

Successes in computational fluid dynamics during the last three decades

J.S. Shang

*Department of Mechanical and Materials Science, Wright State University, Dayton, OH
45435-0001, USA*

Abstract

A glance back on significant accomplishments in computational fluid dynamics for aerodynamic application has been performed to highlight the outstanding achievements by pioneers of this discipline. It is an ardent hope that this abridged literature review will aid to reaffirm excellence in research and to identify knowledge shortfalls both in fluid dynamics and its modeling and simulation capability. The future modeling and simulation technology needs, as well as potential and fertile research areas are offered for consideration.

Introduction

1. Historical perspective

The development of computational fluid dynamics (CFD) can be traced back as far as the early 1900s. The pioneering efforts by Richardson [1], Courant, Friedrichs, and Lewy [2], Southwell [3], von Neumann [4], Lax [5], as well as Godunov [6] address the fundamental issues in numerical analyses for CFD. It is immediately clear that a major portion of these efforts was focused on one of the most difficult problems in resolving the discontinuous fluid phenomena in a discrete space—the Riemann problem [7]. As it will be seen later, it remains the most studied problem in CFD. However, if one is interested in viscous flow simulation, Thom [8] probably obtained the first-ever numerical solution by solving the partial differential equation for a low speed flow past a circular cylinder. For a scholarly description of the CFD historical perspective, the books by Roache [9] and Tannehill, Anderson, and Pletcher [10] are highly recommended.

In the early 1940s, finite-difference methods for solving partial differential equations were put to use in practical problems at Los Alamos National Laboratory with the first electronic computer. These works were strictly limited to atomic weapon system development and wartime technology. The applications widened to include fluid dynamics when the ENIAC was installed at Aberdeen. The advent of the computer has revolutionized a wide range of scientific research; however, fluid dynamics is the most affected by this

revolution. The computational physicist can now add insight and independent views to hasten the maturation of the previously unsolvable nonlinear problems. At the very beginning, the approach of CFD is to solve the governing equations in discrete space with uncompromising rigor. By imposing the proper initial and boundary conditions and without ad hoc simplifying approximations, the computing simulation is an imitation of a physical experiment.

Harlow first proposed the celebrated particle-in-cell (PIC) method in 1957 at Los Alamos National Laboratory [11]. This method uses a combination Lagrangian–Eulerian description of the fluid motion. In discrete space, the solving procedure consists of fixed Eulerian cells through which the fluid moves. The fluid is represented by Lagrangian mass particles with a fixed mass of fluid. The sum of the particle masses within the cell is the mass of the cell. The calculation proceeds through a sequence of finite time steps. After the particle transport is completed, final values of internal energy and velocity are obtained from the new total mass, momentum, and energy in the cells. The sum of these final values of the system is then checked for conservation before advancing to the next time level. In short, the PIC method has demonstrated to be well suited to study the time dependent and multi-dimensional fluid motion. The effectiveness of this method is demonstrated through the applications to shock interaction by Evans et al., supersonic wakes by Amsden and Harlow, as well as to hypersonic sharp leading edge flows by Butler [12–14].

The development of this numerical procedure was accompanied by exhaustive proof in order to illustrate the range of validity of the approximations. The PIC method actually set the standards for the future development of all CFD algorithms and numerical procedures. The detailed derivation of all pertinent formulations and extensive discussions on computational accuracy and limits of applicability become the accepted tradition in CFD research. At that time, the computed resource was severely limited and allowed only a small number of representative calculations in an investigation; and yet the experience has shown that the extensive and detailed information obtainable from CFD is

immeasurable. The complementary contribution to better understand the basic physics with experiments and theoretical analysis is fully appreciated.

A fluid dynamic problem of great concern for aerodynamic performance is that of flow separation at which point the boundary-layer approximation breaks down. Lees and his students [15] led the first few well-known applications for complex aerodynamic problems involving boundary-layer/shock-wave interaction. His basic approach is built on the integral momentum equation and his incisive insight on the self-similar boundary layer. The interacting boundary solution method eventually adopted the boundary-layer code developed by a CFD pioneer, Davis [16]. Davis actually solved the multi-dimensional compressible boundary-layer equation based on the physics by a combined implicit-explicit, finite-difference approximation. He solved the rapidly changing and steep flow field gradient across the boundary layer by the tridiagonal Thomas algorithm, and the relatively slow varying streamwise variation by a forward differencing scheme. His numerical procedure for solving the compressible boundary-layer equation is accurate and robust.

The separated flow solution was recoverable by a trial-and-error method; the final solution is the numerical result that passed the saddle point at flow separation. In this connection, the triple deck theory of Stewartson [17] has provided a scaling law for the interacting boundary layers and demonstrated that the singular point of flow separation in the interacting boundary layer is indeed removable. This scaling law was successfully incorporated into the interacting laminar boundary-layer method to provide insight into the evolution of the separating flow structure [18].

For inviscid flow in the supersonic domain, the method of characteristics has been developed to a very high level of sophistication for three-dimensional flows. In fact, Rakich [19], another pioneer of CFD, devised a complex three-dimensional network of grid points to describe the intersections of the Mach cone and stream surface. The bicharacteristics that describe the compatibility conditions are partial differential equations containing cross-derivatives normal to the characteristics. For steady supersonic blunt body simulation, a set of initial data is needed for the hyperbolic equation system. These initial values, downstream of the limiting characteristics, may not be available for complex aerodynamic shapes, thus limiting its applications. However, this limitation was removed by the work of Moretti and Abbett [20]. They solved the time-dependent Euler equation by a finite-difference method, and the flow field was obtained as the steady-state asymptote. Their work has made two very important contributions to CFD; first, the time marching formulation permits the unsteady Euler equation retaining the hyperbolic formulation even for the subsonic flows. Second, they demonstrate that the Rankine-Hugoniot shock jump condition can be captured by the finite-difference

approximation. Meanwhile, the vortex lattice method derived from the small perturbation theory was advanced to application for inviscid subsonic flows over aircraft [21]. This simple yet elegant method is still in use for commercial aircraft design and becomes a classic example in engineering that followed the axiom that was frequently attributed to Einstein, "keep it simple but not simpler".

The first coherent and structured CFD organization solely for aerodynamic application was the brainchild of Dean Chapman, then the Director of Aeronautical Science Directorate of the NASA Ames Research Center. He successfully recruited and nurtured a large group of devoted talent for CFD. During that time, a rare genius in digital computer design, Seymour Cray made high-speed computers commercially available such as CDC6400 and CDC 7600. The combination of talent and support infrastructure led to a revolutionary advance in computational aerodynamic research. It was an unprecedented, and still never duplicated, amount of attention to detail and encouragement by organization leaders at the national level to a technical endeavor. For example, any CFD presentation from the Ames Research Center to a professional society was reviewed and rehearsed by the then Center Director, Hans Mark. It remains a shining case study of how to develop cutting edge technology in any arena. The research leadership role was entrusted on the shoulders of Harvard Lomax and Robert MacCormack. They carried out their duty faithfully and exerted their effort to achieve a new culture for scientific excellence. Therefore, it should not be surprising that a large group of legendary scientists were trained and got their baptism in CFD. The group of luminaries includes William Ballhaus, Richard Beam, Steven Diewert, C.M. Hung, John Kim, Paul Kutler, Parviz Moin, Earll Murman, Thomas Pulliam, Joseph Steger, Robert Warming, Helen Yee, and many others. The impact of the Ames Research Center to the CFD community extends worldwide; distinguished scientists such as Kozo Fujii and S. Obayashi of Japan, Rizzi of Sweden, as well as Wolfgang Schmidt of Germany have either an extensive visiting tour or sustained collaboration with scientists at the NASA Ames Research Center.

Equally important, the Ames Research Center has not only set the standard for scientific research, but also established the collaborative culture in the CFD community. The close working relationship among researchers at the center and a large group of constantly circulating visiting scientists through the center actually created a close-knit CFD community. A tradition of hard working, generously sharing, and strong mutual support was achieved and maintained in a very competitive environment. One cannot help but remember the long working hours, the endless toiling, but exciting challenge for gaining new knowledge, and the wonderful times together with respected colleagues. This goodwill and unwritten mutual esteem have been sustained and are

apparent in all international symposia, even today.

The successful activities at the NASA Ames Research Center inspires similar activity at other NASA science and technology centers such as the Langley and now Glenn Centers. The military service branches also appreciated the need to develop this modeling and difficult interdisciplinary investigations in penetration mechanics and electromagnetic energy deposition for aerodynamic control. For this reason, this fundamental numerical algorithm is still taught in most CFD classes.

MacCormack's lasting contribution to CFD is also reflected strongly in shock-boundary interaction problems. The physics of viscous–inviscid flow interaction must be recovered from solving the Navier–Stokes equations. The early works in compression ramp and shock-boundary interactions by Hung and MacCormack [28], Horstman et al. [29], and Shang and Hankey [30] have provided a better basic understanding of the boundary-layer separation and exposed the weakness of rudimentary turbulent closure models.

The very few early solutions by solving the Reynolds-averaged Navier–Stokes equations were for shock-boundary-layer interaction over a two-dimensional compression ramp including flow separation. The comparison of the numerical simulation and a Schlieren photograph is depicted in Fig. 1 to show that the numerical results indeed capture the essential feature of this fundamental aerodynamic phenomenon. In this connection, Knight

[31] also first applied this numerical technique to simulate realistic high-speed inlets for analyzing the performance of air-breathing engines. A sustained research effort in shock-boundary interactions has been maintained for the past 30 years, and recently David Dolling has summarized all these efforts in an excellent review article [32].

In the 1970s, even a three-dimensional hypersonic compression corner problem was successfully simulated using the MacCormack explicit method [33]. The computational domain of a strong hypersonic

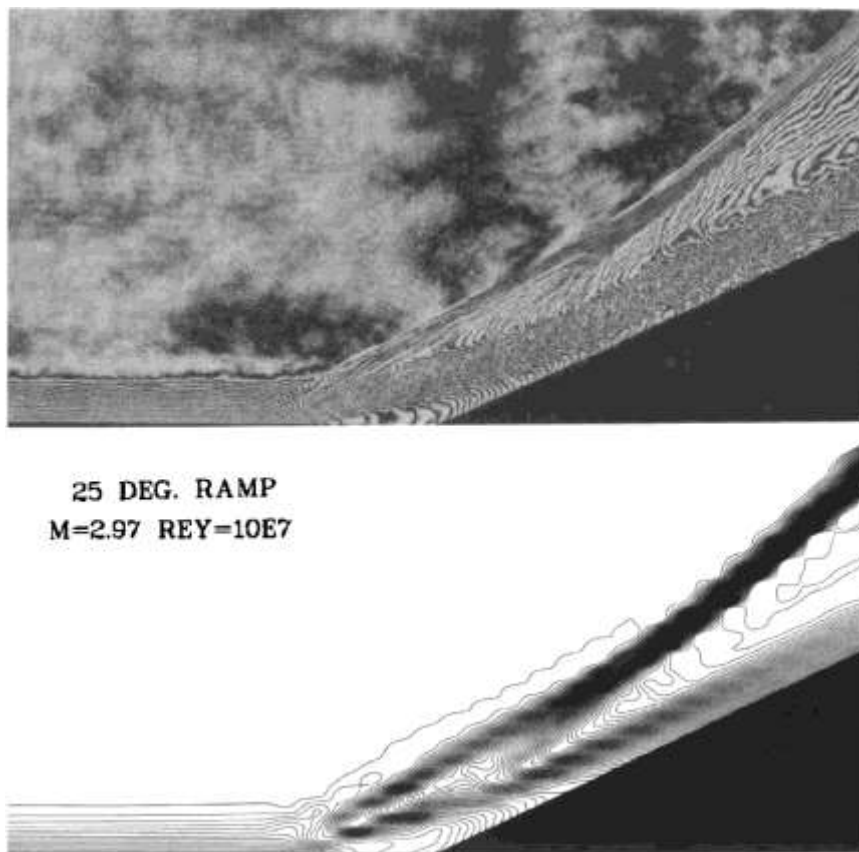


Fig. 1. Shock-boundary-layer interaction over a compression ramp.

shock-boundary-layer interaction was confined in a frustum of a rectangular pyramid by a mesh system of $(8 \times 32 \times 36)$ bounded by a wedge and a flat plate. The mesh system consisted of a measly 9216 points, but it already occupied the complete memory capacity of the CDC 7600 computer. A physically meaningful

solution was obtained by invoking the salient feature from the hypersonic equivalence principle—the dominant flow perturbation occurs mostly in the cross flow plane. The numerical results reached impressive agreement with experimental measurements in heat transfer rate and surface pressure distribution. Equally

important, the triple-point shock structure was captured at the intersection of the wedge shock and the induced shock from the sharp leading edge flat plate (Fig. 2). From this calculation, the hot spot of the corner was also identified as the penetrating inviscid stream at the shock triple point. Although these types of numerical computations resolved only the essential feature of interacting flow field, it began to become a powerful tool in aerodynamic research.

Another previously unsolvable nonlinear transonic flow phenomenon has also attracted a lot of research efforts. The basic physics of transonic flow emerges from the fact that a flow disturbance must propagate in drastically changing domains of dependence. If one optsto study transonic flow using the Euler equations, the governing nonlinear partial equations system changes from the elliptic, parabolic, and hyperbolic type corresponding to whether the flow field exists in the subsonic, transonic, or supersonic flow regimes

respec- tively. Aside from the unknown and uncertain well- posed boundary condition criterion for the discrete approximation, there is ambiguity as how to best satisfy the directional signal propagation according to the eigenvalue of the differential system.

A breakthrough in transonic flow simulation is attributed to Murman and Cole [34]. Their novel approach was the first to use a combination of central and windward difference approximations to satisfy the domain of dependence. The transonic small disturbance theory was used to solve the flow past thin airfoils with imbedded shock waves. The governing equation is a mixed elliptic–hyperbolic differential equation that was solved by a separate difference formula in the elliptic and hyperbolic regions to account properly for the local domain of dependence. Their accomplishment again reinforces the fundamental rule in algorithm

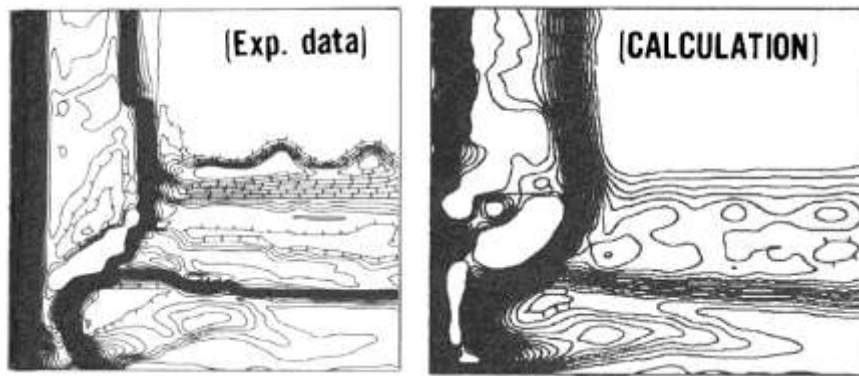


Fig. 2. Triple shock structure in a 3D corner, $M=12.6$.

development—the most accurate and efficient numerical procedure for problem solving is the one that best mimics the physics.

During the same time frame, Jameson [35] started to develop a widely used explicit numerical procedure for transonic flows and initiated an illuminative career and became one of the most respected leaders in CFD. The most remarkable achievements by Jameson are his emulation of the shockless transonic wing, multigrid algorithm development, and his ingenious aerodynamic optimizing techniques. His numerous contributions to transonic airfoil and wing designs have no peer and equally impressive is his natural ability in nurturing young talents and bringing out the most creativity from them.

The venturing of CFD into practical applications was greatly aided by the body orientated coordinate genera- tion technique introduced by Thompson [36]. He ranks among all pioneers in CFD and uniquely possesses an unfailing courtesy of southern gentry. His work indeed has opened a new avenue for CFD applications to practical and complex configurations ahead of any other physics-based simulation discipline such as computa- tional electromagnetics (CEM). For structured grid computations, the grid generation by solving partial elliptic [36], hyperbolic [37], and

algebraic [38] equations is the cornerstone for application to complex configura- tions.

Since a major portion of engineering applications is time dependent, some numerical simulations with bodies of relative motion have to be obtained from a moving grid. When the governing equations are mapped onto a moving computational domain and solved by a finite-difference technique in the strong conservation form, the geometrical conservation law by Thomas and Lombard [39] must be observed to eliminate computational errors. In essence, the geometrical con- servation law stresses the coupling between the numer- ical algorithms and the moving grid metric calculations. This requirement arises from a mathematical identity in the metrics evaluation and must be satisfied simulta- neously with the governing equation. The geometrical conservation law has provided a solid foundation for extending CFD applications to the moving frame of reference.

As the complexity of CFD simulations has increased, efforts were focused on accelerating the numerical convergence rate and stability of the numerical algo- rithm to reduce the required

computing resources. It has been known for quite a while, that the implicit schemes, in general, possess the more favorable stability property for solving linear partial differential equations [40,41]. This class of algorithms is commonly referred to as the ADI (alternating direction implicit) scheme, and indeed it is unconditionally stable when applied to three-dimensional parabolic and elliptic partial differential equations and two-dimensional hyperbolic systems. Since the discrete system of equations must be solved simultaneously, a matrix inversion procedure is required. The inversion process not only needs a much greater computer addressable memory, but also may incur round-off error. However, the gain in computing stability has frequently compensated for the additional resources required over that of explicit

schemes. The pioneering contributions by Briley and McDonald who used the ADI scheme to solve the Navier–Stokes equations were first published in 1970 in a laboratory report and a year later in more accessible sources in 1971 and 1974 [42,43]. Beam and Warming made sustained and substantial contributions to the factorized implicit numerical algorithms. They first presented their work in solving the compressible Navier–Stokes equations in 1977 and published it a year later [44]. This algorithm has been subjected to systematic development by an exceptional group of individuals, such as Pulliam, Steger among others, to become the most widely used numerical procedure in the CFD community for the next few decades [45].

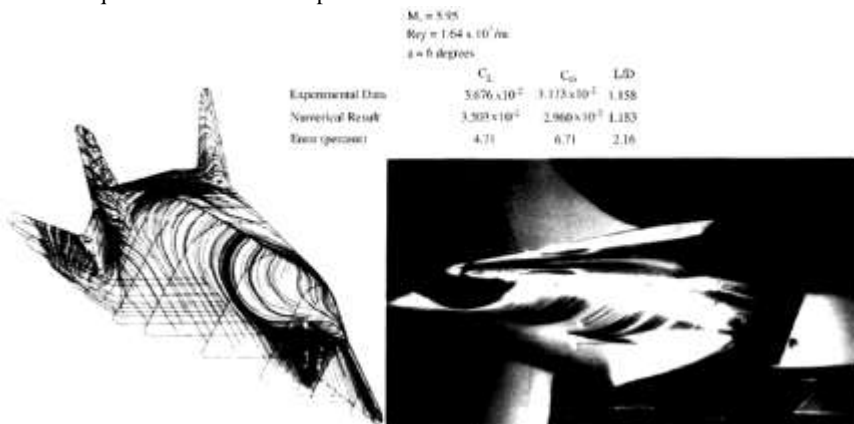


Fig. 3. Reentry vehicle X-24C-10D simulations.

An insignificant event in research that reflects the ingrained tradition of peer review and the open debate amongst the CFD community is probably worth sharing. At the AIAA 1977 Summer Meeting in Albuquerque, Briley, Warming, Lomax, and Shang got together for a technical exchange on the development and relative merits of ADI schemes. One cannot help but feel proud about the open and earnest discussion and the sense of fairness in the CFD discipline. This feeling prevailed and in 2001, when McDonald became the Director of the NASA Ames Research Center, he bestowed the coveted J. Allen Award to Dick Beam and Bob Warming for their accomplishments in developing the factored implicit numerical procedures.

The search for high computing efficiency reflects an impressive creativity in the CFD community. The Newton quadrature scheme probably has the fastest convergence rate known to us, but the scheme also requires that an initial estimate of the solution must be within a convergence tolerance. The overall convergence rate of an equation system is closely tied to the spectral radius of its eigenvalues and the elimination of error residue from its initial estimate. To achieve a fast convergence rate of an iterative approach to a steady-state asymptote for the Navier–Stokes equations, a new strategy is required. Brandt

met this need by introducing the multi-grid method [46]. The basic idea is to filter out the low-frequency numerical error by interpolating the finer grid result to a coarser grid, and to obtain the correction to the fine grid by an up-sweeping process. This method has exhibited a substantial improvement of rate of iterative convergence. The attraction of the multi-grid iterative technique also lies in its broad range of applicability to CFD problems.

The introduction of the implicit and iterative algorithm, grid generation techniques, and physically based

approximations such as the parabolized [47] and thin-layer [45] Navier–Stokes equations greatly enhanced the range of CFD applications. Some early CFD applications in aerodynamics include the transonic airfoil by Levy [48], aileron buzz by Steger and Bailey [49], airfoildynamic stall by Tassa and Sankar [50], scramjet flow field by Drummer and Weidner [51], boundary-layer instability by Fasel [52], bodies at high angle of attack by Helliwell et al. [53]. Shang and Scherr in 1985 eventually simulated the aerodynamic performance of a complete reentry vehicle (X-24C) on the Cray 1 computer using the MacCormack explicit scheme on the grid generated by Steger’s hyperbolic grid generator [54]. The computed surface shear stress map and oil film

pattern on a scaled X24C model is depicted in Fig. 3.

2. Achievements in the eighties

2.1. Finite-volume methods

The finite-volume formulation of the macroscopic conservation law is intrinsic in the Eulerian frame of reference. The concept of conservation laws is actually defined for an arbitrary control volume. The variation of dependent variables within the control volume, whether they are mass or components of momentum or internal energy, are balanced by the flux across the control surface of this volume. The basic formulation uses the integral form of the Navier–Stokes equations. The finite-volume formulation rigorously enforces the conservative law both on each elementary cell and for the complete control volume of the flow field. This formulation is less susceptible to singular behavior of a geometrical shape than the metrics of coordinate transformation in the finite-difference approximation. The first numerical result of this formulation for the Navier–Stokes equations is attributed to MacCormack and Paullay [55], but Rizzi and Inouye first coined the term [56] finite-volume method. However, the finite-volume method was not widely used until the 1980s. Thomas and Walters [57] and MacCormack [58] implemented this formulation for the Navier–Stokes equations by an implicit Gauss-Seidel relaxation algorithm, which led to a group of robust numerical procedures as the mainstay of present CFD applications.

The basic formulation of the finite-volume scheme requires the reconstruction of the flux vector normal to the elementary volume; it is therefore natural to introduce the windward differencing approximation that had been consistently advocated by van Leer [59]. Furthermore, the reconstruction process on the control surfaces also easily permits the development of high-resolution procedures. The seminal contribution by Harten [60] for the high-order reconstruction process, and the contributions to windward approximation and total variation diminishing (TVD) scheme, and the contribution to the monotone scheme by Osher and Chakravarthy [61] should be noted.

2.2. Characteristic-based methods

Using the compatibility condition to solve the steady, supersonic Euler equations was at the very beginning of aerodynamic research [5,6]. In fact, it was the genesis of the method of characteristics since 1929 by Busemann [62], and was developed further to include rotational flow by Ferri in the late 1940s [63]. However, predicting a multi-dimensional flow field that contains shock waves and contact surfaces was presented in a landmark paper by Godunov [6]. He treated discontinuities of the hyperbolic differential systems by assuming a piecewise continuous data distribution within a control volume and by solving

the Riemann problem across each cell interface. The flux vector is computed by the windward approximation to satisfy the governing equation in an integral conservation form. By solving sets of Riemann problems over the entire computational domain, this approach honors the physics of domain of dependence using the correct database according to the directional propagation of wave motions.

In 1973, Boris and Book introduced the flux correction approach [64], and independently a few years later, Steger and Warming [65] introduced the flux-splitting method to the CFD community. In this outstanding work of Steger and Warming, they have shown system-

3. Outlook

In any human endeavor, the knowledge sharing among peers and passing from generation to generation is paramount to mature a scientific discipline to a new horizon. The education and training for CFD were strongly emphasized from day 1. There is a wonderful tradition in the aerospace industry of using workshop to bring new technology to the community. In the early 1970s, numerous CFD workshops were held either by government agencies or professional societies such as AIAA and ASME to compensate for the lack of textbooks. The workshop usually consisted of lectures and a few sample computer codes. In fact, it was the way one learned the basics in CFD at the very beginning. A lot of successful stories were originated from this type of training process.

Over the years, a series of excellent textbooks began to appear [9,10,128] and the learning process was also formalized. In most universities, CFD was offered in two to three consecutive classes; the syllabus roughly divided into the basics concepts of CFD, the classic algorithms, and numerical methods used. Professional societies have also sustained the seminar series and the self-study option. Most new generation CFD users educated under these more rigorous education programs tend to have a better grasp of the basics and benefited greatly from their formal training.

Now the most common practice for those who are proficient with workstations and PCs is to use Math Libraries or commercially available software packages. The computed results are displayed or analyzed with canned graphic software. However, the best practice shall still be derived from understanding the underlying physics and judiciously choosing a numerical procedure to achieve the best simulation. The computing error can be simply eliminated or alleviated by well-posed initial/boundary conditions and grid density refinement. However, the error incurred by using the inappropriate governing equation or initial/ boundary conditions is uncorrectable. This required judgment can only be nurtured through rigorous

education and training.

The future direction of CFD is easily determined from two overriding perspectives—faultless scientific foundation and practical application needs. It is too well known that the weakest link in CFD as a scientific discipline is

the inadequate description of turbulence. This critical research arena requires long-term vision, sustained support, and rigorous peer review. The pioneering efforts using DNS and LES have opened research avenues for all to follow.

Modeling and simulation needs in aerospace engineering are clearly reflected by the unresolved and least understood problems in fluid dynamics, which are unsteady bifurcation and vortex interaction [92]. All these physical phenomena are nonlinear and have a strong element of time dependency associated with them. In the present context, bifurcation is defined as the transition between different dynamic states of fluid motion. The separated flow, laminar-turbulent transition, control surface buffeting and fluttering, lifting surface dynamic stall, inlet unstart, combustion instability, propulsive system surge, and rotating stall compressor all belong to this category. These phenomena are the aerodynamic performance pacing items, therefore they must be conquered with a concerted effort. As far as the vortex interaction is concerned Kuchemann has best described the importance of vortex dynamics in fluid dynamics—vortices are the sinews and muscles of fluid motion. Any future improvement in aircraft performance must rely on a better understanding and more accurate description of vortex interaction.

Equally important for future needs is system engineering. There is an urgent need to sustain the further development of interdisciplinary CFD capability. This ability to solve the show-stopping system issue and to weed out the unproductive ideas at the onset by interdisciplinary modeling and simulation tools will drastically shorten the design cycle and push CFD research for the unforeseeable future. In this sense CFD is not a mature technical discipline. However one should always bear in mind for future pursuit the two axioms from lessons learned; first, keep it simple but not simpler; it is truly an invaluable gift from Einstein. Second, research in CFD must return to basics to affect the widest applications; any basic research accomplishment will have a greatly enhanced value if it can be applied effectively.

Conclusion

Narrating a technical endeavor spanning nearly a century by an aerodynamicist and with a limited knowledge, numerous as well as significant contributions to CFD will be unintentionally overlooked either by author's limited exposure, personal bias, fading memory, or combination of these. Most importantly, the present effort only reflects a personal experience in scientific discipline that is vast; please

accept my sincere apology for any omission.

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