

CS&E@CIT 2006
Workshop on the Frontiers of Computational Science and Engineering at Caltech

Saturday, November 18, 2006, 8:30am-4pm
 Rock Auditorium, Broad 100

Hosted by the Center for Advanced Computing Research



The goal of this workshop is to highlight the broad range of CS&E efforts at Caltech, and to identify some specific actions to help build and support the campus CS&E community. This is intended to be a forward-looking workshop, with the main theme being what can we do together to assume leadership in some approaches to e-Science? A related theme is how can CACR best serve the Caltech community as a catalyst, matchmaker, or forum for exchange of ideas and experiences across many different disciplines in CS&E?

The format is eleven 15-minute talks by current practitioners of CS&E at Caltech. After lunch, there will be two panel discussions on commonalities and strategic directions. The speakers have been asked to cover some of the following specific questions:

- Briefly describe their CS&E activities
- What is going well and not so well in their CS&E approach
- What are some outstanding challenges
- Do they see any potential interactions with other CS&E groups on campus, and
- What are the impacts of CS&E on Caltech's education mission?

The focus is not the provisioning and operation of high-performance computing facilities, although this will necessarily be a topic of discussion. Rather, the primary intent is to explore ways that e-Science and CS&E can have a broader impact at Caltech.

Final Agenda

8:30- 9:00	Coffee
9:00 - 9:15	Opening Remarks: Ideas Behind this Workshop George Djorgovski, Prof. of Astronomy and co-Director CACR
9:15 - 9:30	CACR: Its History, Status, and Future Plans Mark Stalzer, Executive Director CACR
9:30 - 9:45	Multi-Scale Modeling and Simulation of Materials Michael Ortiz, Prof. of Aeronautics and Mechanical Engineering
9:45 - 10:00	DANSE: Distributed Data Analysis for Neutron Scattering Brent Fultz, Prof. of Materials Science and Applied Physics
10:00 - 10:15	Modeling of Functional Changes and Enzymatic Reactions in Cells Mary Kennedy, Prof. of Biology
10:15 - 10:45	Coffee Break
10:45 - 11:00	Networking and Grids for High Energy Physics and the Large Hadron Collider Harvey Newman, Prof. of Physics
11:00 - 11:15	How to Build a Virtual Observatory Roy Williams, Member of Professional Staff CACR and Director NVO
11:15 - 11:30	Simulation of Extreme Spacetimes Lee Lindblom, Senior Research Associate TAPIR
11:30 - 11:45	Integrated Large-Scale Modeling and Simulation at JPL: A Recent Appraisal Rich Doyle, Manager Mission Info Tech, Interplanetary Network Directorate
11:45 - 12:00	Spectral-Element and Adjoint Methods in Computational Seismology Jeroen Tromp, Prof. of Geophysics and Director Seismological Laboratory

12:00 - 12:15	<p>First Principles Prediction of Materials and Proteins</p> <p>William Goddard, Prof. of Chemistry, Materials Science, and Applied Physics</p>
12:15 - 1:15	Lunch
1:15 - 2:15	<p>Panel Discussion: What are the Commonalities?</p> <ul style="list-style-type: none"> • Moderator: Richard Murray, Prof. of Control & Dynamical Systems and Director Info Sci & Tech • Kimberley Douglas, University Librarian • Brent Fultz • Mary Kennedy • Jeroen Tromp
2:15 - 2:30	Coffee Break
2:30 - 3:30	<p>Panel Discussion: Strategic Trends and Future Directions</p> <ul style="list-style-type: none"> • Moderator: George Djorgovski • Mani Chandy, Prof. of Computer Science • Rich Doyle • Mike Gurnis, Prof. of Geophysics and co-Director CACR • Vincent McKoy, Prof. of Theoretical Chemistry • Barbara Wold, Prof. of Molecular Biology and Director Beckman Institute
3:30 - 3:45	<p>Summary Comments</p> <p>George Djorgovski and Mark Stalzer</p>
3:45	Adjourn