COMPUTATIONAL SCIENCE AND ENGINEERING (CS&E) Taking Its Place alongside Theory and Experiment as a Way of "Doing Science"

The digital computer was invented for numerical calculation, specifically to compute solutions to problems that are too lengthy to be solved "by hand.'' Computational Science and Engineering (CS&E) describes the use of computers to solve problems in science and engineering. It is an enterprise that permeates the entire breadth of science and engineering, with computation taking its place alongside theory and experiment as a way of "doing'' science. It is also an enterprise that is thoroughly interdisciplinary, drawing on computer science and mathematics for its methodology as it addresses scientific problems.

Three dramatically new aspects of CS&E are the ability to:
- Simulate complex systems
- Construct approximate solutions to problems that cannot be expressed directly in terms of analytic formulas
- Store, manipulate, and analyze complex sets of data

These characteristics of CS&E are exemplified by numerical weather prediction and climate modeling. People observe the weather and most rely on weather forecasts generated by national governments. Although people grumble about the reliability and accuracy of the forecasts, they have improved markedly over the past 20 years, due mostly to better simulation.

How does numerical weather prediction work? Physical principles lead to systems of equations for fluid flow in the atmosphere. These, together with databases of topographical information provide the starting point for numerical weather prediction. Researchers cannot expect that these equations can be solved in closed form. Instead, the atmosphere is "discretized''—broken into small units and the physical principles are used to predict how these units change over a short time.

Beginning with the current weather observations, repeated time steps are taken to produce forecasts farther into the future. The computational science that enters into weather forecasting includes:
- How current observation details are used to initialize the simulations
- How the atmosphere is discretized
- How physical laws are applied in the simulations
- How the reliability of a forecast is assessed

Note that these issues would remain even if the observations of researchers were entirely accurate and their

Academic Programs

Cornell has a long history of contributions to computational science and engineering—both in areas of application and in methodologies that support the enterprise. The programs in Computing and Information Science are bringing greater coordination to academic activities in CS&E across the university. The first step has been to organize and offer a set of mini "tools'' courses that introduce students to computational techniques. However, graduate students pursuing computational science and engineering can benefit from more extensive training in CS&E methods. Therefore, planning is underway to establish a CS&E graduate minor for Ph.D. students. The goal of this minor is to establish a strong technical foundation in CS&E for students pursuing CS&E research or careers.

Computing and Information Science sponsorship is helping to bring stronger computational science into an Integrative Graduate Education and Research Traineeship (IGERT) program in Nonlinear Systems. During a five-year span, this NSF–funded program provides 30 graduate student fellowships (each for two years) to participate in education and training activities that transcend disciplinary boundaries. Nonlinear dynamics is a central theme in the program, which draws participants from more than a dozen graduate fields. The proposed focus areas for the next three to five years are in:
- Networks
- Gene regulation and signal transduction
- Moving machines and organisms
- Biological pattern formation

In each of these areas, faculty groups will mentor research projects that bring computation together with theory and empirical data. An important part of the program is a course on computational methods offered by CIS.

knowledge of the physical laws of processes, such as cloud formation, was perfect. Because the atmosphere is turbulent and unstable, researchers expect numerical errors in the forecasts to grow and that there will be a finite time horizon for accurate predictions.

Computing methods pull together CS&E research on scientific problems that initially seem to have little in common with one another. Researchers find that abstract concepts rooted in computer science and mathematics often lead to accurate, efficient methods of solving large classes of problems. For example, models of physical processes such as atmospheric circulation are often formulated as differential equations, which relate the rates of change of different quantities in space and time. Mathematical theory helps researchers understand how many solutions to equations of different kinds to expect and how these solutions depend on parameters appearing in the problem. Computer science helps researchers to develop data structures and algorithms that can be used to compute (approximate) solutions. Numerical analysis helps researchers to understand and improve the accuracy of these solutions. Techniques for visualization help researchers to condense and interpret the information in the solutions. Systematically organizing information in specialized databases helps to analyze the information further with statistical methods, for example. Each of these aspects of computational science and engineering has its own community of experts, and each community contributes to the solution of complex problems like weather prediction.

CS&E research at Cornell takes place in many departments, centers, and institutes. In particular, the Cornell Theory Center has been a leader in parallel computing technologies since its inception in 1984 and continues to provide large-scale computing resources to the Cornell research community. The Center for Applied Mathematics and its Graduate Field in Applied Mathematics have nurtured CS&E since their inception 40 years ago. To give a sense of the broad, diverse research in CS&E, research vignettes of three "founding members'' of the Faculty for Computing and Information Science follow.

John M. Guckenheimer
Professor of Mathematics

- **Mathematical theory** helps researchers understand how many solutions to different kinds of equations to expect and how these solutions depend on parameters appearing in the problem.
- **Computer science** helps researchers to develop data structures and algorithms that can be used to compute (approximate) solutions.
- **Numerical analysis** helps researchers to understand and improve the accuracy of these solutions.
- **Techniques for visualization** help researchers to condense and interpret the information in the solutions.
- **Systematically organizing information in specialized databases** helps to analyze the information further with statistical methods.