CMPS 445-01 Parallel & Distributed Computing

3.0 hours credit, 45 contact hours.

Instructor: Shizhong Yang, Room E105 of Thurman Hall
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Textbooks:

1. (Recommended) High Performance Computing Programming and Applications by John Levesque, CRC Press, 2011, ISBN 978-1-4200-7705-6.
2. Reference book: Programming Massively Parallel Processors, David B. Kirk and Wen-mei W. Hwu, Morgan Kaufmann, 2010, ISBN: 978-0-12-381472-2.

Specifics:

A. Course Description: This course covers basic parallel programming environment, parallel programming paradigms and implementation (MPI and programming), focusing on a subset of widely used contemporary parallel programming models, and providing application in materials design, and biomedical research. Topics include Dell Linux cluster, parallel programming principles, MPI, GPU and CUDA, performance tune up of parallel codes in material science and biomedical research, and result data analysis and processing. Applications are drawn from diverse areas of science and engineering

B. Prerequisites: Two semesters of calculus and some experience in programming, CMPS 190 or equivalent and MATH 135, knowledge of Linux/Unix systems, algorithms, basic programming language.

C. Is a selective elective.

Course Learning Outcomes:

Each student by the time of graduation will demonstrate:
1. An ability to analyze a complex computing problem and to apply principles of computing and other relevant disciplines to identify solution (ABET Outcome-1),
2. An ability to apply computer science theory and software development fundamentals to produce computing-based solution (ABET Outcome-6).

Topics:

The students will participate in the programming of real application problems. The problems will vary from semester to semester and will be chosen for intrinsic interest and being easy enough to partially solve and enjoy. A sample problem could be similar to calculate Pi using Monte-Carlo method and compare the efficiency when implement on LONI machines.

Linux/Unix programming environment:
vi/make; Account login/allocation/HPC job running;
MPI & code parallelization
GPU & CUDA
Topics in computational material and biochemistry include:
Program/code optimization
VASP simulation/Perl
MedeA simulation/layered servers
ICM docking/NAMD simulation
CHARMM/AMBER11 simulation
Result visualization
Recent advance in computational bioinformatics
Recent advance in computational materials design

Course Requirements:

There will be assignments/projects and two tests. Several presentations are required. A term paper will be assigned at an appropriate time. Students are expected to attend all lectures, attempt all assignments, and take all tests. Excessive absences will affect your final grade. Assigned tests can only be made up after documented medical excuses are presented. No late homework.

Course Work:

	Approx. weight in grade
Assignments, projects	10%
Midterm	40%
Final	40%
Attendance	10%

Grading:

90%-100%	A
80%-89%	B
70%-79%	C
60%-69%	D
59% and less	F