Research Directions in Mechanics
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Research Directions in Computational Mechanics

U.S. National Committee on Theoretical and Applied Mechanics

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EXECUTIVE SUMMARY

Computational Mechanics: The Subject

What is it that engineers and scientists do that accounts for the remarkable advances in transportation, communication, manufacturing, and technology since the beginning of the industrial revolution? Without doubt, one of the most import ant things they do is to model natural phenomena. They develop conceptual and mathematical abstractions to simulate physical events. According to the late John Von Neumann, "The sciences do not try to explain, they hardly even try to interpret, they mainly make models. By a model is meant a mathematical construct that, with the addition of certain verbal interpretations, describes observed phenomena. The justification of such a mathematical construct is solely and precisely that it is expected to work."

Many of these mathematical models are based on fundamental scientific laws, axioms of physics exacted from centuries of research on the behavior of mechanical systems under the action of natural forces. Today this subject is referred to simply as mechanics - a term that encompasses broad fields of science concerned with the behavior of fluids, solids, and complex materials. Mechanics is vitally important to virtually every area of technology and remains an intellectually rich subject taught in all major universities. It is the focus of research in schools of mechanical, civil, and aerospace engineering, and engineering science and mechanics, as well as petroleum and chemical engineering and applied mathematics and physics. Time and again, investments in mechanics re search have produced enormous dividends to the industrialized world.

All mechanics models are characterized mathematically by very complex expressions, many of which, until the advent of electronic computation, stood outside the reach of the scientific and engineering communities. Over the last three de cades, however, the computer has made it possible to solve many problems of mechanics, dramatically expanding the capabilities for mathematical modeling. It has made possible the detailed analysis and design of a multitude of new products and an understanding of many natural phenomena elevated the standard of living throughout much of the world. There now exists a new and growing body of knowledge connected with the use of computational methods and devices to analyze the mechanics models--computational mechanics.

Major Industries and Technological Areas Affected By Computational Mechanics

Several major technological areas are heavily dependent on the continued growth of computational mechanics. These include manufacturing process and product simulation, space exploration and defense, environmental phenomena, and fundamental scientific research. Further comments on each of these areas follow.

Manufacturing: Computer Simulation of Materials, Processes, and Products

Many of the great industrial achievements made in the United States in recent years have been possible because of the appearance of new and innovative manufacturing processes that take advantage of new materials. The design of most of these processes would not have been possible without detailed computer simulated material behavior under anticipated lifetime conditions and the products' desirable features.

Of the myriad examples that could be cited, the following are some of the manufacturing applications of computational modeling:

1. *Plastics and injection molding*. Computer simulations of molten plastics and the formation of plastic parts represent a tool used with increasing frequency in a growing number of manufacturing applications.
2. *Computer chips and components*. The design and analysis of computer chips, computer components, microchip interconnections, and the overall integrity of computer boards subject to mechanical and thermal effects require computer modeling of the anticipated stress, deformation, and temperature in the design of stable and robust computer parts.
3. *Biomedical devices*. Prostheses, artificial organs, hospital equipment, and other devices that must function reliably in life-threatening circumstances are manufactured under conditions simulated by computer modeling techniques.
4. *Sheet metal forming*. Simulations of residual stresses, cracks, fatigue life, and other properties of metal products produced in sheet metal formation are widely used, particularly in the automobile and aircraft industries, for the design of parts fabricated from sheet metal.
5. *Crashworthiness of automobiles*. Recent advances in simulation of automobile crashes have made it possible to test automotive designs at a fraction of the cost and time required to do full-scale vehicle testing.
6. *Conventional aircraft and aerospace vehicles*. Perhaps no industry is more dependent on computational modeling than the modern aerospace industry. It relies on computer simulations of high-speed flow around aircraft and space vehicles as a key design tool. It is virtually impossible to check the performance of hypersonic aircraft and spacecraft by full scale testing, and the only means to determine the merits of specific design iterations is through computer simulation.
7. *Combustion phenomena*. The design of internal combustion engines, solid propellant rocket motors, and thermal energy conversion processes is now being done through numerical modeling of the underlying fluid mechanics and chemical reaction phenomena.

Space Exploration and Military Defense

The use of computational mechanics in contemporary aerospace industries is essential in the design and control of space stations and space vehicles. Detailed computer simulations play a crucial role in the behavior assessment of these space structures in orbit. Similar types of computer simulations are under way to study the design and performance issues in orbital mechanics, submarine technology, and the function of other defense systems in simulated real-life environments. For instance, advances have been made in computer simulation of the mechanics of nuclear and nonnuclear explosions, and the impact of projectiles (e.g., birds and meteors) on military and nonmilitary targets. It is hoped that computer modeling can displace the expensive testing of such events.

Environmental Phenomena

Computational mechanics is increasingly important in simulating both large- and small-scale phenomena affect in the environment, for instance, pollution control. The dispersion of contaminants in the atmosphere, food agricultural products, aquifers, and oceans and estuaries is governed by physical processes that can be modeled. Computational mechanics will play a fundamental role in developing the mechanisms to control, contain, and abate environmental pollution. Computational mechanics is also being applied to fossil energy recovery and conversion. Computer simulation of oil and gas fields and implementation of advanced oil recovery methods could help increase current oil supplies. Simulation of chemical processes, fluidized bed, energy structure behaviors, and related technologies could significantly enhance energy conservation efficiencies.

Fundamental Scientific Research

There is a growing use of computational mechanics techniques as a fundamental research tool. This ranges from the use of computer modeling for design of study experiments of new material to the materials performance response to stress: damage, and deformation under various loading condition Events that occur on submicrosecond time scales are difficult to study in depth in a laboratory but can be modeled computationally and studied on whatever time scale the investigator chooses. On the other hand, events that take place over centuries cannot be studied in practical laboratory experiments but can be modeled on a computer. This includes the study C environmental phenomena such as planetary atmospheres, geological processes, earthquakes, and ice flows, as well as star galaxies, and various astronomical events. These examples emphasize the importance of modeling physical events.

Significance of Computational Mechanics to National Interests

Computational mechanics is an integral and major component in many fields of engineering design and manufacturing. Major established industries such as the automobile, aerospace, chemical, pharmaceutical, petroleum, electronics, and communications, as well as emerging industries such as biotechnology, rely on computational mechanics-based capabilities to simulate and model complex systems for the analysis, engineering, design, and manufacture of high technology products. Detailed discussions of specific areas are given in the Appendices.

Recently, an Office of Technology Assessment (OTA) paper "Seeking Solutions: High-Performance Computing for Science" (April 1991), was requested by the Senate Committee on Commerce and Transportation and the House Committee on Science, Space, and Technology to examine high performance computing as part of the infrastructure proposed by the White House Office of Science and Technology Policy's (OSTP) National High-Performance Computing and Communications initiative. In the OSTA paper, high performance computing is portrayed as playing an increasingly significant role in all sectors of our economy, including manufacturing, service, agriculture, government, national security and defense. The paper states that: " .... concern for the Japanese challenge in high performance computing goes beyond the competitiveness of the U.S. supercomputing industry. Computational simulation in engineering design and manufacturing is becoming a major factor in maintaining a competitive posture in high technology industries… It is in the availability and application of high-performance computing to increase productivity and improve quality where the greatest future economic benefits may lie."

The OTA paper has been reinforced by a recent report from the National Research Council's Board on Mathematical Sciences titled, "Mathematical Sciences, Technology, and Economic Competitiveness" (1991). Advances and capabilities in computational and mathematical modeling (computational mechanics) have been determined to have a direct connection to economic competitiveness. These advances and capabilities represent the tools of international competition and are important for maintaining America's supremacy in science and engineering. This is particularly significant at this time in our history, when our economy has been labeled as "an economy going nowhere," and our ability to commercialize our technological capabilities in biotechnology industries is questionable. The trends for our high technology industries have been unfavorable, as illustrated in Figure 1. These trends, identified in a 1987 report from the Council on Competitiveness, titled *Picking Up the Pace*, for several key industries, clearly show that as a nation we have been doing a poor job in commercializing our science and technology base.

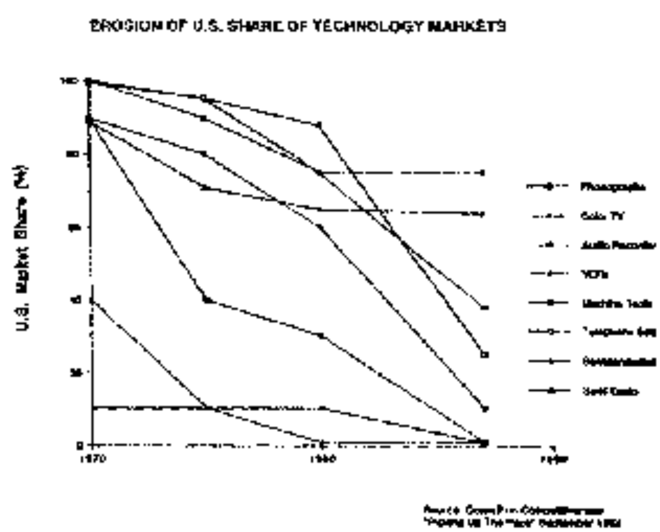

FIGURE 1: Erosion of U.S. Share of Technology Markets

Of particular concern to this report are trends in the computer industry. Computational mechanics play a large role in the software used by this industry. For example, a CRAY survey of supercomputer use in engineering showed that 10 percent is used in crashworthiness simulation (described in Appendix 2), and 30 percent is used in computational fluid dynamics (Appendix 12).

Software development in these fields is a native technology whose further development and application to industrial problems is inextricably and symbiotically linked to the health of the computer industry, for leadership in software is a vital element in the export of computers. Figure 2 shows that despite the U.S. computer industry's continuing heavy investment in R&D, the U.S. share of the world's computer systems market fell from about 60 percent to 40 percent between 1983 and 1989, while Japan's share rose from 8 percent to 22 percent, and Europe's share grew from 10 percent to 15 percent. Furthermore, Figure 3 illustrates that in 1990 the computer systems industry's trade balance was zero for the first time.

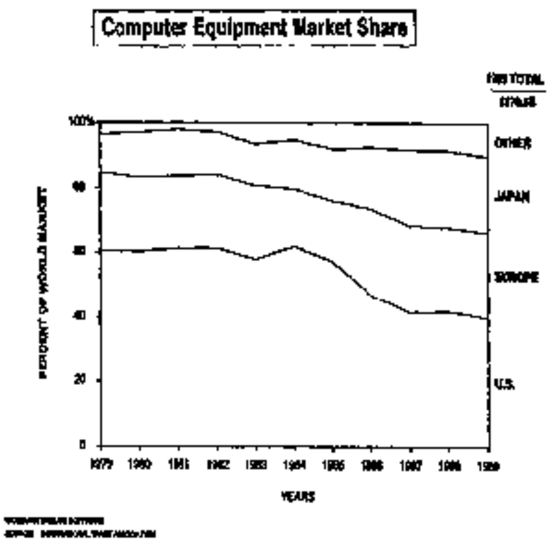

FIGURE 2: Computer Equipment Market Share (from a report prepared by the Computer Systems Policy Project(CSPP), "Perspective on U.S. Technology Policy, Part I: The Federal R&D Investment."

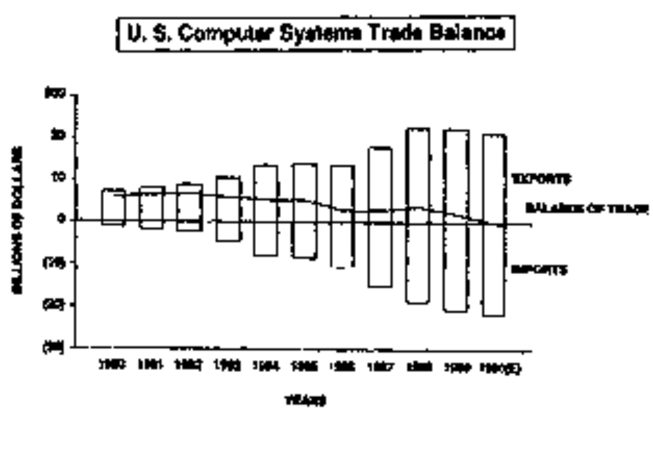

FIGURE 3: U.S. Computer Systems Trade Balance (from a report prepared by the Computer Systems Policy Project (CSPP), "Perspective on U.S. Technology Policy, Part I: The Federal R&D Investment.")

In March 1991 the National Critical Technologies Panel, organized under the direction of OSTP, issued a report that identified 22 technologies that, according to the panel's chairman, Dr. William Phillips, "are considered essential for the U.S. to develop in the interests of the nation's long-term security and economic prosperity."

The critical technologies identified in this panel's report are listed in Table 1 in six broad categories. It is important to note that one category, Information and Communication, is directly related to many of the R&D activities in computational mechanics, while the remaining five (and most of their individual technologies) are linked to developments and applications from the field of computational mechanics.

TABLE 1

MATERIALS • **Materials synthesis and processing** • **Electronic and photonic materials** • **Ceramics** • **Composites** • **High-performance metals and alloys**
MANUFACTURING • **Flexible computer integrated manufacturing** • **Intelligent processing equipment** • **Micro- and nanofabrication** • **Systems management technologies**
INFORMATION AND COMMUNICATIONS • **Software** • **Microelectronics and optoelectronics** • **High-performance computing and networking** • **High-definition imaging and displays** • **Sensors and signal processing** • **Data storage and peripherals** • **Computer simulation and modeling**
BIOTECHNOLOGY AND LIFE SCIENCES • **Applied molecular biology** • **Medical technology**
AERONAUTICS AND SURFACE TRANSPORTATION • **Aeronautics** • **Surface transportation technologies**
ENERGY AND ENVIRONMENT • **Energy technologies** • **Pollution minimization, remediation, and waste management**

The High-Performance Computing and Communications Initiative

The High-Performance Computing and Communications (HPCC) initiative represents a major strategic investment for the nation that is expected to yield both economic and social returns. This initiative can have substantial impact on the field of computational mechanics, if a concurrent investment is made in computational mechanics that can lead to significant progress in the efforts critical to this nation's needs.

The HPCC initiative represents an ambitious and welcome opportunity to reverse the trends in our high-technology industries and, in particular, in our computer systems industry. This 5-year, multibillion-dollar program offers great opportunities for development and application of the technology associated with computational mechanics. Indeed, many of the goals, strategies, and proposed programs, embodied in Grand Challenges, will depend on the successful implementation of the technological capabilities afforded by computational mechanics.

The goals, strategy, and program components of the HPCC program are presented in Table 2.

Among the various components of this program, the one most pertinent to computational mechanics falls within the largest--Advanced Software Technology and Algorithms (ASTA), which represents 41 percent of the proposed funding.

One of the subcomponents of ASTA--Computational Techniques--is described as follows:
Computational techniques: The focus of the HPCC program on scalable parallel computing systems dictates that significant advances in computational techniques will be needed. The design and theory of algorithms are as important as hardware or networking improvements in reaching teraflop computational performance. Research in computational techniques will include parallel algorithms, numerical and mathematical analysis, parallel languages, computational models, and program refinement techniques.

The various activities of the HPCC initiative will contribute to a number of "grand challenge" problem areas. The grand challenges are defined in the 1987 OSTP report, titled A Research and Development Strategy for High Performance Computing, as fundamental problems in science or engineering with broad implications, whose solution would be facilitated by the application of high performance computing resources.

Table 3 indicates how many research directions in computational mechanics contribute to resolving the grand challenges of the HPCC initiative. It is clear that without significant advances in computational mechanics, successful resolutions of these challenges will be impossible.

Computational mechanics is closely related to several research initiatives of title U.S. government and the national needs identified in these initiatives. Appendix 6 describes how computational mechanics can be used to design new materials and to predict the life and failure of existing materials. However, significant progress in modeling is needed before this potential can come to fruition.

Following this section, a summary of research directions in computational mechanics is presented, in which the basic research areas that feed these applications are discussed. If the field is to progress over the next decade, these basic research areas require sustained attention and support.

TABLE 2

Goals: Strategic Priorities

- Extend U.S. technological leadership in high performance computing and computer communications.
- Provide wide dissemination and application of the technologies both to speed the pace of innovation and to serve the national economy, national security, education, and the global environment.
- Spur gains in U.S. productivity and industrial competitiveness by making high performance computing and networking technologies an integral part of the design and production process.

Strategy: Integrating Priorities

- Support solutions to important scientific and technical challenges through a vigorous R&D effort.
- Reduce the uncertainties to industry for R&D and use of this technology through increased cooperation between government, industry, and universities, and by the continued use of government and government-funded facilities as a prototype user for early commercial HPCC products.
- Support the underlying research, network, and computational infrastructures on which U.S. high performance computing technology is based.
- Support the U.S. human resource base to meet the needs of industry, universities, and government.

Program Components

- High Performance Computing Systems
- Research for Future Generations of Computing Systems
- System Design Tools
- Advanced Prototype Systems
- Evaluation of Early Systems
- Advanced Software Technology and Algorithms
- Software Support for Grand Challenges
- Software Components and Tools
- Computational Techniques
- High Performance Computing Research Centers
- National Research and Education Network
- Interagency Interim NREN
- Gigabits Research and Development
- Basic Research and Human Resources
- Basic Research
- Research Participation and Training
- Infrastructure
- Education, Training, and Curriculum

Relevance of Computational Mechanics Major Technical Areas to the Grand Challenges of HPCC

GRAND CHALLENGE PROBLEMS

	Weather	Materials	Semiconductors	Superconductors	Vehicle Signature	Turbulence	Vehicle Dynamics	Nuclear Fusion	Combustion	Enhanced Oil & Gas Recovery	Computational Ocean Sciences	Vision	Anti-Sub. Warfare
ADAPTIVE METHODS AND ERROR ESTIMATION	•	•	•	•	•	•	•	•	•	•	•		•
PROTOTYPE TEST SIMULATION	•	•	•	•	•	•	•	•	•	•	•	•	•
PARALLEL COMPUTATION	•	•	•	•	•	•		•	•	•	•		•
AI IN MATH MODELING	•	•	•	•	•	•	•	•	•	•	•	•	
ENVIRONMENTAL CONTAMINATION AND [illegible]										•	•		
MATERIALS RESEARCH		•	•	•									•
STRUCTURES AND STRUCTURAL DYNAMICS			•										•
NONLINEAR EQUATIONS AND BIFURCATION	•	•	•	•	•	•	•	•	•	•	•		
UNCERTAINTY AND STOCHASTIC PROCESSES	•	•			•	•					•		•
CHEMICALLY REACTING FLOW AND COMBUSTION					•	•			•				
NUMERICAL MODELING OF TURBULENCE	•					•			•		•		•
GENERAL CFD	•		•			•	•		•	•	•		•
NONLINEAR DYNAMICS OF MULTIBODY SYSTEMS		•							•	•	•		
MANUFACTURING PROCESSES			•		•							•	•

TABLE 3: Relevance of Computational Mechanics Major Areas to the Grand Challenges of HPCC

Concluding Remarks

In its assessment of computational mechanics in the United States, the committee has identified the following broad areas that require focused research and financial support over the next decade:

1. *Adaptive methods for nonlinear problems*. Adaptive methods that allocate computational resources to the portions of a simulation where it is most needed are crucial to the types of computation on the leading edge of mechanics. Simulations of manufacturing processes, crashworthiness, and materials failure all require that adaptivity be feasible. Research is required in the fundamentals of error analysis and control for nonlinear problems, strategies for implementing adaptivity in mechanics problems, and treatment of various classes of mechanics problems by adaptive methods. Particular difficulties are foreseen in the implementation of adaptive strategies on massively parallel computers. Promising opportunities are also seen in the exploitation of artificial intelligence and knowledge-based systems in controlling adaptivity and other aspects of algorithm performance.

2. *Optimal control of computational modeling*. This is a new area of research that draws on the use of artificial intelligence and knowledge-based systems, methods of a posteriori error estimation, adaptive methods, and parallel computing to optimize and control the computational process, making it as efficient and reliable as possible. These component subjects are expected to be important areas of research for at least the next 10 years.

3. *Structures and materials*. The computational modeling of new materials as well as the behavior and control of structures composed of such materials constitute one of the most important and exciting areas of research for the next decade. New advances in computer modeling techniques and a better understanding of the micromechanics of structural materials bring within the realm of possibility the actual design of new structures that exhibit special strength, fatigue life, stiffness, and fracture resistance. The role of computational mechanics modeling in these areas is an essential one; however, many basic problems must be resolved to achieve these goals.

4. *Computational fluid dynamics (CFD)*. This field, which includes traditional computational fluid dynamics, combustion, hypersonics, chemically reacting flows, environmental pollution and contamination modeling, weather prediction, direct numerical simulation of turbulence, and turbulence modeling, has suffered from a flawed philosophy advocated in the past by some agencies that the size and speed of available computers will drive the advances in CFD, making research on methodology of secondary importance. Recent developments

prove that a contrary philosophy is needed for the healthy growth of CFD over the next decade. True advances in these subjects will result from interdisciplinary research in fluid dynamics, computer science and engineering, and numerical analysis in which all aspects of CFD modeling are addressed. In particular, many traditional approaches to CFD modeling are now obsolete. There is a need for considerable research that will develop effective techniques to overcome the extensive list of long-standing open problems.

5. *Reliability of computational modeling*. The issue of computational mechanics reliability will be of special concern during the next decade. A variety of research areas will impact this issue, including the development of theories for probabilistic methods, uncertainty and stochastic processes in mechanics, a posteriori error estimation, post-processing, and knowledge-based systems. The use of hierarchical modeling concepts also emerges as an area that requires research to provide a basis for testing the models' reliability.

6. *Interdisciplinary parallel computing*. To achieve higher levels of computational power, such as computer processing speeds in the teraflop range, hardware designers are increasingly turning to massively parallel computers. The efficient utilization of these computers will require fundamentally new concepts in computational mechanics algorithms.

7. Research in parallel computing techniques in computational mechanics must be done by interdisciplinary teams with expertise in computational mechanics, numerical analysis, and computer science. Interaction among computer scientists, engineers, numerical analysts, and hardware developers is essential to achieving advances. Parallel programming constructs targeted for computational mechanics must be developed and new programming languages and software tools must be standardized. New languages must have capabilities rich enough to address readily the complexities commonly found in computational mechanics. The design and development of special hardware to optimize performance for particular mechanics computations should also be undertaken.