

**Workshop on Biomedical Computing HPCS Needs
Agenda - January 17, 2003**

Science and Technology Associates, Inc.
4001 N. Fairfax Drive, Suite 700
Arlington, VA 22203
Phone: 703.522.5123 Fax: 703.522.0367

- 09:00 – 09:15 Introductions
- 09:15 – 09:30 HPCS Overview, Bob Graybill, DARPA
- 09:30 – 10:00 HPCS Biomedical Computing Requirements Overview, Kay Howell, FAS and Gerry Higgins, SimQuest, LLC
- 10:00 – 10:45 *Protein Structure Prediction*, Giri Chukkapalli NPACI UCSD
- 10:45 – 11:30 *Image-based Computational Hemodynamics*, Juan Cebral, GMU
- 11:30 – 12:15 *Application of Quantum Chemistry to Biology*, Stan Burke, ABCC, NIH
- 12:15 – 1:00 Lunch
- 1:00 – 1:30 *Digital Imaging – Visible Human Datasets*, Brian Athey Univ. Michigan
- 1:30 – 2:00 *Bioinformatics Computing Center Issues*, Brian Athey, Univ. Michigan
- 2:00 – 2:45 *The Biomedical Informatics Research Network (BIRN)*, Bret Peterson, NCR, NIH
- 2:45 – 3:30 *Massive in Silico Screening of Chemical Databases for Countermeasures of and Chemical Weapons*, Yuan-Ping Pang, Mayo Medical School
- 3:30 – 4:15 *Conformational Analysis of the Acyl Pocket Loop in Acetylcholinesterase Computed by Monte Carlo Methods with a Generalized Born Model of Solvation*, Louis Carlacci, AHCRC
- 4:15– 5:00 General discussion and wrap up

Workshop Objectives:

For the application areas to be discussed, characterize the computational and architectural requirements, including:

- | | |
|---|--|
| ☒ Computational requirements | ☒ Memory access patterns |
| ☒ I/O performance | ☒ Compiler speed |
| ☒ O/S speed and stability | ☒ Batch and interactive mgmt capabilities |
| ☒ Platform porting strategies and experiences | ☒ Performance across multiple architectures/sy |
| ☒ Code size | ☒ Key algorithms and algorithmic improvement |