Memorial University of Newfoundland

Scientific Computing

CMSC6950 Computer Based Research Tools and Applications

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Intercession 2016
Lectures: MW 0900–1200
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Course Description

Using computers in research computing requires a diverse set of skills and tools for the research to be effective and efficient. The goal of this intensive intercession course is to increase your level of proficiency with using computers to do research in science. The pace and scope of this practical course will be adaptive based on the previous experience of the students.

Computing in research often gets applied with one of two approaches. Some researchers develop new code and have to consider the technical details of numerical analysis and software engineering. Other researchers use proven applications that provide a predefined user interface and have established work flows. This course sits at the interface between those approaches and will cover how to build new programs from other software and libraries. It will also develop automated of research work flows for passing data between different software applications.

Textbook

- Anthony Scopatz, Kathryn D. Huff.
  Effective Computation in Physics: Field Guide to Research with Python.
  O'Reilly Media, 2015.

  Available on-campus through the MUN library at
  `http://proquestcombo.safaribooksonline.com/book/physics/9781491901564`

Evaluation

- Assignments 60%

- Final exam 40%

Lecture Topics

1. Command line and shells

2. Python Scripting

   (a) Introduction to Python
   (b) Regular Expressions
   (c) NumPy and Arrays

3. Software Development

   (a) Revision Control (`git`)
   (b) Building Software (`make`)
   (c) Debugging and Profiling

4. Analysis and Visualization

   (a) 2D plotting (`matplotlib`)
   (b) Movies and Animations

5. Working with Data

   (a) Data Structures
   (b) Files and Formats
   (c) Databases

6. High Performance Computing

   (a) Introduction to the ACEnet facilities
   (b) Parallel Programming
   (c) GPGPU Programming

Miscellaneous

Memorial policies on academic misconduct apply. All submitted work must be original or properly referenced.