CPS 5401

Introduction to Computational Science

Fall 2012

The University of Texas at El Paso

Shirley Moore

http://www.cs.utep.edu/svmoore/

http://svmoore.pbworks.com/

CPS 5401 is an introduction to basic computational science skills including UNIX, scientific programming using high level languages, parallel computer architectures, parallel programming paradigms, and numerical algorithms.

Course #:	CPS 5401
Course title:	Introduction to Computational Science
Credit hours:	4
Term:	Fall 2012
Time & location:	Tuesdays and Thursdays, 6-8pm, CCSB 1.0202
Prerequisites:	Instructor approval
Course fee:	None
Instructor:	Shirley Moore
Office location:	Chemistry and Computer Science Building 2.0204
Contact information:	Phone: 915-747-5883 Email: svmoore@utep.edu Fax: 915-747-5030 WWW: http://www.cs.utep.edu/svmoore/
Office hours:	5-6pm Tuesday and Thursday or by appointment
Required textbook:	Georg Hager and Gerhard Wellein, *Introduction to High Performance Computing for Scientists and Engineers*, CRC Press, 2011
Online textbook:	Cleve Moler, *Numerical Computing with MATLAB*, http://www.mathworks.com/moler/chapters.html , 2004

Course Objectives

The course will cover three major aspects of computational science in three parts:

- Part I will consist of a practical introduction to UNIX, scientific programming using high level languages, parallel computer architectures, parallel programming models, and current trends in high performance computing.
- Part II will cover performance and scalability issues, performance evaluation and optimization, and a more detailed treatment of parallelization issues, including hybrid programming models and locality optimization.
- Part III will cover broadly useful numerical algorithms and their parallelization including dense and sparse linear algebra, FFTs, and PDEs.

Course Activities and Grading

Your grade for the course will be based on the following:

- 20% homework
- 10% quizzes
- 40% projects
- 30% midterm and final exams

Late and Make-up Policies and Re-submissions

- Assignments submitted within one week after the deadline will suffer a reduction of one letter grade (e.g., An assignment that would otherwise receive a grade of "B" will receive a grade of "C").
- Assignments may be re-submitted for re-grading up to one week after initial grades are released. Up to one half the credit lost on the original submission can potentially be recovered. Students are not required to re-submit. Late assignments may not be re-submitted.
- Quizzes may not be made up. Exams can only be made up with a valid excuse.

Attendance Policy

This is a challenging course and attendance is essential for success. Although attendance will not be taken, please try not to be absent unless absolutely necessary.

Classroom Conduct

Cell phones, ipods, headphones, etc. may not be used during the class, quizzes, or exams. Laptop computers may be used only for taking notes or as directed for class activities. Food and drinks other than water bottles should not be brought to class.

Accommodations for Students with Disabilities and Exceptional Circumstances

Individuals with disabilities have the right to equal access and opportunity. Please contact Dr. Moore the UTEP Office of Disabled Student Services (DSSO) if you have a special circumstance such that an accommodation would be helpful in permitting you to excel or demonstrate mastery of the material covered in this course.

Academic Honesty Policy

Make sure you understand the UTEP academic honesty policy. Students are encouraged to share ideas, but you must do your own homework and you must write your own code for the projects (you may copy code that is on the course website). If homework or program code is suspected of being duplicated or copied, you will receive an incomplete for the assignment, and your case will be referred to the Dean of Students for adjudication. If the instructor has reason to believe that you have cheated on a quiz or exam, your case will be referred to the Dean of Students for adjudication.

Course Topics

- UNIX (3 sessions)
  - Logging in and account setup
  - Shell and environment variables
  - File system
  - Job control
  - Shell programming
  - Makefiles
- Scientific programming languages (3 sessions)
  - General concepts
  - Fortran 90/95
  - C and C++
- Parallel computer architecture (4 sessions)
  - Cache-based microprocessors
  - Memory hierarchies
  - Multicore processors
  - Multithreaded processors
  - Vector processors
  - GPGPUs
  - Shared memory computers
  - Distributed memory computers
  - Hierarchical (hybrid) systems
  - Networks
- Parallel programming paradigms (4 sessions)
  - Data and functional parallelism
  - Shared memory parallel programming with OpenMP
  - Distributed memory parallel programming with MPI
  - Hybrid parallelization with MPI and OpenMP
  - PGAS languages
  - GPU programming models
- Performance optimization (3 sessions)
  - Single node profiling and optimization
  - Parallel profiling and tracing
  - Data access optimization
  - Efficient OpenMP programming
  - Locality optimizations on ccNUMA architectures
  - Efficient MPI programming
  - Topology and affinity in multicore environments
- Scalability (1 session)
  - Scalability and efficiency metrics
  - Strong vs. weak scalability
  - Communication models
- Dense and sparse linear algebra (4 sessions)
  - Vector and matrix products

    - LU factorization
    - Cholesky factorization
    - Triangular systems
    - Band and tridiagonal systems
    - Iterative methods
- Eigenvalue problems (1 session)
- Fast Fourier transform (1 session)
- Numerical optimization (1 session)
- Partial differential equations (1 session)