CMSC6920 Applied Scientific Programming Outline

Winter 2017

Instructors
Dr. Christopher Rowley (Chemistry, crowley@mun.ca)
Dr. Entcho Demirov (Physics, entcho@mun.ca)
Dr. Alexander Bihlo (Mathematics, abihlo@mun.ca)

Class Meetings: SN-2041, Fridays 2 PM – 5 PM, as scheduled by the instructor

Goal: Students will be taught a variety of scientific computing techniques to solve example problems in a number of science disciplines by doing three separate projects.

Structure: There will be approximately 3 hours of classroom time per week. The course will be divided into 3 one-month modules, each taught by a different instructor.

Prerequisites: Students will be expected to hold a B.Sc. or B.Eng. degree, or equivalent, with a strong computational orientation, and have demonstrated knowledge of a computer language such as Fortran, and/or C and/or C++, and/or Matlab, and/or Python.

Grading scheme: The course grade will be principally determined by marks received on the three projects, as well as any additional assignments and tests. The final grade is determined from each module equally.

Module 1. (Rowley): Stochastic Modeling in C++
This module will introduce C++ programming for scientific computing, covering data types, logic, loops, mathematics, and memory allocation. We will then cover basic algorithms, such as random number generators. There will be an applied project to simulate a 2D Ising model using the Metropolis Monte Carlo algorithm. The first component of the evaluation will be based on components your completion of short programming assignments and participation in class discussions of these assignments. The second component will be based on your completion of the requirements of the term project.

Module 2. (Demirov): Climate Modeling
The basic principles of ocean and atmosphere modeling will be formulated. The module will introduce the continuous equations of climate dynamics and numerical methods used in present day climate models. A student-written energy balance model and pre-written 3-D coupled atmosphere and ocean model will be used to study the characteristics of present day climate and climate change. The applied project will be to study computational aspects and efficiency of climate models and physical principles of climate change.

Module 3. (Bihlo): Geometric Numerical Integration
Almost all equations arising in practical applications (such as physics) typically possess geometric properties that are worth preserving in the course of a numerical integration. Such properties can include conservation laws (or first integrals), Hamiltonian structures, symmetries, variational principles, monotonicity, etc. Discretization schemes that numerically capture such geometric properties of differential equations are
termed geometric numerical integrators. In this module we are focusing on several examples for geometric numerical integrators (and comparison against standard numerical schemes) with applications to some important physical models, such as the solar system, point vortex dynamics on the plane and on the sphere, and the equations of molecular dynamics.

**Statement of Inclusion: Students with Disabilities**

Memorial University of Newfoundland is committed to ensuring an environment of understanding and respect for the dignity and worth of each student and also to supporting inclusive education based on the principles of equity, accessibility and collaboration. Students who require physical or academic accommodations are encouraged to speak privately to the instructor so that appropriate accommodations can be made in order that you may participate fully in the course. All conversations will remain confidential.

**Absences Due To Heath Issues**

If you are unable to submit a report or assignment on time due to a health issue, you must verbally declare to the instructor that you require an alternative means of evaluation within one week of the missed requirement. An alternative means of evaluation and new due date will be assigned.

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