# Future of CACHE

## Saturday, August 8, 2009

Hotel Boulderado
2115 Thirteenth Street
Boulder, Colorado 80302

- **8:30 AM** **Warren D. Seider, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA 19104-6393**

  ***40-Year Cache Evolution – Emphasis On Last 15 Years***

  The role of CACHE during its first decade in stimulating computing in ChE courses will be traced very briefly. This will lead into its second decade, with an added focus on research conferences, as well as the use of authorware and more personalized computers. The 1990's brought PCs, and GUIs, and more active use of educational modules in ChE courses. Also, CACHE integrated members of the molecular modeling community to provide JAVA simulations and a web-based textbook over the Internet, as well as a series of FOMMS Conferences. A similar involvement of CFD experts led to the cooperative development of FLOWLAB, a collection of teaching modules for use with FLUENT. Throughout the 1990s to present day, through POLYMATH, CACHE has played an important role in providing a student-oriented interface for implementing an increasingly sophisticated set of numerical methods – linked to MATLAB and EXCEL – and used with leading ChE textbooks. In the 2000s, CACHE created a comprehensive web site, and as work in systems biology became more active, CACHE facilitated the first FOSBE Conferences. And, more recently, CACHE hosted discussions of the ChE role in the NSF Cyber-Infrastructure initiative.

- **8:55 AM** **Robert H. Davis, Dean & Tisone Professor, College of Engineering and Applied Science, University of Colorado at Boulder**

  ***Several Things that CU is Doing to Make Engineering Education Attractive***

  Higher education in the United States is in tension. On one hand, there are increasing numbers of young people seeking college degrees. On the other hand, public support of higher education is waning. The future of engineering education is of particular importance, as the U.S. National Academies have recommended an investment in engineering education for the national good and yet interest in pursuing engineering study has declined over the past 25 years.

  The College of Engineering and Applied Science at the University of Colorado (CU) has initiated several programs aimed at increasing the attractiveness and accessibility of engineering education, including

  1. The Engineering GoldShirt Program
  2. An Engineering Honors Program
  3. A freshmen Engineering Projects course
  4. Engineers Without Borders
  5. Partnerships with regional school districts
  6. The Earn-learn Program

  This presentation will discuss the challenges and successes of those programs. It will conclude with some thoughts on the future of engineering education.

- **9:20 AM** **Phillip R. Westmoreland, NSF and University of Massachusetts Amherst After 8/16/2009:Department of Chemical and Biomolecular Engineering and Executive Director, NCSU Institute for Computational Science and Engineering, North Carolina State University, Raleigh, NC 27695**

  ***The Future of ChE and CACHE: Our Role in Computational Science and Engineering***

  The nature of computing in engineering is on the cusp of significant change, and CACHE is in a distinctive position to help not only in chemical engineering but also across the breadth of engineering.

  My experience is that while today's engineering students are the most computer-savvy ever – as far as crafting content and learning to use whatever software they get. Ironically, they are possibly the most computer-illiterate since the 1960's in being able to develop codes or even to work knowledgably with code developers.

  We are in the early stages of a dramatic shift in computing paradigms, a term I do not choose lightly. Throughout CACHE's history, we have seen increases in the size and speed of problem solutions. The basic ideas of coding have evolved rather smoothly, shifting to object-oriented programming and reasonably straightforward adaptation to parallel processing. In the 25 years of widespread PC use, their speed increases have come largely from faster clock speeds. Now, multicore, hyperparallel computation is about to become the rule rather than the exception. Dual-

- **9:20 AM** **Phillip R. Westmoreland (cont'd)**

  and quad-core computers behave conventionally as far as programming, although it is amusing to become able to run Windows and Mac on the same Intel Core Duo! However, supercomputers are moving to having hundreds of thousands of processors, and you can now buy your own 960-processor desktop computer (exploiting GPUs) for under $8,000. Not only our programming but our basic algorithms and even our approaches to debugging must change.

  Traumatic changes, I expect, but offering great promise. Simulations of manufacturing, healthcare, and new products that now are inconceivably challenging will become routine. Stochastic methods will have new prominence. Biological, chemical, and physical problems that now have no parallel solution methods will be forced to innovate and find now approaches.

  CACHE has a special role in these impending changes because of its central emphasis on education. We face new questions about what computing expertise all engineers should have, and we can also address the needs of those who must become computing experts. The advances will be tied increasingly to collaborative interaction with computer scientists, much as ChEs have partnered with and incorporated modern physical chemistry, materials science, and biology. More than ever, the students we aid will need to stretch beyond the university, helping the educational community build computational thinking into K-12 education and into longterm workforce development. The challenges are big, but the history and position of CACHE point to great things it will dare to do in the future.

- **9:45 AM** **Robert P. Hesketh, Professor and Chair, Chemical Engineering, Rowan University**

  ***Introducing Undergraduates to Advanced Computational Software using Practical Problems***

  This paper presents techniques that have been employed at Rowan University Chemical engineering program to introduce undergraduate students to advanced computational packages. The software used at Rowan is COMSOL Multiphysics. This package is used in the undergraduate reaction engineering and transport phenomena courses.

  The software package is introduced to the students through a series of self paced tutorials. There are 4 tutorials in chemical reaction engineering and a second semester fluid mechanics course as well as 8 tutorials in transport phenomena. These tutorials start with a summary of the problem and the equations necessary to model the equipment or phenomena. This is followed by step by step instructions on how to use the program to solve the problem. The tutorials end by asking the students to solve several modifications of the initial problem.

  In using this software over several years it was determined that these tutorials were essential for getting the students to use the software. Many of the tutorials in the COMSOL package are based on relatively complex



- **9:45 AM** **Robert P. Hesketh (cont'd)**

  geometries and phenomena and were deemed by the students as too difficult for beginners to use. These self-paced tutorials were introduced to allow students the ability to compare known solutions with the solutions obtained from COMSOL Multiphysics. In many of the tutorials the analytical and POLYMATH solutions are compared with the COMSOL solution. This allows the students to gain confidence in the use of this tool as well as gives them the ability to determine problems with the software.

  In this presentation, several examples will be given of the self-paced modules. An explanation of how they are used in the class room and evidence of their success will be presented. In addition, it will be shown how the undergraduate courses have been transformed from courses based only on analytical solutions to a major emphasis on computational solutions.

- **10:10 AM** **Lawrence B. Evans, Co-founder and Chief Executive Officer, Rive Technology**

  ***The Evolution of Computing in Chemical Engineering: Some Perspectives and Future Directions***

  In the last forty years since CACHE was founded we have made a remarkable journey. None of us who gathered in 1969 would have dreamed that we would be meeting here in 2009 to celebrate such a successful organization.

  In this talk I would first like to describe the forces that have driven the advances we have made, including: the incredible increase in computing and communications power driven by Moore's law, advances in our ability to model the physical and chemical world, improvements in the way we interact with computers, and the increasing need to bring value and to solve problems for society.

  Then, I would like to speculate on how these forces might evolve and what the trends would mean for our future. Finally, I would like to share some lessons I have learned from working as part of a wide range of organizations, including MIT, CACHE, AIChE, Aspen Technology, and now the start-up company, Rive Technology.

- **10:35 AM** **Round Table Discussion**