Computational Science and Engineering at UC Davis

Final Report of the Committee on Computational Science and Engineering

Committee Chair:
Joel E. Keizer, Institute of Theoretical Dynamics

Acting Committee Chair:
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Other Committee Members:
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Winston Ko, Physics
C. William McCurdy, Jr., Lawrence Berkeley Lab., Applied Science
David M. Rocke, Graduate School of Management
William P. Thurston, Mathematics

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Preamble

This Report concerns the future of *computational science and engineering (CS&E)* at the University of California, Davis. CS&E is a rapidly developing area with particularly strong connections to the sciences, engineering, and mathematics. CS&E is concerned with the development of computational models as an alternative way to help understand complex physical and biological processes—or to model entirely abstract processes, encountered in mathematics and computer science. CS&E involves diverse areas such as Monte Carlo simulations of random processes; algorithm development for the analysis of massive and multidimensional data sets; numerical algorithms for the solution of differential equations characterizing a wide variety of physical phenomena; development of methods for the analysis of biomedical diagnostics; computational molecular biology; visualization and virtual reality rendering for the study of large and complicated three-dimensional structures; digital image analysis, compression, and transmission; and computational techniques in relation to the study of discrete mathematics, including cryptography and combinatorics. A significant portion of UC Davis faculty and researchers is actively involved in a variety of CS&E fields and the development of algorithms and methods for solving large-scale problems impacting the future of the research process and teaching in science and engineering. It should be the objective of this Initiative to create an environment at UC Davis that will enable world-class education and research in CS&E.

The Committee is convinced that CS&E will play an important if not a dominating role for the future of the scientific discovery process and engineering design. We provide three examples:

- **Computational Physics.** National needs in the areas of numerical simulation, data exploration, and large-scale high-bandwidth communication have led to the creation of the so-called *Accelerated Strategic Computing Initiative (ASCI)* of the Department of Energy. Three major DoE laboratories—Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Sandia National Laboratory (SNL)—are spearheading revolutionary computational methods to simulate complex physical processes and the behavior of materials under extreme conditions. CS&E is vital for the success of ASCI[1].

- **Computational Neuroscience.** With today's high-resolution imaging technology it is possible to produce brain scans that reveal thoughts, moods, and memories—as clearly as a traditional X-ray image reveals bone structure. We are now able to observe a person's brain registering an event or experiencing

[1] We would like to point out that areas like numerical analysis and numerical linear algebra are crucial components of the foundation for CS&E. These areas are relevant for the development of practical algorithmic solutions to a variety of CS&E problems, not only problems in computational physics. It will be crucial for the development of CS&E to build in numerical areas such as numerical analysis and numerical linear algebra early on.

a painful memory. We can generate a static map of the human brain and can observe the electrical processes as they occur over time. Neuroscientists are beginning to develop models of the human brain that are direct results of this latest high-resolution imaging technology. The next step is the development of algorithms that simulate the observed brain activity patterns. Again, computational science and engineering methods will play a key role in advancing this area of research.

- **Computational Biology.** One of the most complicated processes currently being studied by scientists in a variety of disciplines, and primarily in molecular biology, is the so-called *folding problem.* The molecular structure of complex protein molecules is believed to greatly impact the eventual function of these proteins. It is crucial to understand the time-varying process of process folding itself, and computational techniques are of fundamental interest to (computational) molecular biologists to better understand the relationship between the structure of protein molecules, the folding process that leads to a final structure, and the function of the protein.

These examples do not represent the Committee's "priority areas" for CS&E, but they demonstrate that computation is becoming a key element in diverse fields. While most UC Davis disciplines that would greatly benefit from computation are not yet fully utilizing its power, we believe that the teaching and research components of this Initiative will help craft the kind of computation-oriented environment that will allow our university to remain competitive and become a national leader in CS&E in the next century. It is obvious that computational methods are a key component of the modern research process throughout the science and engineering fields. To be competitive as a research university in the 21st century, UC Davis will have to make significant investments in its computational infrastructure enabling efficient research on large-scale problems. The research aspect of this Initiative is to be viewed as at least as important as the teaching component.

The teaching, development, study, and application of computational methods is already crucial for a large variety of disciplines at UC Davis. To ensure the competitiveness of UC Davis in science and engineering education and research UC Davis must substantially strengthen and focus its efforts concerning CS&E in the coming years. The main objective of the CS&E Initiative must be the creation of an educational and research environment that is both attractive and accessible to students[2],

[2]It is reasonable to expect that some basic training in computer science principles—e.g., knowledge of a high-level programming language and algorithmic problem solving—would be de facto prerequisites for all CS&E students. Currently, Computer Science cannot accommodate the demand for lower-level computer science instruction on campus. (This is mainly due to the relatively small size of the Computer Science faculty. But the campus has by now recognized this problem and made a commitment to make substantial FTE resources available to Computer Science to remedy the current situation.) In general, one can think of two scenarios: (i) A CS&E unit would develop and

current faculty, and faculty to be hired. Linking this objective to the established and highly visible programs of UC Davis in the sciences and engineering should allow a maximum degree of leverage through potential joint appointments for new faculty hires.

One must be careful not to confuse CS&E with the established discipline of computer science, with its focus on the *organization, design, analysis, theory, programming, and application of digital computers and computing systems*[3]. Nonetheless, the rapid growth of CS&E has been triggered by key hardware and software developments in computer science and engineering. It will be crucial for the success of the CS&E Initiative to foster a strong relationship with the Computer Science Department as well. Computer Science will play a significant role in the basic preparation of both graduate and undergraduate students minoring or specializing in CS&E. Moreover, the Computer Science Department already has a dedicated sub-group of faculty working on CS&E problems (e.g., visualization/computer graphics, computational biology, medical informatics, database/information systems, combinatorial optimization, cryptography, and other fields) and thus would be a natural home for several of the FTEs or joint CS&E appointments resulting from the Initiative.

To accomplish the desired major impact of CS&E on the campus, it will be crucial to have a strong interaction with all CS&E-impacted and -interested science and engineering units. CS&E is a field that must not be viewed in isolation from applications or as a field that could thrive by merely looking inward. CS&E must reach out to science and engineering in order to justify its existence, improve and strengthen ongoing computing-based efforts, and promote an increase in the utilization of CS&E across science and engineering in general. It is the view of the majority of the Committee members that UC Davis needs a CS&E facility and that it should couple CS&E activities and the tackled science and engineering applications very closely. Without this coupling there would be the danger that departments and units across campus might initiate their own independent CS&E-like activities, and this would surely deprive a potential CS&E unit of students, interactions, and funding. The development of CS&E on campus must not be done in isolation from the campus community at large. Only this will ensure the success of a centralized CS&E effort, an effort that would be accepted broadly, would minimize the risk of duplicating efforts, and would lead to the desired interdisciplinary faculty interactions in CS&E.

Another important aspect of the development of CS&E relates to the existing *Graduate Group in Applied Mathematics (GGAM).* This Graduate Group consists of

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offer its own introductory computer courses or (ii) sufficient resources are made available to Computer Science to guarantee immediate and universal access to existing lower-level computer science courses.

[3]UC Davis General Catalog, 1998–99, p. 222.

approximately sixty faculty members and was formed to train applied mathematicians to carry out research in the physical sciences and engineering. GGAM aims at satisfying the need for applied mathematics education as it relates to science and engineering applications. GGAM offers MS and PhD degrees, and students may be supervised by any faculty member of the Group. The areas represented by this Group span a wide variety of fields, currently including population biology, atmospheric sciences, continuum mechanics, optimization and control, theoretical chemistry, computer and engineering sciences, mathematical physics, scientific visualization and geometric modeling, and mathematics. GGAM should play an important role in the development of CS&E. The reason for this is that the "three pillars" of CS&E are (i) science and engineering applications; (ii) methods of applied mathematics; and (iii) computer science techniques for practical algorithm implementation. The development of CS&E should build on these three components and ensure that more and improved interactions will result. Moreover, the *Graduate Group in Statistics* could play a similarly important role in this context. Both applied mathematics and statistics principles are of crucial importance for algorithm development to solve CS&E problems.

There is no lack of funding opportunities in CS&E. Examples are large-scale programs such as the *Accelerated Strategic Computing Initiative (ASCI)*, the *Next Generation Internet Initiative*, and the *Information Technology for the* 21^{st} *Century* program. ASCI is the result of a nuclear test ban treaty prohibiting the U.S. from testing nuclear devices. ASCI is concerned with the development of large-scale CS&E technology allowing the computer simulation of the behavior of nuclear devices. ASCI and the other cited programs require a major involvement of academic institutions, which is a significant asset concerning the development of CS&E at UC Davis.

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1 What Is CS&E?

Most science and engineering fields are not intrinsically defined by the use of computers or computation—but computers and computation are becoming more and more important to enable scientific and engineering progress. Computational methods provide a powerful means for investigating scientific problems or achieving engineering design objectives. Computer science is a distinguished discipline in the sense that it is centrally concerned with questions that address issues of computation, e.g., the design and analysis of algorithms, the development of computer networking technology, the study of parallel computer architectures, or the analysis of algorithm complexity.

The Committee interprets CS&E as the field concerned with the development, analysis, and utilization of computational methods for practical science and engineering problems. The rapidly increasing importance of CS&E is due to the widespread and growing realization that computation can greatly augment or replace some of the traditional means for scientific investigation and engineering design. Computation is now widely available throughout the physical sciences and engineering, and it can provide a relatively inexpensive alternative for traditional scientific investigation, i.e., theoretical and experimental investigation. Computation is not just a relatively inexpensive alternative, but it also provides a third distinct mode of investigation (adding to theory and experimentation). Computation can also lead to insights that are difficult or impossible to gain otherwise. The massive amounts of data being produced cause additional problems: How to organize these massive amounts of data? How to "mine" and analyze them? How to define what to look for in the data and how to visualize them?

Ideally, a person in CS&E should be focused on at least one specific field utilizing computational methods, and should be active in that field or closely follow the computational problems and activities in that field. Equally important, that person should make substantial contributions to the development, analysis, or application of computational methods that benefit that field. Many CS&E fields can have impact on and relationships with several application areas. This, for example, is the case with visualization, which, broadly speaking, is concerned with the development of rendering technology for the analysis of scientific and engineering data. The same is true for a variety of other CS&E fields concerned with the development of algorithmic methods that are applicable to a large number of applications.

CS&E is much broader than the traditional numerical-based computations, which are of fundamental interest in *scientific computing.* CS&E methods are not exclusively numerical, and they are not necessarily based on "deep mathematics." CS&E also overlaps with computer science, but it differs from it in the sense that a strong connection to an application area is a "must" for CS&E. Many computer science departments support research and education in CS&E fields, which, for example, includes the study of scientific computing libraries, data visualization, or methods simplifying parallel computing for specific application domains.

2 The Role of CS&E at UC Davis

2.1 What CS&E Should Not Be

Many efforts exist on campus today concerning the more effective incorporation of computational tools into teaching and research. Some of these efforts have translated into the development of courses that teach the use of specific computational tools and specific software packages. Examples for this include the use of GIS in geography and the social sciences, GEANT for Monte Carlo methods applied to experimental design (in particle physics), CAD/CAM in landscape architecture, CAD in automotive and aircraft design, BLAST in molecular biology for sequence searching, MAPMAKER for QTL linkage analysis in genetics and evolution, and IBM Data Explorer in hydrologic science—just to name a few. It is desirable that departments and programs throughout the campus employ and teach the usage of these computational tools. The use of specific software packages can have enormous impact on certain scientific fields, but the teaching of such tools is not the major thrust for the CS&E Initiative.

The CS&E Initiative's hiring focus *should not be* the hiring of faculty who would teach the use of or introduce software packages, or to provide instruction in basic computer usage. It is legitimate to expect that each individual current faculty member incorporate computational tools into teaching and research whenever appropriate, regardless of departmental affiliation. The teaching of specific software packages should be incorporated into current courses by adding specific laboratory sections introducing these packages. The need for the teaching of application-specific software tools can be explained partially by the fact that exposure to such tools will make a student more competitive for the job market. It should remain, or become, the responsibility of the respective departments to incorporate the teaching of software tools into their courses, which, in turn, should make these courses more attractive to students. This should be reflected by the hiring efforts of the individual departments, which should favor candidates with experience in area-specific software tools. But CS&E FTEs should not be used to hire this faculty type, a faculty lacking interest or in-depth expertise in developing and analyzing computational tools.

In addition, there currently exists a general need for the preparation of large numbers of professionals with traditional computer science and computer engineering training. This fact is very much driven by current needs of the computer industry. It cannot and should not be the mission of CS&E at UC Davis to prepare this type of professional. This is, and should remain, the responsibility of the Computer Science and the Electrical and Computer Engineering Departments. The campus must provide sufficient support to ensure that high-quality training of a steadily increasing number of computer scientists/engineers will be possible. CS&E faculty hires should be able to contribute to teaching both traditional computer science/engineering and CS&E courses. However, student (and industry) demand for "mainstream CS&E education" will continue to grow at an extraordinary pace, and this should translate into continued and expanded support for Computer Science and Electrical and Computer Engineering over the coming years.

2.2 What CS&E Should Be

Faculty members hired under the CS&E Initiative should be those who can make important scientific contributions to the development and study of computational methods. CS&E faculty should do *research* concerning the development, study, and application of computational methods, with a contribution to application areas.

In their research, CS&E faculty are usually motivated by particular applied problems to be solved, the specific model being used in a computer simulation, or certain implementation aspects of algorithmic methods. Computer scientists/engineers, on the other hand, are mainly concerned with the development of better computer and computing infrastructure technology or, when involved in applied efforts, by generalization and problem abstraction. The key areas of interest to a "traditional computer scientist" would include the development and generalization of algorithms to make them applicable to a large class of problems, the design and analysis of complex data structures useful for a wide range of problems, or the complexity analysis of algorithms. It would be desirable to hire new CS&E faculty who are able to make contributions to these fundamental and "traditional" areas of study and to relate them clearly and strongly to CS&E application domains.

A typical CS&E faculty member's educational background and professional experience are rooted in application areas of computational methods or in computer science, computer engineering, or (applied) mathematics. CS&E faculty members, then, can teach students about the development of application-specific computational methods—possibly including the use of existing tools based on these methods—and the algorithmic design and analysis of these methods from a computer science or computer engineering perspective. The CS&E Committee strongly recommends the aggressive recruitment of the type of scientist who is clearly an active participant in state-of-the-art CS&E technique and algorithm development. CS&E teaching and research efforts should be driven by existing and emerging areas utilizing computational methods, keeping particularly strong UC Davis areas in mind, including computer science, computer engineering, computational/applied mathematics, or computational statistics.

The Committee is of the opinion that a strong CS&E program would have a positive impact on computer science or computer engineering education and research efforts as well. The symbiotic nature of the fields of CS&E and computer science or computer engineering would most likely lead to collaborations between CS&E faculty members and other computer scientists and computer engineers. It is reasonable to expect that several CS&E faculty would have an interest in and qualify for joint appointments[4] and could also contribute to basic computer science and computer

[4] According to current campus regulations, a faculty member with a formal joint appointment in

literacy teaching efforts. On the research side, the creation of a wealth of fundamental computer science research problems is a natural side effect of all CS&E efforts. Computer scientists/engineers should be able to gain from this substantially. In fact, we are convinced that existing research efforts in computer science or computer engineering would greatly benefit from an exposure to large-scale computational problems addressed by CS&E faculty. Synergy would most likely characterize the evolution of the relationship between CS&E and Computer Science and, to some degree, Electrical and Computer Engineering.

The Committee is also convinced that a strong CS&E program would have a positive impact on science education and research efforts as well. As CS&E becomes the "third arm" of science and engineering (the other arms being the "theoretical arm" and the "experimental arm"), there would be more collaboration between CS&E faculty members and science. It is important to have several CS&E faculty with joint appointments in the science fields who could contribute to the corresponding courses associated with the particular specialty areas. On the research side, solving problems with common computational roots, e.g., data mining, yet with wide-ranging connection to the science field of current research, ranging from genome research to cosmology, would make CS&E truly exciting.

The creation of a "home" for CS&E faculty—in the sense of co-locating CS&E faculty in a common physical location—is highly desirable. The Committee believes that the co-location of CS&E faculty members holds the potential to fuse major CS&E research efforts and could also be a major factor in attracting outstanding new faculty members. In general, such a home should stimulate communication and should mix CS&E faculty and students with diverse backgrounds and interests concerning office space and research space arrangements. Several Committee members have participated in NSF research centers before, and one of the main benefits of these centers is the provision of a truly interdisciplinary environment. Currently, CS&E education and research efforts are found in different departments and units across campus, and there is little coordination among the (relatively few) computational groups and efforts. Regardless of CS&E's eventual organizational structure, a home would allow the campus to streamline its CS&E efforts and build neeeded CS&E infrastructure in and around this home.

multiple departments has full voting rights in all departments he/she is a member of and also has to execute all duties of a faculty member in all departments. Furthermore, all departments vote on the jointly appointed faculty member's merit and promotion cases. (See also *UC Davis Academic Personnel Manual*, UCD-220H Academic Review Process–Joint Appointments.) A related issue is the appointment of CS&E faculty members with partial appointments at one or multiple of the national laboratories. In this case, the current merit and promotion regulations are definite obstacles for having faculty seek joint appointments. Currently, work conducted at a national laboratory would not be an asset for merits and promotions. The campus will have to investigate seriously how it should alter its current practices to value and encourage joint appointments, particularly appointments that involve national laboratories. This issue has implications far beyond CS&E, and it is a problem that deserves campus attention at the highest level.

This Initiative is likely to lead to a significant number of joint faculty appointments, which could be appointments in multiple UC Davis departments or joint appointments with the national laboratories. The Committee is, to some degree, concerned about current regulations concerning joint appointments at UC Davis. Concerning the hiring process for CS&E, obstacles related to joint appointments should be eliminated as much as possible. Job expectations should be clearly defined by the departments involved in joint appointments, and the environment that a jointly appointed faculty member would be exposed to should be inviting; the conditions have to be such that a joint appointment carries significantly more advantages than disadvantages for a faculty member. This is particularly important for jointly appointed junior faculty.

3 How the CS&E Initiative Relates to Departmental Plans

The Committee has solicited input from various UC Davis departments, divisions, centers, and schools with a strong interest in the future development of CS&E. We have asked several UC Davis departments to provide input concerning these questions:

- How does the CS&E Initiative fit into your departmental plan and priorities?
- What are the names, areas of expertise, and affiliations of people your department would consider outstanding senior candidates, appropriate to be hired under the *Target-of-Excellence* program?
- Which universities, in your view, are the producers of strong new CS&E PhDs?
- How would appointments of CS&E faculty contribute to your department's teaching responsibilities and curricular development?
- What resources—e.g., retirement FTEs, space, or other forms of commitment—could a department provide to CS&E hires?

The responses we have received are summarized in the following sections.

3.1 College of Agricultural & Environmental Sciences

3.1.1 Environmental Science and Policy

[Comments were provided by Professor Alan Hastings.] Environmental Science and Policy is very interested in expanding efforts in ecosystem modeling, which would be a field that is highly appropriate for the development of CS&E. For example, ecosystem simulations do require computational biology techniques for the simulation of complicated cellular structures.

3.1.2 Land, Air and Water Resources

The use of computing resources varies dramatically among the faculty in Land, Air and Water Resources (LAWR). Some faculty are interested in only the most basic uses of a Mac or PC, while others have considerable expertise in computer modeling, visualization, and programming. Recognizing this great diversity, LAWR provides these comments concerning the CS&E Initiative:

- **Desirable Priorities for CS&E.** Two items were identified: (i) Continued instruction of introductory FORTRAN is quite important to atmospheric science (AS) and hydrologic science (HS) programs. (ii) Easier access to introductory C programming courses is highly desirable.

- **Faculty.** LAWR did not have the resources to develop a list of potential high-caliber faculty candidates in the available time.

- **Teaching.** LAWR can identify at least four ways in which CS&E appointments would contribute to departmental teaching programs. (i) The continuation of ENG5 or an equivalent introduction to FORTRAN is a prime concern. FORTRAN remains the primary tool our students use for computation that they write themselves. A Hydrologic Science (HS) faculty member complained that ENG5 was hard to get into. LAWR uses ENG5 as a base for several courses in AS, and it is a requirement of the AS major. (ii) Some students feel that the C language has become important to learn as a means to improve their job prospects. Yet, access to courses concerned with this subject matter has in the past been very restrictive. (iii) Hydrologic science (HS) faculty have an interest in having a course in environmental visualization and manipulating data structures. One HS faculty member has tried to develop such a course recently. (iv) The AS program has a high level of computational fluid dynamics expertise. There are potential benefits from some coordination with the existing AS program.

- **Resources.** As indicated in item (iii) in the previous paragraph, LAWR faculty have a lot of expertise in CS&E-related fields.

3.2 College of Letters and Science

3.2.1 Chemistry

The degree to which a CS&E Initiative would fit into the Chemistry departmental plan and priorities will depend strongly on the end focus of the Initiative. An Initiative directed more towards the computer science side of things, such that the main focus becomes the development of generic algorithms which are divorced from specific scientific applications will have virtually no overlap with our departmental plans and priorities (and for this reason we feel that creating a CS&E unit within Computer Science is risky, as it will likely direct the Initiative toward generic problems). If, however, the focus of the Initiative is on the development of discipline- and application-specific algorithmic and methodological improvements, with a strong effort to promote interdisciplinary fertilization of these ideas, then the Initiative will provide an excellent complement to the departmental plan and priorities. Indeed, research focused on the development of new computational methods for solving chemical problems is already a strength in our department (three faculty), and our departmental plan already calls for the hiring of one additional faculty member in this area. Additionally, two campus initiatives currently figuring prominently in the Chemistry Department's long-range hiring plans, the *Structural Biology* and the *NEAT Initiatives*, encompass the study of highly complex systems which are ripe for computational investigation, yet which are sufficiently challenging that solving them will require the creation of new computational methods and algorithms. The combination of the draw of the CS&E Initiative and CS&E FTEs could enable us to bring in senior CS&E-chemistry hires in either, or preferably, both of these two areas, making UC Davis a powerhouse in the development of computational methodologies for the study of complex systems. Finally, we note that CS&E hires tied to these campus initiatives will be able to foster both computational (with other CS&E faculty) and scientific (with experimental researchers also involved in these initiatives) collaborations.

The Chemistry Department would be interested in hiring senior faculty members who combine computational algorithm development with a focus on solving specific scientific problems, especially those connected with the initiatives noted in the previous paragraph. A list of potential senior hires is: Ron Elber, Hebrew University of Jerusalem (global optimization and reaction path following in biomolecular systems); Jim Doll, Brown University (imaginary time path integral Monte Carlo methods); B. Monte Pettit, University of Houston (grand canonical molecular dynamics and new methods of analysis for biomolecular systems); Robert Wyatt, University of Texas (parallel computing and matrix decomposition methods for reactive scattering problems); William Swope, IBM Almaden Research Center (molecular dynamics algorithms for liquids); Garrison Sposito, UC Berkeley (computational methods for the study of soil minerals); Michael Treacy, NEC Princeton (computational methods for modeling complex crystalline frameworks); and Martin Head-Gordon, UC Berkeley (methods for reducing basis set scaling for large electronic structure problems).

Chemistry foresees two main needs in the computational instruction of our undergraduate majors, neither of which can be accomplished with the currently available departmental resources (including FTEs, teaching release time for course development, computer hardware, and technical staff support for computing resources). First, all chemistry majors will need a great deal more exposure to a variety of commercially available chemical software packages in order to be competitive in tomorrow's job market. While we recognize that this is not, and should not be, the focus of the CS&E Initiative, we feel that joint CS&E-Chemistry FTE could contribute significantly to the development and instruction of commercial software-based laboratories and courses. Second, and more closely tied to the spirit of the CS&E Initiative, is the realization that the job opportunities for students with training in general scientific modeling are continually expanding. In particular, students with computational and modeling training in one scientific discipline are often hired to model problems in a related or different scientific discipline. Thus, we think it would be a great advantage to chemistry majors to provide them with the option to take advanced undergraduate coursework in general scientific modeling. We anticipate that this coursework would be taught by CS&E faculty and would include, after a foundation of basic programming skills, exercises in which the students develop programs designed to model and solve various scientific applications. To make these courses accessible to a broad range of undergraduates, they should include applications from a variety of disciplines, but these applications should require no more than the introductory coursework in those disciplines to be understood.

Given the nature and depth of the Chemistry degree, a CS&E minor would have to require, at the very most, a maximum of six courses. Even this number of courses would most likely impact the time to degree for many chemistry majors and would not be particularly attractive. Since eliminating the requirements in the current Chemistry major is not a viable option (the only flexibility afforded by the ACS certification is in undergraduate research, which we strongly believe should not be replaced by CS&E or any other coursework), we suggest to consider the possibility of a combined Chemistry-CS&E major in which advanced CS&E coursework would replace some of the advanced Chemistry requirements, e.g., some of the advanced experimental laboratory courses.

The Chemistry Department is not able to make a commitment of any resources to the CS&E Initiative at this time, in part because the focus of this Initiative is not yet crystallized.

3.2.2 Economics

The Department of Economics supports the CS&E Initiative but is not in a position of directly participating in it now. Although Economics is a quantitative discipline it has traditionally been more a user of CS&E technology rather than a generator. Notable exceptions where Economics has actually been a generator are: (i) general equilibrium models of the economy where systems of equations are solved using an algorithm proposed by Scarf, an economist, in the 1960s; (ii) some techniques for macro-economic models of the economy; and (iii) computationally intensive methods for nonlinear regression, notably the recently proposed method of simulated moments (McFadden, Packes, and Pollard, 1989) and indirect inference (Gourieroux, Monfort, Gallant, and Tauchen in the 1990s).

The most likely area where a new hire might have interest in the CS&E Initiative is in econometrics but even there, there is only a small chance that the person would be interested. Most hiring in economics departments is directed to areas of economic interest rather than to specific tools.

The development plan of the Economics Department at Davis does not involve fields which would require especially sophisticated computational techniques. Future CS&E faculty will have little overlap with current Economics faculty, and it is not likely that the situation will change with future recruitment. In particular, since no economics department concentrates on producing CS&E types, no Target-of-Excellence candidates come to mind. If the Department hired someone of interest to CS&E it would be by coincidence.

We are sorry not to have any resources to offer CS&E hires. The Economics Department, like other Division of Social Science departments, has insufficient office space and resources for its own faculty.

We hope that the CS&E Initiative will be of interest to other departments, more dependent on developing new computational techniques than Economics. It may well be that the future development of economic research will call one day for a fruitful interaction between CS&E and Economics, but at this point it is premature.

3.2.3 Geology

The geological sciences increasingly are addressing complex processes that require the means to work with very large data sets and to conduct high-resolution numerical simulations of complex, strongly nonlinear physical systems. Graduate students and undergraduate majors need to be prepared to address complex natural systems and their interaction with man-made hazards using advanced computational methods. Students in the geology program and the geophysics minor would take courses in scientific computing offered by CS&E faculty. Areas of geological sciences that could benefit from the development of the CS&E Initiative include seismology, geodesy, geodynamics, geophysical fluid dynamics, quantitative geomorphology, and modeling of hydrological systems.

Although we do not explicitly incorporate CS&E positions in our most recent departmental plan, our plan includes appointments in geophysics, quantitative geomorphology, and other areas that would benefit from and interact with CS&E faculty.

3.2.4 Mathematics

The Department of Mathematics provided these comments concerning the CS&E Initiative:

- **CS&E Initiative and Departmental Plans and Priorities.** The Department of Mathematics has strong and internationally acclaimed research and educational programs in computational mathematics. These activities go beyond the traditional strength in numerical analysis and scientific computation, and have influenced current research in wide areas of mathematics including geometry, topology, analysis, discrete mathematics, and mathematical physics.

  The main lines developed in the Department's preproposal for Provost Grey's Initiatives have also been incorporated in this year's Academic Plan of the Department. There are two aspects of direct relevance to the CS&E Initiative. The first is discrete mathematics, an area that has gained enormously in importance because of its manifold applications to problems of computing and which has been developing rapidly itself due to the availability of fast computers. The second is a focus on experimental mathematics, i.e., research in mathematics involving novel uses of computing for the discovery and understanding of mathematical structures. Both are a high priority. Mathematics also wishes to further develop existing strength in the Department in the areas of scientific computation, fluid dynamics, image and signal processing, and mathematical biology, which are three more areas explicitly covered by the CS&E Initiative. Thus, the CS&E Initiative is the natural context for the realization of our plans. Moreover, the core areas of mathematics play an increasingly important role in an ever wider range of technological applications. One can hardly imagine a program in the area of CS&E without a strong mathematical component.

- **Hiring.** Exciting hires in CS&E that would have a strong and positive impact on the Department's programs include Neil Sloane, AT&T (coding theory), John Conway, Princeton (discrete mathematics), Ron Graham, UCSD, and Richard Stanley, MIT (both combinatorics), Peter Shor, AT&T (quantum computation), Hendrik Lenstra, Berkeley (applied number theory), Charles Peskin, Courant Institute, NYU (mathematical biology), and Ronald R. Coifman, Yale, Vladimir Rokhlin, Yale (both computational harmonic analysis).

  Strong PhD programs in computational sciences exist at Yale, Stanford, Brown, UCLA, MIT, Michigan, Wisconsin, Rice, Cornell, Texas, Maryland, Courant, Illinois, Purdue, and Florida, and in mathematical biology at Utah and Boston University.

- **CS&E and its Relation to Teaching.** CS&E-oriented appointments are expected to bring wider variety and deeper expertise in related areas into the Department's teaching programs at both graduate and undergraduate levels.

- **Resources.** The Department has requested to the Dean of MPS seven FTEs in discrete mathematics and 3 three FTEs in scientific computation for the period 2000–2006. The Department has also requested office and additional space for its needs. However, at this point, the Department is not in the position to commit any resources to the Initiative.

3.2.5 Physics

The Department of Physics provided these comments concerning the CS&E Initiative:

- **CS&E Initiative and Departmental Plans and Priorities.** In our December 1998 Academic Plan, we have earmarked our next two hires in the hopper (cosmology and high-energy experiment) to be in the data-intensive computational science area. We plan to leverage these two CS&E-participating hires to obtain two more half-GFTE joint appointments with CS&E. We will also commit two RFTEs to the CS&E Initiative to leverage two more half-GFTE appointments with CS&E [GFTE=growth FTE, RFTE = retirement FTE].

- **Hiring.** Senior faculty examples include Ed Bertchinger, MIT (astrophysics), Davis Cutts, Brown (high-energy physics, experimentalist), Leif Lonnblatt, CERN (high-energy physics, theoretician), David Ceperley, UIUC (quantum

Monte Carlo methods), E. (Tim) Kaxiras, Harvard (materials physics: surfaces). Institutions to be targeted for recruitment should include Georgia Tech, LSU, Oregon State, UC Berkeley, Northwestern, Ohio State, Caltech, and Boston U.

- **CS&E and its Relation to Teaching.** The normal course load in Physics is three podium courses per year: on the average one graduate, one small- and one large-enrollment undergraduate course each. A CS&E-participating faculty member will teach each year two physics courses and one CS&E course or one computational physics course, cross-listed with CS&E. A faculty member jointly appointed with CS&E will teach one physics course and two CS&E courses, including a large-enrollment course, per year.

- **Resources.** Physics will commit RFTEs as well as positions in the hopper. Physics has no space to commit.

3.2.6 Statistics

The Division of Statistics expects that there would be many opportunities for collaboration and joint ventures in teaching and research involving the Division and a formally organized group in CS&E. Our recently submitted plan for the further development of Computational and Graphical Statistics calls for the addition of five new faculty positions over the next seven years. We envision at least two of these positions being allocated to joint appointments with other units. We believe that an affiliation with CS&E would be among the more likely possibilities, and we would welcome the opportunity to plan a joint search with CS&E if and when the Initiative is authorized.

The mention of potential joint Target-of-Excellence hires is also very appealing. Individuals that come to mind would include Colin Mallows and Daryl Pregibon from AT&T, Y. Vardi from Rutgers, and D. Nychka of North Carolina State. All four are world-class researchers with strong profiles in computational aspects of Statistics, and each would have, we believe, the seniority and record of accomplishment that would qualify them for a targeted recruitment. Finally, with regard to academic institutions currently producing new PhDs with strength on the interface of Statistics and Computational Science, we would mention U. Washington, U. Chicago, Stanford U., and Carnegie Mellon.

3.3 College of Engineering

3.3.1 Applied Science

The Department of Applied Science of the College of Engineering has had a long and distinguished tradition of computational science, built largely around the computational facilities of LLNL and LBNL. Nearly 40% of the Department's graduates have specialized in computational physics, and their training in massively parallel techniques for computation of "real-life" problems (like weather prediction, biology, material damage, crack formation, etc.) has been superb. The Department's students have no problem finding positions after graduation.

To further this end, the Department voted several years ago to initiate a search for more top-notch faculty in this area. To the Department's delight, the Department succeeded in recruiting two of the best computational physicists in the country in the range of first-level full professor this year (1999). These two candidates were aggressively sought after by LLNL and LBNL and will take half-time appointments at these national laboratories. This year's entering class of graduate students is fully 50% interested in computational science. In addition, our efforts in computer media and communications, which involve Computer Science and Electrical and Computer Engineering, bring Applied Science squarely into the center of the Engineering College's computational efforts.

3.3.2 Civil and Environmental Engineering

The Department of Civil and Environmental Engineering provided these comments concerning the CS&E Initiative:

- **CS&E Initiative and Departmental Plans and Priorities.** Computational methods development for modeling physical systems forms the backbone of much of the research being conducted by CEE faculty. CS&E-related activities in CEE may be roughly grouped into three categories: (i) modeling of transport phenomena, including environmental fluid dynamics, subsurface flow, and atmospheric mixing; (ii) modeling of chemical reactions in complex systems, including aqueous and atmospheric environments; and (iii) computational solid mechanics, including simulation of the response and failure of all types of structures and materials subjected to many kinds of loading. In all of these areas, it is essential to note that CEE faculty have historically been engaged in the development and implementation of novel computational methodology, and not merely in the use of existing codes. To the above list of three broad disciplines may be added the rapidly-evolving field of information technology as it relates to the collection and manipulation of data relevant to civil engineering systems. Examples include traffic flow data in large urban areas, and remotely sensed hydrologic data. Some, but by no means all, of these research activities are related to the "classical" pursuit of solving complex boundary value problems by computational means. Many involve the manipulation and visualization of large data sets associated with large-scale data collection, for example. The CEE faculty expect that CS&E-related research activities in the CEE Department will continue to broaden in scope in the future. Accordingly, sustaining an environment in which the CEE Department has the ability to add faculty members with CS&E-related backgrounds is considered to be of extremely high priority.

- **Hiring.** In the very recent past, Professor Ian King retired from the CEE Department, leaving a large disciplinary void in the area of computational fluid dynamics. The Department considers it to be of the highest priority that this void be filled as soon as possible. Professor King's replacement is envisioned to primarily focus on the construction of numerical, probably finite element-based, models for complex fluid flows. While this person would likely be a user of sophisticated visualization tools, the person would not necessarily be directly engaged in the creation of such tools. In the computational solid mechanics area, a search is presently under way to replace a recent departure at the junior level. Due to a number of retirements in recent years, the faculty in CEE actively engaged in this discipline are all quite young. A new senior faculty member to provide leadership is considered important. Historically, the CEE Department has been very strong in computational solid mechanics, and has made many widely known research contributions. On the UC Davis campus, the expertise in computational solid mechanics within CEE is of vital importance to a number of units outside the CEE Department, both in relation to teaching and research.

  Our list of Target-of-Excellence individuals includes Phil Gresho, LLNL (computational fluid dynamics); Mary Wheeler, UT Austin (subsurface and atmospheric transport); Clint Dawson, UT Austin (transport phenomena); Tom Russelli, U. Colorado at Denver (transport phenomena); J. N. Reddy, Texas A&M (computational solid mechanics); and Brian Moran, Northwestern (computational solid mechanics). Our list of institutions includes UT Austin (computational solid and fluid mechanics), Northwestern (computational solid mechanics), Stanford (computational solid mechanics), Caltech (air quality modeling), and Carnegie Mellon (air quality modeling).

- **CS&E and its Relation to Teaching.** At the undergraduate level, many CEE course offerings have a strong presence of computational methods. For this reason, CEE undergraduates are required to take EAD 115. For some time, many CEE faculty have felt that we should be teaching one or more computational methods courses designed specifically for our needs. However, the pressures of covering the broad curriculum that we now teach has prevented us from making new course offerings of this kind. At the graduate level, the 212A-B-C series of courses, which cover the finite element method for both solid and fluid applications, usually have the largest enrollments of any graduate offerings in the CEE curriculum. In fact, students from many other departments in the College of Engineering as well as students from, e.g., Mathematics and Geology often take these courses. Additional CS&E-oriented faculty would be invaluable in enriching our offerings with other, more specialized courses that include, e.g., visualization and parallel computing.

- **Resources.** Depending on the individual, the area of expertise, and the circumstances, the CEE Department would be open to fostering collaborations with CS&E-oriented faculty. For example, a small fractional appointment (0.1 to 0.2 FTE) of one of our faculty with CS&E orientation with a CS&E unit, reciprocated with a small fractional appointment of a CS&E-faculty member in another area of interest to the Department can be envisioned. For example, if the computational solid mechanics search presently under way, the replacement of Ian King, or some future growth FTE in remote sensing yields an individual of interest to CS&E, and the Department desires some expertise to work on visualization or parallel computing, then an exchange of FTE may be possible. In the area of parallel computing, one of our faculty will be assembling a PC processor-based parallel computing platform that may ultimately have from 60 to 100 Pentium-type processors. A CS&E faculty with research interests in that type of computational environment could have the opportunity to collaborate in the use of this system when working on problems of common interest. Under these circumstances, the CEE Department would consider it desirable to distribute the costs of additional system development and support appropriately across all participants in the collaborative effort.

3.3.3 Computer Science

The CS&E Initiative and the Departmental Plan of Computer Science — Priorities and Hiring. The Department of Computer Science (CS) is a very active participant in CS&E activities today, and it is highly committed to this Initiative. CS research can be divided into two broad categories: basic (or "core" CS research) and applied. Core CS research deals with the development of technologies to build computers that are faster, cheaper, and easier to use. But computational methodologies are becoming an integral part of research in many fields, e.g., in biology, mathematics, physics, chemistry, the arts, and dozens of branches of engineering. This development has already been recognized by CS. The boundary between CS and other disciplines is getting blurred, and strong interdisciplinary research is needed to achieve the most effective results on these "boundary problems." Besides the CS&E Initiative, CS expects to play a key role in some other interdisciplinary campus Initiatives such as the Genomics/Bioinformatics and ArtsVision Initiatives. CS is supplying faculty expertise to all three of these campus Initiative committees, including the Chair of the Bioinformatics Subcommittee on Genomics and the Acting Chair of the CS&E Initiative.

Several CS faculty members contribute to CS&E and are highly accomplished leaders in their CS&E subdisciplines, e.g., Professors Bernd Hamann and Ken Joy in visualization and computer graphics; Professor Dan Gusfield in computational biology; Professor Alan J. Laub, Dean of Engineering, in scientific numerical computation; and Professor Michael Gertz in database and information systems. Another CS&E faculty member, Professor Nelson Max—who teaches, does research in, and supervises graduate student research in computer graphics and visualization—is expected to hold a joint appointment in CS in the near future. Our commitment to the field of CS&E is strongly demonstrated by the fact that two out of our three new faculty hires during the current academic year (1998/99) are CS&E-oriented faculty. One of them is Dr. Kwan-Liu Ma, who works in computer graphics and visualization; he is a 1993 PhD graduate from the University of Utah comes to us from NASA/ICASE. The other new CS&E hire is Dr. Zhaojun Bai, who works in numerical analysis and scientific computation; he comes to us from the faculty of the University of Kentucky.

Our Departmental Plan calls for the hiring of several additional CS&E-oriented faculty over the next several years. Potential CS&E areas in which we can add strength include computational biology, information systems, more hires in areas closely linked to or supporting visualization and computer graphics, and emerging "digital" disciplines such as computer music.

CS&E and its Relation to Teaching. CS offers a wide range of courses in computer graphics and visualization at both the undergraduate and graduate levels (ECS 175, 177, 178, 275A/B, 277, 278, 279). ECS 175 is very popular and is usually offered every quarter. One of our new hires, Dr. Ma, is expected to introduce a new graduate course in visualization during 1999/2000. Dr. Bai's hiring will enable us to revitalize our course offerings in scientific computation. He will offer a new course in scientific computation during 1999/2000. In the coming years, we expect that Dr. Bai will also be able to introduce courses on this subject at the undergraduate level. In the computational biology area, Professor Gusfield has taught ECS224 for several years and has recently introduced a new course, ECS 124, to be offered for the first time during 1999/2000. In the database and information systems area, we offer several courses (ECS 165A, 165B, 167, 168, 265). New hires are expected to introduce new courses and expand our graduate offerings in the years ahead.

Resources. CS is planning to add 16 growth FTE positions by the year 2005/06. Several of these positions will be earmarked for CS&E disciplines. Currently, with a faculty size of 19, the resources in CS are running at capacity, e.g., space, or are running out of capacity, particularly technical support. We expect that, due to our planned growth, there will be additional space (and financial support) made available to CS to recruit the new faculty hires.

3.3.4 Mechanical and Aeronautical Engineering

At the present time, the Department of Mechanical and Aeronautical Engineering (MAE) considers itself to be one of the leaders on campus in CS&E fields. This leadership is the result of the strong and fundamental efforts that exist in MAE in Computational Fluid Dynamics (CFD), Energy Systems Design, Computed-Aided Design (CAD), Computed-Aided Manufacturing (CAM), Computational Mechanics, and real-time control and optimization of physical systems. The MAE Department is both internationally and nationally recognized for its excellence in engineering and scientific computation, and the Department plans to build its future around this excellence and other CS&E-related subjects.

The MAE Department considers the CS&E Initiative as an opportunity for both growth and joint appointments. It is MAE's expectation that MAE can play a key role in attracting faculty for the CS&E Initiative, and MAE has many faculty members who would be interested in joint appointments. The current research areas in which the MAE Department excels are directly related to the CS&E Initiative, and MAE should play a significant role in teaching, facility development, and research opportunities. It should also be pointed out that the CS&E Initiative is an excellent opportunity for the College of Engineering to develop strong ties with the other colleges on the Davis Campus. The need for strong multi-disciplinary interactions between the College of Engineering and the Biological and Physical Sciences is growing rapidly, and the MAE Department is committed to developing these activities.

The MAE Department fully endorses the CS&E Initiative, and it is committed to actively participate in the development of the multi-disciplinary teaching and research in a potential new division for CS&E. MAE feels that the CS&E Initiative should be one of the top priorities of the UC Davis campus, and it should be closely connected to all of the colleges and departments on campus that would benefit from its activities.

3.4 Inter-College Programs: Division of Biological Sciences

3.4.1 Neurobiology, Physiology, and Behavior (NPB)

The NPB Academic Plan notes that computational neuroscience is developing into a key component of contemporary neurobiology because it successfully integrates cellular, systems, and cognitive levels of analysis. The plan notes that the Institute for Theoretical Dynamics (ITD) makes UC Davis a particularly attractive place for active computational researchers, with NPB maintaining a long-term commitment to this field.

The Section offers advanced courses in computational neurobiology at the undergraduate and graduate levels, and is proposing recruitment of a computational neurobiologist whose research focuses on the analysis of the dynamics of neural circuits and systems. The Section will recruit for a person with a primary focus on the theoretical and analytical aspects of neurobiology, with preference to candidates with a practical interest in experimental work. Close links for this recruit include various colleagues at ITD and Bruno Olshausen (Psychology) at the Center for Neuroscience. Several other NPB faculty have strong interests in modeling and would also form synergistic interactions with this researcher.

3.4.2 Molecular and Cellular Biology (MCB)

MCB's Academic Plan highlights computational technology as a technique that has led to major paradigm shifts in the area of biochemistry. As such, it is an area the

Section considers essential to its program, and one that will interface with current strengths in biochemistry and with the Center for Functional Genomics and Bioinformatics.

The MCB Section anticipates retirements of the majority of its faculty who currently teach in the biochemistry curriculum, and anticipates a need for, and the opportunity to conduct, at least two recruitments in the area of bioinformatics/computational structural biology. Candidates will research evolutionary (i.e., phylogenetic), functional, and structural relationships amongst members of a particular protein superfamily, utilizing the vast amount of sequence information available through the various genome projects. Technical approaches will include mathematical, statistical, and computational biological methodologies (e.g., the development of novel methodological approaches for mining of multiple databases) as well as approaches using biochemical/molecular biology for experimental assessment of functional implications of theoretical predictions. This research will ultimately encompass the newly emerging discipline of "systems biology" (i.e. the integration of protein sequence, three-dimensional structure and relevant biological data to understand the interplay of groups of genes in biological processes).

Two recruitments are proposed over the next three years. One candidate is expected to take a leadership role (possibly a senior hire) in campus-wide efforts to strengthen the infrastructure and intellectual developments in the areas of computational biology, genomics, and bioinformatics. A second candidate in the area of computational structural biology at a more junior level is also proposed. This individual will develop tools/approaches for protein structure prediction, protein folding, protein evolution, and/or protein-protein and protein-ligand interactions of relevance to biology, medicine, and/or agriculture. These candidates are expected to utilize any number of computational approaches, including, but not limited to, molecular simulations, genetic algorithms, and/or neural networks.

3.5 Professional Schools

3.5.1 Graduate School of Management

[Comments were provided by Dean Robert Smiley.] As I described briefly to the overall committee this winter, the Graduate School of Management is involved in computational science. The involvement ranges from simulations carried out by our management science and statistics faculty, which Professor Rocke is involved in, to empirical work on financial data, which requires both speed and high volume storage.

We also have teaching needs in the area of information technology. Our requirements are probably a bit different from most departments, however. After teaching a level of basic familiarity with hardware and business related software, we teach how to manage (configure, purchase, maintain, etc.) an information system. Hiring in this area is one of our most pressing needs, but we do not now have any vacant FTEs.

I am not familiar enough with the field at present to indicate who might be hired under the Target-of-Excellence Program, but I do know that Stanford, Rochester, NYU, and Arizona have a reputation for strength in the area. Joint appointments with Engineering would certainly be worth pursuing.

As a young school, I do not foresee any retirements until about 2007 or later. At that time or earlier if a resignation occurs, we would be interested in investigating the possibility of a joint hire. If we continue to be partially successful in obtaining additional space in AOB IV (we currently occupy about 3/4 of the building), we could provide space for someone appointed in our school.

3.5.2 School of Medicine: Biological Chemistry

The Department of Biological Chemistry likely is not able to provide help for or commit resources to this Initiative. According to the department's response, most of the research in Biological Chemistry is not computationally intensive.

4 Academic Plan for CS&E

The academic plan for CS&E should have several key elements, of which we present some below. These elements also impact the development of facilities and organizational structures to support teaching and research; projected needs for faculty FTEs, staff researchers, and technical and administrative support; different options concerning the organizational structure for undergraduate and graduate CS&E training, including curricular development; plans for collaborations with LBNL, LLNL, and potentially SNL; and the relationship between the academic plan for CS&E and the Stage 1 Initiative concerning the *Center for Functional Genomics and Bioinformatics*. We begin with a discussion of organizational structures for CS&E.

4.1 Possible Organizational Models for CS&E Education

The Committee members have discussed various options concerning an organizational structure for CS&E. We briefly summarize these options in the following subsections. The *Recommendations* section in this report lists the preferred choice of the majority of the CS&E Committee members.

4.1.1 Model 1: Establishment of a Graduate Group in CS&E and the Distribution of FTEs across Existing Units

Graduate Group. The establishment of a Graduate Group in CS&E is reasonable and desirable. The Graduate Group would allow better coordination of CS&E graduate education and linking CS&E faculty from different departments together to do interdisciplinary research. The Graduate Group would immediately develop a curriculum for a graduate degree and possibly a graduate area of emphasis for CS&E. A CS&E seminar series would allow the Graduate Group to create more awareness about CS&E and its significance for the future of this campus.

Distribution of CS&E FTEs across Existing Units. Concerning the distribution of CS&E FTEs across existing units, the question one has to answer is: Would the distribution of existing and new CS&E faculty across existing departments, coupled with the establishment of a Graduate Group, suffice to achieve the desirable impact that the CS&E Initiative should have? The answer is probably "no." The distribution of FTEs does not seem desirable, since it would most likely not lead to the evolution of a coherent educational and research thrust in CS&E.

4.1.2 Model 2: Concentration of CS&E FTEs in a Small Number of Existing Departments

In addition to creating a CS&E Graduate Group, this model would distribute CS&E FTEs in a few departments. To establish critical mass and coherency and to attract faculty, students, and funding, the CS&E Initiative could place a significant number of CS&E FTEs into a small number of existing administrative units. The one commonality that ties together people in CS&E is their commitment to develop, study, and use computational methods for one or multiple application domains. The unit on campus that has as its primary commitment the development and study of computational tools is Computer Science. Other units, for example Mechanical and Aeronautical Engineering, have a strong commitment to the development and application of computational tools as well, but are not primarily driven by computation. To foster the desired coherent educational and research thrust for CS&E a significant number of FTEs could be designated for a few units, e.g., Computer Science and Mathematics. New faculty should have their focus clearly on computation, should be expected to contribute to and feel comfortable with core fields in their respective home departments, Computer Science, for example, and have strong links to the disciplines driving their computational interest. Joint appointments for CS&E faculty would seem attractive and desirable under this model.

4.1.3 Model 3: An Independent Unit (Division) for CS&E

In addition to creating a CS&E Graduate Group, this model would lead to the creation of a new, independent organizational structure for CS&E. Model 3 for CS&E at UC Davis would be the establishment of an independent structure responsible for coordinating all educational efforts in CS&E.

Potential Problems with a Unit for CS&E, Coupled with an Undergraduate MAJOR in CS&E. Concerning the profile of a CS&E faculty member, close ties with at least one application area and a certain degree of sophistication in computer science, preferably coupled with, for example, a background in applied mathematics or statistics, are essential. Concerning the student body, it is reasonable to assume that the number of students sufficiently prepared to master demanding material concerning the development and study of CS&E methods is relatively small. The amount of training enabling a student to take CS&E courses—the kinds of courses that would not merely teach the application of tools but actually deal with the underlying concepts and their study—is substantial. This is particularly clear for material concerning scientific computing (including, as its core, numerical analysis and numerical linear algebra), multidimensional data mining algorithms, or optimization methods. Thus, one should be concerned about the number of undergraduate students who would qualify for and benefit from CS&E courses. Hence, the establishment of an undergraduate major might become a long-term goal of this Initiative, but there would be serious problems one would have to overcome: (i) defining a pool of CS&E courses large enough to provide the number of credit hours needed for a major; (ii) creating mechanisms that would link the CS&E course material to applications in which the CS&E methods taught are relevant; and (iii) ensuring that the courses of such a CS&E major would not be de facto duplicates of existing courses.

Students with an already established background in scientific and engineering applications of CS&E, computer science, and possibly mathematical methods would be primary target groups for CS&E course material. To equip undergraduate students with the required high degree of sophistication prior to their taking CS&E courses, one would have to revise existing undergraduate curricula and requirements substantially to prepare students accordingly. An undergraduate CS&E major without a serious connection to specific applications of CS&E might duplicate, to a large extent, course material from Computer Science, Mathematics, or Statistics. This is not desirable. CS&E certainly should not lead to a "watered-down version" of these three existing programs, or others.

Thus, the inherent interdisciplinary nature of CS&E is an obstacle for the establishment of an undergraduate major. A CS&E curriculum, by its very nature, should expect some knowledge of application-specific problems and basic requirements concerning possible computational solutions. Given the wide range of application domains, what would be common to the CS&E curriculum, faculty, and students in a CS&E undergraduate major? Most likely, the commonality would be rather generic mathematical and computer science methods and problem solving skills, applicable to a variety of computational problems encountered in science and engineering disciplines. On the other side, there is the danger that a major might focus on highly similar applications, and one would have to ensure that such a major would not just teach software packages and tools or evolve into a "second Computer Science Department." Unless the faculty of an independent unit responsible for CS&E course delivery are focused on highly similar aspects of CS&E, there would hardly exist any intellectual core to hold this unit's faculty members together. The commitment, then, should be the use and development of computation as a tool to enable scientific discovery through computation.

Potential Advantages of a Unit for CS&E, Dedicated to an Undergraduate MINOR and Graduate Education. An alternative to the establishment of an undergraduate major in CS&E within a department-like structure would be the development of CS&E to support double majors, minors, designated areas of emphasis, etc. This could, possibly, be implemented within existing departments representing application areas of CS&E or within Computer Science. An administrative structure facilitating double majors, minors, designated areas of emphasis, etc. would be needed, and the campus would have to implement mechanisms that would encourage undergraduate students to pursue such dual proficiencies. Improved future job competitiveness would be an important argument to attract student attention to such programs. Students would major most likely in a science or engineering field, computer science, or mathematics, with a specialization in CS&E.

A divisional administrative structure to support undergraduate minors and a graduate major in CS&E should be considered strongly. For example, this model could be implemented by the creation of an independent Division of CS&E hosted in Computer Science or—and this is the option favored by the CS&E Committee—in the College of Engineering. This is analogous to the *Division of Statistics*, hosted in the College of Letters and Science. This model ensures that the educational and intellectual interests of other colleges are protected. Courses, minors, and majors that such a Division would offer *should be accessible to the general campus student body* as much as possible. This aspect should be paramount concerning course delivery—regardless of what type of organizational structure for CS&E is chosen in the end. If universal access to CS&E courses were guaranteed, such a division would be attractive to the campus at large. If a Division of CS&E were eventually placed in a particular college, e.g., Engineering, it would be pivotal to ensure that students from across campus would have equal access to CS&E courses. Major resources would have to be committed to a new Division of CS&E, in terms of space, computing resources for educational laboratories, and administrative and technical support. The College of Engineering and the campus would have to make significant investments to make this model work.

Placing a Division of CS&E in the College of Engineering would locate it in the same college as Computer Science, which should be positive in the context of course coordination and minimizing the danger of course material overlap or duplication. The creation of a Division within an existing department, i.e., Computer Science, could potentially lead to internal conflicts as a result of competition for resources. One would minimize this danger by creating an independent Division of CS&E in the College of Engineering.

Some Committee members see a danger for possible duplication of efforts. The mission of Computer Science might, in the end, have serious overlap with the goals set forth for the CS&E Initiative. This should be avoided. Furthermore, one has to assume that hiring priorities would have to be changed to some degree by departments heavily impacted by CS&E expansion. To foster more widespread and more enthusiastic support concerning expansion in CS&E areas, one might promote joint appointments: Model 2 could foster joint faculty appointments and could thereby make the hiring of CS&E faculty attractive—both to the department(s) where CS&E appointments are concentrated and to the application domains in which CS&E faculty would be appointed jointly. The CS&E faculty members would define and coordinate a graduate program and, most likely, minors or emphasis areas in CS&E together with faculty from all disciplines with an interest in computation.

4.1.4 Model 4: An Independent Department for CS&E

The final possibility is the creation of a full Department of CS&E within one of the Colleges. This possibility would have most of the characteristics of the divisional structure, but would differ in its internal administrative configuration (Department Chair vs. Associate Dean) and reporting structure. It would still be important to encourage joint appointments and to maintain collaborative links with other departments and research centers. Newly developed graduate programs should still be within a Graduate Group whose formation could begin as early as the Fall Quarter of 1999.

Regardless of whether a Department or a Division of CS&E would be chosen, it would be important to consider carefully the phasing and time-line for their establishment. First, one should solicit interest from UC Davis faculty in transferring to this new unit. Such appointments could be a full FTE or fractions of FTEs. Considering the original establishment of Computer Science in the early 1980's as example, the Committee on Academic Personnel could appoint an ad hoc committee to screen faculty applications and act in lieu of a faculty to recommend for or against appointments. These recommendations would then proceed in the same way as a similar request by a currently appointed faculty member to join an existing department. This step could be completed during the Fall Quarter of 1999.

The initial group of faculty established in the first step may not form a departmental critical mass, so it may be necessary to constitute a larger, temporary group of faculty to act for the Department concerning, for example, personnel and curricular issues. Besides the faculty actually appointed in the Department, additional faculty could be appointed for a limited term to this temporary body to ensure disciplinary balance. (This mechanism was used in 1979 to begin the establishment of the Graduate School of Management.)

By the Fall Quarter of 2000, recruitment for the first group of outside faculty in CS&E could begin, and, by this time, an initial set of courses would have been developed and approved by the Academic Senate. A full minor curriculum could be implemented by the Fall Quarter of 2001 at the latest or possibly by the Fall Quarter of 2000, depending on the size and composition of the initial group of faculty.

The majority of the Committee favors Model 3 with its emphasis on minor and graduate education as the near-term goal and Model 4 as the long-term goal for this Initiative. (See also section 5 and Recommendations section.)

4.2 A Center for CS&E

Independently of the final organizational structure of CS&E as it relates to the teaching mission, the Committee recommends the immediate creation of a *Center for CS&E* that would become the primary home for current and new CS&E faculty, the place for research coordination and computing laboratories. Current CS&E faculty are dispersed over the whole campus, and the Committee strongly believes in the idea of physically co-locating current CS&E faculty, researchers, and students. The Center should be responsible for those efforts that would benefit from centralization and a center environment, i.e., all heavily computing-oriented CS&E research projects. It should provide an interdisciplinary research environment with computation as its focus and could also help with the development of educational efforts in the early phases. The development of such a Center could occur in multiple stages.

The first stage of development of a Center would bring together current CS&E

faculty at UC Davis, who could also immediately initiate, for example, a *Program in CS&E*, i.e., current faculty would draw from existing programs and majors to coordinate CS&E-related course material and also institute new ones[5]. Such a Program should be viewed only as a transitional step in the sense that it would merely be supporting the creation of the eventual organizational structure for CS&E education on campus. The *Center for Image Processing and Integrated Computing (CIPIC)* and the *Institute of Theoretical Dynamics (ITD)* could serve as the basis for the development of a CS&E Center on campus[6]. (Several members of GGAM are associated with ITD.) With a small augmentation of existing administrative support in these two Organized Research Units (ORUs), the Center (and its potential educational Program) for CS&E could immediately begin to develop computer facilities and research and teaching opportunities for current CS&E faculty and students. The Center's associated faculty members would also be actively involved in recruiting and hiring new CS&E faculty[7]. We recommend the recruitment of a small number of senior computational scientists with an international reputation as soon as possible to help with the development of the Center and, possibly, the steering of curricular efforts.

The second stage of development of a CS&E Center would be signaled by the final establishment of the organizational structure for CS&E. At this point, the Center's mission should focus on CS&E research and possibly research integration into educational efforts, but the further development of key curricular aspects of CS&E should become the responsibility of the particular unit implemented for CS&E education. At the end of the first stage of the Center's developments, the Center should have a permanent space allocation, preferably in the Academic Surge Building to facilitate interactions with existing research units located in that building. We propose that new faculty hired under the CS&E Initiative would have their primary office and research space in the Center, while their formal (possibly joint) appointments would reside with the potential unit for CS&E and possibly other departments. The Center would function as the catalyst for computational science on campus, and the Center should also become the home for non-tenured CS&E researchers, visiting faculty, or visiting researchers from industry and national laboratories participating in interdis-

[5] A first step would be to seek approval of a graduate curriculum for CS&E, to be offered through the Graduate Group in CS&E. A Program in CS&E would require the addition of courses in support of minors. CS&E minors would be offered through the CS&E Program. The *Women's Studies* program at UC Davis is offering both a minor and a major, which is built around a faculty core that is highly diverse and whose members, in some cases, have official appointments in Women's Studies. Women's Studies could serve as a model for the creation of similar CS&E educational efforts during the early stages of curricular development.

[6] CIPIC's, ITD's, and CS&E's envisioned missions would complement each other. The development of CS&E on campus should take advantage of the significant expertise and infrastructure that exists in CIPIC and ITD.

[7] The Center would *not* be the final organizational unit responsible for CS&E curricular development. Only during the very early stages of curricular development the Center's affiliated faculty would steer, together with departments having an interest in CS&E, the key components for future CS&E education.

ciplinary efforts[8]. In the following, we address issues pertaining to the establishment of a CS&E Center.

- **Initial Focus Areas.** A small number of new CS&E focus areas that would be targeted for support by the Center should be identified. These should not overlap with programs currently supported by campus ORUs or other research units on campus, but should build on emerging new CS&E efforts building on existing areas of excellence, e.g., computational astrophysics and computational molecular biology.

- **Massive Data Problem.** A severe problem that is impacting all CS&E fields is the problem of dealing with massive amounts of data to be modeled, to be stored, to be transmitted, and to be analyzed for scientific discovery. The progress in imaging and computing technology is "flooding" all CS&E fields with data, and it will be crucial to invest in areas such as data modeling, data organization, database and information system technology, multimedia, high-speed networking, data analysis, visualization, and other fields addressing massive data problems. For example, there is a need for data modeling, including meta-data modeling, which is particularly important in interdisciplinary applications. It is crucial to describe data in terms of data formats and data models such that the structure and meaning of the data can easily be understood by and shared among different groups. There exists a definite need in this area concerning both teaching and research[9].

- **Computing Mission for UC Davis.** The Center could be responsible for the development and maintenance of the high-performance computing and massive data storage infrastructure of UC Davis. Nevertheless, there is no agreement among the Committee members whether a CS&E Center should or should not take on this responsibility. This would require a strong commitment to supporting permanent personnel, such as technical staff for computer maintenance, system management, and training.

- **Resource Requirements.** Initially, the Center and associated current faculty would be concerned with the establishment and administration of new CS&E

[8]The *Center for Neuroscience* could serve as a model for the development of a CS&E Center. In the case of the Neuroscience Center, research and teaching efforts are coordinated through the Center for the campus, and faculty from various disciplines work and, in some cases, have appointments with the Center. The Neuroscience Center offers a *Program in Neuroscience* leading to a graduate degree with neuroscience being the area of emphasis. A center setting is highly attractive for both informal seminars and distinguished lecturer series. The creation of an atmosphere that is lively, that is inviting, and that is stimulating communication would be a crucial consideration for the design of a CS&E Center.

[9]The NSF has identified the massive data problem as particularly important. Evidence for this is a recently announced NSF initiative, called *Large Scientific and Software Data Set Visualization* (NSF 99-105).

research efforts, bringing together current CS&E faculty. The Center would become the home for current CS&E faculty and new faculty hired under the Initiative. The amount of space, amount (and source) of start-up funding, and amount of the annual budget for the Center must be estimated realistically. In the first stage of the Center's development, resources should be made available based on the assumption that about 15 current UC Davis faculty members in CS&E would be spending a significant amount of their time in the Center. During the second stage of the Center's development, resource commitments should be growing steadily, based on the assumption that the number of Center-affiliated faculty would reach about 45 after a period of about six years—considering the fact that most of the new CS&E faculty would have joint appointments[10].

4.3 Faculty Recruitment

Substantial numbers of growth and retirement FTE faculty appointments would be required to make this Initiative successful. In addition to supporting the need for graduate education and leading research programs in CS&E, faculty hired under this Initiative should be expected to help with the delivery of existing courses with large student enrollments, e.g., introductory computer science courses, and the development and delivery of new CS&E courses, in the context of both undergraduate and graduate education.

Concerning a hiring strategy, one could build CS&E by implementing either a *top-down* or a *bottom-up* approach. The top-down approach would be based on the model of identifying leading and internationally recognized CS&E faculty, attempting to recruit them to UC Davis, and providing these faculty with the means to define and shape CS&E. The bottom-up approach would be centered around the idea of bringing together current CS&E faculty from the campus and recruit additional faculty that would complement the current faculty. The Committee believes that there are advantages and disadvantages to both strategies. Hiring a few senior faculty during the early stages of CS&E development might be advantageous. Realistically, it would not be easy to hire senior faculty in CS&E as it is still an emerging and relatively young discipline. The initial hiring of senior people could provide the visibility and leadership needed to make UC Davis a leader in CS&E. In addition, CS&E faculty members should qualify for joint appointments linking at least two departments. A campus committee consisting of current CS&E faculty should, in close collaboration with individual departments, identify priority areas targeted for hiring during the first

[10]The number 45 is based on the following assumptions: (i) There are currently about 15 faculty members on campus who define themselves primarily as CS&E faculty; and (ii) a new faculty member hired under the CS&E Initiative would, on average, consume only 50% of a CS&E FTE, since this faculty member is likely to also consume 50% of an FTE in another unit where the faculty member would contribute to non-CS&E efforts. This would likely be true even for a divisional or departmental model for CS&E. This explains the total number of potentially 45 CS&E faculty members.

rounds of recruitment. Individual departmental plans should be considered in hiring new CS&E faculty. New faculty should be able to contribute to existing departments as much as to the CS&E Initiative itself. We discuss specific recruitment issues in the following paragraphs.

- **Requested Number of FTEs. We recommend the allocation of a total of 15 FTEs for the recruitment of new faculty members under the CS&E Initiative, over a six-year recruitment period.** A typical CS&E faculty appointment would, in most cases, be a joint appointment between the organizational unit responsible for CS&E and another department. Flexibility will be required concerning such joint appointments, and it is reasonable to expect that new faculty could have any percentage of their appointment be counted as CS&E. Therefore, the requested number of FTEs would eventually lead to a much larger number of new faculty members with a CS&E component to their interests. The majority of new faculty appointed under the CS&E Initiative should be able to contribute to the needs of all the units in which they would hold appointments and the development of CS&E in its own right[11].

- **Role of Current UC Davis CS&E Faculty.** The UC Davis faculty members involved in the preparation of this CS&E Initiative report represent only a fraction of current UC Davis faculty interested in the teaching of or research in CS&E areas. We suggest that a faculty committee be formed as soon as possible with the responsibility of coordinating and overseeing the early phase of recruiting in CS&E and handling other issues, like curricular development. This would be necessary during the transitional period eventually leading to a formal CS&E unit.

- **Student Demand for CS&E.** Initially, courses supporting an undergraduate minor in CS&E (and a graduate minor or major) in CS&E should be developed in close collaboration with those disciplines interested in having their students minor in CS&E or impacted by the teaching of new CS&E courses. Of course, in order to have a Graduate Group in CS&E, there must be a graduate major in CS&E. The involvement of Computer Science would be crucial in this process. It is reasonable to expect that between 5% and 25% of all undergraduate students in the sciences and engineering disciplines (depending on their primary field of study) would have an interest in minoring in CS&E. It is much harder to estimate this for other disciplines. The Committee assumes that departments would change their current undergraduate curricular requirements in order to foster the minor option in CS&E. Pursuing a minor in CS&E should not impact the amount of time it takes a student to graduate. The percentage of graduate

[11] To help alleviate current problems in the delivery of fundamental computer science courses at the undergraduate level, a relatively large number of CS&E FTEs should be dedicated to CS&E hires who could contribute to Computer Science's undergraduate educational mission.

students in the physical sciences and engineering disciplines with an interest in adding CS&E as an area of emphasis or to pursue a graduate degree in CS&E should also lie between 5% and 25%.

- **Retirement FTEs.** CS&E is an evolving area, and the number of FTEs becoming available from retirement of faculty already working in this area is likely to be very small over the next six years. It is recommended that those departments and divisions having a strong interest in CS&E identify retirement FTEs that could potentially be used to leverage this Initiative.

- **Joint Appointments with LLNL and LBNL.** LLNL and LBNL have a strong interest in closely working with UC Davis, for a multitude of reasons—the major ones being access to students and university research. Faculty and students, on the other hand, gain insight into large-scale applied problems, students become more competitive for summer internships, and the campus obtains access to high-performance computing environments through collaborations. LLNL, LBNL, and faculty candidates who interviewed with UC Davis in the past often articulated a strong interest in joint university-laboratory appointments. This should be fully exploited when recruiting new CS&E faculty, and the campus should view this type of joint appointment positively.

- **Fields Targeted for CS&E Recruitment.** The Committee recommends—considering existing CS&E strengths and perceived future needs of UC Davis—this list of fields to be targeted for CS&E faculty recruitment (not ordered according to priority): (i) *generic areas:* numerical analysis, numerical linear algebra, and numerical methods for solving differential equations; Monte Carlo methods; discrete and experimental mathematics; machine learning, encompassing data analysis, data mining, clustering, classification, pattern recognition, neural networks, genetic algorithms, and feature extraction; optimization, including combinatorial optimization; visualization and virtual reality; information and database systems, with an emphasis on scientific and engineering data modeling; and algorithm development concepts for CS&E; and (ii) *application-specific areas:* biofluid dynamics; bioinformatics and structural/functional genomics (leveraging the Initiative for a Center for Functional Genomics and Bioinformatics); computational biology, including computational molecular biology; computational neuroscience; computational physics/cosmology; ecosystem modeling; and digital arts, e.g., virtual reality for design, computer graphics animation in relation to the performing arts, or computer music[12].

[12]The CS&E Committee envisions the establishment of new and strengthening of existing connections between CS&E and UC Davis arts programs. In fact, Computer Science has in the past received applications from faculty with an interest in the application of computer technology to the arts. It would require careful coordination between the arts and primarily computing-oriented units to hire faculty who could effectively contribute to both traditional computing fields and the arts.

A serious CS&E effort would eventually involve a several campus units, and it would be important to coordinate the prioritization of fields targeted for CS&E recruitment with all units carrying out actual science and engineering applications. The responses provided in section 3, entitled *How CS&E Relates to Existing Plans at UC Davis*, provide a first guideline for ranking the listed generic and application-specific CS&E areas according to the needs of the various units affected by and interested in the CS&E Initiative.

4.4 Development of a CS&E Curriculum

CS&E educational efforts should have a student's interest at heart, i.e., the main emphasis should lie on the preparation of a competitive student who understands fundamental CS&E methods, knows how to apply these methods to a particular application area, and is competent to generalize or adapt these methods to practical computational problems encountered in applications in one's future career. A CS&E curriculum and "typical" CS&E courses must be fundamentally different from a computer science or computer engineering curriculum and computer science or computer engineering courses. We outline various aspects in the following.

The Committee anticipates that there will be a need for CS&E education beyond science and engineering. It can be foreseen that even students in such diverse fields as art, management, and economics will become more and more interested in enrolling in undergraduate CS&E courses and pursuing a minor degree in CS&E.

There are several undergraduate and graduate programs that could be supported by CS&E faculty members. Some possibilities are outlined below, keeping in mind that the actual curriculum would be designed by the CS&E faculty after it is formally organized.

- **Undergraduate Minor.** Based on discussions with numerous faculty, it is evident that a need for an undergraduate minor in CS&E exists on campus today. The undergraduate component of CS&E development must address this need, and the goal should be the creation of such a minor. It is clear that the need for a minor in CS&E exists throughout the science and engineering disciplines—and other fields should follow soon.

  The set of courses that students with a minor in CS&E would have to take would initially be developed and administered, possibly, by the Program in CS&E and later by a potentially independent Division for CS&E. The Program

The Committee hopes that it will be possible to evaluate faculty candidates with an interest in the application of computer technology to the arts more favorably in the future. The CS&E and the *ArtsVision* Initiatives should closely work together concerning recruitment efforts of digital arts faculty. These faculty could promote state-of-the-art computational techniques in the arts and, at the same time, push computational technology by working on challenging digital arts problems like, for example, digital dance.

or Division would be coordinating courses that apply to a broad spectrum of applications. A total of about 20 to 24 credit hours constitutes a minor. The set of courses defining a potential CS&E minor would be defined by CS&E faculty in consultation with the departments whose students would most likely take advantage of the CS&E minor. Departments with an interest in seeing their students minoring in CS&E should allow and prepare for changes in their respective curricula. In this context, it would be very important that the affected departments would be open to the idea of having CS&E become the primary home for the preparation of their students in computational methods.

This is an attractive possibility and is likely to be popular with physical science, biological science, earth and environmental science, and engineering majors, as well as selected social science majors. We envision a two- or three-course introductory sequence to be taken by sophomores or juniors that would introduce computational methods and theory applicable in a variety of areas. Unlike the computer science introductory curriculum, there would be an equal concentration on floating-point problems as well as integer problems, but with a rigorous foundation in the theory of algorithms. The total course requirements might be six courses; the remaining three or four courses would be chosen from a list containing courses taught by CS&E faculty in several departments.

Prerequisites would again be determined by the CS&E faculty. Clearly this would include mathematics at least through calculus, and probably also linear algebra, differential equations, and vector analysis. Some knowledge of programming would be required, but the exact prerequisite computer science courses need to be specified; it might include a data structures course and algorithms course, or both. This would be co-determined with the computer science content of the core sequence, so that students would have an adequate conceptual background in computer science for the remainder of the curriculum. It is very likely and desirable that discrete mathematics will play a significant role as well.

- **Masters Program.** The organization and development of the graduate curriculum would be the responsibility of the CS&E Graduate Group. To facilitate curricular development the Chair of the Graduate Group would, in close consultation with other campus units, define a Masters program in CS&E or an area of emphasis in CS&E.

  A Masters Program would be conducted by a graduate group and would focus on students with a background in science or engineering who wish to pursue a computationally oriented career but whose undergraduate background is not yet sufficient. The potential topics would be similar to those for the undergraduate minor, but the coursework would be more extensive and the majority of it would be offered at the graduate level. Students would be expected to have a greater background in mathematics and computer science than for the undergraduate minor, and students would need to make up these courses if they were admitted without having taken them. To attract students to the Program, it would be crucial to keep prerequisites concerning mathematics and computer science courses minimal.

- **"Graduate" Area of Emphasis.** This would be a kind of mixture between the previous two programs. The coursework would be at the graduate level, but would not be as extensive as for a Masters degree. It is not clear what the demand for this option might be, but it could be implemented with very few if any additional courses than those required for the first two options.

- **PhD Program.** This would be an objective for the longer term. A Graduate Group established for the Masters Program and the area of emphasis could develop a PhD program provided that there is student interest and a demonstrated need for the graduates.

- **Courses.** Courses would be selected from existing graduate courses, and new courses would be developed by new and current faculty. Courses would be cross-listed. Besides any introductory sequence, the hiring of a substantial number of CS&E faculty will result in many new courses, many of broad interest to students in a variety of graduate and undergraduate programs. What these courses would be depends on specific recruitments, but some possible areas would be the ones listed in section 4.3 under *Fields Targeted for CS&E Recruitment*.

4.5 Computer Science Instruction and CS&E Education

The current and predicted future increase in demand for computer science education, driven by student and industry needs, still exceeds the increase in supplied teaching resources, both from a faculty and an instructional laboratory perspective. The Committee is aware of the recent efforts of the campus to help reduce this problem by allocating additional resources to Computer Science. Unfortunately, the UC Davis student populace is still experiencing difficulties in enrolling in certain Computer Science courses that are in very high demand. While the Committee realizes that this is a major reason to call for the expansion of computational-oriented education in all departments throughout campus, the Committee strongly believes that core computer science training is, and should remain, the responsibility of the Computer Science Department.

The Committee is of the opinion that the establishment of a CS&E unit could help reduce, at least to some degree, the demands on Computer Science and, at the same time, prepare students with a potentially stronger emphasis on the applications of computational methods. It must be ensured that the potential implementation of a new CS&E unit—with its educational mission being the delivery of computational methods courses—does not duplicate efforts of Computer Science. There exists a strong industry need for core computer science education that emphasizes—and Computer Science is the appropriate place to provide this type of education.

To meet the demand for core computer science education, it has been suggested to expand resources in departments other than Computer Science. The Committee believes that this would not be in the interest of students and not in the interest of the campus as a whole. It is more appropriate to focus on the quality of computer science instruction, to leave core computer science education as Computer Science's obligation, and to meet the increasing demand for computer science instruction by supporting Computer Science directly, and by favoring a CS&E hiring process that would attract CS&E hires who would be qualified for and interested in contributing to core computer science teaching. CS&E faculty candidates with dual interests and backgrounds in non-computer science disciplines as well as computer science should also be considered favorably for future hiring. They could equally contribute to both delivery of computer science courses and CS&E courses. This approach would also take into account that Computer Science is housed in Engineering, while half of its students are in another college. Dual appointments of CS&E-focused faculty members between Computer Science and another department would allow multiple departments to grow and would help reduce the strain put on computer science education. Computer Science is open to expansion in application-oriented directions favoring faculty candidates with a strong CS&E interest.

4.6 Connections with LBNL and LLNL

Additional opportunities for research and educational development would be provided by building on the existing strong associations with the two national laboratories closest to UC Davis, LLNL and LBNL. In collaboration with the campus deans, CS&E would be responsible for the development of mutually beneficial efforts like the ones listed in the following.

- **Faculty Recruitment.** The recruitment of CS&E faculty with joint appointments with either LLNL or LBNL should be fully exploited.

- **Formal Academic Collaboration.** The creation of formal academic connections and collaborations between CS&E and computational research centers at LLNL and LBNL, e.g., the *Center for Applied Scientific Computing (CASC)* at LLNL and the *National Energy Research Scientific Computing Center (NERSC)* at LBNL, should be enabled.

- **Computational Resources.** The campus should foster the joint development of computational resources, such as high-performance computing infrastructure, high-speed optical networks, or massive data storage and data visualization environments.

- **Student Fellowships.** LLNL and LBNL should, in close collaboration with UC Davis, consider the expansion of student fellowship opportunities, such as the UC Davis-LLNL *Graduate Student Employeeship Program*, to foster more joint supervision of doctoral students.

Potential. Beginning with John von Neumann's work at LANL using early computers to solve differential equations, the national laboratories have been home to many of the largest computing facilities and leading programs in CS&E in the United States. A number of those major facilities and programs are now part of the national infrastructure in CS&E and involve university collaborations and outside access to computing resources at the Department of Energy (DoE) laboratories at Berkeley, Livermore, Los Alamos, Argonne, Oak Ridge, and elsewhere.

The University of California is a contractor for the DoE and operates three of these Laboratories: LBNL, LLNL, LANL. At UC Davis we therefore have a major opportunity to exploit a special relationship with those institutions to enhance the CS&E Initiative. In particular, the caliber of scientists and engineers we want to recruit to the faculty positions associated with this Initiative will find these positions much more attractive if they are accompanied by the chance of a close association with one of the laboratories.

The future of CS&E at UC Davis is dependent in large measure on our faculty's ability to attack the large-scale problems that characterize modern applications of computing in science and engineering. The forefront of research in almost all areas is focusing on complex systems in lieu of the simple models of earlier efforts. The areas of multi-component materials, complex biological systems, climate and global systems, total simulation of combustion engines, total engineering modeling of automobiles, and many other problems are emerging as "big science" for which both large teams of researchers and major resources are necessary for progress. Even computer science research itself benefits from proximity to this scale of computational application, where, for example, the large data sets now being used in visualization and imaging drive a new class of algorithms and approaches.

Opportunities. At UC Davis we already have the mechanism in place for joint appointments between any of the three UC-operated national laboratories and the campus itself. There are faculty currently holding such appointments with various fractions of their positions divided between UC and national laboratories. We even have a department resident at LLNL, Applied Science, and various disciplinary centers which encourage such appointments. In addition, a number of faculty have DoE contracts and are thereby naturally connected to programs at the UC-operated laboratories with which they collaborate.

The national laboratories also benefit from this relationship. Many of the best researchers are more comfortable with the more open and free research environment that a university faculty position can provide them. It is an advantage to the national laboratories to be able to recruit such people to become part of their research programs on the part-time basis that a joint appointment allows. In fact, there are many examples where primary intellectual leadership is exercised in national laboratories by faculty members from the UC campuses.

As part of the CS&E Initiative, it is therefore strongly recommended that many of the associated faculty positions be leveraged by joint appointments with the UC-operated national laboratories. These joint appointments will need to be negotiated by the deans and department chairs involved in recruiting these faculty, and such arrangements will have to be made in advance in order to have both institutions agree to share the costs of the positions and to jointly recruit candidates.

Barriers and the Need for Changing the University-Laboratory Interface. Typically, a UC campus and a UC-operated national laboratory in which joint appointments are held share the costs of the faculty salary and benefits. These arrangements allow faculty to gain access to both the high-end computing resources they need and the stimulus of large teams working on complex problems. They do not, however, always function smoothly. The problems originate from the requirement to serve two masters, from different and often incompatible cultures.

The principal difficulty is that the teaching and service (and some research) activities of a faculty member in his or her university position may not be of interest to the national laboratory, and conversely the service, program development, and administrative activities associated with a laboratory position may be of little relevance to the merit review of a university professor. In effect, if a faculty member with a 50% appointment initiates and manages a large research program funded by the DoE in one of the national laboratories, few of the associated administrative and national service activities are relevant to tenure and promotion. Moreover, if the same faculty member publishes work in areas not related to his or her DoE research, serves on university committees, and develops a program funded by NSF, none of those activities affects performance evaluations in the national laboratory.

The reduced teaching load and lessened ability to perform service activities in the university that must accompany a joint appointment may become additional liabilities for the faculty member. As a result, it is difficult to see how a faculty member's career, especially that of an assistant professor, is not put at risk by a joint appointment with a national laboratory—even though both appointments are within the UC system and are actually with the same employer.

It can be foreseen that some CS&E faculty hires, most likely at the senior level, would be quite interested in using a joint appointment with a national laboratory to take on a leadership role in the applied laboratory environment by heading groups of professionals and defining major research programs. Currently, this type of organizational or professional competence is not valued by our academic merit and promotion process to a large degree. Joint appointments with national laboratories would be more attractive to faculty if the university evaluation process were to value the laboratory work component more, which, in turn, would excite a jointly appointed faculty member to execute a true leadership role at the laboratory. One should also keep in mind the actual leverage of university and national laboratory finances that would result from this type of joint appointment.

If UC Davis is to avoid missing a major opportunity in developing this Initiative, the campus must move to address these fundamental structural problems. At stake is the ability to effectively extend the number of faculty positions in the Initiative. An attractive mechanism for joint appointments, with a single set of criteria for merit evaluation, and career development advantages in place of the current disadvantages, will ensure an opportunity for UC Davis to become a major player in this field almost overnight.

4.7 Relationship with Center for Functional Genomics and Bioinformatics

In the area of computational biology, there may be some overlap between the CS&E Initiative and the Stage 1 Initiative for the Center for Functional Genomics and Bioinformatics. This overlap will permit recruitment of faculty who assist development in both areas. It will be important to follow these principles:

- **Joint Review of Faculty Candidates.** We propose that appointments overlapping the CS&E and the Center for Functional Genomics and Bioinformatics Initiatives be reviewed jointly in order to coordinate recruitment across the campus.

- **Avoiding Duplication of Effort.** Potentially overlapping positions need to be identified, and the leaders of the two Initiatives should decide jointly what constitutes a duplication of effort and ensure that duplication will not happen.

The CS&E Initiative includes the subarea of computational biology. *Computational molecular biology*, for example, is closely aligned with bioinformatics, although there is no definition of the two fields that is completely agreed on. Computer Science, ITD, and Mathematics contributed preproposals that include some aspects of computational molecular biology, and ITD contributed a preproposal that includes other aspects of computational biology. Clearly, hiring plans in computational molecular biology should be coordinated as much as possible with hiring plans in bioinformatics. One has to avoid redundant hiring and leverage the efforts of both groups as much as possible.

While there is no perfect way to distinguish between the fields of computational molecular biology and bioinformatics, there is a distinction in the kinds of people who might be hired under the two initiatives. In both cases, it is essential that the people we hire be active in developing methodology, and yet be closely aligned with its application in one or more specific biological subareas. However, it is natural to expect that people hired under the Bioinformatics Initiative might have a greater orientation to the biological applications, while the people hired under the CS&E

Initiative might have a greater orientation to methodological issues. This reflects both the differences in the flavor of the two initiatives, and the fact that people have to be housed in specific departments and sometimes teach in areas other than their research specialty. Still, it may turn out that faculty hired in bioinformatics may have their primary training outside of biology, while faculty hired in computational biology may have their primary training in biology.

The Genomics/Bioinformatics Initiative proposal is not yet completed, and the final direction of that proposal may depend on current hiring efforts in genomics. Hence, it is not clear what hiring decisions will be made in bioinformatics in the short run. It is important, however, that decisions in computational biology under the CS&E Initiative not be held up, waiting for clarity on bioinformatics. Excellent people can be recruited in computational biology who will mesh well with whatever direction the Bioinformatics Initiative ultimately takes.

5 Concerns Regarding an Independent Unit for CS&E (Daniel Gusfield)

I have serious reservations about the final recommendation to form a "department-like" structure for CS&E, either a division or a department. These comments apply as well, or maybe more, to an "above-department" division along the lines of the current Division of Statistics. Some of my earlier comments have been incorporated into the main body of the Report, but I would like to collect them in one place.

1) Computational science is ultimately about doing science, engineering, or mathematics with the aid of computation. Computational science develops and applies computational methods in (usually) traditional scientific fields that are not themselves fundamentally defined by involvement with computation. The computation augments, or in some cases replaces, more traditional laboratory or theoretical work. There is a growing realization that computation can lead to insights in many scientific fields that would not be obtained from theory or experiment alone. I am deeply committed to that view and to seeing its further development.

The success of computational science will be measured by the impact of the computational work in the application areas. Computational science is not limited to any specific scientific domain, nor any specific set of computational techniques.

2) The use of computation in many scientific fields is increasing and will increase even without a focussed initiative. However, there is a need and an opportunity to accelerate this process at UC Davis by reserving a substantial number of future FTEs for people in a variety of sciences who incorporate sophisticated computation into their work, and who develop new computational methods as well as use existing ones. By increasing the number of faculty at UC Davis who use and develop computational methods in their various scientific fields, UC Davis will help shape the future of computation in science, engineering, and mathematics. Other mechanisms, such as a graduate group, undergraduate minors, and a center to increase interaction and to coordinate joint research, funding, seminars, graduate advising, courses on material that crosses many scientific fields, etc. are also vital to the success of computational science campus-wide.

3) Computational science requires the non-trivial integration of one or more traditional scientific, engineering, or mathematics specialties with the deep application of mathematics or computer science (and often both). That integration, and an outward-looking orientation, is at the heart of what successful computational science should be. It is not expected that many undergraduates will master the prerequisite scientific, mathematical, and computer science background to then, as undergraduates, study computational science material, truly distinct from the background material. Moreover, much of the background material is taught in existing undergraduate courses. It is therefore the Committee's view that the educational focus of computational science be at the graduate level, although survey courses on computational science are desirable in order to stimulate interest in the field and encourage undergraduates to study the needed background material. No large undergraduate major in computational science can be expected, and the number of undergraduates who will be prepared to take a serious, advanced course on computational science, will be quite limited.

4) Given the wide range of scientific disciplines and of computational techniques that should make up successful computational science, the need for the computational scientist to be integrated into a traditional science as well as a computational field, the lack of a large undergraduate major and limited audience for advanced undergraduate courses in computational science, I do not see that a department-like structure for computational science is desirable.

The danger is that a department-like structure will separate computational scientists from the traditional sciences that provide a key part of the justification for computational science. And given the wide range of specialty scientific areas that individual faculty would focus on, it is not clear what "intellectual glue" will hold the faculty of such a unit together, unless (and this is highly undesirable) the unit narrows the range of supported computational techniques or application areas. Further, it is unclear that such a department could teach true computational science courses to sufficient numbers of students to justify the anticipated number of FTEs. It is undesirable to replicate courses from Mathematics and Computer Science that form the needed undergraduate background for computational science, and the demand will be limited for the advanced undergraduate courses that fall into the true domain of computational science. Duplication of courses could lead to unproductive friction between CS&E and existing units that would reduce the cooperation between the units and hence retard the central goal of developing CS&E at UC Davis.

Any plan for a CS&E unit should have a clear charter to avoid duplication of effort with existing units, and a detailed accounting of how its teaching resources match undergraduate demand.

5) I believe there are two possible models for computational science that can succeed. In one model, hires of computational scientists (people who develop computational tools for their work in a traditional scientific field) are placed in existing departments, aided by the development of a computational science Center to coordinate campus-wide efforts, jointly develop undergraduate minors, and a graduate group. This approach clearly avoids the problem of separating computational scientists from their areas of application. In this model, hires would teach courses in their home departments unrelated to computational science, in addition to developing specialty courses in computational science, either for their home department or for a wider audience. Because computational science would only be a part of their teaching load, the potential imbalance between the number of proposed new computational scientists and the student demand for true computational science courses, would be avoided. This model is consistent, as an example, with the anticipated physics hires mentioned in Section 3.2.5.

In the second model, computational scientists who wished to be organized into a unit more focussed on computation than on their applied science, would be housed in a Division of the Computer Science Department. The one commonality that would tie together such people is their commitment to use and to develop computational methods to do science. The only entity on campus that has a fundamental commitment and orientation to computation, and to the development of non-trivial computational tools, is the Computer Science Department. Therefore, if there is to be a concentration of such people into a single unit, the Computer Science Department is the natural home. The faculty in such a Division would be people capable of teaching mainstream computer science courses as well as computational science, and hence this would again avoid the teaching imbalance problem.

6 Conclusions

UC Davis should build on existing strengths. The CS&E Initiative should focus on people with strong connections to a diverse range of application domains. Many of these will relate to the representation, analysis, and exploitation of large data sets, not necessarily being numerical data. The focus cannot be exclusively on numerical computation or scientific computing. It is desirable to foster stronger connections between CS&E faculty and areas which have not traditionally exploited computational methods to the degree that the physical and, particularly, the engineering sciences have. UC Davis should build the future development of CS&E on existing strengths, considering computational needs and evolving opportunities on campus, likely with a substantial emphasis on the biological sciences. One of our goals should be to quickly become distinguished nationally in CS&E.

The CS&E Initiative should initially build on and expand traditionally strong CS&E programs. The campus should identify existing strong CS&E programs on campus and expand these first. This would allow UC Davis to achieve true national and international excellence in a few of its already strong CS&E fields.

The CS&E Initiative should emphasize high-quality research. The CS&E Initiative should focus on people who develop, analyze, and apply computational methods for applications. These people should have close connections to at least one application. High-quality research should be the desired outcome of expansion and investing in CS&E.

CS&E faculty should qualify for joint appointments. To establish critical mass and coherency and to attract faculty, students, and funding, the Initiative should place the majority of current and new faculty in a few primary CS&E units. To emphasize the interdisciplinary nature of CS&E most new faculty hires should qualify for joint appointments.

The creation of an undergraduate major in CS&E is not reasonable. The Initiative should not include the development of an undergraduate major. This, coupled with the creation of a new, independent unit for CS&E, might lead to a superficial treatment of CS&E. The creation of an undergraduate major could be viewed as a potential long-term objective, but there is no consensus among the Committee members on this subject.

CS&E will prepare our students for tomorrow's careers. The establishment and continued expansion of CS&E course development over the coming years is viewed by the Committee as a necessary process to prepare our university's students for careers in science and engineering of the 21st century. Departments with an interest in and need for the development of CS&E courses—either to keep their majors attractive or to make their graduating students more competitive—must allow for more flexibility in curricular course requirements imposed on their students. Revised curricular requirements should reflect that departments favor CS&E components in their students' course plans.

7 Recommendations

Based on majority consensus, the Committee makes the following recommendations concerning the future development of CS&E at UC Davis:

- **Development of a Division of CS&E hosted in the College of Engineering.** This is the organizational structure that the majority of the CS&E Committee favors. The establishment of an independent *Division of CS&E in the College of Engineering*, possibly initiated via a Program in CS&E, would (i) ensure that duplication of effort (with Computer Science) would be minimized—as a result of both CS&E and Computer Science being in Engineering—and (ii) ensure that both CS&E and Computer Science would control resources such as space and administrative and technical support independently. The Division's role concerning curricular development would be the formation of a Graduate Group in CS&E and the fostering of minors or emphasis areas in CS&E. Faculty in the Division could have joint appointments in departments representing applications for CS&E, and there could be a smaller number of faculty whose primary appointments would be in these other departments. The CS&E Division would differ from Computer Science in its commitment to a significant connection to application areas of computational methods—and in several other practical aspects. The Division should financially be independent.

  Just like the Division of Statistics is hosted in the College of Letters and Science, this model would serve the interests of students and faculty from all colleges. The campus would have to make major resource allocations available to the Initiative, i.e., to the College of Engineering, to enable the creation and support of the new Division. It is reasonable to expect that faculty would have varying percentages of appointments in the Division. The Division would have to serve the entire student body of UC Davis, and it would be imperative to mandate that the Division provide mechanisms enabling equal chances for access to its courses and programs. This concern must be resolved in order to generate wide-spread campus support for such a divisional model. The Division should financially be independent, i.e., the budget of CS&E should be separate from the budgets of other units, even if CS&E were initially affiliated with or coordinated through another unit. The Division of CS&E could evolve into a full Department of CS&E.

  (One Committee member, Professor Daniel Gusfield is not in favor of this recommendation, see section 5.)

- **Development of a Center for CS&E.** Regardless of the final organizational structure for CS&E education, the campus should consider the creation of a *Center for CS&E*, whose primary function would be to provide a desirable home for CS&E research efforts. The Center could serve these primary purposes: (i) it could be the place where the majority of interdisciplinary CS&E research efforts are performed and administered; (ii) it could play a leading role in the development of graduate education in CS&E and an enabling role during the initial development of undergraduate education in CS&E; and (iii) it could organize seminars and invited lecture series. Overall, the environment provided by the Center should be inviting and attractive to faculty and students from diverse CS&E fields to promote a lively atmosphere. The Center should be the primary coordinating institution for the campus's major CS&E research efforts. The Center should have its own independent budget, which must be sufficient to carry out its mission, including the functions listed as (i), (ii), (iii), and (iv).

Computational science and engineering education and research will play a substantial role in the university of the 21$^{\text{st}}$ century. UC Davis is in an ideal position to distinguish itself and become a national leader in CS&E by coupling the investments in CS&E with existing areas of excellence.

The Committee believes that the desired and anticipated expansion of Computer Science at UC Davis should foster the hiring of faculty with a strong background and interest in both CS&E and computer science. This will help the campus's need for growth in CS&E education and Computer Science's need to deliver core computer science education.

8 Cost Estimate

Our cost estimate is based on the assumption that 15 FTEs would be allocated to CS&E faculty over a six-year period. We assume that these 15 FTEs would be distributed as follows: four full professor, five associate professor, and six assistant professor FTEs. Start-up funds for both junior and senior faculty hires in CS&E would, in general, be substantially less than those typically needed for "traditional laboratory scientists." A CS&E faculty member would require start-up funds primarily for computer systems, massive data storage systems, high-speed (optical) networks, parallel computer systems, graphics workstations, powerful PCs, and possibly large-scale stereo projection systems required for virtual reality applications. The following table summarizes our cost estimate.

	Office Space [sq. ft.]	**Lab. Space [sq. ft.]**	**Start-Up Funds [$]**
Four Full Professors, Step IV			
Individual:	280	1,500	500,000
Sub-Total:	1120	6,000	2,000,000
Five Associate Professors, Step II			
Individual:	210	900	300,000
Sub-Total:	1050	4,500	1,500,000
Six Assistant Professors, Step III			
Individual:	210	600	200,000
Sub-Total:	1260	3,600	1,200,000
Total:	**3,430**	**14,100**	**4,700,000**

Office Space refers to the office space required for a faculty member and associated researchers. We assume that a full professor would require office space for two research associates, while an associate and assistant professor would require office space for one research associate (required office space per faculty member: 140 sq. ft, required office space per research associate: 70 sq. ft.). What we call *Lab Space* would effectively be the combined space required for students and computing equipment. We assume that *Start-Up Funds* would encompass the costs of an individual faculty member for computer hardware and software and potentially networking needs.

In addition to these costs, one would have to consider the permanent costs for *administrative support*, *technical support*, and other forms of *permanent maintenance* of a CS&E Center and a CS&E Division. It seems reasonable to assume that the costs for these items, on a per-faculty basis, would be similar to those of a unit like Computer Science. Besides these costs, there would also be the costs to support the basic administrative office infrastructure that would be required for a Division of CS&E.

Considering potential joint appointments with national laboratories, it is be reasonable to expect that the start-up requirements of a new faculty member also working at a national laboratory would be relatively lower as a result of the existing infrastructure provided by the laboratory.