MODULE 1.1

Overview of Computational Science

Many significant applied and basic research questions in science today are interdisciplinary in nature, involving physical and/or biological sciences, mathematics, and computer science. For example, *Nature* reported that John Krebs, chief executive of Britain's Natural Environment Research Council, considers that the environment "requires a 'new breed' of scientist, and new ways of problem solving that cut across traditional disciplines" and that Britain expects a shortage of "environmental scientists with mathematical, computational and statistical skills." (Masood 1998)

The Human Genome Project "has created the need for new kinds of scientific specialists who can be creative at the interface of biology and other disciplines, such as computer science, engineering, mathematics, physics, chemistry, and the social sciences. As the popularity of genomic research increases, the demand for these specialists greatly exceeds the supply. . . . There is an urgent need to train more scientists in interdisciplinary areas that can contribute to genomics," according to Francis Collins in an article in *Science* (Collins et al. 1998).

Computational science is a fast-growing interdisciplinary field that is at the intersection of the sciences, computer science, and mathematics. There is a critical need for scientists who have a strong background in computational science. Much scientific investigation now involves computing as well as theory and experiment. Computing can often stimulate the insight and understanding that theory and experiment alone cannot achieve.

This field of computational science combines computer simulation, scientific visualization, mathematical modeling, computer programming and data structures, networking, database design, symbolic computation, and high performance computing with various scientific disciplines. Computer simulation and modeling offer valuable approaches to problems in many areas, as the following examples indicate.

1. Scientists at Los Alamos National Laboratory and the University of Minnesota wrote, "**mathematical modeling has impacted our understanding of HIV pathogenesis**. Before modeling was brought to bear in a serious manner, AIDS was thought to be a slow disease in which treatment could be delayed until symptoms appeared, and patients were not monitored very aggressively. In the large, multicenter AIDS cohort studies aimed at monitoring the natural history of the disease, blood typically was drawn every six months. There was a poor understanding of the biological processes that were responsible for the observed levels of virus in the blood and the rapidity at which the virus became drug resistant. Modeling, coupled with advances in technology, has changed all of this." Dynamic modeling not only has revealed important features of HIV pathogenesis but has advanced the drug treatment regime for AIDS patients (Perelson and Nelson 1999).

2. Boeing Airline engineers completely designed **The Boeing 777 jetliner** using three-dimensional computer graphics. "Preassembly" of the airplane on the computer at every stage of the design process eliminated the necessity of a costly, full-scale mock-up and reduced error, adjustments, and revisions by 50 percent (Boeing). The pilots that fly these and other large airplanes train on sophisticated, computer flight simulators, which enable the pilots to practice dealing with dangerous situations, such as engine fire and wind shear.

3. From the 1960s, numerical **weather prediction** has revolutionized forecasting. "Since then, forecasting has improved side-by-side with the evolution of computing technology, and advances in computing continue to drive better forecasting as weather researchers develop improved numerical models" (Pittsburgh Supercomputing Center 2001).

4. Researchers at the University of Washington's School of Fisheries are employing mathematical modeling to examine the **impact on fish survival of the removal of four dams** on the lower Snake River. Another team at the University of Tennessee's Institute for Environmental Modeling is using computational ecology to study complex options for **ecological management of the Everglades**. Louis Gross, Director of the Institute, says that "computational technology, coupled with mathematics and ecology, will play an ever-increasing role in generating vital information society needs to make tough decisions about its surroundings" (Helly et al.).

5. A group of engineers and computer scientists at Carnegie Mellon University and seismologists from the University of Southern California and the National University of Mexico is building three-dimensional computer simulations of **ground motion during earthquakes** to predict how areas, such as the Greater Los Angeles Basin, will behave during such a disaster. Using powerful parallel-processing computer systems, one simulation indicated a complex pattern of basin ground motion with some sites experiencing nine times greater motion than others. With such information, scientists can predict the damage in an area (Pittsburgh Supercomputing Center 1997). Seattle, Washington is another area prone to earthquakes. The National Tsunami Hazard Mitigation Program has an extensive simulation modeling effort to assess the hazards of **tsunami threats** after earthquakes in the Puget Sound region so that officials can plan and mitigate their dangers (Koshimura and Mofjeld 2001). With computational models, others have studied the **economic impact** of disruption to the water supply caused by an earthquake in the Portland, Oregon region and appropriate responses to minimize the consequences (Rose and Liao).

Such collaboration among scientists, mathematicians, engineers, and computer scientists is indicative of much computational science research and practice. The fruits of these researchers' models and simulations are a deeper understanding of complex systems, a better foundation for important decisions, and a revolution in scientific advances that are helping people all over the world.

Projects

1. Investigate three applications of computational science involving different scientific areas and write at least a paragraph on each. List references.
2. Investigate an application of computational science and write a three-page, typed, double-spaced paper on the topic. List references.

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