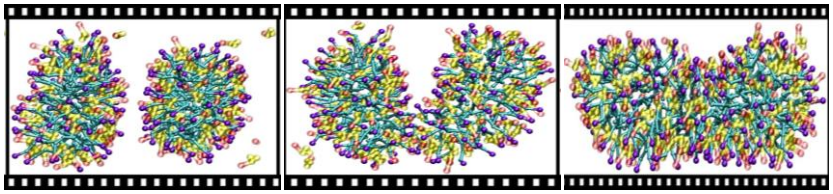

Scientific Exploration through Simulations (SETS)

Summer Workshop at Syracuse University

July 9-12, 2012, 201 Link Hall, Syracuse University

Objectives:

This workshop represents a key activity associated with the National Science Foundation supported project, OCI-1135486, "CI-TEAM Demo: Scientific Exploration through Simulation (SETS): Cloud-Enabled *in silico* Design and Discovery of Energy Materials in STEM Education". The goal of the workshop is to introduce and provide hands on training to K-12 teachers and students in state of the art, open source computer simulations that help understand molecular structure/dynamics and molecular-scale phenomena in physical, chemical and biological systems and their relevance to the energy field. The role of such simulations in design and discovery in various fields of engineering and technology will be emphasized through examples derived from contemporary research. SU researchers, teachers and student participants will work collaboratively to test/evaluate the software components and develop mechanisms (e.g. home works, projects) to help integrate the computer simulations into the school curricula in AY 2012-13. Students will have the opportunity to continue their participation in the project throughout the school year. A follow up workshop is planned for the summer of 2013 to evaluate the effectiveness of the pedagogical mechanisms developed and implemented in AY 2012-13 as well as to seek ways to expand the scope of the CI-TEAM project.

Each participant will receive a certificate of attendance. Subject to meeting employment eligibility requirements, a stipend of $200 will be provided to each student participant.

Participants

SU Professors:

R. "Suresh" Sureshkumar (Biomedical and Chemical Engineering)
Steve Chapin (Electrical Engineering and Computer Science)
Ari Chakraborty (Chemistry)
Shikha Nangia (Biomedical and Chemical Engineering)
Scott Shablak (Education, Project Evaluation)

SU Doctoral Student:

Abhi Sambasivam (Biomedical and Chemical Engineering)

SU Undergraduate Students:

William Stahl (Computer Science)
Chelsea Stephens (Biomedical Engineering)
Stephen De Salvo (Chemical Engineering)

High School Teachers:

Sally Mitchell (East Syracuse Minoa)
Mehriban Sirin (Syracuse Academy of Sciences)

High School Students:

Somil Aggarwal
Alec Beaton
Tyler Buchman
Snigdha Chatterjee
John Drogo
Jessica Fink
Tionna Knight
Lan Pham
Venice Magunga
Bilgenur Sirin
Kayla Vidal

Notes:

- Each participant has an account set up on the SU computer network. The userid is g-<first initial><last name>. For instance, the userid for Sally Mitchell is g-smitchell. Passwords will be given at the time of registration.
- Each participant will be able to log on to the high performance computer cluster "prophet" housed in SU's Green Data Center. Userids and passwords will be given at the time of registration.
- **Students are encouraged to bring their Chemistry textbook**.

Program

Monday July 9, 2012

Activities:

- Setup, Orientation, Workshop Objectives
- Introduction to Computer Simulations
- Building and Analyzing Small Molecules using AVOGADRO

9 **AM**	Arrival and registration (Link 121) Ms. Lynore de la Rossa will greet the students/teachers. Name tag, file folder and note pad/pen will be provided. Complete paperwork required to process stipends. Go to Computer Laboratory in Link 201
9:30-10	Login and Setup (Abhi, Will, Stephen)
10-10:30	Introduction—CI Team and Participants CI Team Workshop—Objectives and Overview (Ari) (Presentation followed by Q&A)
10:30-10:45	Break
10:45-Noon	Introduction to Computer Simulations: Applications (Presentation followed by Q&A)
Noon-1 **PM**	Lunch **(Room TBA)** Meet with Project Evaluation Team
1-2:15	Building and Analyzing Molecular Structures using AVOGADRO (Abhi, Stephen, Ari) --Introduction --Installation on home computers/laptops -- Features/options, documentation --Building simple molecular structures ---Water, Carbon Dioxide, Ammonia etc. --Equilibrium structure: energy minimization principle
2:15-2:30	Break
2:30-3:45	Exploring with AVOGADRO (Abhi, Stephen, Ari) --Students identify molecules of their choice --Explore their structure/geometry --Save the work, print the files --Each student submits their work to Abhi
3:45-4:15	Discussion and feedback (Ari and SU team, teachers and students) --Notes (Abhi)

Tuesday, July 10 2012

Overview:

- Building and Analyzing Small Molecules using AVOGADRO
- Introduction to Molecular Dynamics (MD)
- Visualization of MD Simulations using Jmol

9-10:30 **AM**	Exploring molecular structures using AVOGADRO: beyond simple molecules (Abhi, Ari) ---cyclic molecules, alkanes, alkenes, aromatics, isomers, polymers, amphiphiles, among others
10:30-10:45	Break
10:45-Noon	Exploring molecular structures using AVOGADRO: beyond simple molecules (Abhi, Ari) ---Students build and analyze a molecule of their own choice from the above class ---Save the work, print files, submit work to Abhi
Noon-1 **PM**	Lunch, Informal Discussion
1-2:15	Introduction to Molecular Dynamics* (Shikha) ---Basic concepts (F = ma) ---Force fields (What contributes to F and how to represent them?) ---Applications in science and technology ---How are the equations solved to obtain trajectories? ---Time and length scales ---Computational requirements ---Introduction to the MD computational interface (GROMACS) ---Q&A
2:15-2:30	Break
2:30-3:45	Visualizing MD simulations VMD* (Shikha, Abhi, Stephen) ---Installation (home computers/laptop) ---Features/options, documentation ---Building and analyzing complex molecular structures --- DNA, Proteins, Molecular Assemblies ---Visualization of MD trajectories
3:45-4:15	Discussion and feedback ---Notes (Abhi)

Wednesday, July 11 2012

Overview:

- Linux Operating System (to prepare for GROMACS)
- Performing MD using the GROMACS Interface: Molecular Systems

9-10:30 **AM**	Linux Tutorial* (Stephen, Will, Steve, Abhi) ---Basic commands ---Directory/file creation, deletion etc. ---vi file interface
10:30-10:45	Break
10:45-Noon	Students explore the Linux OS (Stephen, Abhi, Chelsea, Steve) ---Logon and access their home directory ---create a vi file based on specification given ---edit, save the file ---submit printout to Stephen
Noon-1 **PM**	Lunch, Presentation on SU Admission Process (Kathleen Joyce)
1-2:15	Performing MD Simulations: GROMACS Interface* (Shikha, Abhi, Stephen) ---Intro and demo ---Prepare a periodic box of water ---Insert a small protein (e.g. albumin) ---Run dynamic simulation to equilibrate system ---Collect/visualize data
2:15-2:30	Break
2:30-3:45	Exploring the GROMACS Interface* (Abhi, Stephen, Shikha) ---Preset examples ---Water/Hexane, Water/Hexane/Surfactant ---Surfactant Self-Assembly (CTAC/Water) ---Visualization
3:45-4:15	Discussion and feedback (Shikha to lead)

Thursday, July 12 2012

Overview:

- Performing MD using the GROMACS Interface: Molecular Systems
- Beyond the Workshop--Pursuing Computational Research
- Beyond the Workshop—Integration of Software Tools into Curriculum

9 **AM**—Noon (with a 10 minute break as needed)	Exploring the GROMACS Interface—Contd. (Abhi, Stephen, Shikha) Student/teacher teams design and perform their own simulation ---Protein-water system ---SDS Surfactant ---Ethanol-Water Mixture
Noon – 1 **PM**	Lunch, Discussion with the Project Evaluation team
1-2 PM	Exploring the GROMACS Interface—Contd. Student/teacher teams design and perform their own simulation. ---Create a system of molecules in water and observe their dynamics ---Save the work, print documentation and submit
3-3:00	Pursuing computational research at SU (Suresh to lead discussion)
3:00-3:15	Break
3:15-4:00	Incorporation of software tools into school curriculum in AY 12-13 (Sally, Mehriban to lead discussion)
4:00-4:15	Closing remarks (Dean Laura Steinberg); Group Photo

* Lectures need to be videotaped.

** Professional and in house pictures of workshop activities will be taken for reporting purposes.