

CPSC 8810/ECE 8930

High-Performance Computing for Computational Science and Engineering Shuangshuang Jin

Class Location/Meeting Time:

RHDANX 109/ZGEC 106

Tuesday and Thursday 9:30am-10:45pm, January 13 to April 28, 2022

Instructor: Dr. Shuangshuang Jin

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(Charleston)

Course Description

“High Performance Computing (HPC) most generally refers to the practice of aggregating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation.”

With the increasing demand, scale, and data in computational science and engineering, fast modeling and simulation plays a significant role in providing real-time monitoring, analytics, and decision making. This course is designed to provide instruction in the formulation, design, analysis, implementation, and application of HPC approaches in science and engineering.

Multithreading, Open Multi-Processing (OpenMP), Massive Programming Interface (MPI), and CUDA/OpenCL/OpenACC programming on a variety of shared, distributed, or hybrid memory architectures will be introduced as the parallel programming tools. Popular parallel scientific libraries and advanced computational frameworks (e.g., SuperLU, PETSc, Julia, RAPIDS, etc.) will also be introduced to facilitate fast and efficient parallel application development to tackle large-scale complex real-world problems.

Extensive case studies on the intersection of HPC with energy systems will be provided in this class, spanning from the parallel development of standalone power system applications (e.g., power flow, dynamic simulation, contingency analysis, state estimation, etc.), scalable power grid frameworks (e.g., GridPACK, GridLAB-D), to co-simulation infrastructure, an analysis technique that allows simulators from different domains to interact with each other by exchanging values through the course of the simulation (e.g., HELICS, an open-source cyber-physical-energy co-simulation framework for energy systems, with a strong tie to the electric power system.)

The transformative HPC techniques and hands-on parallel programming experiences learned from this class can easily be applied to solve large-scale real-world computational-critical problems in another discipline for in-depth research and development purpose.

Prerequisites: Working knowledge of C/C++ and Linux system. Working knowledge of data structures, algorithms, and linear algebra. Prior knowledge or experience with distributed or parallel computing is a plus.

Course Objectives

- Achieve breadth of learning through introductory lectures on HPC methods and techniques
- Achieve depth of learning through case studies in applying HPC approaches in science and engineering
- Learn multidisciplinary aspects of computation and develop parallel computational thinking and programming skills

Course Outline

Topics covered will include (subject to change):

- Basics of HPC and its application to CSE
- HPC programming interfaces
 - OpenMP
 - Pthreads
 - MPI
 - GPGPU
 - OpenACC
 - CUDA
 - OpenCL
 - Hybrid parallelism
 - MPI+OpenMP
 - MPI+CUDA
 - OpenMP+OpenACC
- Advanced libraires, computational frameworks, and open-source tools
 - BLAS/LAPACK
 - PETSc
 - Julia
 - RAPIDS
- HPC application case studies on Power & Energy Systems
 - GridLAB-D
 - Dynamic simulation
 - GridPACK
 - T&D Co-Simulation
- Discussions & Teamwork
 - Paper digest
 - Term project
 - Presentation
 - Technical writing

Course Materials

- No textbooks are required.
- Slides, online resources, papers, and reading materials will be made available to students during the class.

Laptop Requirements

- Having access to a laptop during class time is critical
 - Working with supercomputing resources in class
 - Working on in-class electronic quizzes on Canvas

Grades

- Graded Components
 - Term Project/Presentation/Essay: 90%
 - Attendance and participation: 10%
- Grading Scale
 - *A*-Excellent indicates work of a very high character, the highest grade given.
 - *B*-Good indicates work that is definitely above average, though not of the highest quality.
 - *C*-Fair indicates work of average or medium character.
 - *F*-Failed indicates that the student knows so little of the subject that it must be repeated in order that credit can be received.

Course Policies

- Attendance: Attendance is encouraged. Substantial project information will be provided in class lectures.
- Academic Integrity: Cheating or plagiarizing on any work for this course will receive no credit for that work. Further action will also be taken if necessary.
- Late-work: An assignment submitted 24 hours of the due date will only be eligible for 80% of the maximum number of point allotted; An assignment submitted 24 to 48 hours of the due date will only be eligible for 50% of the maximum number of point allotted; Assignments submitted more than 48 hours after the due date will not be accepted.
- Re-grade: All requests for re-grades must be submitted within one week of the graded assignments being returned.
- Accommodations for students with disabilities: If you have a documented disability that requires an accommodation, please contact me so we can set up an appointment to discuss your needs. Or contact: Student Disability Services, G20 Redfern, 864-656-6848.
- Mobile Devices: Please refrain from using mobile devices during our class sessions.

Important dates:

- First Class: Thursday January 13, 2022
- Last Day to Add a Class: Wednesday January 19, 2022
- Last Day to Drop a Class without a “W” Grade: Wednesday January 26, 2022
- Last Day to Drop a Class without a Final Grade: Friday March 18, 2022
- Spring Break: Monday March 21 – Friday March 25, 2022

- Final Exams: Monday May 2 – Friday May 6, 2022
- Wednesday Feb 2, 2022: Last day to apply for May graduation