Computational Science and Engineering

In Computational Science and Engineering (CSE) mathematical models and computational methods are developed and used to study and solve problems in science and engineering. Research in CSE is thus inherently interdisciplinary and requires domain expertise in the natural or engineering sciences; mathematical modeling and analysis; construction and analysis of numerical algorithms; software development and implementation, often on large-scale parallel and distributed computers; validation; and analysis/visualization of results. Generally, know-how in CSE is distributed throughout the departments within the Faculty of Science and Technology.

A more detailed discussion of the CSE area can be found at http://www.siam.org/students/resources/report.php

Examples of Present CSE Research Areas at UmU
Examples of research projects 2009 at Umeå University (UmU) that can be characterized as CSE are:

• Development of numerical solution methods for problems modeled by partial differential equations with applications in industrial and medical fluid dynamics, and acoustic/electromagnetic wave propagation.
• Development of network models and computer simulation techniques for simulation of evolution processes.
• Development of statistical or data mining techniques with applications in bioinformatics.
• Systems biology of plant and mammalian biology integrating experimental sciences in chemistry, biology and medicine with bioinformatics, mathematics, data driven modelling and visualization.
• Visual and interactive multiphysics simulation for engineering, design and training simulators.
• Mathematical modeling in ecology and evolution.
• Development of theory, algorithms and state-of-the-art software tools for matrix computations in computer-aided control system design and analysis.

In the final section a more detailed description of these CSE areas is given.

CSE Related Research Organizations at UmU
Interdisciplinary research organizations are now established at UmU. These joint efforts all aim at creating interdisciplinary environments in, or closely related to, the CSE area.

• Modeling Science Lab
• UMIT Research Lab
• Computational Life Science Cluster (CLiC)

Furthermore, High Performance Computing Center North (HPC2N) provides state-of-the-art computational and grid infrastructure as well as leading expertise in high-performance and parallel computing.
The study plan in CSE

The study plan in CSE was created based on many reasons of which some are listed below:

- CSE relevant projects appear at most departments of the faculty. A typical example could be a trained computer scientist who applies mathematical modeling, physical simulations, anatomy, and biochemical imaging to study skeletal muscle dynamics. This new way of doing research requires integrative thinking and close interaction between different scientific disciplines.
- CSE projects do not in general fit into the requirements of the other study plans at the faculty. The broad skills needed for a CSE researcher are cross-disciplinary, which may be in conflict with the required broad knowledge in the domain area which is normally required for a PhD in a particular field. The new interdisciplinary CSE PhD therefore helps to avoid “dilution” of the previous more specialized study plans. degrees. The CSE study plan therefore complements to existing PhD degrees that still serves their original purpose.
- The degree PhD in CSE will in many cases better reflect the actual expertise and training of PhD candidates in this interdisciplinary field.
- The CSE study plan provides a structure to improve quality; exploit synergy effects, for instance joint courses and seminars; exchange of knowledge; and bring people in different departments with similar interests together.
- The CSE study plan plays an important role for the future development of the new interdisciplinary research organizations mentioned above.
- Many sources of funding now require interdisciplinary projects. Therefore the CSE study plan creates a strategic advantage for UmU in the competition for future funding.
- CSE research centers and PhD programs are now established at leading universities around the globe and the field is rapidly growing and gaining recognition as an important scientific mode of investigation, along with theory and experiment. To take part of and contribute to this development it was important for UmU to establish the CSE study plan.
- The CSE study plan gives critical mass in the number of students and thus better economy and motivation e.g. for arranging joint courses.

PhD Curriculum

There is one CSE study plan, common for all departments with specializations in: Biology, Chemistry, Computing Science, Mathematics, Mathematical Statistics, and Physics. The PhD thesis work is devoted to an application within the discipline of specialization. The specializations in Computing Science, Mathematics, and Mathematical Statistics will involve significant aspects of an application in science or engineering but is characterized by development of CSE software tools, models, and methods to a higher degree than specializations in other disciplines.

The doctoral students will be encouraged to apply for participation in the National Graduate School of Scientific Computing (NGSSC). NGSSC is funded by the Swedish Research Council (Vetenskapsrådet) and provides and funds training in mathematics and computations for Swedish PhD students. Participation in NGSSC will also provide the students with a national network of fellow students devoted to CSE. The department of Computing Science and HPC2N have developed and given several NGSSC courses.
Examples of CSE Projects at UmU

Computational Partial Differential Equations
The most complete mathematical models for phenomena in the physical, biological, and medical sciences are given in terms of partial differential equations. Before the advent of computers, these models were often quite useless in themselves, since these equations cannot in general be solved “analytically”. The explosive development of computers and efficient numerical methods to exploit the hardware is increasingly making partial-differential-equation modeling into an indispensable tool in scientific inquiry and engineering design. Using numerical techniques, we may study the behavior of the system and also study techniques to control or optimize the system behavior. For instance, we may among millions of possible configurations find the geometric shape of a mechanical component so that the strength is maximized subject to given weight and load conditions. Recent developments in massively parallel computer resources provide the possibility of solving very complex problems involving different types of physics coupled over different scales. However, emerging computer architectures also demand the development of new methods that decouple the underlying problems as much as possible in order to make optimal use of the parallel computing capacity. Another important current trend is to study the effects of uncertainty in input data or the model itself using statistical techniques. In short, research in this area is interdisciplinary and depends on a combination of mathematics, statistics, numerical analysis, computer science, and knowledge of modeling the application field.

Complex Networks
Many systems in nature and society consist of large numbers of interacting units – financial markets, bird flocks, car traffic, nervous systems, Internet, etc. The key to understanding such systems lies in the interaction between the agents. From all the interaction, global properties emerge. The study of emergent phenomena is the broader context of our research. Our approach is to construct mechanistic models - mathematical models where the units are represented individually, including their interactions and response to the environment. These models can be investigated mathematically or computationally, or form tools for analyzing data. Our research concerns both more theoretical, methodological questions and specific questions about concrete systems. Frequently, the units of complex systems are interacting via a network. Such networks, both in nature, society and technology can often be described as being, to some extent, random, but also having structure. Typically, the functionality of a networked system is related to dynamic systems on the network (flow of merchandise in trade, data packets in the Internet, electric pulses in the nervous system, etc.). In such cases, the network structure tells us something about the behavior of the dynamic system. One central question in much of our group’s research is to relate the dynamic functionality to network structure.

Mathematical Ecology
Mathematical and computational models are increasingly recognized as important tools for understanding complex ecosystem. Major advances during the last decades have brought us to a point where modeling cannot only be used to elucidate general patterns, but also to describe, understand, and predict the dynamics of specific systems. Two important examples of such advances are the theory of physiological structured population models that makes it possible to formulate and
analyze ecologically realistic models and the development of eco-genetic and adaptive dynamics modeling techniques that greatly facilitate the study of evolutionary processes. While these developments have opened up new frontiers on the interface between the life sciences and the quantitative sciences, the demand for expertise in both the theoretical and empirical domains often necessitates an interdisciplinary approach. The scientific efforts at Umeå University are focused on interdisciplinary collaborations where mathematical and computational modeling is used to explore ecological questions and on methodological advances in ecology and evolution.

Bioinformatics and Computational Modeling
Biology, including medicine, has to a large extent become an information science and bioinformatics and data mining are now a prerequisite for all experimental and applied biology, including drug discovery, vaccine development and high-throughput technologies. In fact, computational modeling is now accepted as a third mode of science, along theory and experiment. Bioinformatics is a multidisciplinary discipline that solves problems in life science using computer science, mathematics and statistics. Therefore, a successful bioinformatician generally needs knowledge in life science, computer science and statistics. Computational Life Science Cluster (CLiC) at Umeå University, provides a critical and missing link in computational modeling and informatics for experimental sciences, e.g. at Umeå Centre for Microbial Research (UCMR) and Umeå Plant Science Center (UPSC). CLiC encompass approximately 30 researchers (principal investigators, doctoral students and postdocs) that are physically co-located and include six different departments at both Faculty of Science and Technology and Medical Faculty. This interdisciplinary competence makes CLiC unique. Our core expertise is in A.) high throughput technologies, B.) Network modeling, databases and visualization and C.) Structural biology and sequence analysis.

Visual Multiphysics
Visual multiphysics concerns modeling, numerical simulation and visualization of multibody systems, e.g., involving rigid articulated bodies and viscoelastic solids with dry or wet friction, fluids and gases, and complex materials like sand and organic tissue. These are building blocks for realizing complex systems of vehicles, robots, bio-mechanical systems and the complex environments in which these exist and operate. Among the application areas are visual interactive simulation software for vehicle operator training, surgical simulation, design and virtual prototyping, computer and video games, learning and education, 3D animations, and CAD/CAE. The rapid development of computing hardware, e.g., many-core processors, GPU-computing, and of model and data standardization raises big challenges for the field. The research ranges from fundamental aspects of temporal and spatial discretization of the physical world, to 3D computer graphics and haptics, topological analysis of the system, algorithms for adaptive resolution and parallel computing. It is also a complimentary field in many other research groups, as well as one of the areas for strategic recruitment and growth within UMIT.
Computer Aided Control System Design

Computer Aided Control System Design (CACSD) is a broad interdisciplinary field that concern the study of algorithms, computers and software to be used as enabling technology in control engineering. Since several years a research program at Computing Science, funded by the Swedish Foundation for Strategic Research (SSF), is focusing on the development of theory, algorithms and state-of-the-art software tools for matrix pencil computations in CACSD applications. Outgoing from generalized state-space (descriptor) systems, which, e.g., arise from modeling interconnected systems (electrical circuits) and mechanical systems (multi-body contact problems), several critical ill-posed computational problems encountered in the analysis and synthesis of descriptor systems are considered. Examples include computing subspaces and canonical structure information of the associated system pencil, various matrix equations (Sylvester, Riccati), and complicated nearness problems (distance to uncontrollability/unobservability). For large-scale systems, these problems are fundamental in model reduction applications. Presently, much attention is put on periodic systems, i.e., models that originate from applications with a periodic or seasonal behavior, and the corresponding challenging structured high-dimensional matrix problems. Most recently, numerical methods for solving periodic Riccati differential equations have been developed and evaluated.