Computational Science and Engineering

What is Computational Science and Engineering?

Advanced computation and simulation in science and engineering constitute an important area in rapid growth in many leading industrial nations. The background for this is the continuing development of efficient computer hardware that has been seen over the past few decades which in turn has imposed an exceptional activity in the progress of vector and parallel computing, numerical algorithms and visualization. The consequence is that new vistas have been opened for realistic computer simulations of mathematical models in engineering and science. We will here use the term *Computational Science and Engineering* or CSE for those activities in science and engineering where computers play a significant role. The importance of CSE has been realized in many countries like USA, Japan, Australia and several European countries. A variety of research programs have been initiated and funded within the fields of high performance computing and its applications, algorithm design, and scientific visualization.

Ingredients of CSE

The use of CSE is ubiquitous in applications, like e.g. solid and structural mechanics, fluid mechanics, optimization in processing and production technology, technological design, aerodynamics, meteorology, electromagnetism, chemistry, physics, medicine and so on. The field of CSE is vast and relies on methods which are interdisciplinary. There is a common core of numerical methods, mathematical analysis and modeling and aspects of computer science.

- *Mathematics* play a central role, a very large and important class of mathematical models in engineering are formulated by means of partial differential equations, including complex geometries and boundary conditions, phenomena occurring on different time scales etc. The prior mathematical analysis of the model is paramount to a successful numerical simulation.
- The most popular *numerical methods* for partial differential equations include finite -difference, -element, -volume, and spectral methods. In most cases these discretization techniques lead to a system of algebraic equations that needs to be solved, and to overcome the vast computational challenges in solving such equations, it is necessary to develop and use algorithms that can take advantage of the potential of parallel machine architectures. Modern numerical methods also include grid generation techniques, convergence acceleration, error estimation and adaptivity. It is important to keep in mind that the fast development of new computers and machine architectures causes a dynamic change in optimal numerical methods. Algorithms that were popular ten years ago may have become obsolete in view of today's technology.
- Obviously, the modeling and design of software for these simulations is complicated by the existence of a large variety of machine architectures and numerical algorithms that are tailored for particular applications and computer hardware. It is necessary to make use of modern methods for design and modeling of such software, in recent years there has been a significant increase in the activity of developing object oriented numerical software, the aim being to overcome the difficulties of writing portable and reusable code. Finally, when large scale

simulations are performed on problems with complex geometries, there is a need to be able to interpret the results of the simulations. The recent development of advanced visualization equipment is of great importance in CSE, and the task of utilizing this equipment in an optimal way is considered an inherent part of the field.

CSE is apparently multidisciplinary with dynamic activity of great complexity. The aim of this activity is to improve the quality of computer simulations in applications. To exploit the potential for such improvements in full, it is necessary to use state of the art techniques from a variety of fields. The time when it was possible for engineers to acquire sufficient depth knowledge in all aspects of computation seems to be a bygone era. On the other hand, to succeed in breaking computational barriers within a particular application area, detailed knowledge of the nature of the physical problem is required, knowledge that can only be achieved through experience with computation and observation of physical phenomena where they occur, either in the real world or in a laboratory. Ideally there should thus be a symbiotic relationship between engineers, mathematical and numerical analysts and computer scientists. We have tried to picture the ingredients of CSE *as traditionally seen by the engineer* in the figure below. The application is in the center of his attention, but in order to solve the computational problems involved, he needs elements of mathematical modeling, numerical analysis and computer science. In the modern setting, sometimes denoted *the third paradigm*, the generic aspects of computation are put in focus.