Course Overview
Computational Science is an interdisciplinary field that seeks to simulate real-world phenomena. Simulations involve using mathematical models and computer models to generate data, which is then analyzed to assess the models, to make predictions, or to estimate. Simulations can require enormous numbers of computations, so it is with recent advances in computational power and applied mathematics that Computational Science has become an integral part in doing modern science. For example, in computational pharmacology, simulations are run to test new drugs before using live specimens, providing for the development of more accurate drugs. As future practitioners, you may not be implementing simulations, but at minimum this course will enhance your computational skills, expand your understanding of ways mathematics and computer science are used in modern science, develop extensive data-analysis skills, and be fun.

Course Objectives
This course will introduce students to:

1. Some essential elements of computational science;
2. A variety of experimental designs;
3. Appropriate statistical analyses for these designs;
4. Essential computer literacy skills.

Learning Outcomes:
By the end of this course, students should be able to:

- Use descriptive statistics to summarize and visualize data (Obj 1, 3, 4)
  - Compute measures of center and spread
  - Use technology to build useful histograms, bar charts and scatter plots
- Simulate random processes (Obj 1 - 4)
- Build a confidence intervals (Obj 1, 3, 4)
• Single population proportion
• Difference of population proportions
• Single population mean
• Difference of populations means

• Appropriately apply and interpret hypothesis tests on population means and proportions (Obj 1 - 4)
  - Z-test on a single population mean
  - t-test on a single population mean
  - Z-test on a single population proportion
  - Z-test on a difference of two population means
  - t-test on a difference of two population means
  - Z-test on a difference of two population proportions

• Appropriately apply ANOVA in the following cases: (Obj 1 - 4)
  - 1-Way ANOVA
  - Two-Factor ANOVA
  - Data Transformation Scenarios

• Appropriately apply Non-Parametric Statistics including: (Obj 1 - 4)
  - Mann-Whitney U
  - Wilcoxon Rank Test
  - Statistical Bootstrap Methods

• Multiple Regression and Correlation (Obj 1 - 4)
• Goodness of Fit (Obj 1 - 4)
• Contingency Tables (Obj 1 - 4)
• Have a qualitative understanding of the mathematics models utilized in the above (Obj 1)
• Have a general understanding of Experimental Designs relevant to the above (Obj 2)
• In their respective cases, use Python, Excel or SPSS to execute the above (Obj 4)

Assessment will be conducted via in-class assignments, homework, and exams.

Attendance
Students are expected to attend all classes. If you miss a class, you are responsible for any assignments or announcements made.

Homework
Homework problems will be assigned each day, with some problems to be collected and graded. Unless otherwise noted, homework will be due at the beginning of the next class period. Homework that is too late (instructor’s discretion) won’t be accepted. Exams will be strongly influenced by all
assigned problems, so it is to your advantage to learn how to do all assigned homework. Collected problems will be given integer scores between 0 and 4: 4 = essentially flawless; 3 = minor errors, but no major errors; 2 = one major error; 1 = at least two major errors; 0 = no attempt or the solution is unintelligible.

**In-Class Work**
Some assignments will involve completing work in class, and as with homework, some of these will be collected and graded, using the same grading scheme as above.

**Projects**
You will complete a project during the semester. The goal of the project is to allow you to apply methods of computational science to an issue of your interest. In the project you will choose the issue of study, supply your own conjecture, design the experiment, simulate the experiment, and then present, analyze, and interpret the data appropriately. Simulations that strive for creativity and realism will be rewarded. The project will be completed in three parts, with each part a prerequisite to the next, i.e., Part II cannot be done without Part I being completed first. Late assignments will be accepted if and only if acceptable written documentation is provided. The due dates of the individual parts are given below.

<table>
<thead>
<tr>
<th>Project</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Part I</td>
<td>February 16</td>
</tr>
<tr>
<td>Part II</td>
<td>March 23</td>
</tr>
<tr>
<td>Part III</td>
<td>April 25</td>
</tr>
</tbody>
</table>

**Exams**
There will be three comprehensive 2-hour exams. Exams and will measure both your conceptual understanding of the material and your problem solving skills. I expect the first two exams will given on February 23 and April 6. The third exam will be given at 11:00 am on Monday, May 8. If you miss an exam, acceptable written documentation for the absence must be supplied to be eligible for a make-up.

**Academic Honesty**
All work on assignments, quizzes and tests is expected to be your own and represent your ability in course content. The Carroll University Academic Integrity Policy is located in your student handbook. Please familiarize yourself with this policy. If a student violates this policy in any way, the instructor or College reserves the right to impose a sanction of failure on the assignments/assessment or failure in the course.

**Grades**
The grading scheme is as follows:
<table>
<thead>
<tr>
<th></th>
<th>Percent</th>
</tr>
</thead>
<tbody>
<tr>
<td>Homework</td>
<td>35%</td>
</tr>
<tr>
<td>Project</td>
<td></td>
</tr>
<tr>
<td>Part I</td>
<td>3%</td>
</tr>
<tr>
<td>Part II</td>
<td>3%</td>
</tr>
<tr>
<td>Part III</td>
<td>9%</td>
</tr>
<tr>
<td>Exam I</td>
<td>15%</td>
</tr>
<tr>
<td>Exam II</td>
<td>15%</td>
</tr>
<tr>
<td>Exam III</td>
<td>20%</td>
</tr>
<tr>
<td>Total</td>
<td>100%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Percent Interval</th>
<th>Grade</th>
</tr>
</thead>
<tbody>
<tr>
<td>[92, 100]</td>
<td>A</td>
</tr>
<tr>
<td>[88, 92)</td>
<td>AB</td>
</tr>
<tr>
<td>[82, 88)</td>
<td>B</td>
</tr>
<tr>
<td>[78, 82)</td>
<td>BC</td>
</tr>
<tr>
<td>[68, 78)</td>
<td>C</td>
</tr>
<tr>
<td>[58, 68)</td>
<td>D</td>
</tr>
<tr>
<td>[0, 58)</td>
<td>F</td>
</tr>
</tbody>
</table>

Final day to drop: April 5.

Carroll Portal (LMS)
This course will use the Carroll Portal for various purposes, including for your grades. Keep track of your grades, and notify the instructor should you spot an error.

Final Notes
1. Special accommodations for this course may be granted via direct orders from the Walter Young Center (WYC). It is your responsibility to notify the WYC of your special needs. (They will require certain forms of verifiable documentation or diagnoses.) Such accommodations will be made only after the instructor has received notification from the WYC, and will not be given retroactively for previous assignments or exams.

2. The instructor and the College reserve the right to modify, amend, or change the syllabus (course requirements, grading policy, etc.) as the curriculum and/or program require(s).

Tentative Schedule
- (1 week) Review descriptive statistics and simulation of random processes
- (1 week) Confidence intervals for single and difference of population means
- (2 week) Hypothesis tests on population means and proportions
- (2 weeks) Regression and correlation, including multiple regression
• (1 week) 1-Way ANOVA
• (1 week) Two-Factor ANOVA
• (1 week) Data transformation scenarios
• (2 weeks) Non-parametric statistics
• (1 week) Goodness of fit
• (1 week) Contingency tables