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Edited by
S. Abarbanel
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Progress and Supercomputing in Computational Fluid Dynamics

Proceedings of U.S.-Israel Workshop, 1984

Earll M. Murman
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PREFACE

The present volume, with the exception of the introductory chapter, consists of papers delivered at the workshop entitled "The Impact of Supercomputers on the Next Decade of Computational Fluid Dynamics." The workshop, which took place in Jerusalem, Israel during the week of December 16, 1984, was initiated by the National Science Foundation of the USA (NSF), by the Ministry of Science and Development, Israel (IMSD), and co-sponsored by the National Aeronautics and Space Administration (NASA), the Office of Scientific Research of the U.S. Air Force (AFOSR), Tel Aviv University and Massachusetts Institute of Technology.
The introductory chapter attempts to summarize what transpired at the workshop.

The genesis of the workshop was an agreement between NSF and IMS, signed in the spring of 1983, to conduct a series of bi-national workshops and symposia. This workshop represented the first activity sponsored under the agreement. The undersigned were selected by their respective national bodies to act as co-coordinators and organizers of the workshop.

The first question that we faced was to decide upon a topic. In the past few years the field of CFD has mushroomed and consequently there have been many meetings, symposia, workshops, congresses, etc. dealing with all aspects of CFD. The smaller workshops and symposia have by and large been specialists' meetings. Among them they have covered the whole spectrum--from the mathematical theory of hyperbolic conservation laws through numerical simulation of turbulence to numerical boundary conditions in CFD. We thought that the time was ripe to pause and present to the community a sort of "State of the CFD-Nation" report consisting of two elements: technical papers by leading researchers and an attempt to assess where the field is going. It was decided that the technical papers should represent diverse areas and in fact we relished the idea of having theoreticians and practitioners (such as code-developers) meet together. We had two reasons for this--the first was that this is hardly ever done in small meetings and secondly the diversity was necessary for our second aim of assessing where are we going. The theme of this assessment, "The Impact of Supercomputers on the Next Decade of CFD," was selected since, from among all the factors driving the field and progress in our understanding of it, the coming Supercomputers are particularly important at this juncture.

The undersigned have enjoyed their involvement in this undertaking. All participants were very cooperative in meeting deadlines, being present at all sessions, and in presenting work that is at the cutting edge of their research. We would like to thank them all for their splendid cooperation. As with all such meetings, the "nitty-gritty" of organizing the event determines the welfare of the undertaking. Many people contributed to the success of the workshop--we would like to thank them especially; Ms. Ellen Mandigo at MIT, who coordinated the travel of the U.S. participants and the manuscripts; Ms. Sara Marcus at Tel Aviv University, who coordinated the arrangements for the workshop on the Israeli side; the Kennes company, which was in charge of the hotel and meeting facilities arrangements; and the Birkhauser Book Publishing Co. of Boston.

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TABLE OF CONTENTS

Progress in Scientific Computing, Vol. 6
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IMPACT OF SUPERCOMPUTERS ON THE NEXT DECADE OF COMPUTATIONAL FLUID DYNAMICS

Earll M. Murman
Saul S. Abarbanel

Introduction

A small group of CFD researchers from the United States and Israel gathered in Jerusalem during December 1984 at a workshop entitled "The Impact of Supercomputers on the Next Decade of Computational Fluid Dynamics." The background of the workshop attendees ranged from CFD code developers to applied mathematicians to computer experts. During the workshop the participants presented and discussed results of their current research. They then engaged in discussion of the workshop theme. This article attempts to summarize their observations and speculations on what the impact of supercomputers will be on CFD during the next decade. First, however, we briefly summarize the papers in these proceedings and the current status of CFD.

The Present

Supercomputers and CFD have affected every aspect of fluid dynamics to some degree during the past decade. Perhaps the area which has experienced the most dramatic impact is the field of attached flow aerodynamics, typical of design point conditions for transport aircraft. In this situation the fluid flow is well behaved by design. Separated and unsteady flow are avoided. The turbulent flow models applicable to attached boundary layers are acceptable (though not perfect). There are no chemical reactions or phase changes taking place. The major challenges lie in solving the nonlinear inviscid flow equations (primarily transonic) and dealing with the complex geometry. During the past decade, the capability of the computers and algorithms has developed enormously in this one particular subdiscipline. In some instances they are as much utilized as wind tunnel testing, although by no means supplementing them.

In most other fields of science and engineering, many of the more difficult fluid dynamic phenomena which are absent in attached flow aerodynamics are of paramount importance. For example, turbomachines are dominated by three-dimensional viscous and unsteady phenomena which affect heat transfer and performance. In many devices for propulsion and chemical processes, multicomponent chemical reactions and turbulent mixing must be modeled. High performance aircraft and helicopters are strongly influenced by vortical and unsteady effects. Low drag bodies are dominated by the prediction of transition. Separated, unsteady wakes of automobiles influence their fuel consumption and handling capabilities. In large scale geophysical fluid dynamics, coriolis forces and stratification effects are dominant. These lead to multiple time scale wave phenomena. Unstable stratification produces turbulent, buoyant mixing. Turbulent flow is present in virtually every situation, yet can only be adequately modeled for the simplest of flows like attached boundary layers and jets. This does not exhaust the list, but the point made here is quite clear; only the tip of the iceberg has been seen by the progress made in attached flow aerodynamics. The biggest challenges are yet to come. The papers in the proceedings give one assessment of where the field stands in this respect.

The Papers

Fernbach's paper gives a comprehensive overview of the current performance of supercomputers and what is on the horizon. This field is now very active following a dormant period in the 70's. The basic message is that computer speed and main memory will both increase by about two orders of magnitude in the next decade. Also, all future supercomputers will be a combination of vector (pipeline) and parallel (multiprocessor) architectures. Algorithms will have to adapt to and exploit these architectural features to achieve the stated machine performance. Thompkins' paper demonstrates that supercomputing does not necessarily have to be done on supercomputers. It makes an interesting case for the need of personal-sized supercomputers with speeds about one order of magnitude slower than the mainframes, but with comparable memories. The idea of using higher level languages for multiprocessor applications is brought out by Thompkins. Navier-Stokes results are also presented for turbomachine cascades, illustrating the state of the art for CFD applied to these flows. The paper by Jameson, Leicher, and Dawson demonstrates one way that the current generation of algorithms for inviscid external flows can be modified for multi-processor architectures.

The paper by Steger and Buning provides an overview of current issues regarding the computation of inviscid and viscous aerodynamic flows. In addition to a number of interesting results which are presented, the experience of these authors using the current generation of supercomputers is recorded. Vectorization of implicit algorithms is explained. The need for good graphical postprocessing of large data bases turns out to be mandatory. A similar message is given in the paper by Murman, Rizzi and Powell, which compares two independently obtained solutions for leading edge vortex flows for delta wings. This paper also illustrates that this class of compressible flows is relatively unexplored compared to shock wave dominated flows.

Several papers present new algorithms for the Euler and the incompressible or compressible Navier-Stokes equations. Since the solution of these equations will become more frequent with the higher power of computers, this is an important topic for the future. The paper by Walters and Dwoyer introduces an upwind differencing line relaxation algorithm for the Euler equations. McCormack presents a new algorithm for the compressible Navier-Stokes equations which has some similarities to the algorithm of Walters and Dwoyer. Turkel presents methods for accelerating the convergence to a steady state solution of the Euler or Navier-Stokes equations by using preconditioning to alter the time consistency of the equation set. The paper by Glowinski considers finite element methods for the incompressible Navier-Stokes equations and presents a number of results concerning entry to ducts and the subsequent internal flow. Remarks are also included on finite element methods for compressible Navier-Stokes equations and applications on supercomputers. Israeli gives an algorithm for the parabolized Navier-Stokes (PNS) equations. Brandt and Ta'asan present the latest multigrid algorithms for quasi-elliptic systems which arise from discrete approximations to the Navier-Stokes and related equations. The importance of algorithms, such as multigrid methods, which have convergence rates (spectral radius) independent of the number of mesh points will be mentioned later.

Perhaps no problem is more central to fluid mechanics than the prediction of transition and turbulent flows. Three papers deal with this topic. Brachet, Metcalfe, Orszag and Riley present new results for instability of free shear flows based upon direct computations of the Navier-Stokes equations. Numerical experiments such as these can lead to new theoretical understanding of instability of rotational flows. Ferziger's paper gives a comprehensive overview of current and future approaches to turbulent flow computations using direct simulations of the Navier-Stokes equations, large eddy simulation, and turbulence models. Wolfshtein considers the latter topic in much greater detail. These two papers point out the capabilities and shortcomings of current turbulence models. The importance of having accurate algorithms is stressed by both authors.

Papers by Sulem and by Michelson illustrate how numerical results can be used to understand the nature of the solutions to partial differential equations. The use of spectral methods for problems which require high accuracy is receiving increased interest. The presentations by Abarbanel and Gottlieb, and Gottlieb and Tadmor consider some basic issues regarding the resolution of extreme gradients by spectral methods. The paper by Browning and Kreiss illustrates that many fluid problems with multiple time and length scales are exceedingly difficult to compute, even with "unlimited" computer power. It is important to understand that the powerful new supercomputers will only yield useful results if the mathematical and numerical analysis formulation is carefully done. The paper by Sever is another illustration of this.

The Next Decade

During the next decade supercomputer power will increase dramatically. The directly addressable high speed memory capacity will increase by about two orders of magnitude, from 2-16 Mwords to 256 Mwords or 2 million words to 256 million more. Processor speed will increase an order of magnitude from about 100 MFLOPS to 1000 MFLOPS, or perhaps more. It is likely that the corresponding parameters of smaller computers will increase by similar factors. These estimates are important because history has shown that whenever an important parameter is varied by an order of magnitude, new discoveries are made. The difficulty is to have some feeling as to what those discoveries might be. The participants realized, of course, that forecasting the future is more of a "guestimate" than an exact science. It is interesting to note, however, that during the panel discussion almost everyone subscribed to the idea that the new supercomputers will not only allow tackling bigger problems, but will also lead to a better understanding of the physics of some complex problems such as turbulence, vortical flows, and chemically reacting flows.

In the remainder of this article we summarize the feelings expressed by the attendees concerning four questions which were posed by the panel.

Impact of Supercomputers on CFD

In the field of aerodynamics, the preliminary design of transport aircraft will primarily be done on supercomputers. The modeling and computing capability will be basically in place. Unlike earlier predictions that computers will make wind tunnels obsolete, few people subscribe to that viewpoint now. What is more likely to happen is that the use of wind tunnels by researchers and design engineers will change. Less and less of the exploratory design will be done by tests as predictive methods become more reliable. This has already happened in several instances with the current generation of computers. The next generation will provide enough resolution and speed that a realistic model of an actual cruising transport aircraft can be computed.

The capability to model "off-design" or "unclean" aerodynamic flows will increase. These are flows which are separated, unsteady, vortex dominated, and the like. Such flows are of great importance for maneuvers of high performance aircraft or for emergency situations for transport aircraft. The loads developed in these regimes often determine the required strength of the aircraft components. The same phenomena often dominate rotary wing and rotating machinery aerodynamics. Capacity of computers and algorithms up to now has not been adequate to support a frontal assault on this class of problems. The payoff for analysis of unsteady, separated, vortical flows will be much greater than for the clean flows representing cruise aerodynamics. This is because little theory has ever been developed for them.

The complexity of problems which the researcher and the engineer will be dealing with will grow in some proportion to the new computer power. This will have a number of impacts on the daily life of the fluids mechanician. Problems under investigation will have many length and time scales. Analysis of results will be more challenging. It will be harder to understand the solution due to the number of interacting physical phenomena present. This is illustrated by the paper of Brachet, Metcalfe, Orszag, and Riley. New methods of analyzing and presenting results will have to emerge in order to deal with this. Graphical output is crucial, and maybe artificial intelligence types of technology will help out.

One difficulty which can be foreseen is the problem of verifying the accuracy or fidelity of a computed result. Up to now, it has generally been possible to compare computed results with theory for limiting conditions. For example, a transonic wing calculation can be compared with linear wing theory for low Mach numbers, or a Navier-Stokes solution can be compared with a laminar boundary layer. But as the computations move into more nonlinear flows, the past theoretical framework will become less and less applicable. Comparison with experiment is essential, and independent computations of the same problem by different researchers will be necessary. Perhaps a renewed interest in theory will result from this need.

Impact of Supercomputers on Basic Sciences

As one participant stated, the great masters of fluid mechanics in the past solved all the linear problems and left us with only the non-linear ones. Since most fluid mechanic problems are nonlinear, we can speculate that the ability to model highly nonlinear problems with powerful computers will lead to many new discoveries. Another participant thought that the impact of supercomputers will influence the basic way we think about physical problems. New information will be discovered from numerical experiments and provide insight for modeling. In this sense, computational experiments are akin to laboratory experiments which have provided insight and ideas throughout the history of fluid mechanics and other scientific disciplines.

In the past, computational methods have made a major impact on our ability to compute and understand potential flows and inviscid flows dominated by shockwaves. One can conclude that these classes of flows are well understood both from the physical and algorithmic points of view. Although the ability to analyze shock dominated flows has been a major step forward in fluid mechanics, much is left to be done. For example, only limited CFD studies have been done for vortical flows, and little is understood about the algorithm requirements for inviscid rotational flows. Many studies have been done for two-dimensional separated flows, but only limited studies for three-dimensional separated flows. Although efficient algorithms for steady flows are under development, indications are that the flows these algorithms are to be applied to may be unsteady in nature. See for example Thompkins or Murman, Rizzi and Powell.

Perhaps no area is more tempting to speculate on than the field of turbulence. This is an area in which progress has been relatively stagnant since Reynolds introduced all the unknowns without introducing any new equations. In the past decade, computational models and laboratory experiments have opened a new look at turbulence. The idea of organized or coherent structure has emerged. On the other hand, mathematicians have shown that solutions to fairly simple dynamical systems have chaotic behavior. An interesting question which was posed is "What will be the resolution of the speculation that there is both determinism and chaos in nonlinear equations?" Computational experiments could provide a framework for helping to answer this question.

Another area which will probably be strongly influenced by more powerful computational approaches is the coupling of chemical reactions and heat release to fluid flow problems. Even fairly "simple" reactions involve many species with many time scales of reactions. In the past, computers simply were not large enough to tackle many of these problems. Rate constants are always an uncertain factor in such calculations. Perhaps being able to model the experimental conditions under which the rate constants are measured will lead to more accurate measurements of their values.

One issue on which there was quite a difference of opinion is the degree to which modeling will be required prior to computing. On the one hand, many participants felt that the time was upon us to tackle the full three-dimensional Navier-Stokes equations, possibly adding models only for subgrid scale turbulence. Others felt that the past practice of selecting simplified sets of equations such as inviscid or parabolized viscous will still be prudent. It is likely that some level of modeling will always be required as computer capability will never be big enough to solve a complex problem from first principles. In fact, for most problems this is unnecessary. The question is, will the type of modeling appropriate for the future be different from that used in the past when computer memory, speed, and accessibility were much more limited?

Impact of Supercomputers on Algorithms and Languages

An important issue regarding algorithms arises from the multiprocessor and vector architectures of supercomputers. Algorithms which cannot be efficiently used on these architectures will be of limited utility. Many fluid mechanic problems are solved using time dependent integration procedures for initial boundary value problems. Both