Computational Science for the Undergraduate Environment

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Abstract -- Computational Science, defined as the intersection of mathematics, computing, and science, can be naturally integrated into existing undergraduate mathematics and science curricula. The interdisciplinary nature of computational science integrates ideas from applied mathematics, computing, and visualization to solve problems from diverse areas in science, engineering, and finance. Supported by grants from the National Science Foundation and Battelle, Capital University is creating a comprehensive program culminating in a minor in Computational Science. The program is designed for the undergraduate Liberal Arts Environment. Components of the program could also be easily integrated into existing engineering curricula. The curriculum provides a collection of courses defined as core and electives. Core courses educate students in modeling using various computational science tools, while electives provide more in-depth understanding in the Computational fields of: biology, chemistry, environmental science, psychology, and neuroscience.

Index Terms – computational science, curriculum, modeling, visualization

Work in Progress

Computational Science is an emerging and rapidly growing interdisciplinary field at the intersection of mathematics, computing, and science. It is a new discipline that investigates ways of using mathematical modeling, computing, and visualization to solve complex scientific problems. It is considered to be the third methodology in the development of scientific knowledge, alongside theory and experimentation. Its true interdisciplinary nature integrates concepts from applied mathematics (calculus, matrix/linear algebra, ordinary differential equations/ partial differential equations, statistics, numerical analysis) and computer science (programming, parallel computing, visualization) into the solution process of problems from the disciplines of physical/life/behavioral sciences, engineering, and finance.

Funded by a grant from the National Science Foundation (CCLI-EMD, DUE 9952806), and supported by a grant from Battelle, Capital University is in the process of designing a comprehensive undergraduate program culminating in a minor in Computational Science. The program is for mathematics, science, and pre-engineering majors. Since modeling is an integral part of any computational experiment, and since (applied) mathematics is the core of modeling, all courses have a mathematical component. One of the goals of the program is to present mathematics within the context of science problems, and also to demonstrate how computing technology (symbolic, numeric, parallel, graphical/visualization) should be used to solve problems from various scientific disciplines.

The curriculum consists of core and elective courses. Core courses include: i) two courses in Computational Science (using Maple/ Mathematica/ Matlab to solve science related problems, numerical computations of mathematical techniques, and topics in visualization); ii) a course in computational and Applied Mathematics (integrating ideas from the fields of linear/ matrix analysis, difference/ differential equations, and numerical analysis); iii) a capstone team-based undergraduate research experience. Elective courses include: i) two courses in parallel and high performance computing; ii) a course in scientific visualization; iii) an array of courses designed as Computational X (X = Biology, Chemistry, Environmental Science, Neuroscience, Physics, Psychology.) Each course consists of a collection of modules/ case studies which follow the scheme: problem, background (science, math), model, method, implementation, assessment. Furthermore, conceptual questions are integrated into each module as well as homework and student projects.

The structure of the program will be presented, outlining each course, and the integration of the minor into existing curricula will be analyzed. Also, specific modules (enzyme kinetics, models of infectious diseases, self-esteem, satellite surveillance) from the Computational Science I course will be presented. The content of other courses will also be provided.