Education Plan

Objective: Significantly increase literacy/interest of US students in modeling and high-performance computing.

- Undergraduate:
  - Undergraduate research (SURF)
  - Advanced technical electives

- Graduate:
  - Advanced courses on predictive modeling and simulation (C&SE)
  - Research workshops
  - Seminar series
  - Short courses on HPC, programming
  - Summer internships at the Labs

[Links to Engineering and Computer Science](engineering.purdue.edu/Engr/Research/SURF/)
[Computer Science and Engineering](www.cse.purdue.edu)
Fall 2008 PRISM Seminar Series

August 22: Peter Schultz, Sandia, NM
NCN/PRISM “From Density Functional Theory to Defect Level in Silicon”

September 19: Jim Allen, Sandia, NM
“Challenges of Micro-System Product Development”

October 3: Jayathi Murthy, Purdue
"An Introduction to PRISM”

October 17: Rahul Bidkar, ME, Purdue
“Gas Damping of Microcantilevers at Low Ambient Pressures”

October 31: Michael Eldred, Sandia, NM
“Nonintrusive Polynomial Chaos and Stochastic Collocations Methods”

November 14: Habib Najm, Sandia, Livermore

December 5: Alex Pothen, CS, Purdue

Discussion and pizza on Fridays at Birck 1001
High Performance Parallel Scientific Computing Workshop

- Organizers: Alejandro Strachan and Faisal Saied
- 1 ½ hands-on school on September 4-5
  http://www.cri.purdue.edu/hppsc.cfm
- 40+ student and staff participants.
- Speakers from the Labs
  - Blaise Barney, LLNL, “Overview of HPC at the NNSA/SC National Labs”
  - Steve Plimpton, Sandia, Scalable Algorithms group.

- Introduction to HPC
- Fundamentals of parallel processing
- MPI
- Hands-on exercises using LAMMPS
- Guest lectures
Computational Science and Engineering (CS&E)

• Interdisciplinary graduate specialization program started in 1995
• Over 50 MS and PhD students and 137 faculty in 2007 including 6 PRISM members
• 14 core courses in HPC architectures, parallel algorithms, programming, and visualization
• Over 60 relevant CSE courses in disciplines ranging from computational biology to nuclear engineering
• Enrich program with more topical courses

https://engineering.purdue.edu/CSE
CS&E Courses from PRISM Faculty

- **CS525: Parallel Computing (Grama)**
- **MA692D High Performance Computing (Dong)**
- **MA598B Numerical Methods for Stochastic Computations (Xiu):** Mathematical framework for stochastic equations and available numerical techniques. UQ approaches.
- **AAE 590D: Molecular Gas Dynamics (Alexeenko):** Kinetic theory of gases; direct simulation Monte Carlo (DSMC) and deterministic methods for solution of Boltzmann equation.

https://engineering.purdue.edu/CSE
UNM Contributions
Deborah Sulsky

• The High Performance Computing Center (HPC) offers local resources for code development, testing and education. [http://www.hpc.unm.edu](http://www.hpc.unm.edu)

• The Computational Science and Engineering (CSE) Certificate involves course work in parallel computing and a computational thesis. [http://www.hpc.unm.edu/education/cse-program](http://www.hpc.unm.edu/education/cse-program)

• A new Nanoscience and Microsystems (NSMS) PhD degree has started. Leveraging of IGERT support possible to involve additional students in this project.

• New Mexico Computing Applications Center (NMCAC): Encanto is an SGI Altix ICE cluster with 1792 nodes, each with 8 2.66GHz cores.

• UNM has partnered with SNL and others to establish the National Institute for Nano-Engineering (NINE) to broaden students' education through multi-disciplinary team research in leading-edge technical areas.

• UNM is an Hispanic serving institution and the only such Carnegie RU/VH Research University giving us a qualified pool of under-represented students.
UIUC Contributions
Narayan Aluru

• Several courses on MEMS are offered for undergraduate and graduate students. Examples include Introduction to MEMS, MEMS/NEMS Theory and Fabrication, Modeling and Simulation of MEMS, etc.

• NCSA offers local resources for large-scale simulations

• Computational Science and Engineering (CSE) Certificate for graduate students interested in Computational Science.

• Beckman Institute and Micro Nano Technology Lab offers experimental and computational resources for micro and nanoscale research

• Molecular and Electronic Nanostructures Research Theme at Beckman Institute hosts a weekly seminar series on micro and nanoscale science and engineering

• MEMS/NEMS Simulation Tools developed at Illinois are available via nanoHUB
MEMS Hub

- Seminar series
- Simulation tools
- Experimental data
- Wiki pages
- Community forum
November 7, 2008:
1-day Workshop at Purdue
“HUBbub about Online Research, Education, and Collaboration: Using the HUBzero Platform for Scientific Computing”
organized by Michael McLennan

http://hubzero.org/

Interactions with Labs

• Collaborations in critical areas
  • Validation data generation, sample fabrication
  • LAMMPS development
  • Linear solver development (PetSC)
  • Summer students
• Joint participation in short courses, workshops, seminar series
• Thesis committees
• Sabbaticals (Purdue Labs)
2008 Sandia Intern: Ryan Tung

- 8 weeks in June-July at Dept 1526, Solid Mechanics in Sandia, NM
- Lab Mentor: Anton Sumali
- Purdue Advisor: Arvind Raman (ME)
- Experiments:
  - Measuring gas damping of the Cantilever Array discovery platform (CADP) from 1mT to atmospheric, to verify squeeze film damping theories.
  - Measuring gas damping of freely suspended AFM beams from 1mT to atmospheric, for verification of 2-d BE method and ES-BGK simulations (Rahul Bidkar)
  - Measuring ODS's of MEMS switch (Peroulis Group) and damping at various pressures.