software. First, software funding is fragile, and there is not always a source. Furthermore, agencies do not have a mechanism to follow through, for example, by assigning responsibility to maintaining the software. When developing a project, MATLAB or Mathematica allows proof of concept, but more time and effort is required to write robust codes with proper documentation.

2 Funding

We will see an increased interest from funding agencies regarding the usefulness in solving problems in applications, such as those arising from energy, pollution, and climate concerns. There is a need for applied research, especially in developing methods and theory that fuse mathematics, statistics, and computer science in applications, but we also need to explain the role of basic research (e.g. fundamental mathematics and computer science). In addition to funding for models and algorithms, funding for software development is an important topic that should get more attention. We must convince the funding agencies to be interested in funding software and then make more progress in integrating software distribution with journal publication.

DOE is the largest funder of physical sciences in the United States. A recent report, "Applied Mathematics at the U.S. Department of Energy: Past, Present and a View to the Future," can be found at the following website:
`http://www.er.doe.gov/ascr/ProgramDocuments/Docs/Brown_Report_May_08.pdf`

3 Educational Issues

CSE is a multidisciplinary discipline, often combining mathematics, computer science and science/engineering departments. However, creating CSE departments is not desirable. Instead, we need to find better ways to support CSE interdisciplinary activities while still having separate disciplines. There are programmatic barriers to overcome, such as departmental issues like student teaching, required course work, and funding, but perhaps the toughest barrier to overcome in conducting interdisciplinary research is the current way in which we "departmentalize" research. The goals, expectations, and desires of each discipline are often different, so keeping everyone happy in interdisciplinary research can be a challenge. Universities are not well suited to support large-scale multidisciplinary research, and federal funding agencies tend to be segmented, making it difficult to receive funding for multidisciplinary research. We need to have feedback between CSE and the individual domain disciplines, and we need to set some professional standards of what is good multidisciplinary research. This will require the support of universities and funding agencies alike. Some programs developed to bridge disciplines include the NSF Grand Challenge that lasted only two years, and the Scientific Discovery through Advanced Computing (SciDAC) program whose mission is to create high performance computing software tools for scientific discovery.

In interdisciplinary CSE research, there is a major need for broad competence and expertise. For example, CSE codes and software can be extremely complicated, and tracking down bugs and strange results may require significant effort and expert knowledge. Thus, we need to create a market of students and researchers who not only have the basic skills and knowledge for conducting interdisciplinary research, but also the formal training and competence in advanced numerics and scientific coding. Major educational reform is needed to introduce computational science on day one, with numerical methods and programming as part of the academic curricula for scientists.

In regards to community concerns, we do not need new journals, but we do need a shift in focus. We are a blend of different communities, and our journals should reflect this. However, writing quality software does not get the merit it deserves, and more support for publishing software is required. One example is ACM Transactions on Mathematical Software (TOMS), which has a high citation rate but slow turnaround.

4 Concluding Remarks

It is no doubt that the future of CSE research is very bright. There are a lot of open problems and challenges in mathematics, computer science and scientific applications research, but key to the successes of this field is effective interdisciplinary research. We as computational scientists should support and strive toward this goal.