Scientific Computing SC 9502
Winter 2017

Instructor: Colin Denniston, cdennist@uwo.ca, office: MC266. If you wish to contact the instructor, please send an email **using your Western email address** and include *SC9502* in the subject line.

First Class time: First official class will be Monday, 9 Jan. in MC260 3:00-4:30pm We will decide on a day/time for subsequent classes at the first class so please bring your schedule along with you. If you cannot make this time please email the instructor with your course schedule so that we can set a time that works for as many people as possible. It is anticipated that we will have 2 lecture hours and 1 hour problem session/tutorial each week.

Prerequisite Requirements: It is expected that students have a working knowledge of a programming language (C or C++ are preferred, although FORTRAN can also be used) and that they have previously tackled mathematical problems numerically (such as in an undergraduate Numerical Methods course). Ask the instructor if you are unsure.

Course Website: Students should check OWL (http://owl.uwo.ca) on a regular basis for news and updates. This is the primary method by which information will be disseminated to all students in the class. The missing of critical information due to your failure to check OWL cannot be used as a basis for appeal.

Course Materials: Notes, supplemental information, and references will be posted on the course website.

Course Description: The course SCIENTIFIC COMPUTING is designed as an introduction to high-level scientific computing. SC 9502 will focus on algorithms and their parallel implementation for solving matrix and differential equations including stochastic differential equations. Applications to quantum chemistry, financial mathematics, and solid or fluid mechanics will be alluded to but not discussed in detail.

The students will be required to implement their solutions on parallel computers. For this purpose, an introduction to MPI and GPU programming will be given. In some cases, programs or routines will have to be designed 'from scratch,' in other cases, it will be required to use existing packages such as BLAS or LAPACK.

Learning Outcomes: Gain skills and experience in scientific computing, and in particular use of HPC systems to solve grid based research problems using appropriate parallel programming paradigms.

Outline:

1. INTRO (2 weeks): Tools of scientific programming: Git, line terminals, accessing HPC systems, basics of MPI.
2. LINEAR ALGEBRA WITH BLAS/LAPACK AND MPI (1 week)
3. PARALLEL NUMERICAL SOLUTIONS OF LATTICE PROBLEMS WITH MPI (2-3 weeks) Review of some finite difference schemes to solve PDE and other lattice problems. This includes implementation of algorithms on parallel computers using MPI and other aspects of practical importance, such as performance evaluation and optimization.
4. PARALLEL NUMERICAL SOLUTIONS OF LATTICE PROBLEMS WITH CUDA (2 weeks) Introduction to CUDA GPU programming and implementation of finite-difference solutions of PDE's using CUDA.
5. PARALLEL NUMERICAL SOLUTIONS OF LATTICE PROBLEMS WITH OPENCL (2 weeks) Introduction to OpenCl GPU programming and implementation of finite-difference solutions of PDE's using OpenCl
6. STOCHASTIC METHODS (remaining time) Introduction to Monte Carlo methods and numerical solutions to stochastic differential equations.

The depth that we will cover some of these topics may depend on the background of the class and the available time.

Evaluation: The grade will be evaluated based on extensive project-like homework assignments. There will be five or six assignments of similar weight (about one every 2 weeks).

No assignments will be dropped from your grade for any reason (If you are sick and the solutions have already been given out or discussed in class, you will have to do a different make-up assignment). Late assignments will be penalized at a rate of 10% per day.

Assignments must …

- be completed independently. Students may not obtain "help" from the problem solutions of another student in this or any previous class here at Western or any other university, or from any "answer key" from the internet. Students may discuss the problems to help each other, but NOT by simply lending solutions. The final solution must be your own work;
- provide complete solutions, including clear explanations and analysis;
- be completed using neat handwriting or typed;
- have each problem beginning on a new page;
- be submitted in person (problem sets submitted electronically or slid under my office door will not be accepted unless specifically arranged with the instructor);
- be stapled together in one group (unstapled assignments are only guaranteed to have the first page marked). Do not submit your assignment in a plastic "envelope".

Addenda

Academic Accommodation Due to Illness

If you are unable to meet a course requirement due to illness or other serious circumstances, you must provide valid medical or other supporting documentation to your Department's graduate chair as soon as possible and contact your instructor immediately. It is the student's responsibility to make alternative arrangements with their instructor once the accommodation has been approved and the instructor has been informed.

Academic Integrity

Students must write their essays and assignments in their own words. Whenever students take an idea, or a passage from another author, they must acknowledge their debt both by using quotation marks where appropriate and by proper referencing such as footnotes or citations. Plagiarism is a major academic offence.

All required papers may be subject to submission for textual similarity review to the commercial plagiarism-detection software under license to the University for the detection of plagiarism. All papers submitted for such checking will be included as source documents in the reference database for the purpose of detecting plagiarism of papers subsequently submitted to the system. Use of the service is subject to the licensing agreement, currently between The University of Western Ontario and Turnitin.com (http://www.turnitin.com).

You should familiarize yourself with University of Western Ontario's Scholastic Offence Policy. The policy describes the university's process for dealing with scholastic offences, including a list of sanctions: http://www.uwo.ca/univsec/appeals_discipline/index.html

Health and Wellness Insert

As part of a successful graduate student experience at Western, we encourage students to make their health and wellness a priority. Western provides several on campus health-related services to help you achieve optimum health and engage in healthy living while pursuing your graduate degree. For example, to support physical activity, all students, as part of their registration, receive membership in Western's Campus Recreation Centre. Numerous cultural events are offered throughout the year. Please check out the Faculty of Music web page http://www.music.uwo.ca/, and our own McIntosh Gallery http://www.mcintoshgallery.ca/. Information regarding health- and wellness-related services available to students may be found at http://www.health.uwo.ca/

Students seeking help regarding mental health concerns are advised to speak to someone they feel comfortable confiding in, such as their faculty supervisor, their program director (graduate chair), or other relevant administrators in their unit. Campus mental health resources may be found at

http://www.health.uwo.ca/mental_health/resources.html

To help you learn more about mental health, Western has developed an interactive mental health learning module, found here: http://www.health.uwo.ca/mental_health/module.html. This module is 30 minutes in length and provides participants with a basic understanding of mental health issues and of available campus and community resources. Topics include stress, anxiety, depression, suicide and eating disorders. After successful completion of the module, participants receive a certificate confirming their participation.