NASA TM-86822

NASA Technical Memorandum 86822

The Impact of Supercomputers on Experimentation: A View From a National Laboratory

Victor L. Peterson

August 1985

NASA

National Aeronautics and
Space Administration

NASA Technical Memorandum 86822

The Impact of Supercomputers on Experimentation: A View From a National Laboratory

Victor L. Peterson, Ames Research Center, Moffett Field, California

August 1985

NASA
National Aeronautics and
Space Administration

Ames Research Center
Moffett Field California 94035

N85-34510 #

THE IMPACT OF SUPERCOMPUTERS ON EXPERIMENTATION: A VIEW FROM A NATIONAL LABORATORY

VICTOR L. PETERSON and JAMES O. ARNOLD
NASA Ames Research Center
Moffett Field, California 94035

Abstract

The relative roles of large-scale scientific computers and physical experiments in several science and engineering disciplines are discussed. Increasing dependence on computers is shown to be motivated both by the rapid growth in computer speed and memory, which permits accurate numerical simulation of complex physical phenomena, and by the rapid reduction in the cost of performing a calculation, which makes computation an increasingly attractive complement to experimentation. Computer speed and memory requirements are presented for selected areas of such disciplines as fluid dynamics, aerodynamics, aerothermodynamics, chemistry, atmospheric sciences, astronomy, and astrophysics, together with some examples of the complementary nature of computation and experiment. Finally, the impact of the emerging role of computers in the technical disciplines is discussed in terms of both the requirements for experimentation and the attainment of previously inaccessible information on physical processes.

Introduction

Computers are playing an increasingly important role in the science and engineering disciplines. They are, in fact, revolutionizing not only the way research is conducted in nearly all fields, but also the way that scientific knowledge and wisdom are applied in the industrial environment, including the search for and recovery of natural resources, the design and manufacture of products, the development of pharmaceuticals, and the production of motion pictures. This revolution, still in its infancy, began about 20 years ago. It is gathering momentum with exponential growth, and it eventually could rival other great events in the course of the evolution of the civilized world. It is crucial for those involved in the pursuit of technical endeavors, including education, to understand how the computer revolution is enhancing the economic and technical value of human resources, and to take the necessary steps to stay at its leading edge. The consequences of ignoring this revolution are not acceptable for a country dedicated to commanding a leadership position in world affairs.

The principal objective of this paper is to provide a brief overview of how computers are beginning to affect the technical disciplines and to discuss how they are changing the requirements for associated physical experiments. This subject will be treated by examining some examples related to aerodynamics, aerothermodynamics, chemistry, atmospheric sciences, astronomy, and astrophysics.

Background

The computer revolution in science and engineering is intimately connected to the development of both computers and numerical methods. Therefore, it is appropriate to review past advances and to quantify future prospects. This review will be limited to top-of-the-line computing engines, commonly referred to as supercomputers. These are the machines that are pacing the development of the computational disciplines, although to be used effectively they must be augmented by appropriate peripheral devices such as front-end computers, terminals, graphics devices, long-term data storage facilities, and communications networks. It is also necessary to have skilled persons trained in the use of supercomputers. There is a shortage of such personnel, and there are only a few universities equipped with supercomputers to provide this training. This must be remedied soon if the growing demand for these specialists is to be met.

The increase in computer speed and cost is shown for some existing and planned machines in figure 1.[1] It is noteworthy that computer speed has grown about four orders of magnitude over a period of 30 years, whereas monthly rental cost has risen by approximately a factor of only 10 in actual-year dollars. In terms of the real value of money, the cost has actually decreased substantially. The exponential growth in computer speed is expected to continue for some time as a result of advances in very-large-scale electronics integration and computer architecture technologies. The increase of computer memory, which is shown in figure 2, has been only about half as large as that for computer speed.[1] The rate of growth is

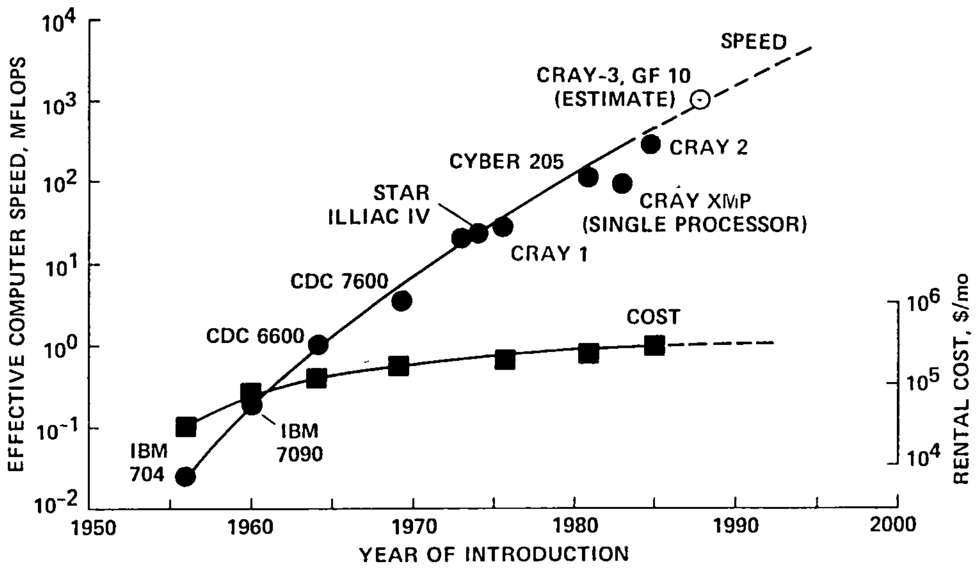

Figure 1.- Increase with time of computer speed and cost.

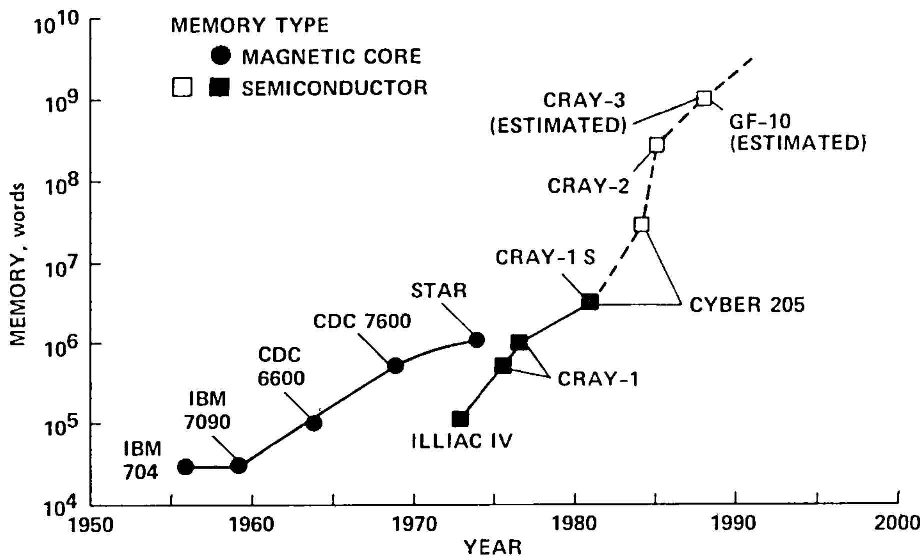

Figure 2 - Increase with time of computer main memory.

expected to be high in the foreseeable future, however. In fact, a Cray-2 computer with a main memory of 256 million 64-bit words is expected to be delivered to the NASA Ames Research Center in the fall of 1985. This capability represents a factor of 8 increase over the 32-million-word Cyber 205 just now being made available. It is almost certain that memory sizes as large as one billion words will be available before 1990.

Improvements in computer performance have been closely paralleled by improvements in numerical methods over the past 20 years. This is illustrated by the data presented in figure 3, which show how the cost of performing a computation has been driven down by the advances that are being made in computers and in numerical methods.[2] In this case, the methods refer to those used to solve two approximating forms of the Navier-Stokes equations governing perfect-gas fluid dynamics, but the results are indicative of methods used for equations governing many other disciplines. Further improvement (several orders of magnitude) in algorithms for solving the Navier-Stokes equations appears to be possible at

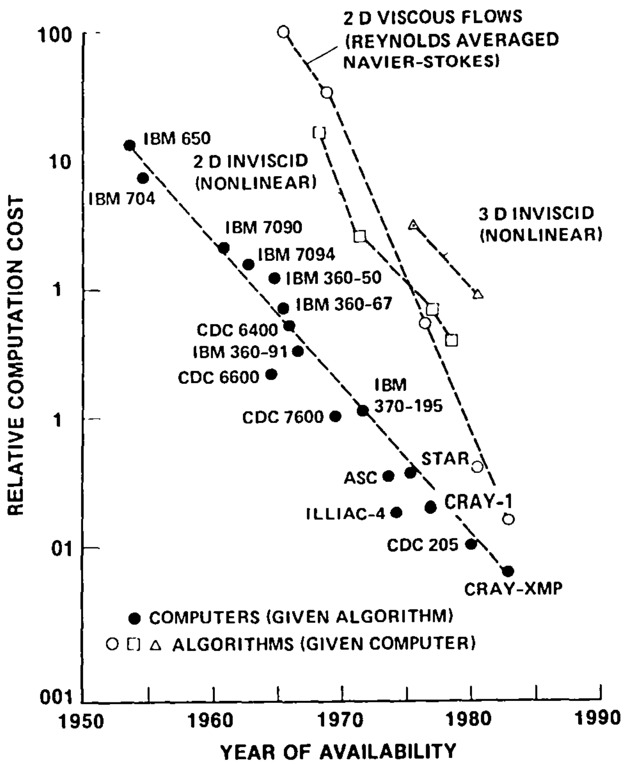

Figure 3.- Comparison of numerical simulatuion cost trend resulting from improvements in algorithms for different forms of the fluid dynamics equations with that owing to improvements in computers.

this time. Results of these improvements in computer and algorithm performance compound to provide a 10^5 reduction, over a 15-year period, in the cost of performing a computation with a given computer code.

Theory and experiment have been used by scientists and engineers in a complementary fashion for many years. In some cases, the physical observation comes first, in other cases, the situation is reversed. Prior to the development of digital computers, however, the role played by theory was hampered by the inability to solve the governing equations for many phenomena. The relative roles of theory and experiment began to change after the introduction of the electronic digital computer. The exact time when these changes begin to occur in a particular discipline is directly related to the complexity of the physics involved and the level of computer power required to solve the governing equations in a reasonable amount of computing time commensurate with the importance of obtaining answers. Thus, different disciplines have different thresholds in terms of computer requirements.

One of the first disciplines to lend itself to practical treatment by the digital computer was the prediction of cannon-shell trajectories. In fact, the ENIAC computer was developed during World War II to calculate ballistics firing tables. Today, problems involving flight mechanics and orbital dynamics are solved routinely without the use of validating experiments. Machines developed in the early 1960s, such as the CDC 6600, were powerful enough to enable research and development of nuclear devices to continue effectively despite the nuclear test-ban treaties. The design of aircraft structures is now done largely using computers, with only minimal proof-testing of the finished product. By 1970 computers were powerful enough to begin tackling nonlinear forms of the equations governing fluid dynamics for simple flow geometries. A little more than 10 years later there were examples of significant geometric design modifications, based solely on computation, being installed on aircraft and committed to flight without the benefit of validating experiments. These are but a few examples of how computers can be adapted for use by various disciplines when they become powerful enough to treat the underlying physical principles with a high degree of precision.

Both technical and economic factors motivate the increasing use of computers in the technical disciplines. While experimental apparatus and advanced instrumentation enhance the ability to observe, computers enhance the ability to reason. Phenomena governed by the laws of physics can be expressed in mathematical form, and computers can be used to solve the resulting equations with a degree of exactness not otherwise possible. In many cases, computers enable researchers to study phenomena that are difficult, if not impossible, to study experimentally. Computers can assist engineers and scientists in meeting increasingly complex demands placed on industrial design and engineering. These demands arise from the need to be competitive on a global scale. There is very little tolerance for design errors despite conflicting requirements of low cost, high quality, energy efficiency, and environmental compatibility. In addition, computers enable industrial product developments to evolve more rapidly to assure economic market success. One by one, the country's major industries are acquiring supercomputers. This expanding market should help control the future costs of large-scale machines.

Unlike many experimental test facilities and instrumentation acquired through discrete purchases and then used for many years without major change, computational equipment requires frequent and continual upgrading to remain current. Supercomputer performance has been increasing by a factor of 10 about every 7 years. Thus, the mainframes should be replaced long before their components are no longer serviceable (typically 15 years). Peripheral devices are also changing rapidly. For example, over a 20-year period, the method of inputting data into the computer has changed from reading punched cards at the site of the computer, to reading punched cards fed in through remote job-entry stations, to the use of "dumb" terminals on the user's desk, to the use of intelligent work stations in the user's office. Likewise, the method of providing computer output has changed from tabular listings, to centralized plotting, to remote plotting, to distributed color graphics devices. Therefore, a modern computing environment requires an annual budget considerably larger than that required to maintain and operate existing equipment, and it requires a careful and continuous planning process to stay abreast of the rapidly changing technology.

The availability of large computers is also affecting the cost of performing experiments. On one hand, the cost is going down because preliminary work done on the computer can be used to guide the conduct of experiments and often eliminates the need to perform measurements for numerous values of the variables. The computer, in effect, provides a great deal of insight into what to expect from the experiment before it is conducted, and it provides a means for interpolating between widely spaced values of the parameters. On the other hand, the cost is going up because computer-generated information provides much more detail concerning the underlying physics than can be obtained from more analytical examination, and thus inspires new experimental requirements. The experimentalist is being forced to conduct more sophisticated experiments that require the development of improved, but costly, test techniques Eventually, the costs associated with experiments in selected fields can be driven down, if not eliminated, as computers become sufficiently powerful to treat situations without appreciable approximation.

Impact of Computers on Selected Disciplines

The degree to which computers are affecting the scientific and engineering process exercised in the various disciplines depends, to a large extent, on the complexity of the underlying physics and the degree of exactness with which available computer power can be used to solve the governing equations. Since the amount of required computer power varies from discipline to discipline, each area of interest must be examined individually to determine the impact. The process involves making an estimate of the computer speed and memory required to solve the governing equations, comparing the requirements with computer capabilities, and then factoring in findings based on past experience. Computers are not yet large enough to treat all situations from first principles so the ability to simplify with models or approximations plays a strong role in most disciplines. Results of applying this process to several disciplines are discussed in this section.

Fluid Dynamics

The Navier-Stokes equations govern the motion of viscous fluids over a broad range of continuum-flow situations, including those of interest in aircraft design. It is not possible to obtain closed-form solutions to these equations for practical engineering problems. However, various degrees of approximation have been worked out over the years to obtain useful results.

Four major levels of approximation to the full equations have been identified.[3] Each level of approximation resolves the underlying physics to a different degree, provides a different level of understanding, and requires a different level of computer capability. These approximations, their capabilities in resolving problems associated with aircraft aerodynamics, and the computer requirements to solve them in a reasonable amount of time (about 15 min) are summarized in table 1 and discussed in some depth in the literature.[2,3] Computer requirements are expressed in terms of the power of a Class VI machine which is defined here to have a processing speed of 30 million floating-point operations per second (MFLOPs) and a main memory of about 8 million words. Computer requirements increase with each higher level of approximation, both because more flow variables are involved and because more panels or grid points are required to resolve the flows to a level of detail that is commensurate with the physics embodied in the approximation. Experience indicates that the Reynolds-averaged form of the Navier-Stokes equations probably will be adequate for most design-oriented problems. The effects of all scales of turbulence are modeled in this level of approximation. The development of these turbulence models is the subject of extensive current research by both computational and experimental fluid dynamicists. In fact, the experimentalists are being guided, to a large extent, by computational research programs which are based either on the application of the large-eddy simulation approximation or on the use of the full Navier-Stokes equations for simple flow geometries. Information presented in table 1 shows that computers having one-tenth the power of a Class VI machine are required to begin to make inroads on the computational treatment of aircraft design problems. Machines of this class, such as the CDC 7600, became available in the late 1960s, but it was not until the mid-1970s that they were generally accessible by the aerodynamicists. Now, of course, Class VI machines, such as the Cray-1 and the Cyber 205, are widely available.

Table 1.- Major levels of approximation to the Navier-Stokes equations with results provided, and computer requirements to obtain solutions in 15 min of computation time.

APPROXIMATION	CAPABILITY	GRID POINTS REQUIRED	COMPUTER REQUIREMENT
LINEARIZED INVISCID	SUBSONIC/SUPERSONIC PRESSURE LOADS VORTEX DRAG	3×10^3 PANELS	1/10 CLASS VI
NONLINEAR INVISCID	ABOVE PLUS TRANSONIC PRESSURE LOADS WAVE DRAG	10^5	CLASS VI
REYNOLDS AVERAGED NAVIER STOKES	ABOVE PLUS SEPARATION/REATTACHMENT STALL/BUFFET/FLUTTER TOTAL DRAG	10^7	30 × CLASS VI
LARGE EDDY SIMULATION	ABOVE PLUS TURBULENCE STRUCTURE AERODYNAMIC NOISE	10^9	3000 × CLASS VI
FULL NAVIER STOKES	ABOVE PLUS LAMINAR/TURBULENT TRANSITION TURBULENCE DISSIPATION	10^{12} TO 10^{15}	3 MILLION TO 3 BILLION CLASS VI

Speed and memory requirements for computational aerodynamics are compared with several existing and planned computers in figure 4. Computers large enough to provide solutions to the Reynolds-averaged Navier-Stokes equations for the flow about a complete aircraft are expected to be available before the end of this decade. That should mark the time when computers will not be just a supplement to the aircraft design process, but they will be an absolute necessity for a country to remain competitive in meeting economic and performance requirements.

An expert group of computational fluid dynamicists, computer and wind-tunnel technologists, and airframe and engine designers were brought together by the National Research Council to assess the impact of computations on the traditional role of ground test facilities over the next 15 years (1983-1998). They concluded that, over the 15-year period considered, the capabilities of the computer as a tool for aircraft and engine design will increase substantially, the unit cost of computation will drop by three orders of magnitude, and the type of testing will change, but there will be no marked change in the requirement for using ground test facilities.[1] This latter conclusion stems from the finding that computation and experimentation play somewhat different roles and have different strengths and weaknesses. On the other hand, computations give considerably greater detail of a flow field than is possible in any wind tunnel. They provide a capability for configuration optimization and for determining the effect of configuration changes before commitment to model construction and testing is made. In addition, computations can provide an alternate source of information often needed to interpret experimental results or to extend them to conditions not obtainable in ground test facilities. On the other hand, ground test facilities provide a ready source of integrated flow information since forces and moments are directly obtained by wind-tunnel balance measurement. In summary, computations and experiments will be used in a complementary rather than competitive mode, and the end result will be products which will maintain the country's preeminence in civil and military aeronautical fields.

Aerothermodynamics

Aerothermodynamics is the extension of aerodynamics into very-high-speed flight regimes where there are significant thermal effects between gas and solid surfaces. As the motion of a vehicle increases to hypersonic speeds (Mach number greater than about 5), shock-heated molecules in the flow exhibit excitation into higher internal degrees of freedom (vibration, rotation, and electronic) and chemical reactions begin to occur. This gives rise to the onset of convective heating and eventually to dissociation of the gas molecules surrounding the vehicle. Additional gas species such as NO, N, and O are formed if the vehicle is flying in air. At even higher speeds, ionization begins causing the appearance of N^+, O^+, and N_2^+. In many instances, the gases will become sufficiently hot to radiate at intensity

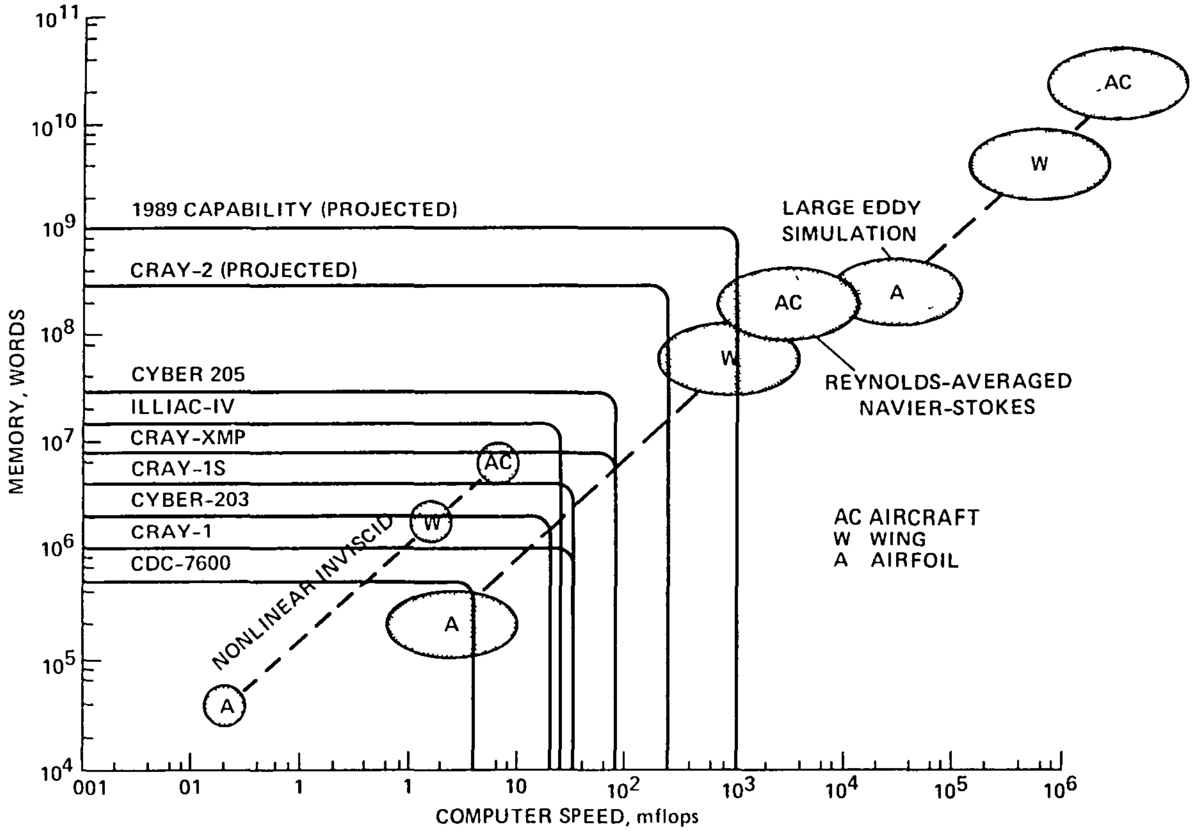

Figure 4.- Computer speed and memory requirements for aerodynamic calculations compared with the capabilities of various machines; 15-min runs with 1985 algorithms.

levels giving rise to the requirement to provide thermal protection against both radiative and convective heating to assure vehicle survival. The gas is generally in thermochemical equilibrium for flight at altitudes below about 40 km in the Earth's atmosphere, but at higher altitudes, the physics are further complicated by having to treat the flow chemistry with finite rates of reactions. All of these real-gas effects must be taken into account to accurately obtain pressures, forces, and heat loads experienced by a vehicle flying at these hypervelocities. Computational treatment of flows involving aerothermodynamic phenomena places greater demands on computer speed and memory than for the treatment of aerodynamics under perfect-gas assumptions because of the need for a more detailed description of the equation of state. These demands are offset, to some extent, by the fact that vehicles designed to fly at hypervelocities generally have simpler geometries than conventional aircraft so that fewer grid points are required to discretize the computational domain.

The impact that modern computers will have on the field of aerothermodynamics can be illustrated by considering the approach contemplated for the design of the next-generation Space Shuttle and comparing it to that used for the existing Shuttle, which was developed in the 1970s. During that decade, the computational approach was in its infancy and computers were not powerful enough to treat the complete vehicle, even with codes based on perfect-gas assumptions. The Shuttle was designed by testing many competing configurations in ground test facilities such as wind tunnels and arc-heated plasma jets. This testing program extended over a period of more than 10 years and it required over 50,000 hours of time in wind tunnels alone. Clearly, this was a highly successful program, but the approach was expensive in terms of time and added weight required to protect against uncertainties caused by not being able to precisely simulate all of the physical phenomena in the ground test facilities. It is likely that the design of the next-generation Shuttle will begin with the calculation of the performance characteristics of many possible configurations using codes based on ideal-gas assumptions. This will guide the selection of vehicle shapes that satify low-speed performance requirements while showing the promise of meeting high-speed requirements. At this point parallel experiments and computations will begin to investigate likely areas of concern related to real-gas effects. Once the real-gas codes are validated by comparison with measurements made at conditions that can be obtained in ground test facilities, they can be used with some degree of confidence to further narrow the number of candidate configurations prior to exhaustive, time-consuming testing. Thus, the burden of "cut and try" optimization will be assigned to the computer and the results will be checked by measurement for those portions of the flight envelope accessible by ground test facilities.

Computer speed and memory requirements for treating real-gas flows about simple shapes typical of planetary probes, ballistic missiles, and orbital transfer vehicles, which will use aerobraking in the Earth's upper atmosphere to replace rocket-motor-assisted maneuvering, are shown in figure 5. Estimates are shown for increasing levels of physical complexity ranging from laminar-flow, ideal-gas considerations to the treatment of chemical and thermochemical nonequilibrium effects with radiation and turbulence physics included The results are based upon using 1985 algorithms, the Reynolds-averaged form of the Navier-Stokes equations, and 15-min solution times.

Aeroassisted orbital transfer vehicles (AOTVs) will fly in a regime in which all of the physical complexities except turbulence are expected to be prominent. The results in figure 5 imply that about 40 hours of CPU time will be required to calculate the flow about this class of vehicle using machines having a speed of 1000 MFLOPs and a memory of 256 million words. This is not considered to be an excessive amount of computing time to provide information vital to the design of an optimized vehicle, but not readily accessible through ground test.

Chemistry

Properties of matter can be calculated by solving the Schrodinger equation, which is the fundamental equation of quantum theory. Interaction energies between species and most physical properties of interest can be calculated for systems composed of as many as 100 atoms using current algorithms and computers. With these

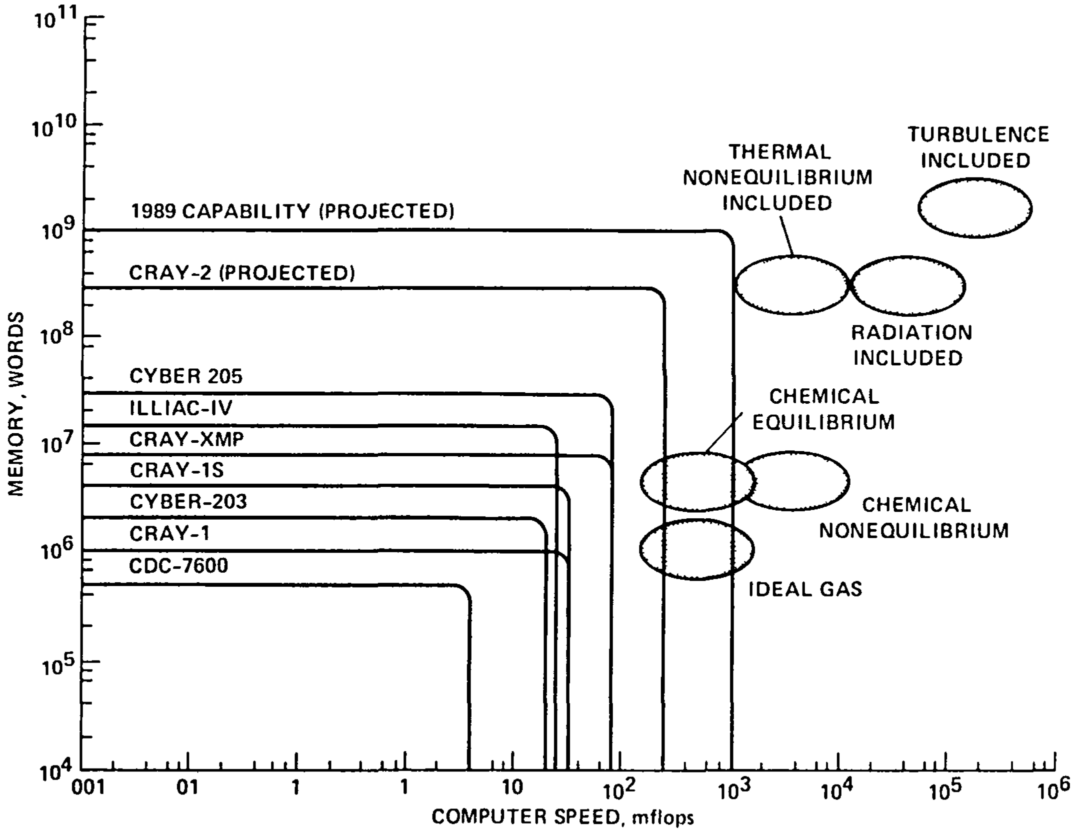

Figure 5.- Computer speed and memory requirements for aerothermodynamic calculations pertaining to planetary probes, ballistic missiles, and orbital transfer vehicles compared with the capabilities of various machines; 15-min runs with 1985 algorithms.

interaction energies, classical and semiclassical mechanics are used to compute collisional properties, including rates of chemical reactions. This field of research is known as computational chemistry, and its applications are as broad as those of chemistry itself. The discussion herein will be limited to problems dealing with atmosphere-entry physics and aerospace materials.

The solution of Schrodinger's equation is usually obtained by a basis-set expansion. Molecular orbitals for the system of interest are written in terms of a set of atomic basis functions, and the expansion coefficients are obtained by minimization of the total electronic energy for the molecule or atomic cluster; the larger the basis set, the more accurate the results. When the energy minimization is accomplished with the total number of electrons in the system assigned in only one way to the molecular orbitals, the result is known as a self-consistent field (SCF) solution. For some systems and some properties, these results are sufficient, as will be discussed later. SCF solutions usually give information on only the lowest or ground electronic state of a system, but this information often is all that is of interest. The SCF solution does not account for the fact that electrons tend to avoid each other in their motions about the nuclei of the molecule. To account for this, the electrons are allowed to occupy the molecular orbitals in many different ways following quantum mechanical rules. This approach is called configuration interaction (CI), and the resulting electronic energies and wavefunctions from whence many properties of isolated systems are derived often are as accurate as those from high-quality laboratory experiments. In general, properties of excited electronic states require the use of the CI approach and this can be computationally expensive.

Atomistic simulation of material properties utilizes the interaction energies obtained either from the quantum chemical solutions or those deduced from measurements. For the former case, quantum calculations are first conducted on an atomic cluster such as 50 or more metal atoms with and without the presence of gaseous impurity species. Effective interatomic forces accounting for two- and three-body interactions are deduced from the potential energy surfaces for the small cluster. These forces are then used as inputs for classical-dynamical-theory calculations for gas-material interactions by considering an ensemble of 10,000 atoms at a point of interest in the material with external (macroscopic) forces connected to the discrete atoms via a set of finite elements.

Computational chemistry currently is being used to provide information required for the calculation of the aerothermodynamic behavior of the AOTVs. For example, the electronic transition probabilities for N_2^+, which contribute importantly to the radiative emission from the hot air, and the rates for the $N^+ + N \rightarrow N + N^+$ charge-transfer reaction, which is an important convective heat-transfer mechanism for nonequilibrium airflows, are being provided by computation. Results based on CI studies are being obtained with reliability levels comparable to high-quality measurements. In addition, emission spectra for the various other radiating species in the flow are being calculated and provided as input to the flow-field codes to predict emission, absorption, and radiative heating. Finally, chemical reaction rates are being computed from first principles by using interaction energies or potential energy surfaces resulting from the solution of the Schrodinger equation at all possible values of the interatomic coordinates. This process involves the simulation of reactive trajectories by solving Hamilton's equations of motion. Many solutions, corresponding to different Boltzman distributions over initial vibrational states (vibrational temperatures) and approach conditions (translational temperatures), are simulated, giving rise to computed reaction cross sections. By averaging these cross sections over the appropriate vibrational distribution, effective rates of reactions can be determined. For endothermic reactions, this can lead to more than an order of magnitude difference in the rate constant, depending upon the degree to which the vibrational temperature is out of equilibrium with the translational temperature (e g., translational temperature of 10,000 K and vibrational temperature of 4000 K).

Another application of computational chemistry is related to the development of new advanced polymers. Many physical properties of polymers depend upon their segmental motions, such as rotations of CH_3 groups about chemical bonds. For example, glass transition and toughness of structural polymers can be understood in terms of such changes on the molecular level. Experiments have revealed a wealth of information on these motions, but the interpretation of the data is often very difficult. An example of how computations can assist with this interpretation involves a recently conducted study of polymethylmethacrylate PMMA, the clear material commonly used for aircraft windows. Torsional potentials for appropriate rotations were computed using a modest basis-set expansion and SCF wavefunctions. The calculated torsional barriers to rotation fell in three ranges and agreed in absolute value with previous measurements. However, assignment of the barrier heights to internal motions deduced by the experimentalists was found to be incorrect. Guidance provided by the calculations permitted appropriate corrections to be made for interpretation of the measurements. This example illustrates the value of a combined experimental and computational approach in the program to develop advanced polymeric materials.

The computational work is having a profound effect on the approach being taken by surface-physics experimentalists. Once it became clear that the computations would be capable of providing detailed and reliable information on the physiochemical properties of small atomic clusters, experimentalists set the goal of measuring these data for very small clusters supported on "inert" substrates. This has recently been accomplished at Ames, and measurements have been made on clusters with as few as six atoms. In other laboratories, clusters of two, three, and more heavy atoms have been seen in free jets and trapped in rare-gas matrices. Thus, the people who are conducting the experiments and those who are using computers are now working on the same "turf" in the field of small particles, and many beneficial results in interpretation have already passed between them. It is expected that these exchanges will increase with time and result in many more unforeseen benefits.

Examples of computer speed and memory requirements for three areas of computational chemistry are shown in figure 6. The first area relates to the gas-phase molecular properties required for nonthermochemical equilibrium aerothermodynamic studies of AOTVs. Radiative properties of molecules such as diatomic nitrogen, for a single molecular geometry, can be calculated on existing computers in less than 15 minutes, although about 50 such calculations are required to provide all of the necessary information. Intermolecular potential surfaces for two diatomic nitrogen molecules, in both ground or electronically excited states, require either substantially larger computers or longer runs since each point on a potential surface requires more than 15 minutes of computing time on today's computers and several hundred points are required to define a surface. Nevertheless, the cost of this amount of computer time is still less than that for measuring required rates of chemical reaction for the four-atom complex in the ground and excited states. Requirements for polymer research are illustrated by the data for vibrational and torsional potentials for polymethylmethacrylate PMMA in the monomer, dimer, trimer, and three-cluster trimer form. Again, these calculations are very lengthy on today's computers, but information is

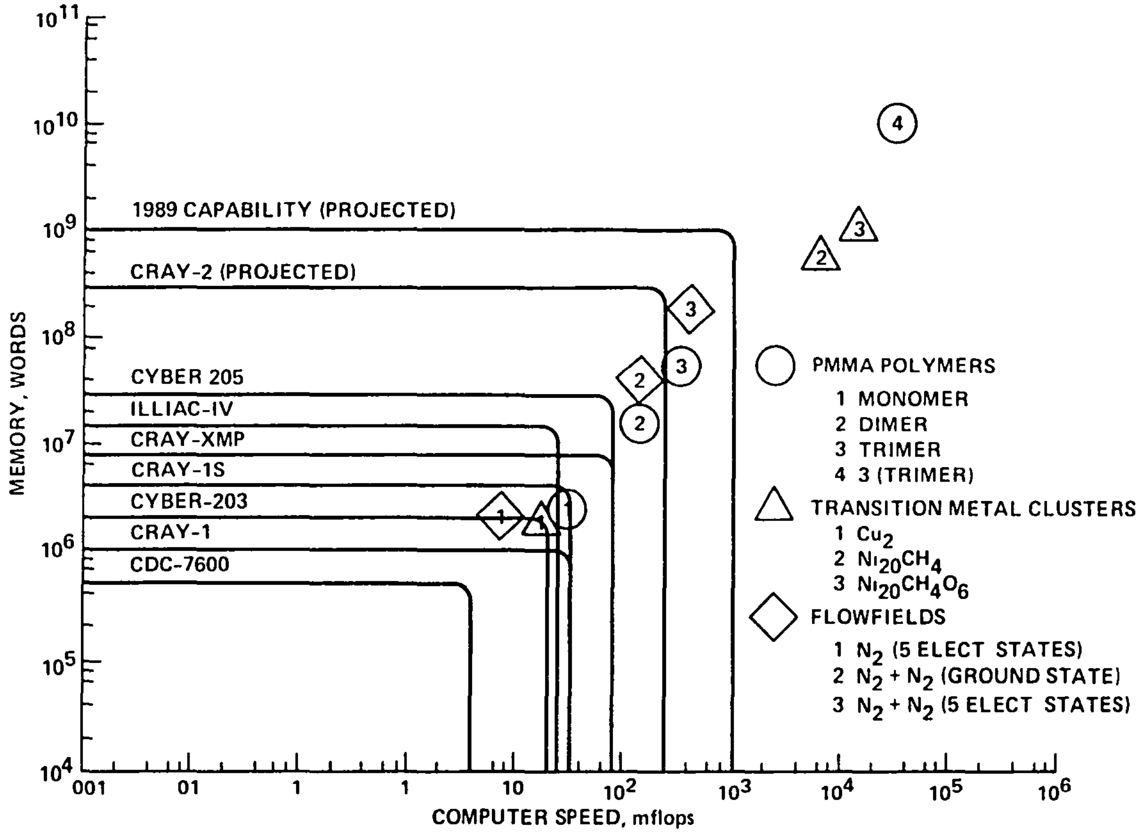

Figure 6.- Computer speed and memory requirements for three areas of computational chemistry compared with the capabilities of various machines; 15-min runs with 1985 algorithms.

provided that cannot be obtained from experiment. Finally, some estimates of computer speed and memory requirements are shown for work on small clusters of metal atoms with focus on developing an understanding of how metals interact with gases. The data for Ni_{20}, with an without gaseous molecules present, correspond to one of several hundred calculations needed to predict the physiochemical properties of small clusters of atoms supported on substrates. Information of this type is pertinent to the understanding of catalysis. It is clear from the results presented in figure 6 that computers much more powerful than those available now will be required to satisfy the future needs of the computational chemist, although considerable information of great value can be obtained economically with existing machines.

As an example of the cost effectiveness of computations in this field, consider the determination of an important electronic transition moment for the C_2 molecule. A summary of 12 different laboratory measurements made prior to 1975 showed that values reported for this transition moment differed by a factor of about 6.[4] The cost of obtaining these measured data is conservatively estimated to be about $600,000. This estimate assumes that each of the 12 experiments cost $50,000 to perform. Today, one computational chemist, spending 3 months and using about 5 hours of time on a Cray-XMP computer ($10,000), can obtain all of the transition moments between the eight lowest states of the C_2 molecule, to within ±15%, and values for the bond-dissociation energy accurate to within 0.1 eV. Fifteen years ago there was no alternative to using shock tubes or similar experimental devices to obtain data of this type; now, the computer is a cost-effective substitute

Atmospheric Sciences

Scientific studies of planetary atmospheres are becoming heavily dependent on the use of large-scale computers for performing complex data analyses, archiving large data sets, and acting to model the physical behavior of the atmospheres over time Models of the atmosphere provide a framework to organize knowledge, define and interpret measurements, predict both short- and long-term weather and climate, and predict environmental impacts resulting from numerous natural and human-induced perturbations. Equations governing the physical phenomena in planetary atmospheres are similar to those describing the fluid dynamics of flows about aircraft, but they must also include the effects of multiphase systems (gas/liquid), radiative transfer, and in some cases, chemical reactions.

Computers are not yet large enough to resolve all of the time-dependent physical processes occurring globally within a planetary atmosphere without the use of approximations and empirically derived information. Therefore, there is a strong interplay between computation and measurement. For example, models of stratospheric aerosol physics and chemistry have been used to guide the selection of instruments and to define critical measurements. Once measurements are made, the models are tested against these data to identify areas of data and model deficiencies. After deficiencies are corrected, the models can be used to predict the consequences of phenomena which are not directly observed, such as those resulting from clouds from volcanic eruptions or meteor impacts in the distant past. Another example involves the use of radiative transfer codes to interpret and extend measurements of the light fields in the atmosphere. Measured light values can be reduced to cloud temperatures and radiative heating rates can be related to atmosphere absorber concentrations.

Examples of computer speed and memory requirements for several selected areas of computational atmospheric sciences research are shown in figure 7. Current supercomputers are adequate for treating three-dimensional localized climate and limited-domain atmospheric models. Much larger machines still are required to extend climate modeling to include complex chemistry, increased range, and greater resolution, and to perform short-term, high-resolution, three-dimensional atmospheric simulations with exchange processes occurring between the stratosphere and troposphere. However, the threshold of required computer power clearly has been crossed for disciplines in the atmospheric sciences.

Astronomy and Astrophysics

Many important insights in modern astronomy have been obtained through large-scale computation. Astronomical phenomena typically combine complex interplays of several physical processes with strong nonlinear effects. Hostile or unattainable environments preclude laboratory studies, and many processes take millions of years to complete. Computation provides a major hope for sorting out and understanding such interacting processes.

The complexities of astronomical phenomena combine with greatly improved observational data to broaden the scope of problems that demand attention and to sharpen the detail sought in interpreting observations. Along with significantly improved accuracy and greatly increased data rates on more traditional observations, qualitatively new kinds of data from space-based observatories and imaging detectors yield a flood of data and introduce new kinds of problems that can be interpreted or solved only with the aid of computers.

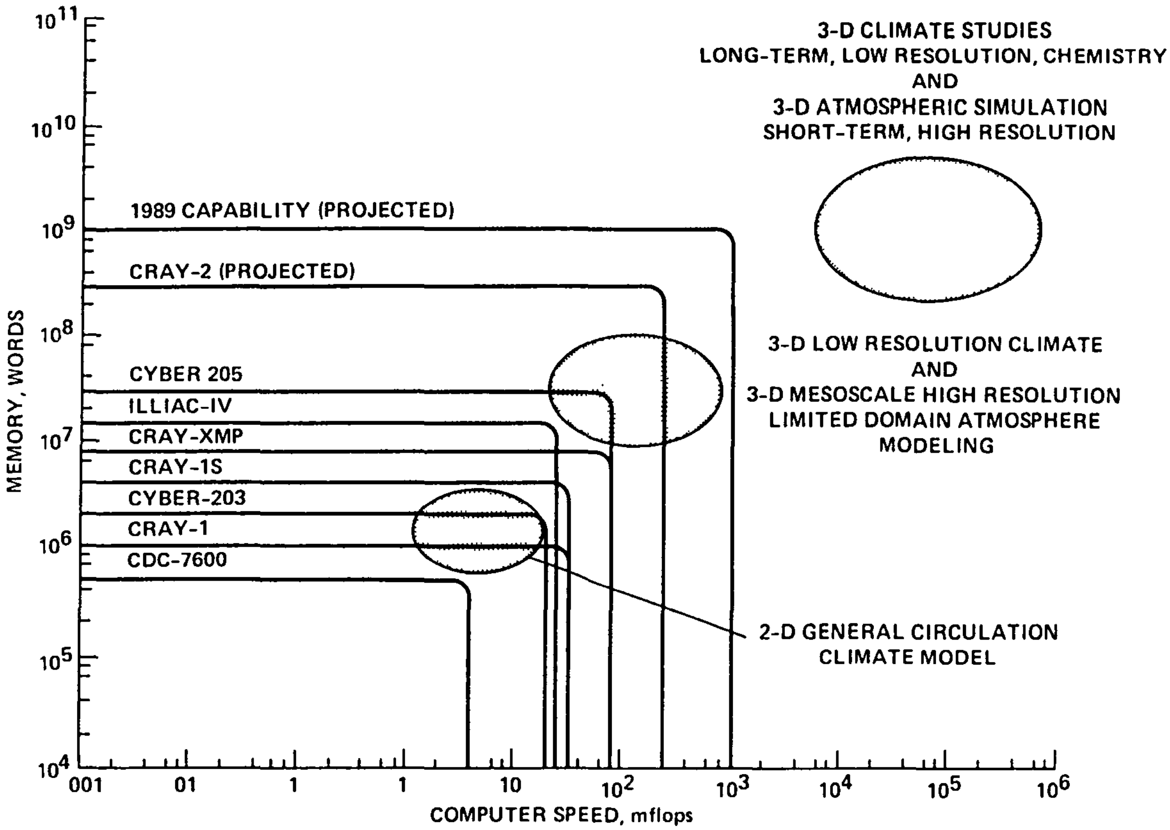

Figure 7.- Computer speed and memory requirements for selected areas of atmospheric sciences research compared with the capabilities of various machines; 15-min runs with 1985 algorithms.

Examples of the use of computers in astrophysics, involving galactic dynamics, are illustrative of current research. Dynamics of galaxies, in which galaxies with three-dimensional shapes that had traditionally been assumed were found to be dynamically unstable when treated by means of numerical experiments conducted with computers. These results led to the suggestion that spiral galaxies are embedded in massive dark "haloes" that are themselves stable and within which the galaxy would be stable. This suggestion stimulated numerous observational studies and now seems to be confirmed by observations of rotation fields in spiral galaxies. Dynamical flow fields in barred spiral galaxies and the shapes and dynamics of elliptical galaxies are other basic properties whose character has been learned from numerical experiments.

These examples illustrate how the computer can be used as an exploratory tool to uncover the dominant physics that govern observed astrophysical phenomena or, even more basically, to study qualitative properties or global stability. The thread of continuity that underlies these examples is the fact that reality is complicated and it cannot be simulated without including all of the relevant physics. Computers now permit increasingly detailed modeling which can result in wholly new understandings. This is a pattern that, through stellar studies, has been repeated over and over again in investigations ranging from the red giants to stellar pulsations, interstellar chemistry, protostellar collapse, and galactic dynamics. Other problems that require the largest and fastest available computers to treat are black hole dynamics, star formation, galactic chemical evolution, magnetic fields and plasmas, radio sources and jets, and supernovae.

Examples of computer speed and memory requirements for computational astronomy and astrophysics research are shown in figure 8. Machines of the CDC 7600 class made possible the solution of two-dimensional models of galactic dynamics and star formation. Current machines permit the move to three dimensions. Even larger machines will allow the simulation of galaxy formation with coupled hydrodynamics and stellar dynamics as well as star formation, including magnetic-field accretion disks and planet formation. It is clear that computers are becoming

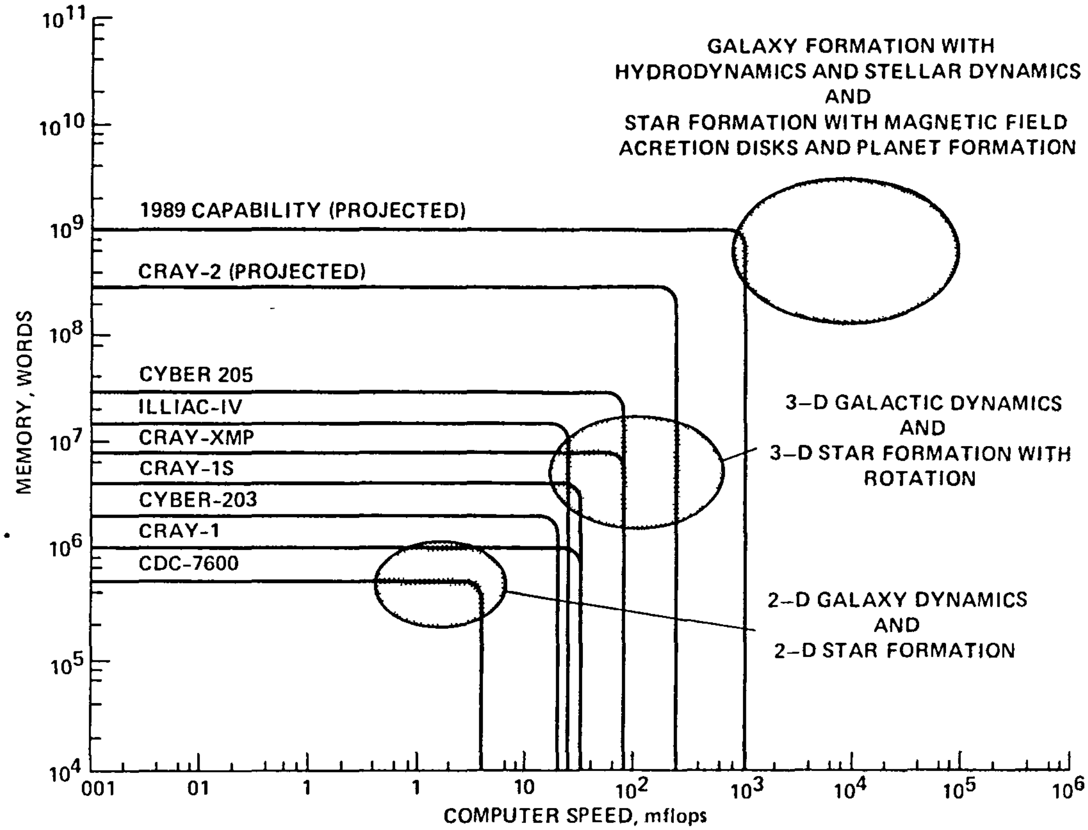

Figure 8.- Computer speed and memory requirements for computational astronomy and astrophysics research compared with the capabilities of various machines; 15-min runs with 1985 algorithms.

indispensable to research in astronomy and astrophysics, and that the need for physical experimentation to provide empirical models and validation will continue into the indefinite future.

Relative Roles of Computation and Experiment

It is clear from the examples presented that while computers are a relatively new tool for the scientist and engineer, they are already becoming indispensable to the research and development process Each of the technical disciplines has a different threshold in terms of the computer speed and memory required for computation to be an important factor, but these thresholds are now being crossed for a wide variety of research and product-development situations. Most of the disciplines still require substantially more computer power before they are fully satisfied; however, the prospects for obtaining this power at reasonable cost in the foreseeable future are very bright.

Experience is beginning to show how this new tool will influence experimentation. In some cases, computation is a cost-effective substitute. In other cases, computation can provide information not readily amenable to measurement. In the general case, however, computation complements experiment and computers are not likely to eliminate the need for experimentation, at least for many years to come. Working together, computation and experiment can provide a greater understanding of physical phenomena and more rapid advances than relying solely on one or the other.

The relative roles of computation and experiment are beginning to change. In earlier years, experiments were performed to establish the variables governing physical phenomena and their interrelationships, and computations were made after the fact either to validate computational methodology or to provide additional understanding of the experimental results. Now, computations are being used to establish these relationships beforehand, and experiments are being conducted either to validate the computations, to provide refinements, or to assist with the modeling of terms in the governing equations that are still too complex to solve from first principles. The development of experiments and the interpretation of results now is heavily dependent on computation Therefore, the experimentalist of the future should receive at least some training in computation to be able to either to perform the computations required to define a good experiment or to be in a position to communicate with others who might be responsible for the computations.

The need for persons trained in large-scale scientific computation in all of the disciplines is growing very rapidly. To satisfy this need, universities, research laboratories, and industrial organizations involved with product development need greater access to supercomputers and the peripheral equipment required to make them effective. This access cannot be provided at the expense of other laboratory equipment since there will be a continuing need for experimentation. In fact, the rapid improvements in computers and computational methodology are placing more stringent requirements on the experimentalists to measure more fundamental quantities with greater degrees of precision. This, in turn, is forcing the test facilities and their supporting instrumentation to become more dependent on computer technology as well. The move toward more dependence on computers is irreversible and ways must be found to adjust to this important revolution.

Conclusions

Computers are changing the approach to the conduct of research and development in many of the science and engineering disciplines. The rapid and continuing growth of their speed and memory enable them to be used to solve, with high degrees of precision, increasingly complete forms of first-principles governing equations. They are, in fact, becoming an attractive complement to, and in some cases a cost-effective substitute for experiment.

Differing complexities of the underlying physics in the various disciplines place different requirements on the power that a computer must have to solve the governing equations in a reasonable amount of time. Thus, each discipline has a threshold of computer power that must be exceeded before the computer becomes an effective tool in that discipline. Research and applications in the disciplines for which this threshold has been crossed, such as fluid dynamics, aerodynamics, aerothermodynamics, chemistry, atmospheric sciences, astronomy, and astrophysics, now are as dependent upon the computer as they are upon physical observation and testing. In fact, many of the experiments in these disciplines are defined by the computations.

The irreversible move toward more dependence on computers is placing new requirements on both human and financial resources. There is a growing need for people with formal training in the use of supercomputers. Universities, industrial corporations, and government laboratories must have increased access to these machines to meet this need. In addition, equipment must be upgraded frequently to remain current. The complementary rather than competitive nature of computation and experiment also means that experiments cannot be abandoned in favor of computation. Thus, laboratory equipment also must continually be supported and upgraded, at least for the foreseeable future.

Computers are an indispensable new tool for the scientist and engineer. This tool will continue to become more powerful with time as hardware, software, and people skilled in their use mature. The effective combination of computation and experiment will contribute greatly toward the maintenance of a competitive position in world affairs.

References

1. National Research Council: Influence of Computational Fluid Dynamics Upon Experimental Aerospace Facilities: A Fifteen Year Projection. National Academy Press, 1983.

2. Peterson, Victor L.: Impact of Computers on Aerodynamics Research and Development. IEEE Proc , vol 72, Jan. 1984.

3. Chapman, Dean R.: Computational Aerodynamics Development and Outlook AIAA Paper 79-0129, Jan. 1979

4. Cooper, D. M., and Nichols, R. W.: Measurements of the Electronic Transition Moments of C_2-Band Systems. JQSRT, vol. 15, Jan. 1975.

1 Report No	2 Government Accession No	3 Recipient's Catalog No
NASA TM 86822		

4 Title and Subtitle	5 Report Date
THE IMPACT OF SUPERCOMPUTERS ON EXPERIMENTATION: A VIEW FROM A NATIONAL LABORATORY	August 1985
	6 Performing Organization Code
7 Author(s)	8 Performing Organization Report No
Victor L. Peterson and James O. Arnold	85377
	10 Work Unit No
9 Performing Organization Name and Address	11 Contract or Grant No
Ames Research Center Moffett Field, CA 94035	
	13 Type of Report and Period Covered
12 Sponsoring Agency Name and Address	Technical Memorandum
National Aeronautics and Space Administration Washington, DC 20546	14 Sponsoring Agency Code 997-21-01

15 Supplementary Notes

Point of Contact: Victor L. Peterson, MS 200-4, Ames Research Center, Moffett Field, CA 94035, (415)694-5065 or FTS 464-5065

16 Abstract

The relative roles of large-scale scientific computers and physical experiments in several science and engineering disciplines are discussed. Increasing dependence on computers is shown to be motivated both by the rapid growth in computer speed and memory, which permits accurate numerical simulation of complex physical phenomena, and by the rapid reduction in the cost of performing a calculation, which makes computation an increasingly attractive complement to experimentation. Computer speed and memory requirements are presented for selected areas of such disciplines as fluid dynamics, aerodynamics, aerothermodynamics, chemistry, atmospheric sciences, astronomy, and astrophysics, together with some examples of the complementary nature of computation and experiment. Finally, the impact of the emerging role of computers in the technical disciplines is discussed in terms of both the requirements for experimentation and the attainment of previously inaccessible information on physical processes.

17 Key Words (Suggested by Author(s))	18 Distribution Statement
Computational physics Computer science Numerical aerodynamic simulation	Unlimited Subject Category - 59

19 Security Classif (of this report)	20 Security Classif (of this page)	21 No of Pages	22 Price*
Unclassified	Unclassified	16	A02

*For sale by the National Technical Information Service, Springfield, Virginia 22161

End of Document