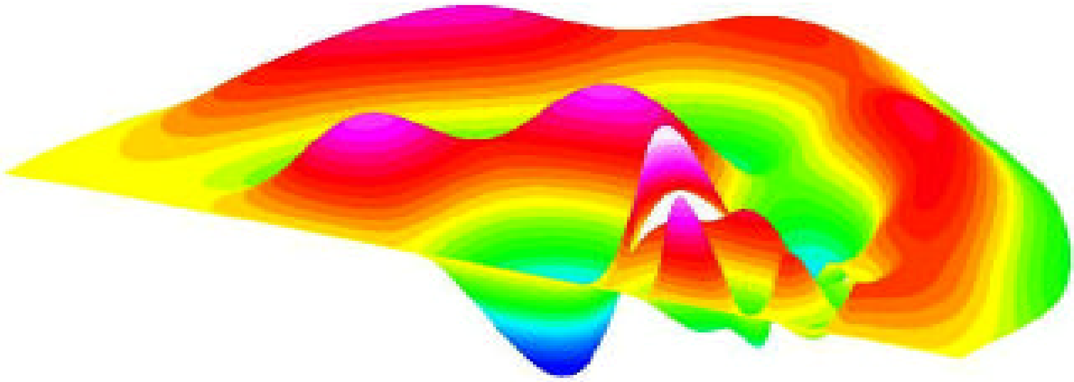

RESEARCH DIRECTIONS IN COMPUTATIONAL MECHANICS

A Report of the United States National Committee on Theoretical and Applied Mechanics
September 2000

Computational Mechanics: A Core Discipline in Computational Science and Engineering

Theoretical and Applied Mechanics (TAM) is the branch of applied science concerned with the study of mechanical phenomena: the behavior of fluids, solids, and complex materials under the actions of forces. Few disciplines have had a greater impact on the industrialized world, enabling technological developments in virtually every area that affects our lives, security, and well being.

Computational Mechanics (CM) is that sub-discipline of TAM concerned with the use of computational methods and devices to study events governed by the principles of mechanics. It is the fundamentally important part of computational science and engineering concerned with the use of computational approaches to characterize, predict, and simulate physical events and engineering systems governed by the laws of mechanics. Computational mechanics has had a profound impact on science and technology over the past three decades. It has transformed much of classical Newtonian theory into practical tools for prediction and understanding of complex systems. These are used in the simulation and design of current and future advances in technology throughout the developed and developing world. These have had a pervasive impact on manufacturing, communication, transportation, medicine, defense and many other areas central to modern civilization. By incorporating new models of physical and biological systems based upon quantum, molecular and biological mechanics, computational mechanics has an enormous potential for future growth and applicability.

Not surprisingly, successful research in CM is usually interdisciplinary in nature, reflecting a combination of concepts, methods, and principles that often span several areas of mechanics, mathematics, computer sciences, and other scientific disciplines as well. As will soon become evident in this exposition, tomorrow's research in CM will be broader than ever before, spanning many new technologies and scientific fields.

Our goal here is to provide a perspective of the major research areas in CM that will be the focus of inquiry during the next decade: what are the research directions in the CM and what are the opportunities for industrial, governmental, university researchers, and those who would implement and apply the research results in computational mechanics?

Computational Mechanics: Societal Benefits

The success of CM will ultimately be judged by effectiveness in solving problems of interest to society and on providing deeper understanding of natural phenomena and engineering systems. The field has been enormously successful to date because of its unprecedented predictive powers, making possible the simulation of complex physical events and the use of these simulations to design engineering systems. This is done through so-called "computer modeling": the development of discretized versions of the theories of mechanics which are amenable to digital computation, together with the complex process of manipulating these digital representations to produce abstractions of the way real systems behave.

Today, a thriving international industry markets computational mechanics software for the analysis, simulation, and design of engineering products and systems. The industry revenues are in the billions of dollars; but the overall impact on goods and services affects trillions of dollars in commerce and product development. In addition, simulation software is used extensively in medical applications, military applications, transportation, and even as tools to complement and validate experimental research and testing.

Some of the applications of CM are well known; others are not. One well-known area in which CM has had dramatic success is with the simulation of crash worthiness of automobiles. Computer-generated simulations of the collision of a vehicle with walls or obstacles, based on fundamental scientific principles on the dynamics of deformable bodies, have replaced hundreds of full-scale tests and saved major automobile manufacturers millions of dollars. More importantly, countless lives have been saved and injuries diminished by improved safety features developed through computer modeling and simulation.

Figure 1 depicts a computer-generated simulation of a full-size car in oblique impact with a cylindrical pole. The entire impact event, which takes place in a thousandth of a second, can be studied in detail in the CM simulation, providing information on deformation, acceleration, forces on models of passengers, energy transfer, and other features of the phenomena that are useful in designing safer and more reliable vehicles.

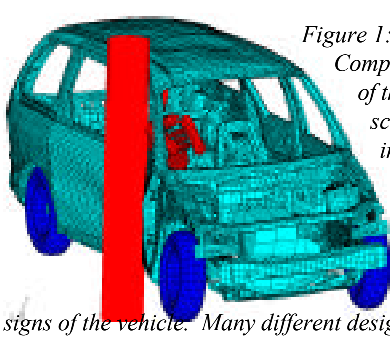

Figure 1:
Computer-generated simulation of the oblique impact of a full-scale model of a van colliding with a cylindrical pole. This simulation models the damage of the vehicle and provides information on passenger safety for various structural designs of the vehicle. Many different design parameters can be varied to determine the effects of each design decision before a single physical test is done.

An exciting CM application area under development is predictive surgery. One example is illustrated in Figure 2, where a computer-generated image of a diseased human aorta is given. The geometry and properties of the living tissue are deduced from MRI imaging and other tests and go directly into computer subroutines that generate a model of blood flow through veins and arteries of the specific human subject. In this example, the flow of oxygenated blood that results from several different options in bypass surgery are calculated and presented to the surgical team so that the best procedure for the particular patient under treatment can be obtained. Many different surgical strategies can be simulated and the results predicted by CM software before a single step in the actual surgery is taken.

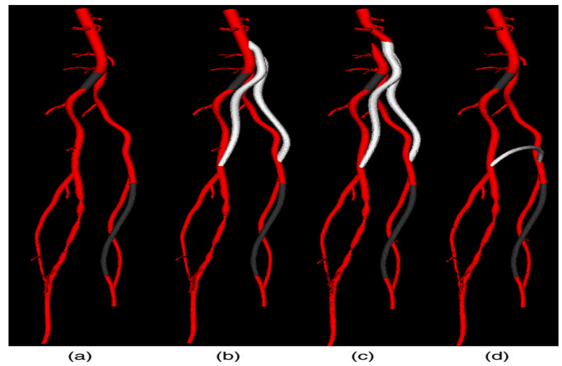

Figure 2a:
A human aorta containing an aneurism, and diseased veins and arteries, shaded gray in the figures, and various bypass surgical procedures for allowing healthy blood flow around the affected area. The blood flow is modeled for each surgical process using principles of fluid mechanics and fluid-structure interactions.

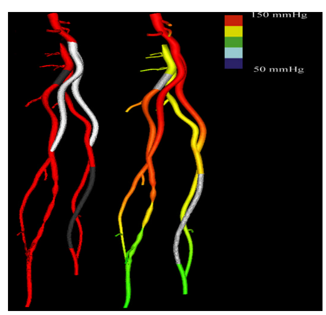

Figure 2b:
The computed flow channels and blood flow from the surgical solutions best suited for a particular patient is selected and modeled in detail using CM principles.

CM has long been used in military applications. One example is in the analysis and design of weapons and armor, such as were the goals of the simulations depicted in Figure 3. There, we observe a computer-generated simulation of a highly complex phenomenon that occurs in micro-seconds: the oblique hypervelocity implates. Here a long list of interactive mechanical phenomena take place, including phase changes of materials, ablations and spalling, shrapnel spraying, thermal effects, and flow – all within the realm of TAM and all modeled using CM technology.

Figure 3a:
A simulation of a metallic rod (a penetrator) impacting and piercing a collection of armor plates in a design of military systems

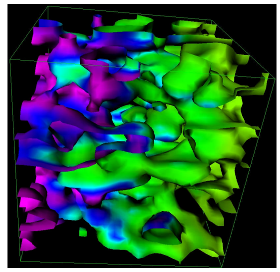

Figure 4b:
A model of the dispersion of pollutants in a porous substrata where biochemical reactions are followed. Various species concentrations shown in different colors within a complex structure.

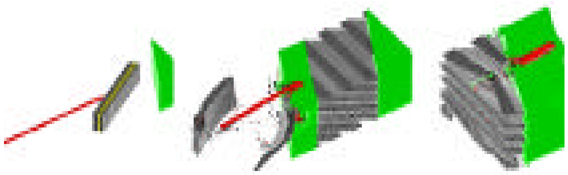

Figure 3b:
A simulation of a hypervelocity impact of a deformable penetration impacting multiple plates of armor. These calculations enable the better design of protective armor configurations.

Applications of CM are not limited to the engineering design of products and systems. Many are concerned with the basic understanding of natural phenomena or with the prediction of natural physical events. Examples in this area include the use of CM methods to study atmospheric changes, ocean currents, surface flow in rivers, subsurface flows in oil reservoirs, or geological phenomena such as the movement and evolution of polar ice caps or the tectonic plates. One such simulation is illustrated in Figures 4a, b. Shown in Figure 4a is a computer-generated model of the topography and substrata of an oil reservoir and the flow of oil, water, and gas in a simulation designed to estimate well production. Figure 4b is a computer visualization of the flow of biological and chemical species in a simulation of pollution remediation in porous media.

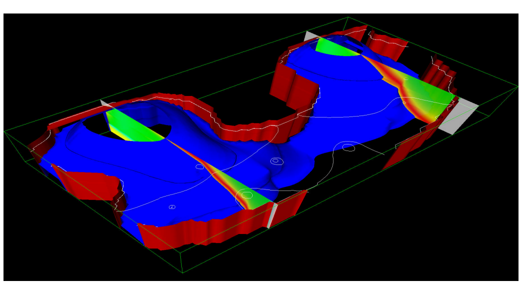

Figure 4a:
Computer-generated 3D map of an oil reservoir and the flow of oil, gas, and water through a complex porous media

Another example of a CM simulation in this general area is indicated in Figures 5a, b. There, we find a simulation of a supernova, the explosion of a star, a billion light years from earth. Fundamental principles of fluid mechanics and gas dynamics, and thermodynamics were used to construct a computational model of this extraterrestrial event, and the remarkable simulations give new information on the structure and the evolution of supernovas, the mass of the system, velocities of debris, and other data that suggest mechanisms for the cause of the phenomena.

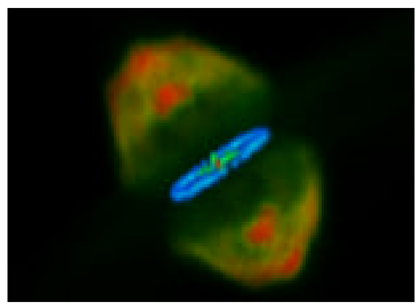

Figure 5a:
Here the theories of gas dynamics and compressible flow of multiphase media are used to model the explosion of a distant star. Colors indicate variations in mass density and temperature.

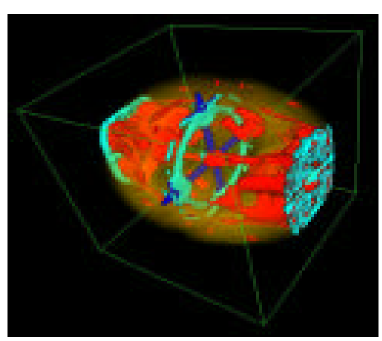

Figure 5b:
A zoom into a closer look at the evolution of the supernova.

Reliability of CM

The question of reliability of computer-generated predictions is one of great concern to specialists in CM. Without some confidence in the accuracy of simulations, their value is obviously diminished. Today, remarkably accurate and reliable simulations are obtained routinely in many application areas while others are, at best, qualitative and capable of depicting only trends in physical events.

This concern for reliability has led to the creation of a challenging technological area labeled simply Validation and Verification: the creation, study and documentation of tools for assessing the predictability of CM-based methods and programs. Validation has to do with determining the appropriateness of the scientific principles and mathematical models used to develop a simulation tool. Verification has to do with determining if the final tool can indeed function as it was intended and if it can correctly produce results consistent with the models upon which it is based.

Validation methods include, when possible, actual comparisons of CM predictions with observations, physical tests and experiments. Even then, such comparisons can be made for only a limited range of parameters and generally not the full range of possibilities embraced by general computational modeling schemes. Modern validation methods also seek to define the limits of various modeling schemes and, ideally, to provide insight as to when these limits are reached and can be overcome.

Verification methods involve the use of benchmark tests developed by experienced analysts over years of work, or implementation of software engineering methods to minimize coding errors and optimize computational performance and program design.

With the rapidly expanding use of CM throughout many areas of science and engineering, "V and V" has become a critical component of today's research in CM. New V and V tools are on the horizon that could dramatically increase the reliability of sophisticated computation modeling. Some of these tools are mentioned later in this exposition.

Computational Mechanics: the Next Decade and the Next Millennium

It may be confidently said that virtually every aspect of our day-to-day lives is affected in some way by CM. Still, the subject is undergoing rapid change and development and many open issues remain.

During the next decade, the field of CM will undergo dramatic changes that will require computational mechanics capabilities not available today. An unprecedented growth in activity and importance is expected that may have been unimaginable only a few years ago. Also, in the next millennium, a paradigm shift in the computational sciences is essential if the needs of industry are to be met.

Perhaps the most remarkable aspect of our vision of CM in the next decade is that CM research will require new interactions of computational methods and devices with a variety of supporting technologies, including imaging, various tomographic modalities, visualization, testing, and laboratory experimentation. In the new CM, "mechanics" will interact with theories of quantum mechanics, molecular dynamics, materials science, biomedical and biological systems, and other disciplines. It will involve the study of microscopic phenomena taking place in pica seconds. A myriad of technological tools need to be integrated into the mechanical analysis, not only for studying engineering materials, but also to study biological systems, submicron devices, and robots. These far-reaching applications will impact predictability, our life styles and personal health and longevity.

Funding Sources: Computer Versus Computational Science

In general, the subtle difference between the terms "computer science" and "computational science", are not recognized but the distinct differences in these disciplines has had a significant impact on the distribution of resources for fundamental research. *Computer science* refers to the science and technology pertinent to the computer, the computational device with which computation is done. *Computational science*, on the other hand, addresses the development of modeling techniques, algorithms, software, and for specific problems in science and engineering. There has been a tendency to promote investment in computer science as the necessary tool with which good computational science can be done, but there has been no comparable support by traditional funding agencies has emerged in the important computational sciences necessary to do important applications. A good example is PITAC, the President's Information Technology Advisory Committee, largely populated by computer scientists as opposed to computational scientists, which after a study of over a year, recommended that federal government invest over a billion dollars into new research in "information technology", principally pure computer science, networking, and hardware. In explaining the value of this program to the US Congress, however, the great benefits of such an investment for doing computational science were stressed, but no funds were allocated to the latter.

In order to meet the needs of industry, renewed emphasis on the computational sciences, and, particularly, CM, is needed. This is not to say that some impressive investments have not been made in this discipline. Indeed, very ambitious programs are underway that will raise the bar in computational modeling. These include the ASCI program (Accelerated Scientific Computation Initiative) which is aimed at displacing traditional nuclear testing and storage procedures with highly-tuned, computer simulations. It remains to be seen whether many of the goals of ASCI are attainable, but the program undoubtedly will create some important advances in CM and related sciences. Such programs also foster a broadening and generalization of all fields supporting computational science, and intrinsically advance supporting technologies to make meaningful simulations possible.

In the pages below, we outline briefly a number of areas with significant research opportunities in CM:

- Virtual Design
- Multi-scale Phenomena, including bridging of molecular to atomistic to continuum models
- Model Selection and Adaptivity
- Very Large-scale Parallel Computing
- Biomedical Applications, including predictive surgery, application of mechanics to the study of cells, bones, nerves, and other biological systems
- Controlling Uncertainty: Probabilistic Methods

Virtual Design

One of the major factors in increasing U.S. industrial competitiveness is the reduction in design cycle time. Such reduction hinges critically on the availability of virtual design, the ability to complete designs entirely in the computer, without making time-consuming prototypes. In virtual design, prototyping is bypassed and prototype tests of normal operations and extreme conditions are simulated on the computer. For example, in the automobile industry, normal operations of the engine and the body, such as ride assessment, stresses in the engine, and car body and airflow around the body and in the engine compartment, are used in designs by computers. Crash and occupant protection that, in the past, required many prototypes, are also simulated in the design process. For Defense Department products, extreme environments, such as live-fire tests are also increasingly simulated.

Although great strides have been made in simulation in the past two decades, virtual prototyping is still more of an art than a science. To develop a virtual prototyping capability, many tests must be performed since many of the physical phenomena can not be modeled on the basis first principles today. Instead, models are tuned to tests, and the technology is not applicable to radically new designs. Specific obstacles to virtual prototyping include the inability to simulate problems with multiphysics phenomena, such as burning and change of phase, fracture and spalling, phenomena involving large disparities in scales, and behavior with a significant stochastic characteristics.

These capabilities are also of crucial importance to our defense. With the rapid development of new concepts of warfare and defense, new weapons and devices must be quickly designed and evaluated. Virtual design and prototyping are essential in this process. For example, with the new emphasis on the soldier and body armor, various protective devices must be evaluated. However, modeling of materials such as kevlar and other new materials in the failure range require a dynamic failure analysis that is beyond the state of our knowledge. These capabilities are also essential to maintaining our nuclear weapons stockpile without testing.

In order to make virtual design a reality in the next decade, radically new computational tools with the ability to handle multiscale phenomena, very heterogeneous materials, and discontinuous behavior, such as fracture and assessment of the range of performance and automatic guidance to improving design, must be available.

Multi-scale phenomena

One of the great strengths of computer simulation over traditional methods of experimental science is its applicability to the study of a complete range of physical phenomena at all possible spatial and temporal scales. This ability of computer simulation to slow down events that take only 10^{-9} seconds and study them in some detail, or to look back into time at the evolution of events that began tens of thousands or hundreds of thousands of years in the past, or to extrapolate to the evolution of events, and make predictions of their structural effects and characteristics many millennia into the future, all are, in principle, achievable with computer simulations. Correspondingly, the study of mechanical events with spatial scales take place at the atomistic level, the motion of dislocations, electrons and protons, the analysis of submicron devices, the study of events with interactions of many different scales, such as turbulent flow, to the characterization of motion of solar systems, galaxies, and systems of gargantuan dimension, are also within the scope of tomorrow's work on CM.

A major challenge to CM for the future is to model events in which these remarkably varying scales are significant in a single system or phenomena. It is then necessary to model *multi-scale phenomena* simultaneously for predictive capability. Analysis of multi-scale phenomena, while apparently beyond the horizon of contemporary capabilities, is one of the most fundamental challenges of research in the next decade and beyond. So-called *scale bridging*, in which the careful characterization of mechanical phenomena require that the model "bridge" the representations of events that occur at two or more scales, require the development of a variety of new techniques and methods. In this area, integration of computational methods and devices with experimental or sensing devices is critical. High fidelity simulation and computational mechanics must involve innovative and efficient use of a spectrum of imaging modalities, including x-ray tomography, electron microscopy, sonar tomography, and many others. Similarly, in modeling phenomena such as climate changes, weather conditions, and the interaction of ocean and atmosphere, satellite-generated data must be incorporated seamlessly into viable computational models to obtain meaningful predictions. Again, the spectrum of computational mechanics must be significantly broadened to include the use of these technologies. Once more, the intrinsically interdisciplinary nature of the subject will be expanded and reinforced.

Model Selection and Adaptivity

Throughout all the mathematical and computational sciences, the first and most primitive step in computer modeling is the selection of the mathematical and computational model itself. Model selection is a largely heuristic process, based on the judgement and experience of the modeler, and on testing and experimentation. But it is frequently purely a subjective endeavor: different analysts may select different models to describe the same physical phenomena. The selection of the model, by which we ordinarily mean the selection of the partial differential, integral or ordinary differential equations, the algorithms, the physical, geometrical and topological characteristics, boundary and initial conditions, etc, is quite often the single most important step in obtaining valid computer simulations of physical events.

In recent years, considerable progress has been made in determining theoretical and computational techniques that aid in model selection. A variety of techniques are under study. Some of these involve embedding a given class of models into a larger class of more sophisticated models in which finer and more detailed representations of the behavior of physical system may be possible. Once such a datum is identified, a notion of modeling error can be made precise, and by various measures, such modeling error can be controlled by adaptive modeling processes. Areas in which adaptive modeling have great promise include the study and characterization of composite materials, unsteady turbulent flows, multiphase flows of fluids, etc. Other techniques for model adaptivity involve the use and integration of test and imaging data, feedback from experiments and measurements, and various combinations of these methodologies.

Model selection is a crucial element in automating engineering analysis and applications are unlimited; the subject could conceivably embrace classes of models including diverse spatial and temporal scales, enabling the systematic and controlled simulation of events modeled using atomistic or molecular models to continuum models. Model selection, model error estimation, and model adaptivity are exciting areas of CM and promise to provide an active area of research for the next decade and beyond.

Controlling Uncertainty: Probabilistic Methods

The random nature of many features of physical events is widely recognized by industry and researchers. The natural stimuli that activate physical systems may be completely unpredictable by deterministic models: the randomness of a gust of wind, the characterization of forces in boundary and initial conditions on mechanical systems, random microstructural features of engineering materials, the random fluctuations in temperature, humidity, and other environmental factors, all make the characterizations provided by deterministic models of mechanics less satisfactory with respect to their predictive capabilities.

Fortunately, the entire subject of uncertainty can itself be addressed in a scientific and mathematically precise way and the random characteristics of nature can be addressed by computational models.

During the next decade, probabilistic modeling of problems in mechanical problems will be a topic of great importance and interest. Including stochastic features into computational models will not only provide realistic simulations of physical events but will also provide the analyst with specific information on the probabilities that can be assigned to predictions. Thus, using probabilistic models of mechanics, the analyst may, for example, determine what the maximum stress will be in a particular machine part under design, rather than upper and lower bounds on such quantities of interest can be expected in view of the uncertainty of the data. What, in particular, is the probability of failure of a sub-system being analyzed and designed? New methods for treating uncertainty will become important in virtually all branches of mechanics: fluid mechanics, mechanics of materials, solid mechanics; it will also promote the development of new computational techniques to analyze uncertainty in engineering systems.

Error Estimation and Adaptivity

The notion of computing estimates of numerical error in computer simulations is not new; serious work in this subject began in the 1980's, and today the notion of a posteriori error estimation is a common topic in university research environments. Error estimation provides a quantitative measure for determining the quality of numerical simulations; it provides a basis for adapting characteristics of discrete models (for example, meshes or approximation orders) so as to improve the quality of results.

To date, most of a posteriori estimation has been confined to a fairly narrow class of problems, largely drawn from linear theory; it has not been fully utilized in the more complex computer simulations used in industry and government laboratories.

It is predicted that a posteriori error estimation and adaptivity will become a common ingredient in all significant computer simulations in CM during the next decade. With a renewed and invigorated interest in reliability of simulations, the calculation of estimates of error in simulations will be as natural a feature of the simulation as any other estimate of physical quantities of interest. An important advance in this area has been the recent discovery of methods to determine upper and lower bounds of local approximation error, so that in any given simulation, once a particular model is selected, computable bounds giving upper and lower limits to computed quantities of interest could be a natural by-product in every simulation. This is a fertile area of research, one in which significant work will be done during the next decade.

Very Large Scale Parallel Computing

One of the most difficult issues facing researchers in CM in the next decade will be purely a conceptual one: the recalibration of their own education, approach, and perceptions to allow them to use efficiently the extraordinary computational tools that will be developed during this period. Today, mechanicians using computational products in engineering analysis and design can routinely develop computational models involving 500,000 to 10,000,000 degrees of freedom. Problems of this size today are being solved on contemporary workstations. Nevertheless, these contemporary models employ rather crude characterizations of materials, geometry, boundary conditions, failure criteria, and many other important features of the system, because it is taken for granted by the modeler that to include these details will result in computational problems so large and complex that they would exceed the capacities of modern computational facilities.

This argument is no longer correct. As the twenty-first century begins, computational devices capable of delivering five trillion operations per second and storing a thousand trillion bytes of data are in use and larger machines are being developed. In a decade's time, machines with capabilities an order-of-magnitude beyond this level may be available. It is probable that such terascale computation capabilities will soon be in the hands of most engineers and mechanicians, thus making possible models with a level of detail and sophistication completely unimaginable only a decade ago.

The proper use of this extraordinary toolkit will itself represent a significant challenge. Included in the challenge is the education of the next generation of engineers and mechanicians who will be expected to not only master the principles of mechanics but also the use of the computational tools available to them.

These new capabilities, and advances in modeling and parallel computation, will ultimately have a remarkable and irreversible impact in education in science and engineering. Simplified models and approximate theories remain important in developing understanding, but students need no longer rehearse only idealized situations: they can now tackle more realistic models. High-speed parallel computing together with the software developments, alluded to elsewhere in this document, will create a revolution in engineering analysis and ultimately in the way it is taught in colleges and universities. Less than a decade ago many feared that access to modern computational methods and machines would breed overconfidence in engineers, at the expense of common sense, judgement and reasoning. Now, the new concern is one of underestimation of the power of modern computational methods and devices and the danger of their under-utilization in important simulations, analysis and design.

Computational Mechanics: Conclusions

CM has become a central enabling discipline that has led to greater understanding and advances in modern science and technology. It has been the basis of numerous important developments in recent years and will continue to be crucial to industrial development and competition, to safety and security, and to understanding the diverse physical and biological systems occurring in nature and in the society. Many research problems in CM await resolution and will provide significant challenges for research in the future. If "the past in prologue", then, in the future, we may anticipate even greater contributions of Computational Mechanics to the advancement of knowledge and to the benefit of a global society.

Acknowledgements

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1. *Research Directions in Computational Mechanics, edited by J.T. Oden, National Research Council, National Academy Press, Washington, D.C, 1991.*
2. *Research Trends in Fluid Dynamics, edited by J.L. Lumley, Andreas Acrivos, L. Gary Leal, and Sidney Leibovich, American Institute of Physics, Woodbury, New York, 1996.*
3. *Research Directions in Solid Mechanics, edited by G. Dvorak, Elsevier Science Publishers, Amsterdam, 1999.*

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- *Figures 5a, b: Professors Chandrajit Bajaj TICAM, and Paul Shapiro, Department of Astronomy, The University of Texas*

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