

Graduate Education in Computational Science and Engineering*

SIAM Working Group on CSE Education†

Abstract. Computational science and engineering (CSE) is a rapidly growing multidisciplinary area with connections to the sciences, engineering, mathematics, and computer science. In this report we attempt to define the core areas and scope of CSE, to provide ideas, advice, and information regarding curriculum and graduate programs in CSE, and to give recommendations regarding the potential for SIAM to contribute.

PII. S0036144500379745

1. Introduction. Computation is now regarded as an equal and indispensable partner, along with theory and experiment, in the advance of scientific knowledge and engineering practice. Numerical simulation enables the study of complex systems and natural phenomena that would be too expensive or dangerous, or even impossible, to study by direct experimentation. The quest for ever higher levels of detail and realism in such simulations requires enormous computational capacity, and has provided the impetus for dramatic breakthroughs in computer algorithms and architectures. Due to these advances, computational scientists and engineers can now solve large-scale problems that were once thought intractable.

Computational science and engineering (CSE) is a rapidly growing multidisciplinary area with connections to the sciences, engineering, mathematics, and computer science. CSE focuses on the development of problem-solving methodologies and robust tools for the solution of scientific and engineering problems. We believe that CSE will play an important if not dominating role for the future of the scientific discovery process and engineering design.

It is natural that SIAM, as the society whose aim is to foster the computational and applied mathematics which is at the core of CSE, should play a role in the growth and development of this new discipline. The objectives of this report are to attempt to define the core areas and scope of CSE, to provide ideas, advice, and information regarding curriculum and graduate programs in CSE, and to give recommendations regarding the potential for SIAM to contribute.

2. Definition of CSE.

2.1 What Is It? CSE is a broad multidisciplinary area that encompasses application (science/engineering), applied mathematics, numerical analysis, and computer science and engineering (see Figure 1). Computer models and computer simulations have become an important part of the research repertoire, supplementing (and in

*Published electronically February 2, 2001.
<http://www.siam.org/journals/sirev/43-1/37974.html>

†For further information contact Linda R. Petzold, Department of Mechanical and Environmental Engineering, University of California, Santa Barbara, CA 93106 (petzold@engineering.ucsb.edu).

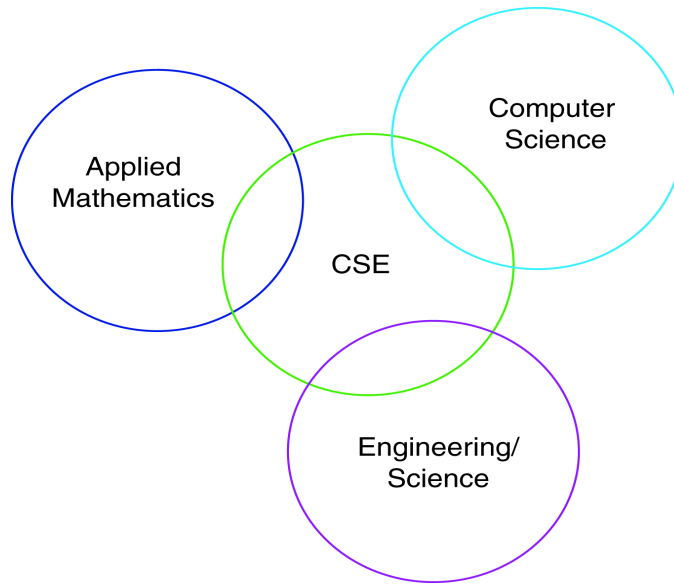


Fig. 1 Relationship of CSE to other disciplines.

some cases replacing) experimentation. Going from application area to computational results requires domain expertise, mathematical modeling, numerical analysis, algorithm development, software implementation, program execution, analysis, validation, and visualization of results. CSE involves all of this.

One point we would like to emphasize in this document is that *CSE is a legitimate and important academic enterprise*, even if it has yet to be formally recognized as such by some institutions. Although it includes elements from computer science, applied mathematics, engineering, and science, CSE focuses on the *integration* of knowledge and methodologies from all of these disciplines, and as such is a subject which is distinct from any of them.

2.2 What Is It Not?

- CSE makes use of the techniques of applied mathematics and computer science for the development of problem-solving methodologies and robust tools which will be the building blocks for solutions to scientific and engineering problems of ever-increasing complexity. It differs from mathematics or computer science in that analysis and methodologies are directed specifically at the solution of problem classes from science and engineering and will generally require a detailed knowledge or substantial collaboration from those disciplines. The computing and mathematical techniques used may be more domain specific, and the computer science and mathematics skills needed will be broader.
- It is more than a scientist or engineer using a canned code to generate and visualize results (skipping all of the intermediate steps).

2.3. Research in CSE. Research in CSE involves the development of state-of-the-art computer science, mathematical, and computational tools directed at the effective solution of real-world problems from science and engineering.

3. CSE as an Emerging Discipline.

3.1. CSE in Science and Industry. Although some researchers have been doing what might now be called CSE research for quite some time, for a number of reasons we appear to be at a critical juncture in terms of the role being played by simulation in science and industry. Historically, simulation has been used as a qualitative guide for design and control, but has often not been expected to provide accurate results for realistic physical systems. Increasingly, simulation is being used in a more quantitative way and is being used as an integral part of manufacturing, design, and decision-making processes and as a fundamental tool for scientific research. Problems where CSE has played and is expected to continue to play a pivotal role include the following:

- *Weather and climate prediction.* Future energy and environmental strategies will require unprecedented accuracy and resolution for understanding how global changes are related to events on regional scales where the impact on people and the environment is the greatest. Achieving such accuracy means bringing the resolution used in weather forecasting to the global predictions, which is not practical currently because of the very large amount of data storage and long computation times that are required. A major advance in computing power will enable scientists to incorporate knowledge about the interactions among the oceans, atmosphere, and living ecosystems, such as swamps, forests, grasslands, and the tundra, into the models used to predict long-term change. Climate modeling at global, regional, and local levels can reduce uncertainties regarding long-term climate change, provide input for the formulation of energy and environmental policy, and abate the impact of violent storms [8].
- *Combustion.* Accurate simulation of combustion systems offers the promise of developing the understanding needed to improve efficiency and reduce emissions as mandated by U.S. public policy. Combustion of fossil fuels accounts for 85% of the energy consumed annually in the U.S. and will continue to do so for the foreseeable future. Achieving predictive simulation of combustion processes will require terascale computing and an unprecedented level of integration among disciplines including physics, chemistry, engineering, mathematics, and computer science [8].
- *Nuclear stockpile stewardship.* While new weapon production has ceased, the ability to design nuclear weapons, analyze their performance, predict their safety and reliability, and certify their functionality as they age is essential for conscientious management of the enduring U.S. nuclear stockpile. Dramatic advances in computer technology have made virtual testing and prototyping viable alternatives to traditional nuclear and nonnuclear test-based methods for stockpile stewardship. Rudimentary versions of virtual testing and prototyping exist today. However, meeting the needs of stockpile stewardship for the near future requires high-performance computing far beyond our current level of performance [1]. The ability to estimate and manage uncertainty in models and computations is critical for this application and increasingly important for many others.
- *Simulation, design, and control of vehicles.* It is now standard practice in the design of mechanical systems such as vehicles, machines, or robots to use computer simulation to observe the dynamic response of the system being designed. Computer-aided design drastically reduces the need to construct

and test prototypes. Simulation is used not only to improve performance, but also for safety and ergonomics. Real-time simulation with operator in the loop and/or hardware in the loop presents substantial challenges for algorithms and software [13].

- *Aircraft design.* Since the early days of computing, computational simulation has been used in the performance analysis and design of aircraft components, such as the analysis of lift and drag of airfoil designs. As computations become more sophisticated and computers more powerful, computational simulation is used as an essential tool in the complete design process. For example, the Boeing 777 was the first jetliner to be 100% digitally designed, using 3D solid modeling. Throughout the design process, the airplane was preassembled on the computer, eliminating the need for a costly full-scale mark-up. CSE will play an increasingly important role in the entire design and analysis process as capabilities improve for such things as numerical modeling of combustion for engine design.
- *Electronic design automation.* Electronic design automation and CSE have long had a symbiotic relationship. Modern electronic systems (most notably the microprocessors that have enabled CSE to achieve its current prominence) are extraordinarily complex. The development of such systems is only possible with the aid of computational tools for simulation and verification of the systems as part of the design process. Computation plays an important role at all levels of electronic design, from simulating the processes used to fabricate semiconductor devices, to simulating and verifying the logic of a microprocessor system or laying out the floor plan of VLSI circuitry.

CSE tools are critical in the exploration of scientific areas such as astrophysics, quantum mechanics, relativity, chemistry, and molecular biology, where experiments are difficult and expensive if not impossible [9], and in analyzing the reams of experimental data and developing models in emerging areas such as the following:

- *Biology.* CSE technologies are rapidly becoming indispensable to the biological and medical sciences. Simulation plays a major role in the conceptual development of medical devices, both those used in diagnostic procedures (electromagnetic, ultrasonic, etc.) and in design of artificial organs (hearts, kidneys, etc.). Biomedical optics depends heavily on computational modeling in detection and treatment in oncology, ophthalmology, cardiology, and physiology. Computational modeling plays a fundamental role in the emerging efforts to combine mathematics and biology in the genomic sciences (genome sequencing, gene expression profiling, genotyping, etc.). In this area one needs large scale simulations with complex computational models to develop new theoretical/conceptual models and understanding of molecular level interactions.
- *Chemistry.* Computational chemistry (CC) is widely used in academic and industrial research. Computed molecular structures, for example, very often are more reliable than experimentally determined ones. According to “Chemical & Engineering News,” the newsletter of the American Chemical Society, CC has developed from a “nice to have” to a “must-have” tool [2]. The main incentive of CC is the prediction of chemical phenomena based on models which relate either to first principles theory (“rigorous models”), to statistical ensembles governed by the laws of classical physics or thermodynamics, or simply to empirical knowledge. In real problem solving situations, these

models are often combined to form “hybrid models” where only the critical part of the problem is treated at the rigorous level of theory. Rigorous theory in the molecular context is synonymous with quantum mechanics, i.e., solving the Schrödinger equation for a molecular complex with or without the presence of external perturbation (photons, electric fields, etc.). There are a number of methods available which provide approximate solutions to the Schrödinger equation (Hartree–Fock and density functional theories, for example). Simulation is used to predict properties of large and complex entities such as a liquid, the folding of a protein in solution, or the elasticity of a polymer. Finally, empirical models most often try to establish correlations between the structure of a molecule and its (pharmaceutical) activity. Simulations and quantum chemical calculations, on the other hand, very often are extremely compute-intensive due to the number of degrees of freedom and the complexity of the terms to be evaluated. The high accuracy required in these calculations sets restrictions with regard to the method used to solve the partial differential equations (PDEs) involved. Further information is available at the website for the International Union of Pure and Applied Chemistry [7].

- *Materials.* The challenge in materials research is to invent new materials and to perfect existing ones by fabrication and processing so that they have the desired performance and environmental response [8]. For example, there are many new and important applications for thin films, including silicon-based microelectronics, compound semiconductors, opto-electronics devices, high-temperature superconductors, and photovoltaic systems. The growth of such thin films, which can be accomplished via processes such as chemical vapor deposition (CVD), is sensitive to many factors in the manufacturing process. Simulation is an essential tool for understanding this process and requires the development of mathematical models and computational techniques. Process control, which is an order of magnitude more computationally complex than simulation, is emerging as an essential tool in fabrication [4]. Recently, large-scale complex computational modeling has been used to design high-pressure, high-throughput CVD reactors to be used as enabling devices in the production of new and exotic materials.
- *Bioengineering.* Historically, engineers have used chemistry, thermodynamics, and transport to design chemical processes. Now these fundamental processes are applied to the understanding of complex biological phenomena that are governed by the same physical laws. Computer models are being used to understand and to develop treatments for glaucoma, to understand and to fabricate bioartificial materials (for example, bioartificial arteries), and for studying the normal and pathological response of soft hydrated tissues in the human musculoskeletal system [11, 10].

3.2. Enabling Technologies for CSE. Growth in the expectations for and applications of CSE methodology has been fueled by rapid and sustained advances over the past twenty years in computing power and algorithm speed and reliability, and by the emergence of software tools for the development and integration of complex software systems and the visualization of results. In many areas of science and engineering, the boundary has been crossed where simulation, or simulation in combination with experiment, is more effective (in some combination of time/cost/accuracy) than experiment alone for real needs.

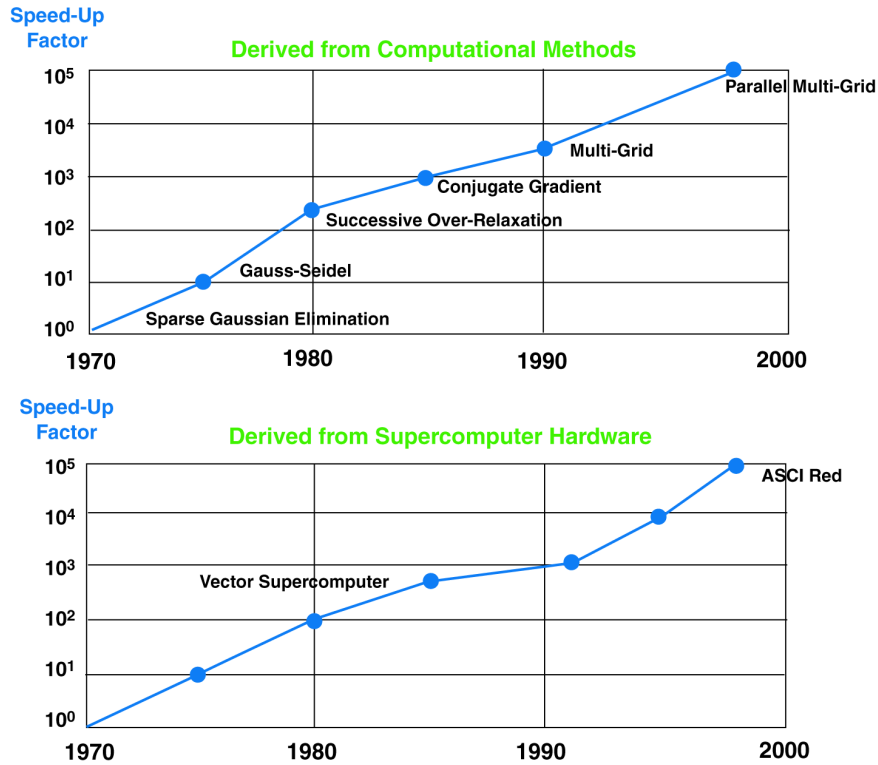


Fig. 2 Comparison of the contributions of mathematical algorithms and computer hardware.

Figure 2 illustrates the contribution of mathematics to the overall speed-up of computational models over the last twenty years compared to the speed-up of computer hardware. This is an updated version of a figure appearing in [14]. Since 1970, production codes at the DOE laboratories have used a sequence of algorithms to solve large sparse linear systems. In many applications, solution of such systems dominates the computation. The algorithms are plotted in the time period in which they were the method of choice against the relative speed of that algorithm on a standard problem, using 1970 as a baseline. The mathematical development of these algorithms occurred many years earlier and underscores the time lag between mathematical discovery and useful implementation of the ideas in production software.

4. CSE Graduate Education.

4.1. Educational Objectives. In addition to a background in mathematics and computer science, a CSE graduate must have a thorough education in an application area (engineering discipline or science). The CSE graduate's mathematical knowledge will be sufficient to model technological and scientific problems. Knowledge of computer science, and in particular numerical algorithms, software design, and visualization, enable the CSE graduate to make efficient use of computers. A graduate knows how to find and exploit software (packages) for a certain task. A CSE student performs interdisciplinary work in mathematics, computer science, and an application area. A CSE graduate is trained to communicate with and collaborate with an

engineer or physicist and/or a computer scientist or mathematician to solve difficult practical problems.

4.2. Curriculum.

4.2.1. Relevant background. We describe below the background that a well-prepared undergraduate will have had before entering a CSE program. It is expected that many students will be strong in several of the areas but may need to acquire expertise in other areas during the initial stages of graduate study.

1. Mathematics and computer science:
 - calculus,
 - basic applied math,
 - linear algebra,
 - real/complex analysis,
 - software design, programming, and testing,
 - data structures and algorithms,
 - numerical analysis.
2. Application area: basic knowledge in an application area such as
 - physics,
 - chemistry,
 - computer science (for example, data mining),
 - fluid dynamics,
 - thermodynamics.

4.2.2. Core Areas for Graduate Curriculum.

1. Mathematics and computer science.
 - Numerical analysis (linear algebra and optimization, ordinary and partial differential equations).
 - Applied mathematics (ordinary differential equations, dynamical systems, partial differential equations, mathematical modeling).
 - Computing (languages, operating systems, networking, and parallel and distributed systems).
 - Data analysis (visualization, statistical methods).

We note that in many institutions there is much redundancy and overlap between courses, for example, in numerical analysis or applied mathematics, being taught in various engineering departments and mathematics. It may be advantageous to have a single core track, perhaps adding special sections for discipline-specific material if that is deemed to be necessary. This has the obvious advantage of cost-effectiveness, enabling even smaller institutions to start a CSE program. Perhaps even more importantly, it gives the students a common educational foundation for the more advanced courses and exposes them to other students and faculty with a wide variety of interests in computer science, mathematics, science, and engineering.

2. Application areas. It is *absolutely essential* that interdisciplinary collaboration be an integral part of the curriculum and the thesis research. Courses should include projects and presentations whenever possible. A CSE graduate should have working knowledge in an application area such as
 - computational physics,
 - physics of the atmosphere and weather forecasting,
 - astronomy,
 - computational chemistry,

- computational fluid dynamics,
- control,
- structural dynamics,
- bioengineering,
- acoustics,
- reactive flows,
- electromagnetics,
- quantum mechanics,
- reservoir engineering,
- molecular biology,
- electronic design automation,
- circuit simulation,
- semiconductor simulation.

Interdisciplinary collaboration can be accomplished via participation in a multidisciplinary research team and/or internship at a national laboratory or in industry.

4.3. Graduate Degree Programs and Models. A list of graduate degree programs that are in place or in progress can be found at www.siam.org/world/compsci/cpsci.htm.

Two general models for the organization of CSE graduate degree programs have emerged. In the first model, a graduate degree is awarded in the new discipline of CSE. Often in this model the CSE program resides within an existing department, usually mathematics or computer science. In the second model, graduate degrees are awarded in the traditional disciplines of mathematics, computer science, science, and engineering, with an area of specialization of CSE. The CSE programs residing in different departments usually share a core curriculum and a basic set of standards for graduation with the CSE specialization. Here we describe several existing programs which illustrate the two models. Further information on CSE graduate programs and CSE education in general is available at www.sgi.com/education/whitepaper.dir/.

4.3.1. MS/Ph.D. in CSE.

CSE at Stanford University. The Scientific Computing and Computational Mathematics Program at Stanford University was established in 1987 and is a graduate degree (MS and Ph.D.) awarding unit comprised of faculty from a variety of departments, including Mathematics, Computer Science, Operations Research, Statistics, Chemical Engineering, Mechanical Engineering, and Electrical Engineering. It was established in recognition of the need for graduate-level training at the intersection of the disciplines of mathematics and computer science, which at the same time draws on applications of fundamental scientific or technological importance.

The core courses, which all MS and Ph.D. students must complete, are two year-long sequences, one in numerical analysis, the other in methods of mathematical physics. In addition, both MS and Ph.D. students must complete a year of courses in a focused application area, a year of courses in computer science (parallel computing or data structures and algorithms are common choices), and further courses in applied mathematics and numerical analysis. The choice outside the core sequences is very broad, allowing the flexibility desirable in a program of this scope, while the core sequences ensure a sound intellectual basis for the program and a commonality among the students.

Ph.D. work falls into two broad categories: theoretical studies of computational algorithms for the solution of problems in applied and computational mathematics and the development and application of novel software for the solution of problems of

scientific or engineering significance. Students in the former category typically work with faculty from computer science, mathematics, operations research, or statistics, while those in the latter category work with advisors rooted in specific application domains; occasional joint supervision of research also occurs and is encouraged.

Of the Ph.D. graduates of the program a significant proportion (roughly 45%) have moved on to academic positions, typically in applied and computational mathematics environments. The remainder are distributed through government labs and industry.

CSE at the University of Texas at Austin. At the University of Texas at Austin, CSE is known as CAM (computational and applied mathematics), but all six departments of the College of Engineering are strong contributors to the program. There are a number of special features of the CAM program at Texas that are noteworthy:

- CSE is an independent academic program leading to the Ph.D. in CAM, which reports directly to the graduate school. It has its own curriculum, although at present all courses are jointly listed, with some offered by participating departments, each with its own oversight committee that is involved in management of the program and its graduate students.
- Fourteen academic departments participate in the CAM program, including Mathematics, Computer Sciences, Aerospace Engineering and Engineering Mechanics, Chemical Engineering, Petroleum and Geophysical Engineering, Electrical Engineering, and Physics. Each member of the CAM Graduate Studies Committee is a faculty member from one of the participating departments.
- There is an organized research center associated with the program called TICAM—The Texas Institute for Computational and Applied Mathematics. The mission of TICAM is to develop, organize, and administer programs in basic and applied research in areas of applied mathematics and computational sciences that deal with mathematical modeling and computer simulation.
- Each student is expected to demonstrate a graduate-level proficiency in three areas. Area A is applicable mathematics. This has traditionally included functional analysis, PDEs, and mathematical physics but could include mathematics or other areas of applicable mathematics. Area B is numerical analysis in scientific computation, including a significant block of course work in computer sciences, architecture, parallel computing, etc. Area C is mathematical modeling and applications. This is an intellectually rich area in which course work may be selected from one or more participating departments. Typical Area C options are acoustics, computational fluid mechanics, electromagnetics, quantum mechanics, kinetic theory, solid mechanics, materials science, and, most recently, computational finance. Students take written exams in all of these areas except Area B where traditionally an oral exam is given. Each student's dissertation is expected to reflect components of all three areas. The Ph.D. Advisory Committees must have representatives from all three areas, as does the Graduate Studies Committee that manages the overall program.
- Faculty in the program hold tenure in one of the participating departments. There is a written document, signed by the deans of the colleges of the participating departments, that guarantees that all participants in the program will be judged in matters of promotion, merit raises, and tenure on the basis of their contribution to the CAM program independent of their contributions to their individual departments.

4.3.2. MS/Ph.D. in Traditional Area, with Specialization in CSE.

CSE at the University of Illinois. The purpose of the CSE option at the University of Illinois is to foster interdisciplinary, computationally oriented research among all fields of science and engineering and to prepare students to work effectively in such an environment.

Students electing the CSE option become proficient in computing technology, including numerical computation and the practical use of advanced computer architectures, as well as in one or more applied disciplines. Such proficiency is gained, in part, through courses that are designed to reduce the usual barriers to interdisciplinary work. Thesis research by CSE students is expected to be computationally oriented and actively advised by faculty members from multiple departments.

CSE is administered by a Steering Committee composed of one representative from each participating department and chaired by the director of CSE. All faculty members affiliated with CSE have regular faculty appointments in one of the participating departments. CSE is sponsored by the College of Engineering, but it is not limited to academic departments within the college. Departments involved include Aeronautical and Astronautical Engineering, Atmospheric Sciences, Chemical Engineering, Civil Engineering, Computer Science, Electrical and Computer Engineering, Materials Science and Engineering, Mathematics, Mechanical and Industrial Engineering, Nuclear Engineering, Physics, and Theoretical and Applied Mechanics.

CSE is a cooperative effort among the participating departments. Each participating department has its own specific requirements for its CSE option, but all are similar and share the common goals of the program. Details are available by accessing the UIUC CSE website [3].

Upon satisfying the degree requirements of the student's graduate department and the CSE requirements, the student is awarded a CSE certificate signifying successful completion of the CSE option. Students must first be admitted to one of the participating departments before enrolling in the CSE option.

All CSE courses are cross-listed with one or more of the participating departments. CSE instruction includes both core and advanced courses. A sampling of CSE courses includes numerical methods, parallel programming, computer architecture, combinatorial algorithms, data structures, software design, computer methods in civil engineering, computational solid and fluid mechanics, finite element analysis, computational aerodynamics, computer simulation of materials, parallel numerical algorithms, scientific visualization, and grid generation.

CSE at Purdue University. The CSE Program at Purdue University is an interdisciplinary graduate program that started in Fall 1995. It offers specializations in computational science and computational engineering in 17 departments across the schools of Purdue. Specializations are offered at both the MS and Ph.D. levels.

The CSE program at Purdue provides students with the opportunity to study a specific science or engineering discipline along with computing in a multidisciplinary environment. The aim of the program is not to produce a student with parts of two degrees, but rather a student who has learned how to integrate computing with another scientific or engineering discipline and is able to make original contributions in both disciplines. The expected course load and examinations for students in this program are roughly the same as for MS or Ph.D. degrees in other disciplines at Purdue, with approximately one-third of the course load and examinations from computing and two-thirds in the student's home department. For students whose home department is Computer Science or Computer Engineering, one-third of the course load will be from outside department application areas.

Specializations at the MS and Ph.D. levels are offered by Agricultural Economics, Agronomy, Biological Sciences, Chemistry, Computer Sciences, Earth and Atmospheric Sciences, Electrical Engineering, Food Science, Industrial and Physical Pharmacy, Mathematics, Mechanical Engineering, Medicinal Chemistry and Pharmacognosy, Nuclear Engineering, Pharmacy Practice, Physics, Psychological Sciences, and Statistics. Students must be admitted both to one of these departments and to the CSE program. The degree is awarded in the home department with the specialization *Computational Engineering* or *Computational Sciences* indicated on the transcript. The program is administered by the CSE Graduate Committee with representation from participating departments. CSE requirements are tailored to the home department's requirements. Students are expected to have a strong interest in computation and its application to science and engineering. Their undergraduate training is expected to have given them a strong foundation in several areas of science, engineering, and computing [12].

4.3.3. CSE Programs in Europe. We discuss CSE programs in Europe separately from those in North America because of the differences in structure of the educational systems, although there is also much in common.

In Europe there are strong activities in CSE. For example, a curriculum was started in 1997 at the Royal Institute of Technology in Stockholm, Sweden. Interdisciplinary application oriented and problem-solving curricula that take into account computer simulation have been introduced into the U.S. in recent years under the label CSE. Related curricula called Industrial Mathematics or Technical Mathematics have been introduced earlier at various places, e.g., in Linz and Kaiserslautern.

Diploma (MS) in CSE at ETH. At ETH Zurich, W. Gander (Computer Science) and M. Gutknecht and R. Jeltsch (Mathematics) took up the discussion on CSE in 1995. They were supported by the Executive Board of the ETH Zurich, which nominated a committee with two more members, W. van Gunsteren (Chemistry) and K. Nipp (Mathematics). In April 1996 this committee worked out a curriculum relying on existing courses at ETH, therefore being cost-neutral without a need for additional personnel. The concept for the curriculum CSE was accepted by the Executive Board ETH in July 1997 and the program began in October 1997. The curriculum is outlined in Table 1. Instead of the usual 4.5 years (9 semesters) of diploma studies at ETH, the CSE curriculum takes only 2.5 years and builds upon knowledge acquired in the first two years of a classical discipline. Candidates for the CSE curriculum must take two years of basic studies in mechanical or electrical engineering, computer science, chemistry, mathematics, and physics at ETH or elsewhere. Depending on their initial studies the students must fill the "gaps" between those first two years of studies and the model undergraduate studies for the CSE curriculum. CSE graduates are able to work on interdisciplinary problem solving in an application area making use of a profound knowledge in mathematics and computer science.

The core courses are theory and numerical techniques for differential equations, optimization, parallel computing, computational quantum mechanics, computational statistical mechanics, software engineering, and visualization/graphics. The specialization fields are physics of the atmosphere, computational chemistry, computational fluid dynamics, control theory, robotics, and computational physics. Further information is available at the ETH CSE website [6].

International Master Program in Scientific Computing at the Department of Numerical Analysis and Computing Science, Royal Institute of Technology (KTH), Stockholm, Sweden. KTH, founded in 1827 and the largest of Sweden's six universities of technology, has extensive inter-

Table 1 *Outline of the curriculum. HWS = hours per week per semester. The core courses are mandatory. One field of specialization has to be chosen.*

	HWS	Short description
Core Courses	37	computational mathematical methods, knowledge in computer science, important application areas, case studies
Field of Specialization	10	work in one computational application area
Elective Courses	12	additional to field of specialization and core courses, also in a computational area
Two Term Papers "Gaps"	12 12	application oriented, computational at least 180 h of work basics for computation and applications
total	83	

national cooperation both in research and education. About 30% of regular students spend one year of their studies at some university abroad, and the KTH Master Programs were started to strengthen internationalization. The programs are given in English with tuition free of charge. A limited number of grants from the Swedish Institute are available to cover living expenses.

The International Master Program in Scientific Computing, hosted by the Department of Numerical Analysis and Computing Science, was initiated in 1996. It is open to students from all over the world with a BSc/BEng or equivalent with a very good background in mathematics and knowledge in numerical methods. Applicants are also required to be experienced in programming and have good overview of at least one application area relevant to scientific computing, such as fluid dynamics, solid mechanics, or electromagnetics. The duration of the program is one and a half years, with one year of courses and projects and half a year of thesis work. The first class was enrolled in 1997 with 8 students. The program now attracts more than 100 applications, and 20 students from more than 10 countries were accepted to enroll in Fall 1999.

In the first week at KTH, the last before official term starts, the students are given an intensive course in the computer environment and MATLAB and C programming. After this immersion the term proper starts with lectures, labs, and project work. The regular courses are as follows.

- First semester:
 - mathematical models, analysis and simulation,
 - applied numerical methods,
 - object oriented program construction for scientific computing,
 - the finite element method,
 - applied nonlinear optimization.
- Second semester:
 - numerical treatment of partial differential equations,
 - computational fluid dynamics,
 - computational physics,
 - computational chemistry,
 - advanced numerical analysis,
 - scientific visualization,
 - algorithms for parallel computation.
- Third semester:
 - high-performance computing.

The thesis work is started at the end of the second semester and completed during the third semester. Through the entire program there are projects within the courses and projects running through several of the courses.

To obtain a Master Degree in Scientific Computing at KTH the students have to pass written exams on the six compulsory courses and at least three eligible courses. All labs and projects must be completed and the thesis must be presented orally in a seminar and as a written technical report. More information about the program can be found in [5].

Impact of educational structure for CSE education in Europe vs. North America. In North America every child goes to high school and graduates at the age of 18. After that many continue with a college education, and some continue their studies at a university. Selections are made by the colleges and universities themselves.

In Europe the selection of university students is often done at an earlier stage. Though there are great differences in the evaluation process, in principle schools of different intellectual level exist in parallel. To enter a school of higher level, an entrance exam has to be passed.

As an example, consider Switzerland. Nine years of school are mandatory. Three levels can be distinguished:

1. Level 1. Primary School: Nine school-years from age 7-16. Children who remain in this school will typically become factory workers or do some other less intellectually challenging work.
2. Level 2. Secondary School: The entrance exam takes place after the first four or five years of primary school. The school also terminates at the age of 16. Typically a graduate of secondary school will continue with a 3–4 year apprenticeship and become a craftsman, such as a car mechanic, an optician, or a bookkeeper.
3. Level 3. Gymnasium: In secondary school (at the age of about 13) another exam can be taken to pass into the Gymnasium. This school takes another six years and finishes with an exam, called *Matura*, at the age of 19. Passing the *Matura* ensures eligibility to every university in Switzerland.

The *Matura* level differs from country to country in Europe. Only about 18% of the children in Switzerland pass the *Matura*. The European mean is about 30% with exceptions like France, with about 50% doing the “Baccalaureat.”

ETH Zurich offers a diploma after 4.5 years of studies. This title is equivalent to a master’s degree in North America.

Students who have completed secondary school and an apprenticeship can take an entrance exam to one of the “Fachhochschulen” (“Universities of Applied Sciences”). These institutions may be best compared with colleges and their diploma after 3 years of studies is generally accepted to be equivalent to a North American BS degree.

4.3.4. Discussion: Structure of CSE Graduate Programs. It is clear that two major models for structuring graduate programs in CSE have emerged, and that both have proven to be successful at various universities. When considering the creation of a new program, the model to be chosen and its chances for success will be highly dependent on local academic strengths and political considerations. Evidently, there is much in common in terms of basic academic content between the two models.

Comparing the two models directly is difficult. We offer a few observations. The degree in CSE may allow a more focused and cohesive program, since this program is often implemented within a single department such as mathematics or computer science, or within a separate academic unit. On the other hand it may be difficult to achieve depth within this type of program, especially in the application areas, or to distinguish this program from applied mathematics.

Since CSE is an emerging area, employment possibilities for students with the CSE degree are not well documented. There is a strong feeling that the current climate is highly favorable towards interdisciplinary work in science and engineering. One argument in favor of the degree in traditional disciplines, with specialization in CSE, is that employers and in particular universities and industry may be more open to this more traditional degree structure.

5. Broadening the CSE Student Experience. It is *absolutely essential* that interdisciplinary collaboration be an integral part of the curriculum and thesis research. There are a number of ways in which this can be achieved.

- Courses should include multidisciplinary projects and presentations whenever possible.
- Participation in a multidisciplinary research team.
- Internship at a National Laboratory or in industry.

The NSF National Partnership for Advanced Computational Infrastructure (NPACIs) in the U.S. has programs in place to assist in CSE education. Two excellent online news magazines provide up-to-date summaries of the activities of the NPACIs: <http://www.npaci.edu/npaci/online/> and the National Computational Science Alliance (NCSA), <http://www.ncsa.uiuc.edu/access/>. The focused education programs are summarized through the cooperative EOT-PACI (Education, Outreach and Training) website for both PACIs, <http://www.eot.org/>. There are Research Experience for Undergraduates (REU) opportunities coordinated through the EOT-PACI and details for applying are provided.

6. Role of SIAM and Update on SIAM CSE Activities. SIAM's first CSE conference took place in Washington, D.C., on September 21–24, 2000, and was highly successful, with approximately 475 attendees representing many areas of science, engineering, and computer science as well as computational and applied mathematics.

To ensure that this conference becomes a regular event and that SIAM will continue to contribute to this rapidly growing discipline, a SIAM Special Interest Group (SIAG) on Computational Science and Engineering has been formed. An open discussion was held at the SIAM CSE meeting on the possibility of forming such a SIAG. Over 250 people attended the open discussion. There was much enthusiasm, and many good ideas were communicated. Steve Ashby of Lawrence Livermore National Laboratory is taking the lead on this effort.

Our recommendations regarding the potential role and contributions of SIAM in CSE education and research include the following:

1. Establish a SIAG on CSE.
2. Define the core areas and scope of this field.
3. Outline ideas for graduate and undergraduate CSE curricula.
4. Hold conferences on CSE.
5. Examine SIAM's existing journals to determine whether there is a place for CSE research as we have defined it and whether there is a need for new journals and publications in this area.
6. Create an electronic CSE bulletin board, which would include
 - a discussion forum,
 - pointers to graduate and undergraduate degree programs,
 - infrastructure for universities, government, and industry to post internship opportunities and for students to post resumes,
 - infrastructure for universities, government, and industry to post job opportunities and for job seekers to post resumes.

7. Publish information of use for CSE education, for example, articles specifically oriented to teaching in CSE programs or courses.
8. Publish CSE textbooks.
9. Publish CSE research books.

SIAM has already begun to take action on many of these recommendations. We expect that as the SIAG on CSE takes shape, SIAM will be well positioned to respond to the needs and to participate in the excitement of this new discipline.

Appendix. The SIAM Working Group on CSE Education. The SIAM Working Group on CSE Education was formed in November 1998 to study the recent developments in CSE graduate education and to give recommendations regarding SIAM's potential role. The Working Group was comprised of Prof. Linda Petzold (University of California Santa Barbara, Chair); Prof. Uri Ascher, University of British Columbia; Prof. H. Thomas Banks, North Carolina State University; Dr. James Crowley, SIAM; Prof. Walter Gander, ETH Zurich; Prof. Leslie Greengard, Courant Institute of Mathematical Sciences, New York University; Prof. Michael Heath, University of Illinois at Urbana-Champaign; Prof. Andrew Lumsdaine, Notre Dame University; Dr. Cleve Moler, The Mathworks, Inc.; Prof. Tinsley Oden, University of Texas Austin; Prof. Robert Schnabel, University of Colorado at Boulder; Prof. Kris Stewart, San Diego State University; and Dr. Anne Trefethen, Numerical Algorithms Group (NAG).

Acknowledgments. We would like to thank our colleagues, Andrew Stuart and Gene Golub of Stanford University, Lennart Edsberg of KTH, Peter Arbenz and Kaspar Nipp of ETH Zurich, the SIAM Education Committee, and the SIAM council and board for their input and advice.

REFERENCES

- [1] Accelerated Strategic Computing Initiative, <http://www.lanl.gov/projects/asci/>.
- [2] Chemical & Engineering News, May 1997.
- [3] *MS/Ph.D. Option handbook*, Computational Science and Engineering, University of Illinois at Urbana-Champaign, M. T. Heath, Director, 1998-1999. Also available from <http://www.cse.uiuc.edu/programs/index.html>.
- [4] Colorado School of Mines, Robert J. Kee website, <http://www.mines.edu/Academic/eng/faculty/rkee/>.
- [5] Computational Science and Engineering, KTH Stockholm, <http://www.nada.kth.se/kurser/master/index-eng.html>.
- [6] Computational Science and Engineering, ETH Zurich, <http://www.cse.ethz.ch>.
- [7] International Union of Pure and Applied Chemistry (IUPAC), <http://www.chem.qmw.ac.uk/iupac/>.
- [8] National Workshop on Advanced Scientific Computing, National Academy of Sciences, James S. Langer, Chair, 1998.
- [9] W. J. KAUFMANN III AND L. L. SMARR, *Supercomputing and the Transformation of Science*, Scientific American Library, W. H. Freeman, New York, 1993.
- [10] Rensselaer Polytechnic Institute, Dept. of Biomedical Engineering, Robert L. Spilker website, <http://www.eng.rpi.edu/~spilker/research.html>.
- [11] University of Colorado, Dept. of Chemical Engineering, Victor H. Barocas website, <http://spot.colorado.edu/~chemeng/faculty/barocas.html>.
- [12] Purdue University, CSE website, <http://www.cse.purdue.edu/>.
- [13] W. SCHIEHLEN, ED., *Multibody Systems Handbook*, Springer-Verlag, New York, 1990.
- [14] *FY 1992 Blue Book: High Performance Computing and Communications*, supplement to the President's Budget, 1992.