Introduction to Scientific Computing Course

CS 471/Math 471, Fall 1997

Brian T. Smith, UNM
Andrew C. Pineda, UNM

Objective Of The Course

- To introduce you to high performance computing system used in science and engineering
- High performance machines nowadays
  - billions of floating point operations/second
  - billions of bytes of random access memory
  - terabytes of online storage
  - levels of memory and multiple processors

Objective Continued

- Use of HPCs to model and simulate complex physical systems to gain insight and understanding on how they behave
- Exposure to tools and techniques
  - programming languages
  - problem solving environments
  - visualization environments
  - basic computing methodologies

Course Approach

- Hands-on experience using local machines
  - lectures to cover basic material
  - lab work to experience the tools
  - exposed to the good, the bad, and the ugly
  - exercises and experiments in labs
  - logbooks written to record your experience

Different Sections--Section I

- For the post-graduate students (Sandia)
  - lecture periods
    - M-W, 4:00-4:50PM Tapy Room 217
  - laboratory periods
    - M-W, 5:20-6:50PM, ESCP Room 109
  - different lecture schedule to accommodate the two case studies and major project
  - lectures assume a different background

Different Sections--Section II

- For UNM under- and graduate students
  - lecture periods
    - T-Th, 4:30-5:20PM, ME Room 220
  - laboratory periods
    - M-W, 5:20-6:50PM, ESCP Room 110
  - more lecture material and more detail
  - case studies are molecular dynamics and advection

Computers Available

- CIRT
  - IBM RS/6000, model 670, AIX 4.1
  - machine names: argo, mirac, pegasus, musca
  - Matlab: on pegasus only
  - SGI Indigo, IRIX 6.2: altair, neptune, europa, venus, pluto
  - SGI Indy: castor, saiph, rigel, spica
  - Modems: 277-9990

Computers Available Cont'd

- AHPCC
  - IBM RS/6000, 370, AIX 4.1: acoma
  - IBM RS/6000, 43P, AIX 4.1: grants, gallup
  - IBM RS/6000, 25T, AIX 4.1: taos, gila
  - IBM RS/6000, 32-node SP1.5: zen01..., chen...
  - HP 715, HP-UX 9.05: isleta
  - Sun Sparc 20, Solaris 5.5: laguna
  - Sun Ultrasparc clone, Solaris ???: ???

AHPCC Cont'd

- Machines
  - SGI Onyx Reality, IRIX 5.3: cochiti
  - SGI Onyx Reality 2, IRIX 6.4: nambe
  - Pentiums,Linux 2.0.27: artesia, deming, ...
  - Modems
    - 277-8393 to 8396, 9033, 9232, 9265, 9095

Lecture Material

- Text
  - An Introduction to High-Performance Scientific Computing, Fosdick et al,
  - Laboratory chapters, Fosdick et al as well as UNM authors
    - ~acpineda/CS471/... on both CIRT and AHPCC machines
  - CSEP Web Text Book, http://csep1.phy.ornl.gov/csep.html

Lecturers

- Brian T. Smith
  - Professor, CS
  - Chief Scientist, HPCERC
  - 277-8249
  - email:bsmith@arc.unm.edu
  - office hours
    - 2:00-3:30PM, M, T, W, Th

Lecturers Cont'd

- Andrew C. Pineda
  - Staff, HPCERC
  - Postdoc, Computational Chemistry
  - 277-8249, -3913 (direct)
  - email: acpineda@arc.unm.edu
  - office hours
    - M-Th. 10:30AM-Noon

Lecturers Cont'd

- Dr. Richard C. Allen
  - Org. 9205, SNL
  - 845-7825
  - email: rcallen@cs.sandia.gov