1 Course Description

This course concerns scientific libraries as the most effective form of communication for advances in scientific computation. We will learn how to design, implement, test, distribute, and maintain a numerical library for the finite element method written in a higher level languages, such as C, Fortran, and Python. Emphasis will be placed solving practical computational problems and providing insight to the user on code accuracy, performance, and tradeoffs. We will also cover basic techniques of algorithm design and implementation, project planning, source management, configuration and build tools, documentation, program construction, i/o, and visualization.

This course will require extensive programming, and familiarity with development tools! Students will learn to write software as a library developer, meaning that they will construct software usable by others. This is a crucial skill for modern computational science, which needs an understandable (modular, hierarchical), extensible, maintainable infrastructure. In particular, this class will construct a finite element library, incorporating the latest advances in FEM, optimizing for leading manycore architectures such as the Intel Xeon Phi and Nvidia Pascal lines, and applied to practical computational problems.

1.1 Infrastructure

Software development practice should be as familiar to modern computational scientists as laboratory practice to physical scientists. Building code, version control, interface design, and debugging should be second nature, and form a firm foundation mathematical modeling and algorithmic experimentation. Moreover, students will learn how to communicate their advances using \LaTeX, obtain DOIs for research products, and disseminate code using hosting sites.

1.2 Texts

There are no required texts for the course, and all material will be provided online as notes and slides by the instructor. The recommended reference texts are The C Programming Language by Brian W. Kernighan and Dennis M.
Ritchie and The \LaTeX Companion by Frank Mittelbach, Michel Goossens, Johannes Braams, David Carlisle, and Chris Rowley, both of which will be available from the book store. In addition, The PETSc Manual, available online, should prove very helpful for the assignments. Recommended texts for foundational FEM concepts include The Mathematical Theory of Finite Element Methods by Brenner and Scott, Discontinuous Galerkin Methods for Solving Elliptic and Parabolic Equations: Theory and Implementation by Riviere, and Automated Solution of Differential Equations by the Finite Element Method from the FEniCS Project.

2 Objective

CAAM 520 students learn to design, implement and manage scientific computing libraries using the C programming language, leveraging their knowledge of applied mathematics, numerical analysis, and algorithmics.

3 Absence Policy

Attendance is not required, however much of the class will be concerned with the discussion and group work which happens during class time. Students who will miss more than 3 classes should consult the instructor.

4 Special Materials

It will not be possible to complete this course without access to a computer for coding and running assignments. If a student does not currently have access, they must contact the instructor and arrange an alternative by the first week of class.

5 Office Hours

Office hours will be held in 3021 Duncan Hall from 1pm–2pm every Tuesday. The instructor will also be available by appointment if that time is unavailable or oversubscribed.

6 Rice Honor Code

In this course, all students will be held to the standards of the Rice Honor Code, a code that you pledged to honor when you matriculated at this institution. If you are unfamiliar with the details of this code and how it is administered, you should consult the Honor System Handbook. This handbook outlines the
University’s expectations for the integrity of your academic work, the procedures for resolving alleged violations of those expectations, and the rights and responsibilities of students and faculty members throughout the process.

7 Disability Support Services

If you have a documented disability or other condition that may affect academic performance you should: 1) make sure this documentation is on file with Disability Support Services (Allen Center, Room 111 / adarice@rice.edu / x5841) to determine the accommodations you need; and 2) talk with the instructor to discuss your accommodation needs.

8 Syllabus Change Policy

This syllabus is only a guide for the course and is subject to change without advanced notice.