

Workshop on Cyberinfrastructure in Chemical and Biological Systems

An NSF workshop on Cyberinfrastructure in Chemical and Biological Systems was held at the National Science Foundation in Arlington, Virginia, September 25-26, 2006.

The workshop brought together research and industrial communities in chemical and biological systems with the Cyberinfrastructure (CI) planning and operational community and focused on:

- (1) next generation strength areas in the U.S. facilitated by CI
- (2) CI technical areas of impact, and
- (3) CI foundations.

The workshop was designed to foster collaboration among several key dimensions of CI and chemical and biological systems. These dimensions included technique and technical integration, academic and industry, infrastructure and application, current and future directions for CI, and current and future economic potential for CI. The workshop will look across a broad diversity of computation and networked-based technologies in order to make recommendations to NSF on future research needs and CI development aimed at researchers and practitioners in chemical and biological systems directions. Further, the workshop will exemplify for the process and systems communities, the value of their roles in investing in CI and CI-enabled research.

Jim Davis was the Organizing Committee chair (jdavis@oit.ucla.edu). Jim is a UCLA Professor of Chemical Engineering and Associate Vice Chancellor of Information Technology and CIO.

The Workshop Organizing Committee included:

Stan Ahalt, Ohio State University, Professor and Director of the Ohio Supercomputer Center (ahalt@osc.edu).

Frank Doyle, UC Santa Barbara, Professor and Associate Director of the Institute of Collaborative Biologies (Frank.doyle@icb.ucsb.edu).

Larry Evans, Aspen Technology, Inc., Founder and Former Chairman of the Board of Directors and Professor at MIT (larry@larryevans.net).

Ignacio Grossmann, Carnegie Mellon University, Professor and Director of the Center for Advanced Process Decision-Making (grossmann@cmu.edu).

Sangtae Kim, Purdue University, Professor and Inaugural Director of the Division of Shared Cyberinfrastructure, CISE, NSF (Kim55@purdue.edu).

The workshop was sponsored and organized in close cooperation with Maria Burka, Chemical and Transport Division and Bruce Hamilton, Bioengineering and Environmental Systems Division within the Engineering Directorate at the National Science Foundation.

For the purpose of this workshop, the definition of Cyberinfrastructure is the coordinated aggregation of software, hardware and other technologies, as well as human expertise to support current and future discoveries in science and engineering and to integrate relevant and often disparate resources to provide a useful, usable and enabling computational and data framework characterized by broad access.

The objectives of the workshop were to: (1) identify and exemplify major application impacts, directions and the potential for CI as it pertains to Chemical and Biological Systems, (2) identify and recommend research areas that aim toward the fulfillment of this potential, and (3) identify associated areas of needed emphasis within the CI infrastructure, education and training, interdisciplinary development, and support and approaches to collaboration.

The two-day workshop encompassed chemical and biological processes, systems biology, pharmaceuticals and metabolic engineering, and will involve energy, environmental, nano- and bioscience perspectives in the process context. The thematic area is generally defined by industries, applications, processes and systems primarily characterized by chemical and biological transformations and material, energy and information flows.

The workshop brought together research and industrial communities in chemical and biological systems involved in smart plant technologies, supply chain management, product and production design and optimization, process management and control, simulation and modeling and data analysis with the CI infrastructure planning and operational community.

Key questions that were addressed at the workshop included:

- (1) What are the future IT-enabled economic drivers for process systems in the U.S?
- (2) How can CI affect or impact these drivers?
- (3) What are the new problems and what are the tools needed?
- (4) What technologies are needed? What are the integration requirements? Where is the expertise, and what is the state of technical capability?
- (5) What are the respective roles of industry, government and academia and how should they interrelate?
- (6) What investments are needed in the CI and what investments are needed in the process systems areas? What should be the source of the investments?

- (7) What partnerships/coalitions are needed?
- (8) How will new and emerging technologies and CI capabilities need to affect organization roles and responsibilities – academia/industry, researcher/research teams, etc.?
- (9) Where are education and training needed?

The results of the workshop will be summarized in a final written report to NSF to be completed by December 31, 2006. The workshop website is at:

<http://www.oit.ucla.edu/nsfci/default.htm>