THE IMPACT OF COMPUTER SIMULATION ON APPLIED SCIENCE

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Up to the 1930's, the development of the applied sciences based on a physical description of natural phenomena was still predominantly in the wake of the mathematics of the eighteenth and nineteenth century. One of the common *modus operandi* consisted in deriving, deductively or inductively, mathematical equations describing physical, engineering or natural systems, and then in exploring properties of those systems by the analytical investigation of solutions of these equations. While this approach has resulted in spectacular advances in a phenomenological description of the world, in the development of industrial machinery and in some mathematical theories of society, the limitations placed by the need to solve these equations "by hand" were enormous.

With the appearance of computers, it suddenly became relatively simple to obtain particular solutions, with diminishing concern both for their possible analytical properties and, as computers grew in size and capability, for the complexity of the object being studied. While there are other factors which, too, may be credited with having helped the spectacular advances in the sciences of the last third of a century, none has had an impact as drastic as that of computers. Although this statement is accepted almost as a triviality today, the impact of computers in general, and of computer simulation in particular has not always been what it was expected to be.

In a somewhat simplistic but not uncommon way, computers were conceived at first as new tools for solving old problems. Indeed, it has been said that Pascal invented his calculating device to ease his father's burden as an accountant, that Charles Babbage conceived of the Analytical Engine as a tool for computing mathematical tables faster and less subject to error than man [1], and Lord Kelvin's remarks about what may be considered as the first differential analyser read as follows:

> "*...and it seems to me very remarkable that the general differential equation of the second order with variable coefficients may be rigorously, continuously and in a simple process solved by a machine*" [7].

But it is perhaps by the uncovering of new modes of research and unforeseen classes of problems, rather than by the crunching away of some of the old ones that the impact of computers has been most significant. Some of this impact has been beneficial to the advancement of science and the welfare of mankind. But some has been much less successful, bringing confusion, dissatisfaction, and (restricting our comments to science alone) possibly a regression in the quality of applied scientific work. The "inside" community of those concerned with computers is generally prone to talk about the not so positive ones. I shall venture to address both.

The traditional sciences had relied essentially on two fundamental modes of research, the experimental and the theoretical, sometimes to the degree of polarization that one finds for instance in physics. Computers have affected this division. More and more disciplines are using computers to simulate complex or large systems, whose equations could be formulated but not solved analytically. In so doing, they have found out that there is a third alternative to the theoretical/experimental dichotomy of the past: this third alternative is the "computational" approach. To wit, the past decade has seen the coining of such expressions as "computational fluid dynamics", "computational physics", "computational mechanics" and the like. "Computational research" is not an extension of either the theoretical or experimental approaches: it is a new way of doing research.

In disciplines which have not had a long past, computer simulation has often been an integral part of their recent development. It is well known, for instance, that aerospace science and industry would not be what they are today if they had not been able to rely heavily on the scientific computation and simulation tools afforded in the past two-and-a-half decades or so. We are all aware of the large computer simulation "laboratories" where characteristics of vehicles are tested from simple components to complete flights and missions, and of the "man in loop" setups where the computer becomes a training tool of extreme sophistication.

"Computational Physics" has become an area of application of computer simulation of great interest. The importance of finding new sources of energy and the difficulties of harnessing nuclear fusion to that effect has resulted in the funelling of significant funds towards the development of computer simulations of the dynamic processes occurring in prototype reactors. The emerging role of computer simulation in physics has received official recognition. Its place may be summarized in a sentence of a recent book by Potter [10]: *"The roles played by mathematical theory, computational physics and experiment are to be regarded as complementary. Each approach can contribute in part to our understanding of physical phenomena."* In addition to the use of "computation toward understanding", mention should also be made of the large effort going into the development of simulations or "codes" designed to analyse the safety of nuclear power plants, indeed a matter of growing public concern.

Weather prediction with the aid of computation was conceived by Richardson in the 1920's [11], and may be well on its way to becoming reality with the occurrence of the electronic computer.

The impact of computers on applied mathematics has been overwhelming. In the precomputer days, a significant part of applied mathematics was concerned with the search for new methods of solution, exact or approximate, of equations describing natural or man-made systems. A major redirection in this activity has been concerned with the formulation of "methods" and analysis of algorithms. For example, Pontryagin's maximum principle and Dynamic Programming (both of the 1950's) may be viewed as sophisticated formulations of methods to solve optimization problems, bearing in mind that all but the simplest applications would be solved by computers. Numerical analysis has grown as a well recognized branch of applied mathematics, and plays a significant role in the development and analysis of computer algorithms for simulation and a variety of other scientific calculations. The role of differential equations, and those aspects of their theory which are of importance have been gradually displaced. Since their introduction toward the end of the seventeenth century, they had remained the almost universal tool used to describe, among other things, the behavior of systems whose state varies continuously with time (dynamical systems). Analog computers are simply differential equation solvers (or differential analysers) and have found their natural application in the simulation of mechanical systems, aerospace vehicles, processing plants and the like to which differential calculus had been long applied. Yet, digital computer simulation starts with a discretization of the time variable, and a transformation of differential equations to algebraic ones. Inasmuch as differential equations have the reputation of being "hard stuff" among the less mathematically inclined scientists, the need to use them has somewhat disappeared as an intermediate tool toward digital computer simulation. One of those who were quick to take advantage of this was Jay Forrester, who left differential equations altogether out of the succession of "soft" system dynamic simulations which he developed. Instead of differential equations, he used "levels" to describe state variables and "rates" to describe their time derivative. E.g., one finds in his book "Industrial Dynamics" (1961) the following:

> *"All memory and continuity from the past to the future exist in the levels of the system... . Rates define the present, instantaneous flows between levels... . The continuous advance in time is broken into small intervals of equal length DT. By definition, this interval must be short enough so that we are willing to accept constant rate of flow over the interval as a satisfactory approximation to continuously varying rates..."* [3] It is almost amusing to

note that this sounds like a rekindling of the Newton/Leibniz feud about the meaning of infinitesimals, brought about by the inability of digital computers to deal with quantities and structures which are not discrete. Forrester's rates are very close in concept to Newton's *fluxions* (see e.g. [16], pp. 200, 201).

The degree of attention (if not necessarily always favorable) given to Forrester's Industrial, Urban and World Dynamics speaks largely for the appeal of a "non-differential analysis" description of dynamical processes to those who had been deniedthe use of this branch of applied mathematics because of the hurdle. Likewise, Bellman's Dynamic Programming [2] is to a large extent a discrete version of the calculus of variations, predicated on the fact that the computer implementation of solutions are to be discrete anyway.

Summarizing, all I have mentioned so far may, by the generally accepted standards, be considered as contributions of computers (or more precisely computer simulation) which have been beneficial to the advancement of the sciences and of their ramifications in our industrial society.

But there have also been casualties. What appeared at first as a general easing of the difficulty of using mathematics by relegating some of it to the computer has brought its own procession of problems. Whereas applied mathematics (not merely applicable mathematics) was utilized with reasonable caution within relatively coherent and mature disciplinary groups, both caution and disciplinary maturity are not any more the appendage of the multitude of published studies describing computer simulations of an ever growing variety of systems. A characteristic of the old scientific establishment is that it has been compartmentalized into a relatively small number of disciplines, and that in each discipline there was an implicit hierarchy of men, structure of peers within which standards of quality were transmitted and carefully controlled. While this state of affairs had its obvious built-in drawbacks, one of its benefits was a closely knit scientific community in which standards were protected and transmitted in a reasonably orderly fashion. With what amounts literally to an explosion in the availability of computers, of the degree of funding, and of the number of those drawing on both, many new sub- and inter-disciplines have emerged with little or no tradition of how to do things (which may be good) and no tradition of how to do things well (which is often very bad).

One reads for instance, in a recent issue of Science [12] the following remarks directed against Environmental Impact Studies, which are all too often conducted by ill-trained scientists:

> *"Many ... have been quick to grasp that the quickest way to silence critical 'ecofreaks' is to allocate a small proportion of funds to any engineering project for ecological studies. Someone is inevitably available to receive the funds, conduct the studies regardless of how quickly results are demanded, write large, diffuse reports containing reams of uninterpreted and incomplete descriptive data, and in some cases, construct 'predictive' models* [read: Computer Simulations] *irrespective of the quality of the data base. These reports have formed a 'gray literature' so diffuse ... that its conclusions and recommendations are never scrutinized by the scientific community at large."*

Given the magnitude that it has taken in certain geographic and disciplinary provinces, the question of this proliferation of "gray" work is more than peripheral to the issue of computers in science. To quote again from [12], *"The advancement of the scientific method is ... in jeopardy."*

It is one of the responsibilities of scientific societies to ensure professional quality and to attempt to prevent, with the limited means which they have, the occurrence of poor quality scientific work. There are many computer simulations and computer "codes" with Environmental Impact or Safety objectives which are developed by the most respectable scientific teams, with all the degree of caution and disciplinary quality that one should expect. That misguided "studies" of the kind described above do also take place is a fact that must be recognized. Given that Administrations, the general public and even sometimes members of the scientific/industrial community are not always able to distinguish between the two creates an uneasy state of affairs in which, unfortunately those who bear most of the guilt stand to lose the least.

Part of the casualty in the growth of computer applications to simulation has been in the "soft" sciences. What was ill recognized at first is that the difficulty was not so much in solving mathematical equations as in formulating them. Or, in the terminology of the trade, the difficulty is with the "modeling" rather than with the computational aspects of the "simulation."

Scientists of the social and environmental sciences who--perhaps simple mindedly--believed that availing themselves of computer simulation would bestow them the rigor and power of exact mathematics that had heretofore been the exclusive province of other disciplines were soon to find out that this was not so.* Whereas computer simulation is capable of giving an exact rendering of a mathematical model, the model itself is often at best a poor mock-up of the real thing. Notions of "soft systems," "fuzzy systems" and "white boxes" were soon to be introduced to describe their universe. But while not bringing them close to answers as often as they hoped for, computer simulation has at least forced them to become more specific in formulating questions. As an example, Forrester's and co-workers'

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* Norbert Wiener made very appropriate remarks on this topic - see [15].

initial work on "World Dynamics" has fostered a significantly large effort in the formulation of assumptions regarding mechanisms of interaction between the different sectors of our society and its habitat. It seems that a clear need exists for more scientists to be trained in the tradition of exact investigations as well as in at least one of the softer disciplines such as the social and environmental sciences. It is also clear that the development of mathematical models and computer simulations of the large and soft systems which are today mankind's concern is in the process of fostering the growth of interdisciplinary schools, in which scientists of different training learn to work together and, maybe more importantly, learn to appreciate the opinion and kind of knowledge of those on the other side of the proverbial fence between the exact and, by inference, the not so exact sciences.

For all its good and all its bad, computer simulation is well past its infancy. As happens with all "tool" disciplines, many of those doing computer simulation who used to identify themselves with computer or simulation Technical Societies identify themselves today with the "end product" disciplines for which computers and simulation are a means to an end, rather than an end in itself. What this brings about is that the most successful and productive aspects of computer simulation have lost their visibility within scientific societies like ours, devoted to the mathematics and computers for simulation rather than in the outcome of simulation studies.

The same dilemma was faced many years ago within mathematics. There seems to have been little question at first that many branches of mathematics were meant to be applied. Differential calculus has been closely associated with the development of mathematical physics, and, much nearer to us, numerical analysis, considered as a branch of mathematics, was defined as the theoretical study of algorithms that were intended to solve real-life problems. But many aspects of applied mathematics and numerical analysis have gravitated toward engineering, physics and other "end use" disciplines, often leaving applied mathematicians and numerical analysts with pursuits which have become more "pure" (i.e. less applicable or applied) than they would like to admit.

The evolution of scientific disciplines is a dynamic process with its own laws, as has been well described by Kuhn [9]. If there were a need to find another example of a dynamic process which is well identified, yet not conducive to modeling and computer simulation, this would be a perfect one.

It is appropriate at this point to attempt to formulate recommendations for the fostering of beneficial aspects of computer simulation, while guarding against the accidents related to a too rapid and uncontrolled growth:

The purely technical aspects of the development of tools follows its own course. Computer hardware, software and algorithmic techniques for solving specific classes of mathematically well defined problems useful to simulation come with a steady stream of innovations which are reported through the classical channels of periodicals and conference proceedings. It would perhaps be well to remind those in charge of the editorial process that we are in the midst of changing values. There is a growing need for authoritative tutorial papers, establishing order in this somewhat voluminous literature, relating to few fundamental principles what appears at first as a multitude of uncorrelated items. Potential benefits of such summarizations are evident.

A large number of computer simulation studies in the classically "hard" sciences associated with industry go unreported: they have reached the status of "standard practice", and fulfill their important role in this modern world. Other than to the end users, their visibility has become apparent primarily to manufacturers who produce the computer hardware and supplies associated with that activity.

It is mostly in the "soft" sciences that caution and corrective action are needed. The responsibility for attempting to guard against the kind of bad scientific work which I have mentioned earlier rests with the traditional scientific establishment: professional societies and Universities. (Some of the remarks by Crosbie in [17] are relevant to this.)

The standards of quality and integrity in scientific work are universal, and their absence easily detected. The recent appearance in the professional literature of a growing number of papers pointing at the weakness of ill-based computer simulation studies attests to the fact that many are aware of the problem. That this awareness will result in a gradual improvement of the situation is hopefully what will take place.

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