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A Commentary on Computational Mechanics

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Introduction

At a recent national scientific meeting, a panel of experts discussed trends in computational methods in mechanics and the physical sciences. One expert, eager to say something profound to get the discussion off on the right track, said something to the effect that "Within the next decade, the only use aerodynamicists will have for wind tunnels is as a place to store computer print-out." This statement reflects two important phenomena that have fallen on the scientific community in the past two decades—the first is physical, political and sociological, and the second is psychological.

The first of these has to do with the significant advances that have been made during recent years in computing machinery, numerical methods, and mathematical modeling. It is an undeniable fact that, in many areas of technology, confidence in computer modeling has put an end to some of the expensive laboratory testing that was so essential a few years ago.

The second thought that our expert's statement provokes is the blatant overconfidence, indeed the arrogance, of many working in the field of computational mechanics. Some refer to this point of view as "the number crunching syndrome" and warn that it is becoming a disease of epidemic proportions in the computational mechanics community. Acute symptoms are the naive viewpoint that because gargantuan computers are now available, one can code all the complicated equations of physics, grind out some numbers, and thereby describe every physical phenomena of interest to mankind. All the major problems of theoretical mechanics can now (or soon will be) solved on the computer.

Our aim here is to discuss both of these phenomena, to amplify on the first, and to describe some trends in research and education in mechanics and computational methods which promote the second. We want to point out that computational mechanics is having an enormous impact on our lives, more than many people realize, and that the benefits of recent advances are important and far reaching. Secondly, we want to point out that computational mechanics can be a "good" science. In the spirit of Shaw, it uncovers more questions than it answers. It is also an intellectually rich and challenging subject, and an important addition to the family of subjects comprising theoretical and applied mechanics. Finally, we want to point out that there are formidable open problems awaiting the creative scientific mind in this field, and that even if some substantial breakthroughs were made, the confidence exhibited by our expert is still not justified.

Computational Mechanics

The advent of electronic computation has had a profound effect on theoretical and applied mechanics during the last two decades. The use of computers has transformed much of theoretical mechanics into a practical tool and an essential basis for a multitude of technological developments which effect large facets of our everyday life. Indeed, in the world's industrial nations, it is almost impossible to go about one's normal activities without coming into contact with some product that has been directly or indirectly the result of computer applications of the principles of mechanics.

There has emerged from the work of recent decades a new discipline, lying essentially in the intersection of theoretical mechanics, computer science, and numerical analysis, which we choose to call computational mechanics. It draws from developments made in each of these disciplines and is nourished by them, but it also stands as a viable branch of knowledge in its own right.

There are four basic components of the field of computational mechanics:

(1) *Theoretical mechanics:* the theoretical study of the mechanical behavior of physical systems and bodies.

(2) *Approximation theory:* the formulation of discrete models, which are approximations of the equations of mechanics.

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(3) *Numerical analysis:* the development of numerical methods to analyze these models.

(4) *Software development:* the development of computer software to implement the numerical methods.

In addition, one might add to this list, (5) *Computer hardware:* the development of computing machines to implement the software. This aspect of computational mechanics is largely in the hands of computer architects who have little interest in mechanics or its applications. Moreover, there is little to say about this subject that has not already been said many times—the development of sophisticated computer hardware has continued to grow at an exponential rate since the late 1950's. There is every reason to believe that this trend will continue; we will not comment further on trends or the status of computer hardware development or research. The comments we make here pertain to items 1 through 4, and particularly items 1, 2, and 3.

Our aim is not so much to summarize existing numerical methods, approximation theories, or the status of theoretical mechanics, but rather to describe what can and is being done in these fields today and point to some obstacles now standing in the way of future developments.

We first must recognize that there are two distinct aspects of computational mechanics, just as there are in mechanics itself. First, there is the mission-oriented and application area; that is the *applied* or *engineering* computational mechanics discipline. The objective here is a practical one: to develop computational techniques that aid in the numerical analysis of various models of physical behavior and to use these analyses to design actual mechanical systems-structures, machines, processes, etc. Usually, the final product of these efforts is a computer program.

Second, there is basic computational mechanics research. Here the goals are to understand the fundamental properties of approximations and of the equations of mechanics, to analyze numerical methods appropriate to study them, and to study techniques for optimizing software to implement these methods.

The contrast between these two areas is analogous to that we see in Numerical analysis, as opposed to numerical Analysis the first aims to study the behavior of solutions to mathematical problems, particularly differential equations, numerically; the second aims at using the techniques of mathematical analysis to study properties of numerical methods. A similar comparison can be made between engineering mechanics and mechanics. In basic computational mechanics, it is impossible (or, if not impossible, at best foolhardy) to separate a study of the mechanical theories describing the phenomena at hand from approximation theory. Physical arguments traditionally have been a guide to the development of sound mathematical models; mathematics (for example, existence theory) and physical experiments are final tests of the validity of the theory. Both are needed to formulate sound discrete models and both provide a starting point for numerical analysis.

It is well known, of course, that what is research to one person may be development (i.e., the assimilation and application of known facts) to another, but we are concerned that much of the activity now being labelled as research in computational methods is, in fact, a sophisticated kind of developmental endeavor which is well outside the realm of good science or mathematics and, in the long run, cannot lead to important scientific achievements.

Applied Computational Mechanics

The brief history of applied computational mechanics is certainly a remarkable success story. Emerging from the empiricism and crude approximate mechanical theories prevalent in the late 1950's, the subject has now reached a level of development where it affects not only the lives of everyone in the scientific community, but also the public at large. New journals on applied numerical analysis appear at increasing rates. International conferences, NATO meetings, symposia, colloquia, are held somewhere virtually every week of the year. International commissions and organizations, some fully supported and representing important industrial nations, have been organized on numerical methods and software. The elements of programming are now being taught to high school students, and every college graduate in engineering and the physical sciences is now expected to know some numerical analysis and programming. A multitude of private companies have appeared which make their livelihood selling computer software for the analysis of engineering problems. .

To further emphasize the point, let us list a few examples of the breadth of computational mechanics in our country:

(1) Computational procedures implemented in computer programs are employed throughout most of the nation's larger manufacturing companies on an everyday basis in the analysis and design of structures and mechanical equipment. Many of the larger companies have installed computer programs on their own in-house computers and organizations with smaller resources now have access to computer programs on a royalty basis furnished by a large number of commercial computing centers.

(2) Every major nuclear industry, and especially all of the nuclear energy laboratories of the federal government, are heavily involved in computer applications of solid, structural, and fluid mechanics in the design of nuclear reactors. The safety and structural integrity of these reactors is a critical aspect of their design and probably could not have been accomplished had there not been significant advances in computational methods during the last ten years.

(3) The major automobile manufacturers in the world now use large scale computer programs as standard operating procedure for the stress analysis, structural design, and dynamic analysis of motor vehicles. The direct application of new ideas in computational mechanics has

resulted in very large savings in the auto industry.

(4) A large portion of the nation's hardware and software development for national defense depends directly on computational methods for mechanics problems. The applications range over such studies as interior, exterior, and terminal ballistics of projectiles; aerodynamics; penetration and impact studies; control of missiles and aircraft; ablation of metals under aerodynamic heating; fracture; the overall structural integrity of water and airborne weapons systems; and satellite dynamics and control.

(5) Since the early 1960's, the computer-based analysis of the mechanical behavior of commercial and military aircraft, ocean liners, oil tankers, and high speed railway systems has been an essential aspect of their design. Without reliable computational techniques, high speed computers, and a number of recent technological advances, the current level of aircraft technology we enjoy would not be possible.

(6) Virtually every aspect of our nation's space program has relied heavily on computer applications of mechanical principles. These range from the stress and stability analysis of the Saturn V rocket and its predecessors, the aerodynamics of space vehicles, the mechanical behaviors of fuels, and the analyses of various material properties to the calculation of optimal orbits and vehicle dynamics of missiles and artificial satellites.

To this list, we could add the heavy use of large scale computers in analyzing modern hydrodynamic models of the lower atmosphere and of the sea to study and predict the weather and the flow of ocean currents; also, problems in water and air pollution are studied using complex models of the motion of rivers, streams, and harbors and of the transmission of pollutants through the atmosphere. We could also add the reliance of the petrochemical industry on computer modeling to simulate oil and gas reservoirs, estimate their capacities, and design recovery methods and storage facilities.

Additional activities could be mentioned, but the essential point is that applied computational mechanics is now an intrinsic part of everyday life in the industrialized world. Hundreds of millions of dollars are invested annually in computational activities of the types described, and these have been very important in providing the high standard of living we enjoy today. More importantly, the continued development of better computational capabilities and more encompassing mechanical theories is essential to our maintaining this standard in the future.

Experimental and Computational Mechanics

Let us return briefly to the question of computational methods as a substitute for physical experiments. During the short span of years in which computational methods developed into an important element of theoretical mechanics, experimental mechanics was by no means dormant—it also enjoyed a period of growth and development unequalled in its history. Modern computing equipment and numerical modeling have brought important new tools to the experimentalist, just as physical experiments and measurements have provided one of the few rational means for testing the validity of many of the computations which led to the achievements listed in the previous section. Modern experimental and computational methods, combined in an interactive way in which one complements the other, represent some of the most powerful tools available for studying many complex physical phenomena. The use of such tools in characterizing materials; testing the validity of mechanical and thermomechanical theories; verifying and evaluating numerical models and their underlying assumptions and limitations; and as a guide to resolve such questions as "at what location in a system and at what time should measurements be taken" can have a significant impact on basic and applied mechanics in years to come.

An Era of Computational Empiricism?

How reliable are numerical experiments as a means for testing the effectiveness of numerical methods? We are reminded of the numerical experiments on nonconforming finite elements in the 1960's. By solving numerically a large collection of sample problems, one group of analysts concluded that their element was "very competitive" as an element for the analysis of plate bending problems. It is now known that that element is divergent! Their deceptively good results arose from particular choices of loading and boundary conditions which, because of special symmetries in the solutions, effectively masked the inadequacy of their element. Then there are the examples of mixed finite elements in the late 1960's, which are numerically inconsistent, but which could produce results which looked reasonable for a specific mesh.

There is also the example of a well-known shell analysis code circulated in the late 1960's and early 1970's and used throughout the United States which employs an inconsistent, and in fact divergent, shell element. Fortunately, many of the applications of this code were accompanied by full scale laboratory experiments which finally were the overriding factor in determining designs of various structural systems.

The picture in the calculation of flow problems is not much better. How reliable are the large hydrodynamic codes? Their accuracy is often established by comparisons with experiments or with special cases for which analytical solutions are known. In the difficult application areas described earlier, the ideal conditions one has in those problems for which analytical solutions are known are practically never present.

In the engineering community of 20 years back, it was understood that the use of classical analytical methods provided very limited tools for studying mechanical behavior and, as a consequence, it was mandatory for the engineer to supplement his analyses with a great deal of judgment and intuition accumulated over years of experience. Empiricism played a great role in engineering design;

while some general theories of mechanical behavior were available, methods for applying them were still under development, and it was necessary to fall back upon approximation schemes and data taken from numerous tests and experiments.

Today it is a widely held view that the advent of electronic computation has put an end to this semiempirical era of engineering technology: nowadays, sophisticated mathematical models can be constructed of some of the most complex physical phenomena and, given a sufficiently large computer budget, numerical results can be produced which are believed to give some indication of the response of the system under investigation.

In the case of linear problems, we now have a relatively broad experience in computing solutions. In general, the reliability of the computed results is seldom questioned as it has been corroborated by intuition, observation, and practical experimentation over a significant period of time. Moreover, error estimates are now available for many of the numerical methods in use and these provide both a priori and a posteriori checks on solution accuracy. It is certainly true that substantial improvements in design, some of which were outlined in the previous section, have resulted from confidence in the use of computers and numerical methods in recent times. The trend today is to continue to press the capabilities of computational methods into areas of nonlinear mechanics in the hope of gaining still further improvements and a better understanding of the response of actual engineering systems.

Unfortunately, in the case of nonlinear problems, few numerical experiments can be supplemented with judgment gained by years of experience. Even worse, many computational empiricists seem to be unaware of the fallibility of their methods. We believe that in the area of nonlinear mechanics, we have, ironically, left one semiempirical era and entered another—the empiricism now is manifesting itself in computations.

There are two major difficulties inherent in the addition of nonlinear analysis capability to the tools of contemporary engineering analysis and design. The first is well known: a numerical analysis of a large scale nonlinear problem is expensive, often 10 to 100 fold that of a comparable linear analysis. Consequently, the choice of an appropriate technique and its effective implementation becomes critically important in the practical analysis of nonlinear problems. Also, for large scale nonlinear problems, few institutions can afford to follow the practice common in linear analyses: solve the problem for several different meshes to test convergence; experiment on the behavior of the solution to changes in material constants and boundary conditions; investigate several loading conditions; and alter the geometry of the problems and compare special cases with known solutions when available. It is rare that this type of numerical experimentation can be done effectively for nonlinear problems.

Also, considering the fact that computational methods are used as a basis for many important decisions which affect our security and livelihood, it is certainly unwise to employ methods whose reliability is not completely verified. This reliability of methods for nonlinear problems is the second major difficulty that faces the developers of nonlinear codes. It makes little sense to invest hours of computing time on a complex nonlinear analysis, only to obtain results which may have little bearing on the actual response of the system at hand. There are many frightening examples which reinforce this point. The use of finite element methods, for example, in the calculation of postbuckling behavior of nonlinear structures can be very sensitive to mesh size—a refinement in what appears to be a reasonable mesh can produce gross changes in the postbuckling response, and the true behavior of the system may be quite different from that produced by what many would consider a reasonable model. In nonlinear evolution problems, examples abound of cases in which a small perturbation of the initial data can produce enormous changes in the response of the system—yet numerical approximations of solutions of problems of this type are ground out daily (many are published) with little evidence that the analyst is aware that his solution may not resemble in any way that experienced by the actual system.

There is much evidence that we are, indeed, in an era of computational empiricism. If we are to leave this era, we must make a conscious distinction between applied and basic computational mechanics and caution the army of enthusiastic users of modern software that much in the way of fundamental research remains to be done before the nonlinear theories of mechanics, in general, can be used with confidence as a basis for analysis and design.

Basic Research in Computational Mechanics—Some Open Questions

Space does not permit us to list all of the important open questions standing in the way of the advancement of basic computational mechanics. The following partial list, however, gives an indication of the flavor of some of the formidable difficulties that remain to be resolved:

(1) *A posteriori estimates: Adaptive mesh refinement Strategies:* Is it possible to measure quantitatively the accuracy of numerical solution by means of testing the solution after it has been calculated? A posteriori estimates for the simplest linear one-dimensional boundary value problems have been established on a rigorous basis, and it is not uncommon for certain a posteriori estimates of accuracy to be used in large scale hydrodynamic calculations, and in the solution of large systems of stiff ordinary differential equations. These, however, are often based on rather shaky mathematical grounds. The development of a posteriori error bounds for difficult two- and three-dimensional problems in solid and fluid mechanics requires computational tools that are not yet available. Once such a posteriori estimates are available, it should not only lend some confidence to some of the methods now in use, but also provide an important ele-

ment in improving solution efficiency. Indeed, the availability of a posteriori estimates would make possible the development of adaptive mesh refinement schemes which could conceivably produce near optimum meshes for the analysis of various boundary value problems. It could solve an old problem: the generation of the best possible numerical solution for a given problem for a given amount of computing time or dollar expenditure.

(2) *Nonlinear elasticity problems:* The numerical analysis of the equations of finite elasticity is in an embryonic stage. Many computer programs for such problems exist, but there is virtually nothing known about their accuracy outside of results produced by numerical experiments. Error estimates and convergence criteria are known for some particular cases, but these are based on assumptions on the regularity and existence of solutions. Unfortunately, means for determining a priori the regularity of solutions for most nonlinear boundary value problems are not known. Even a local analysis of these equations leads to indefinite forms and difficulties with nonuniqueness and instability of solutions. A complete numerical analysis of these problems lies beyond the current state of the art.

We also mention that the key to the study of nonlinear boundary value problems, such as those encountered in finite elasticity, is the availability of an existence theory. Indeed, an existence theory not only provides the basis for an approximation theory but it also provides the only tool outside of physical arguments and laboratory experiments for establishing the validity of a theory itself. To date, a complete existence theory for finite elasticity does not exist and the development of an approximation theory must still be based on a long collection of simplifying assumptions which may or may not be valid for particular problems of interest.

(3) *Elastodynamics:* If the study of numerical analysis of the equations of nonlinear elastostatics is not well established, then the state of the art in elastodynamic problems is even worse. Here it is known that smooth initial data may lead to the development of shock waves, and that multiple solutions can exist. Moreover, not all these solutions may be physically relevant, as positive entropy must be produced across a shock front. How can we model such phenomena numerically? What means do we have to determine that a numerical scheme will not produce in some artificial way an unrealistic solution—one that does have a positive entropy production across shock fronts, but which is only due to some truncation error in the numerical process? Then there are the nonlinear vibration problems, complete with bifurcations and instabilities. How do we determine these various solutions numerically? Which ones, if any, resemble the physical behavior we wish to model, and what is their accuracy?

(4) *Inelastic materials:* When we leave the realm of the mechanics of elastic materials we enter a little explored area of continuum mechanics in which little in the way of a complete mathematical theory is known. Progress in, for example, the theory of finite plasticity has been made in recent years, but few would agree as to what constitutes a reasonable boundary value problem in this area, much less a theory on the existence, uniqueness, and qualitative behavior of solutions of such problems. A mathematically sound approximation theory and numerical analysis of these problems cannot emerge until the problems themselves are well set. One can add to these difficulties all of the computational and mathematical difficulties brought about in modeling phase changes, viscous effects, cracks and singularities, the growth of cracks under dynamic loading, and the identification and implementation of physically reasonable constitutive equations describing these materials:

(5) *Stokesian flows:* Existence and approximation theorems are available for only certain cases of Stokesian flows. The few studies of error and convergence of numerical methods for such classes of problems are typically based on truncation concepts which are invalid for irregular solutions. Bifurcation phenomena in three-dimensional flows are only now being understood and the study of the behavior of numerical approximations of such phenomena is in an extremely early stage of development.

(6) *Compressible flow problems:* Perhaps some of the greatest difficulties in the way of developing an approximation theory and numerical analysis are encountered in the study of compressible flows. The theory of mixed nonlinear partial differential equations is very much underdeveloped. Theories on the qualitative behavior of solutions are known only for special cases and existence theorems for fully developed compressible flow problems are still far beyond the methods of the modern theory of partial differential equations. Since a rational numerical analysis must be based on such theories, the likelihood that problems of this type will soon be treated with numerical confidence is small. The picture is further complicated by the fact that the solution of these equations may be very irregular, i.e., possess shocks and singularities. The development of schemes for handling these difficulties still poses major unsolved problems.

(7) *Non-Newtonian flows: Convection-diffusion problems:* Many of the difficulties one has with Stokesian flows are magnified in the case of non-Newtonian flows. Mathematical bases for many models of non-Newtonian flows are not well set, nor are criteria for constructing theories that will guarantee physically reasonable solutions of the governing equations. Some of the simpler fluids (e.g., Bingham fluids) can be characterized by equations for which there is a reasonably firm mathematical theory for certain choices of boundary and initial conditions, but the development of a corresponding approximation theory and numerical analysis is only in its early stages. Convection-diffusion problems still present numerical difficulties that have not been completely resolved—particularly in nonlinear convection-diffusion processes and/or in cases in which free surfaces are developed which propagate in time.

Concluding Comments

The success of large scale computations has led to some curious situations. As might be expected, it has had some impact on education in engineering and the physical sciences. Many of the general equations of nonlinear solid and fluid mechanics which were laid down in the 19th century are now of more than purely academic interest. They must be understood, expanded, and generalized to provide a basis for modeling many of the various phenomena described earlier. The breadth and scope of some of the applications listed previously should dilute arguments once prevalent in our universities that too much time is spent on the fundamental theories of continuum mechanics and that modern mathematics and numerical analysis is a waste of time for students interested in solving real world problems. Thus, it would seem that the triumphs of applied computational mechanics would heighten the appreciation of most practitioners for the need of more basic work in all of the areas which feed such large scale computational efforts; however, with a few exceptions, the opposite has been true.

The trend in education, particularly in engineering schools, has definitely turned away from the more basic studies in vogue during the late 1960's. In many schools, the basic equations governing mechanical phenomena, if mentioned at all, are too often presented but not taught; emphasis is given to methods to use as opposed to concepts on which to build; on how to as opposed to why.

In many instances, this has produced technicians who practice what some call computer overkill, which refers to the use of existing large sophisticated codes to study systems which could be better understood, at considerably less expense and effort, by the use of much simpler models in the hands of those with a deeper comprehension of the physical phenomena and the basis of the methods available to analyze them.

In other instances, it has created the computerized giant killer, who is ready to launch into the analysis of the most complex physical problems and confidently provide "solutions" which may have significant implications in important technological projects. Alexander Pope's classic line, "A little learning is a dangerous thing" was never more appropriate.

The reasons for such trends in education are complicated. They involve the increasing tendency of university administrations to manage their programs as businesses designed to compete for federal monies; their frequent adoption of short range goals results in training technologists to meet fluctuating industrial needs rather than to provide a basis for learning.

Then there is also the attitude of some educators in engineering and the applied sciences that the phenomena they wish to study are just too complicated to ever warrant the use of modern theories or methods, and that one's only recourse is to reach backward to the semi-empirical methods of decades past. One hears this opinion voiced too frequently by some who are entrusted with the responsibility of directing and conducting basic research and who have some voice in determining directions of educational programs. There is little new about such positions; similar attitudes have always stood in the way of progress in science and technology. In some respects this philosophy is diametrically opposite to that which we have emphasized herein—no confidence as opposed to overconfidence in modern computing capabilities—but it is equally dangerous, for it is not based on penetrating logic but rather on ignorance of the scientific method and confusion as to the purpose and responsibilities of institutions of higher learning. We hope it does not prevail.

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