# The Triad of Theory, Experiment, and Prediction

Bill Buzbee
Scientific Computing Division
National Center for Atmospheric Research
P. O. Box 3000
Boulder, CO 80307

## Abstract

The widespread use of computers is testimony to their importance and has led to philosophical discourses on such concepts as "the information society" and "the cognitive revolution." Some have gone so far as to suggest that the invention of the computer rivals the invention of the wheel. Actually, computers always occur as a part of a larger "system," (so do wheels), and it is these systems that have important philosophical implications. So our goal in this paper is to reflect on the context in which supercomputers are used. In particular, we will generalize the role of supercomputers in science and associated values, discuss the importance of human productivity in the use of supercomputers, and briefly note some of the benefits of integrating supercomputers into national networks.

## Experiment, Theory, and Prediction

Since the time of Bacon (Francis Bacon, 1561-1626), the scientific method has consisted of experiment, theory, and prediction. Experiment involves making careful observations and quantitative analysis of them. Theory involves the discovery/hypothesis of regularities in nature and the development of mathematical descriptions thereof. Prediction involves the application of theory to specific phenomena for development of mathematical models that can be used to predict/understand associated behaviors.

Historically, science has been classified as either experimental or theoretical, so the reader may rightly question the inclusion, or elevation, of prediction to a position of equality with experiment and theory. But philosophers of science have long recognized the role of prediction. For example, Morgenbesser [1] describes science as aiming "at explanation and prediction." Bohm [2] states, "Understanding is now valued as the means to predict, control, and manipulate things. Of course, beginning with Francis Bacon, this has always been important but never so dominant as today." Kuhn [3] describes a developed scientific field as possessing "a body of consistent theory capable of producing refined predictions..." So prediction is a fundamental component of science.

Prediction is generally made possible by the availability of a system of mathematical equations that have time as one of their independent variables and that approximately describes the phenomena under study. If suitable initial conditions can be determined and if the equations can be solved with respect to time, then one has a predictive capability. In modern parlance, the system of equations is called a "mathematical model." Of course, development of such equations is an exercise in theory and experimental measurement of associated physical parameters is often prequisite to solving them. The term "modeling" usually encompasses both the development of the mathematical system and the process of solving it.

On a singularly philosophical note, the efficacy of mathematics in accurately describing nature is truly amazing. In fact, Wigner [4] and Hamming [5] have written treatises on the "unreasonable effectiveness of mathematics." The astronomer Sir James Jeans proposed that God was a mathematician [6]! At any rate, it is fortuitous, perhaps even marvelous, that mankind can develop mathematical systems that describe nature. But solving those systems can be equally challenging and wondrous.

Prior to the advent of computers, modeling was generally limited by human ingenuity in obtaining analytic solutions to the associated mathematical equations--and such is generally impossible. Computers made feasible numerical simulation of models and such is often practical. Thus, computers were an enabling technology for modeling. As a result, today the terms "modeling" and "simulation" pervade the vocabulary of scientists and engineers, and the computer is an ubiquitous tool of them.

## The Role and Value of Supercomputers

By definition, supercomputers are the most powerful computer systems available where power encompasses both processing speed and memory size. Note that this definition is dynamic in time because supercomputers of the last decade are not today's supercomputers, and today's supercomputers will not be the most powerful systems available in the next decade. Although a broad range of computers is used in modeling, use of supercomputers can result in benefits such as treating complexity, reaching beyond experiment, overcoming the limitations of real time, cost-effectiveness, improved response time, and exploration of many design options.

The ability of a scientist to simulate a model is usually limited by the power of the available computer. Put another way, limited computing power may necessitate simplification of the model and thus, failure to obtain the correct result. Herein lies one of the great values of supercomputers--they make possible treatment of complexity in models that is otherwise intractable. In fact, a primary use of supercomputers is to solve problems that cannot be solved by any other class of computing equipment. For example, analysis of huge and/or complex structures is a flagship application of supercomputers within the aerospace, automotive, and petroleum industries. Often, the associated calculations can only be carried out through the use of supercomputers.

Some physical phenomena, such as the circulations in an atmosphere about a rotating globe, either cannot be produced or are difficult to experimentally produce. Computer simulation is often the only avenue for gaining an understanding in these cases, i.e., computer simulation enables us to reach beyond experiment. For example, the injection of greenhouse gases into our atmosphere has the potential to change our climate. Thus, we need a predictive capability whereby we can globally simulate the climate over several decades under various hypotheses about human activity. Such simulations are feasible provided sufficiently powerful computers are used to carry them out.

Many problems of interest take place within either a very short time interval, such as combustion wavefronts, or over a long period of time, such as production of a petroleum reservoir. Both situations can be a challenge if studied by experimental techniques. In the case of a short time period, it can be difficult to experimentally collect detailed information in space and time. In the case of long time periods, the solution may not be of interest by the time it is experimentally solved! One of the advantages of numerical simulation is that it allows us to overcome the constraints of real time. In either case, if sufficient computing power is available, one simply specifies and then anticipates the spacial and temporal resolution of desired results.

When applicable, computer modeling is almost always more cost-effective than traditional laboratory experimentation and prototyping. A good example is the crash analysis performed in the automobile industry. To be specific, it is faster and cheaper. As a result, modeling is rapidly displacing experimentation and prototyping in the practice of science and engineering. But a word of caution is required here. Models are an approximation to reality, whereas experiments usually reflect reality. Put another way, it is essential to validate models via experimentation, so "displacement" is too strong a term. Rather, computer modeling complements and supplements experimentation. The power of supercomputers contributes to cost-effectiveness through the reduction of the number of experiments.

In a competitive economy, the time required to develop and manufacture new products can be critical to market success. Product design is often a result of the exploration of some parameter space. The speed and thoroughness with which this exploration is done may be paced by the power of the computers used in numerical simulations. In those cases, the power of a supercomputer can be a tremendous asset. Even if design time is not a critical factor, the ability to explore many design options can lead to a superior result.

## Scientific Productivity

Historically, supercomputers have been relatively expensive devices and there were few of them. As a result, people went to considerable effort to optimize the use and performance of supercomputers and little concern was given to the economic value of the human capital. Since the advent of electronic computation, the absolute cost of supercomputers has only increased by a factor of two to three, whereas the people cost has skyrocketed. Thus, it no longer makes sense to ignore the cost of people. To illustrate this point, a modern supercomputer costs less than $10,000,000 per year--this is the total annual cost for debt service, operations, power, etc. Typically, there are at least 100 users of the machine and for many organizations, the annual cost of a scientist exceeds $100,000. Thus, the "cost of the users" exceeds the "annual system cost." As a result, management groups of user organizations are paying increasing attention to the productivity of scientists using supercomputers. This has led many organizations to implement time-sharing operating systems on supercomputers because user productivity is maximized. Friendliness and commonality in software is being stressed. Computer-aided software development tools are beginning to emerge. The objective is to keep the scientist focused on science versus waiting in long queues and wrestling with complex and indecipherable software systems.

## Supercomputers and National Networks

Many university scientists must provide their own computing resources from their research grants. As a result, many university researchers only have minicomputers and desktop systems locally available to them. The power of a supercomputer exceeds these machines by one to two orders of magnitude. A problem that requires an hour of supercomputer time is simply not doable using the local systems at many universities. An immense benefit of the national networks is to make supercomputers accessible to a large fraction of the nation's scientists. This greatly extends the range of their research as well as enhances their productivity. Equally as important is that networks make it possible for graduate students to gain experience with supercomputers. All too often we use our past experience to evaluate future possibilities. If students only have experience with a minicomputer or a desktop, they may restrict the scope of their research to problems that can be done on such machines. This practice would obviously be dangerous for our society. So, the combination of supercomputers and networks greatly extends the capability of university scientists and provides vital training for students throughout the nation.

## Synopsis

Computers are an enabling technology for modeling and, as a result, modeling/prediction is becoming recognized as the third arm of science equal in stature to experimental and theoretical science. Supercomputers greatly extend our modeling capabilities by enabling us to treat complexity, reach beyond experiment, and escape the shackles of real time. They also help manage time-critical developments and explore design parameters. The economic cost of scientists and engineers is leading many organizations to put priority on the efficient use of human capital rather than optimizing the performance of supercomputer systems. Finally, the combination of national networks and supercomputers is extending the range of research that university scientists can undertake. This combination is also providing graduate students with the important experience of using the most powerful systems available.

## References


1. S. Morgenbesser, The explanatory--predictive approach to science, B. Baumrin, Ed., *Philosophy of Science: The Delaware Seminar*, Vol. 1, 1961-62, Interscience Publishers, p. 41 (1963).

2. D. Bohm and F. D. Peat, *Science, Order, and Creativity*, Bantam Books, p. 11 (1987).

3. T. Kuhn, *The Essential Tension: Selected Studies in Scientific Tension and Change*, The University of Chicago Press, p. 47 (1977).

4. E. P. Wigner, The unreasonable effectiveness of mathematics in the natural sciences, *Comm. Pure Appl. Math.*, 13 Feb. (1960).

5. R. W. Hamming, The unreasonble effectiveness of mathematics, *Amer. Math. Monthly*, Vol. 87, No. 2, Feb. (1980).

6. J. Jeans, *The Mysterious Universe*, Cambridge University Press, (1930).