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History of Sciences and Ideas / *Histoire des sciences et des idées*

More than a half century of Computational Fluid Dynamics / *Plus d'un demi-siècle de mécanique des fluides numérique*

Evolution of CFD as an engineering science. A personal perspective with emphasis on the finite volume method

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Abstract. Computational Fluid Dynamics—CFD for short—is a comparatively recent development that has made a significant impact in engineering sciences. The foundations of CFD were laid by developments in physics, numerical analysis and matrix theory over the last 200 years or so. It was, however, the electronic computer in the middle of the 20th century that led to its birth and its widespread use. It has now become an invaluable tool for almost every sphere of human activity. A number of researchers contributed to the tools and technology that came to be called CFD but the prime movers were two brilliant scientists—one at Los Alamos National Laboratory and the other at Imperial College, London. The author was a part of the Imperial College group and this is a personal perspective on the evolution of CFD.

Over the last few decades, CFD has made a significant impact in a wide spectrum of engineering and environmental sectors. These include both traditional disciplines such as aerospace, automotive, mechanical and thermal sciences, and newer disciplines and emerging fields of human and social relevance such as biomedical, sports, entertainment, food processing, fire safety, HVAC and energy efficiency. However, a number of challenges remain. For many important applications, we lack both the physics and the mathematical tools to adequately understand the behavior of fluids. The current generation of CFD tools are resource intensive and difficult to use that require a long period of training. Most importantly, except for a very limited set of applications, one cannot rely on the predictions with a high level of confidence.

Computational Fluid Dynamics is now poised on the threshold of a revolution. Recent developments in machine learning, AI, computer hardware, big data, IOT and Virtual Reality tools will lead to design tools with CFD engines that are robust, reliable and easily accessible to a practicing engineer rather than be the domain of a CFD expert. CFD will be a tool that is ubiquitous by its absence—buried inside devices and applications into diverse areas of human activity. This would make it possible for a practicing engineer to effectively visualize a fluid system, interact with its components, conduct CFD simulation, and control its behaviour through dynamic intervention.

Keywords. CFD, Finite volume methods, Machine learning, PINN, AI.

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1. Background

We inhabit fluids, and fluids inhabit us. We're immersed in air and two thirds of the earth surface that we live on is water. Two thirds of the human body is fluid. The solid parts of the earth and that of the human body are actually highly deformable and often behave like fluids.

Computational Fluid Dynamics—CFD for short—predicts the behaviour of fluids, plastics and deforming solids. CFD, in a broader sense, is the science of "*Things That Move*". To understand the physical, biological and environmental world that we live in, we need CFD. Every human endeavour involves fluids and CFD applications span human existence: be it, industry, environment, human body, or the biosphere. CFD tools are critical to aerospace, energy transport, national security, engineering, design, food and chemical processing, consumer electronics, environment, disaster management, life sciences, earth sciences, astronomy, virtual reality, animation and increasingly entertainment. Over the years it has become more a question of what CFD can't do, rather than that of what it can do.

This is a rather subjective and personal perspective of the history of CFD. In that context, my focus is that of a practicing engineer. Therefore, I have emphasised the physics and engineering aspects, rather than the significant developments that have occurred, in parallel, in the fields of mathematics and numerical analysis. I grew up in the remote hills of Himalayas, and never dreamt of participating in the birth of a new branch of engineering science. But I was lucky enough to witness the emergence of CFD at Imperial College. As a footnote, McLeod Ganj, my hometown, became the home to the Dalai Lama and a symbol of rejuvenation of Buddhism. It then played an important role in the human rights movement, and became a prominent place on the political maps of India, China and the US.

The mathematical foundations of fluid dynamics were laid by the 18th Century Swiss mathematician, Leonhard Euler—one of the most prolific mathematicians in history. He developed the Euler Equations that describe the flow of an ideal frictionless fluid in the early 1750's but formally presented to the Swiss Academy later in 1757 [1]. Though this was a monumental theoretical achievement, most flows of practical interest stayed outside the purview of these equations since they ignored friction that plays a very important role in the behaviour of real fluids. In 1821, the French engineer Claude-Louis [2] introduced the concept of viscosity to generalize the Euler equations to deal with the flow of real fluids. Though Navier realized that there were forces between the molecules of fluids, he had no formal concept of shear stress or its relation to the state of the fluid. The next major breakthrough was in the middle of the 19th century by the British physicist and mathematician, Sir George Gabriel [3], who derived a formal mathematical expression that related the stress due to friction (viscosity) to the strain of the fluid. These developments led to the Navier–Stokes Equations that put fluid dynamics on a firm and formal mathematical basis. One unexpected result of these theoretical advances was that whereas the Euler equations were, in many cases, somewhat amenable to analytic solutions, the Navier Stokes equations were intractable except for trivial and highly idealized one or two-dimensional flows in simple geometrical configurations.

The Navier–Stokes equations are now recognized to be one of the most intractable mathematical problems in physics. Despite their broad applicability, no proof is available that a solution always exists in three dimensions and that, if it does exist, it is smooth and unique. The Clay Mathematics Institute [4] has called this challenge one of the seven most important open problems in mathematics and has offered a prize of US$1 million for a solution or a counterexample.

In the absence of analytic solutions, for the rest of the 19th century, the only option available was to focus on certain flows where some terms in the Navier–Stokes equations could be ignored. This then allowed either exact or approximate solutions to the simplified equations. One early example was the case of creeping flows where the frictional force is much greater than the convective inertial force. Stokes [5] formulated equations where the convective terms are completely ignored and the simplified equations are amenable to exact or approximate solutions. Another example is that of the Shallow Water Equations where it is assumed that the horizontal extent of a body is much larger than its vertical depth. This is the case, for example, for large water bodies or the atmosphere at the meso- or global-scales. Order of magnitude analysis then shows that the pressure at any point is hydrostatic in the vertical direction. The vertical acceleration can be dropped and the resulting simplified equations allow solutions for many problems of interest.

The next major advance came at the start of the 20th century when Prandtl [6] introduced the concept of a boundary layer. Many practical flows consist of a dominant direction of flow. Flow in a pipe or that on a flat plate, a jet in ambient surrounding, or the wake behind a cylinder, are common examples. For such flows, he visualized the flow field as consisting of two regions. A boundary layer region where flow gradients are dominant and friction plays an important role, and a far-field region where gradients are negligible and friction can be ignored. He then derived a simplified form of the Navier–Stokes equations on the basis of the order-of-magnitude analysis that applied in the friction-dominated boundary layer. The far-field is then described by the Euler equations. These simplified equations enabled both analytical and approximate solutions for a wide range of applications. Pohlhausen [7] made a major contribution by visualizing the boundary layer to be described by self-similar analytic profiles where the profile parameters can be determined from the known initial and boundary conditions. This led to a rejuvenation of interest in fluid dynamics and great progress was made over the next few decades in solving many problems of practical interest with acceptable approximations.

Many real-life flows of great importance occur in 3 or 4-dimensional space-time domain. They do not have a dominant direction of flow. Examples include flows with separation or recirculation, impinging flows with strong streamline curvature, and flows in complex geometries. Such flows, actually, define the majority of flows encountered in industry and in the environment, and are governed by the complete Navier–Stokes equations. These stayed intractable and evaded all attempts to obtain an analytic or approximate solution, and till the middle of the 20th century, the solution of the complete Navier–Stokes equations stayed a distant dream.

It is in this context that Computational Fluid Dynamics arrived on the scene. What made it possible was the availability of commercial electronic computers starting with the IBM 701 in 1952. It made possible generalized, albeit approximate numerical, solutions of the complete Navier–Stokes equations for a much broader class of practical problems without having to resort to dropping one term or another in the governing equations.

Newton famously stated that If I have seen further, it is by standing on the shoulders of Giants. CFD also stands on the shoulders of mathematicians who, over a period of 200 years, developed the tools that would later form the foundation of CFD. These tools belonged to Numerical Analysis and Matrix Theory. At the start of the 18th century, Brook Taylor [8] introduced the Finite Difference Method (FDM) that laid the foundations of the differential calculus and provided a very convenient tool to convert the governing differential equations into algebraic equations that can then be solved by numerical methods. Next milestone can be credited to Carl Friedrichs Gauss who, over a period of 30 years starting in 1810 [9], made seminal contributions that played an important role in CFD. He introduced both a direct elimination and an iterative method for solution of a system of linear algebraic equations—a matrix. He also introduced the method of weighted residuals. His other important contribution was to develop the Gauss (or Divergence) Theorem that, among other uses, provides an equivalence between surface and volume integrals for a closed volume. This can be used to decrease the order of a differential equation by one. William Rowen Hamilton [10] made important contribution by defining the concept of a Hamiltonian—in the form of minimum energy state for a system—that proved useful in analysis of a dynamical system. Cauchy [11] introduced the method of steepest descent for non-linear equations that is the precursor to the popular Krylov and Conjugate Gradients methods [12] for solving algebraic equations. Jacobi [13] developed a relaxation type of method for solving a system of algebraic equations. A more important contribution of Jacobi was to introduce the concept of pre-conditioning to speed up convergence. Seidel [14] proposed a modification of the Gauss method, today known as the Gauss–Seidel method, that allowed improved convergence in many cases. Chebyshev introduced his polynomials in 1854 that play an important role in iterative matrix solution [15].

In the first half of the 20th century, rapid progress was made in the field of numerical analyses. Variational method and the concept of trial functions for solving partial differential equations, the Rayleigh–Ritz method, was introduced independently by Ritz [16] and Lord Rayleigh [17]. Richardson [18] made some important contributions including the method of polynomial iteration, and a method for improving the accuracy of a solution by extrapolation of solutions obtained with different grids. Boris Galerkin [19] introduced the method of converting a differential equation to its algebraic equivalent through basis functions which forms the basis of the Finite Element Method (FEM). Liebman [20] appears to be the first one to use an iterative method for solving a PDE. His method is essentially a Gauss–Seidel method which had previously been applied to matrices resulting from ordinary algebraic equations. Krylov [21] introduced the concept of Krylov subspace that forms the basis of the currently most successful iterative methods for solution of the iterative equations. Southwell [22] introduced the successive over relaxation method to solve the system of linear equations with significant improvement in speed for a certain class of matrices. Young [23] devised an efficient algorithm to determine the over-relaxation factor for a class of elliptic equations. George Forsyth made important contributions to Numerical Analysis. An excellent summary of methods for solving linear algebraic equations is available, for example, in Forsyth [24].

The 2nd half of the 20th century saw further development of both the direct and the iterative methods for solving a matrix. Much progress was made in developing efficient use of direct matric solvers and Krylov subspace methods for iterative solution reached a point of maturity. Saad [25] has compiled an excellent history of the development of iterative methods.

The field of CFD has mushroomed since the introduction of the electronic computer. However, manual computations of fluid dynamics problems had existed since a few decades earlier. Richardson [26] used a FDM to predict weather. Thom [27,28] obtained a FDM solution for a two-dimensional flow and a flow past a circular cylinder at a Reynolds number of 50. He used the two-dimensional stream-function-vorticity version of Navier–Stokes equations and employed street children as human computers to compute the resulting matrix of equations. Southwell [29] derived the FDM solution for flow past a cylinder up to a Reynolds number of 100. Kawaguti [30,31] explored the problem of flow around a circular cylinder and that in a driven square cavity. Allen and Southwell [32] added the innovation of conformal coordinate transformation to map the infinite domain behind a cylinder into a finite domain. Thom and Apelt [33] made an interesting observation that the range of Reynolds number for flow behind a cylinder could be extended by the use of under-relaxation. Other notable computations were those of Simuni [34] who reported numerical solutions for a range of viscous flow problems. All these researchers reported numerical instability as the Reynolds number was increased. They had employed the central difference scheme, because of its second order accuracy, to discretize their equations. It was left to Courant *et al.* [35] to make a significant contribution by recognizing that the central difference scheme is not the correct choice to get a stable solution for high-speed flows when the flow shows a strong hyperbolic behaviour. They discovered the important role of the upwind, or one-sided, differences, for hyperbolic equations. However, this was not widely known to the rest of the research community working on Navier–Stokes equations till well into the 1960's.

Dorodnytsyn [36], Godunev [37], Gilinski *et al.* [38], Rusanov [39], Yanenko [40] and a number of other Russian scientists, many at the Institute of Applied Mathematics of the USSR (now Russian) Academy of Sciences, contributed immensely to the understanding of the numerical aspects of CFD. The work of Yanenko had particular influence in later years as the Fractional Step Method that he proposed became a very useful option to deal with complex partial differential equations. Unfortunately, much of this work was unknown in the west till well into the 1970's.

Before the advent of the electronic computer the use of numerical methods for fluid flow was severely restricted due to the sheer number of arithmetic computations. However, these explorations made important contributions that highlighted the basic problems encountered in the application of the FDM to Navier–Stokes equations. One interesting fact is that before the advent of the electronic computer a "person" who performed the calculations was called a "computer".

It should be mentioned here that turbulence plays a key, and often controlling, role in the application of CFD. The formal foundations of turbulence were laid by the seminal work of Reynolds [41] half a century after the development of the Navier–Stokes equations. Turbulence is, in itself, a very exhaustive and complex field of research. Significant developments have taken place since the advent of the electronic computers that have resulted in a wide range of approaches to deal with the impact of turbulence on fluid flow. However, the theme of this paper is CFD, hence these important developments in turbulence are not reviewed here. Many exhaustive reviews of turbulence and turbulence models have now been published and these may be referred to by the reader for further information.

2. The basic physics and equations of CFD

The cornerstone of CFD is the law of conservation of a property of the fluid. Consider a closed control volume, V, with a bounding area $\boldsymbol{A}$ and a unit normal n as shown in Figure 1.

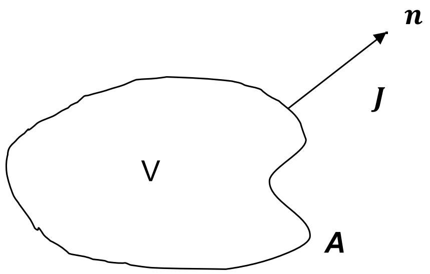

Figure 1. Illustrative control volume.

With $\boldsymbol{J}$ as the net outward flux vector through the area $\boldsymbol{A}$, and G as the net rate of generation, the balance of any given property, Φ, is given by:

$$\int_V \frac{\partial \rho \Phi}{\partial t}\,\mathrm{d}V = -\int_A \boldsymbol{J}\cdot\boldsymbol{n}\,\mathrm{d}A + \int_V G\,\mathrm{d}V \tag{1}$$

Φ here is a property per unit mass of the fluid and ρ is the mass density of the fluid. If we now use Gauss Theorem and, as $\delta V \to 0$, this equation transforms to:

$$\frac{\partial \rho \Phi}{\partial t} = -(\nabla \cdot \boldsymbol{J}) + G \tag{2}$$

Rate of Accumulation = Net Influx through surface + Net Rate of generation.

Fluxes associated with transport processes can be of many types. At this stage we will consider only the most common ones: those due to Convection and Diffusion. Convective flux is due to the motion of the fluid at the continuum scale where the property moves with the velocity of the fluid. The diffusive flux is due to the random Brownian motion of individual fluid molecules that occurs at the molecular or sub-continuum level. At the continuum scale, a net average of this flux is expressed in terms of a diffusivity constant and the gradient of the property of concern. The flux vector, $\boldsymbol{J}$, is then given by:

$$\boldsymbol{J} = \rho u \Phi - \Gamma \Delta \cdot \Phi. \tag{3}$$

In this equation, $\boldsymbol{V}$ is the velocity vector and Γ is the diffusion coefficient. The balance equation then can be written as:

$$\frac{\partial \rho \Phi}{\partial t} = -(\nabla \cdot V \rho \Phi) + (\nabla \cdot \Gamma \nabla \Phi) + G. \tag{4}$$

So, in essence, CFD is really very simple. It is the balance of a property that moves with the fluid. To that extent, it is no different than keeping an account of the bank balance; what is important is to remember the physics behind this process and not the mathematical details.

An important contribution made by Spalding at Imperial College was to generalize this equation to the index format given below to represent any entity that moves:

$$\frac{\partial}{\partial t}(\alpha \Phi) + \frac{\partial}{\partial x_i}(\beta V_i \Phi) = \frac{\partial}{\partial x_i}\left(\Gamma_\Phi \frac{\partial \Phi}{\partial x j}\right) + S_\Phi - \alpha \Phi s_\Phi. \tag{5}$$

Here:

α is the accumulation or Storage Coefficient

β is a specific property of fluid, such as mass density

Γ_Φ is the effective diffusivity Tensor

S_Φ is the source of property Φ

s_Φ is the decay rate of property Φ.

This equation expresses the balance of any property that can move (in continuum approach). This can be fluid itself, heat, mass. electrons, cars, humans, fishes, birds, stars—anything in large enough numbers to be considered a continuum.

3. The origin of modern CFD

Modern CFD started with the advent of the Electronic Computer that became commercially available in the early 1950's. Though there were a few researchers who started solving the fluid flows problems, the birth of what came to be known as Computational Fluid Dynamics (CFD), as we know it today, can be attributed to two brilliant scientists—Frank Harlow at Los Alamos National Laboratory and Brian Spalding at Imperial College. Both worked independently of each other and did not know much about each other's work till the 1970's.

An IBM 701, the first commercially available scientific computer, also known as the Defence Calculator, arrived at Los Alamos in 1953. Soon thereafter, Harlow, leader of the T3 group, started a dedicated exploration of fluid dynamics equations with the Finite Difference Method. The primary interest of his group, was in otherwise intractable fluid dynamics problems related to the US atomic weapons program known as the Manhattan Project. Much of this work was classified and most of the early work appeared as internal reports. Harlow, a physicist by training, had no interest, in commercial applications of CFD. One of the first hints of this work to the outside research community was a paper on the particle-in cell method [42].

An IBM 7090, later upgraded to IBM 7094, arrived at Imperial College, London, in 1962. Unaware of the work at Los Alamos, Brian Spalding at Imperial college, had been trying to get a handle on complex practical problems faced by practicing engineers. His focus was on industrial applications and academic publications. By late 1950's Spalding was already recognized as a major researcher and an expert in the field of combustion. He had made innovative contributions in theoretical and experimental combustion that would lead to the Spalding number or the B factor that is widely used in mass transfer applications today. He was also active in combining the key hydrodynamic, heat and mass transfer concepts of von Karman [43], Kruzhilin [44] and Eckert [45] into a unified framework. He went on to write a seminal book on Mass transfer [46] that has influenced many subsequent researchers. In 1964, he outlined a comprehensive Unified Theory [47] for boundary layers, jets and wakes and with his students [48–51] undertook an extensive in-depth survey of the experimental data to determine the "Universal" empirical constants needed to account for turbulence. He then explored generalized profile methods for numerical solutions of boundary layer flows. His dedication over two decades to explore these concepts and analyse experimental data, proved crucial in developing the Finite Volume Method (FVM) for predicting flows of practical interest that is the most popular method for solving complex fluid flow problems.

It must be emphasised that during these early years, there were other researches who made significant contributions to the development of the technology. These included Barakat and Clark [52], Burgraff [53], Chorin [54], and a few others. However, their focus was mostly on research and on solving specific problems and not on developing generalised CFD methods for distribution to other researchers.

It was Spalding who made CFD a common and popular tool for engineers through publications, training courses and industrial consultancy. He, with his students, published the first books on CFD and incorporated the first consulting company in CFD. Most of the processes that impact practical problems—turbulence, combustion, radiation, wall interactions, multi-phase flows etc. were (and still are) somewhat poorly understood. There is no generally agreed unique mathematical formulation of such processes. Approximations, called models—actually hypotheses—are therefore used to capture some essential aspects of the impact of such processes so that acceptable answers can be obtained for practical design purposes. Spalding boldly ventured into this field—with the philosophy "if it's good enough for design, it's good enough for an engineer"—and derived methodologies that enabled an engineer to gain some insight into complex problems.

In developing the Finite Volume Method (FVM), his group drew expertly and widely on the work by other researchers and added new innovations, explored new avenues and gave the CFD practice a coherent shape that was easy and practical to use for an engineer. Patankar and Spalding [55] had already developed a generalized profile method for solving boundary layer problems that fall in the category of parabolic flows that have a dominant direction of flow. However, a broad range of flows of practical importance fall into the category of elliptical flows with no dominant flow direction. Such flows include those in complex geometries, flows with separation or recirculation, those with strong pressure gradients, and flows with high stream line curvature. Spalding asked two of his students to concentrate on such flows. Runchal started with the separated flows behind a backward facing step and that in a driven-lid square cavity, and Wolfshtein was assigned the problem of the impinging jet on a flat plate. By the end of 1965, Runchal and Wolfshtein came to the conclusion that the parabolic profile method could not be extended to elliptic flows. The only general method then available to tackle the complete form of the Navier–Stokes equations was the method of finite differences. Further development of the profile methods was abandoned at Imperial College and FDM became the method of choice for both parabolic and elliptic flows. Runchal and Wolfshtein [56] published the first general purpose Navier–Stokes solver for two-dimensions elliptic flows and Patankar [57] published a general-purpose solver for parabolic flows.

In 1967, Spalding used his insight to invent a physical rather than a mathematical approach to the FDM. He envisaged the FD grid as a series of Tanks and Tubes as shown in Figure 2 below.

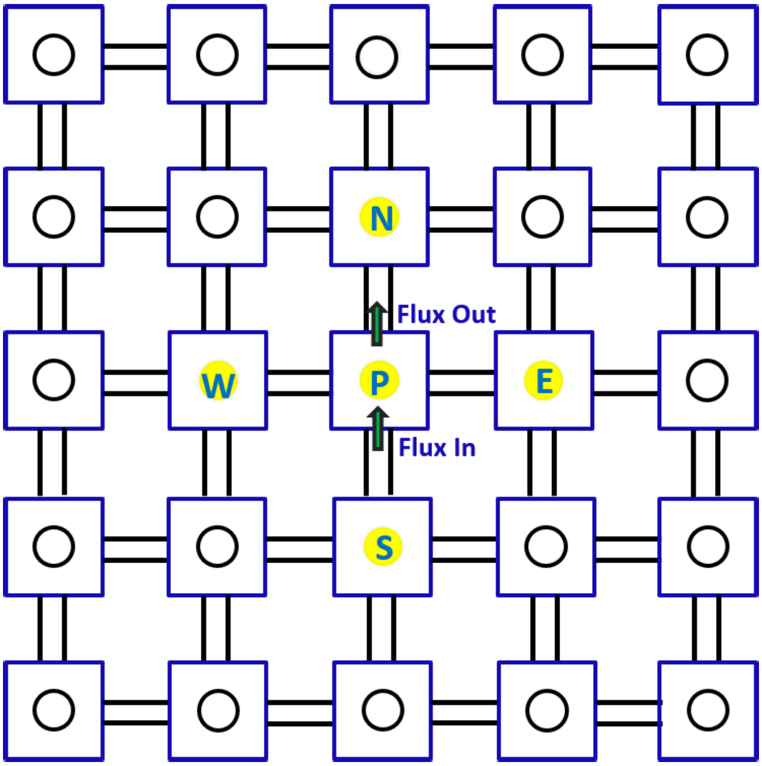

Figure 2. Tank and tube visualization of finite volume method.

With this insight each node of a finite difference grid becomes an independent tank which exchanges fluxes with other tanks by tubes aligned with the grid lines. Though this was a simple conceptual change, it had a profound effect in shifting the focus to physical quantities such as fluxes and amounts of a property rather than mathematical artifacts such as variables, derivatives and basis functions. Runchal [58] realized that the FVM can be generalized by using an integral approach based on Gauss Theorem rather than a differential approach based on the Taylor series which is the basis of the FDM. With these insights, the Finite Volume Method (FVM) was born and the governing equations were reformulated in integral form in terms of accumulated quantities, fluxes, distances, areas and volumes.

Spalding had realized the commercial potential of CFD and a post experience course was organized at Imperial College in 1969, which targeted both academic and industrial communities. He also incorporated the first commercial company in CFD called CHAM in 1969. Based on the work of Runchal, Wolfshtein and Spalding [59, 60], the first ever book on CFD [61] was published by Academic Press. Unlike the focus on intellectual property today, this book contained the full computer code (ANSWER) for solution of the 2-D Navier–Stokes equations which was freely distributed. Spalding had a strict rule that all joint publications carry the names in alphabetic order; Gosman, the editor of the book is therefore listed first.

The extension of FVM to three-dimensional flows came in 1972. Spalding and Patankar [62] developed a three-dimensional velocity-pressure based method—SIMPLE—that revolutionized the field of CFD and established the Imperial College approach as the de-facto standard for solution of the incompressible version of the Navier–Stokes equations. Many researchers have since developed variations of improvements of the SIMPLE approach that have advantages for specific applications. The SIMPLE approach is part of the family of pressure-projection methods which are perhaps the most widely used methods, especially for low Mach number flows [63, 64]. For High Mach number flows the so-called density-based methods are generally preferred [65–67].

Another technology that started soon thereafter was the extension of the Finite Element Method (FEM) to fluids. FEM was originally developed for analysis of structural problems. It employed the minimization principles and Hamiltonian to find the minimum-energy stable state of a system. It was originally applicable only to linear governing equations such as those for structures. Zienkiewicz [68, 69] and his students had considerable success in extending it to fluid flow problems by switching to variational principals. However, FEM, at that time, could not deal with high Reynolds number flows or flows with discontinuities. The path-breaking work in this aspect by Godunov [37] was in the Russian literature and was not yet widely known in the West. FEM also lacked a clear theoretical basis for fluids because a unique minimum energy state does not exist for nonlinear systems. A bigger drawback was that FEM uses global error minimization. There are many systems, such as those with combustion, where a small change or a small error, say in temperature, can lead to orders of magnitude larger error in some other quantity, such as the reaction rate. Local mass balance, therefore, can be very important for these highly nonlinear systems. Today, the differences are semantics since both FEM and FVM have appropriated and borrowed from each other. However, on the practical side, most current commercial codes still use FVM.

As mentioned in the introductory section, turbulence plays a very important role in practical flows. Before the 1960's, the dominant method to deal with turbulence was the Prandtl mixing length model [70] that was based upon the concept of a universal constant (von Karmon constant) and a mixing length that characterized the scale of turbulence eddies. Theoretical foundations of more advanced turbulence models were laid by Chou [71], Prandtl [72], Rotta [73] and Davidov [74]. However, before the electronic computer, it was not possible to make any practical use of these equations. It was but natural that much of the early work on turbulence models occurred at Los Alamos and Imperial College lock-step with CFD. Based upon the Reynolds-Averaged Navier–Stokes (RANS) equations, Harlow and Nakayama [75] developed a two-equation model that allowed characterization of turbulence by a parameter for turbulence kinetic energy (k) and one for a length scale of eddies represented by the rate of dissipation of turbulence (ε). This was the so-called k-ε model. Launder and Spalding [76] generalized this approach and developed "universal" constants that are required for the application of this model. The k-ε model became the de-facto standard for a while. Saffman [77] and Wilcox [78] developed a k-ω model where the length scale is now represented by the vorticity (ω)—essentially a time scale—of the turbulence of eddies. This offered some advantages in representing turbulence near walls. However, turbulence is characterized by a very diverse spectrum of kinetic energy and length scale of eddies. Representation by an "average" energy and an "average" length scale does not do it full justice in most practical applications. An inherent assumption in two-equation models is that turbulence is isotropic or that its anisotropy can be defined by a single constant. This is obviously not the case for most flows near walls or flows with strong pressure gradients or stream-line curvatures. Over the years many turbulence models have been developed to account for complexities of turbulence in practical flows. These include Reynolds-stress models, hybrid k-ε-ω models, LES, ILES, VLES, DES and DNS models, and many other variations. It is outside the scope of this paper to go into the details of these. Excellent reviews of turbulence models are available elsewhere [79–91].

It must be stated here that in the 1960's and 1970's, with the wide availability of electronic computers, computation of flows (and structures) was a very active field. Many researchers made a number of important contributions that made it possible for the Los Alamos and Imperial College groups to develop their generalized approaches. A few of these have been mentioned earlier. In addition to further work on the FDM and FEM, considerable progress has been made in developing the Spectral, and the Lattice Boltzmann approaches to CFD. Further, most of the earlier work in CFD was based on the 1st and 2nd order schemes which stressed stability over accuracy. Since then, many higher order schemes have been developed to improve accuracy with limited computational resources. Also, many significant developments have taken place in numerical analysis and solution of the matrix of equations that result from the application of these numerical approaches. A complete anthology of these is considered beyond the scope of this subjective and personal account.

One interesting fact is that the acronym, CFD, was not coined by either Harlow or Spalding. It was first used by Pat Roache in his famous book called Computational Fluid Dynamics [92].

4. CFD today

Since its introduction only a few decades ago, the field of CFD has mushroomed into practically every aspect of human existence. IMARC [93] estimated that the global commercial CFD market will surpass US$16.0 billion by 2024. Commercial CFD is only a small part of the total CFD activities. The actual CFD market is at least an order of magnitude larger since most of the CFD research and problem solving occurs in government organizations and private R&D departments of large corporations and research organizations that is not directly monetized.

The period since 1970's, has been a period of significant innovation and consolidation. Early use of CFD was mostly for aerospace and defense applications. However soon its potential was realized in other fields. Most flows of practical interest are turbulent. Combustion and chemical reactions play a very important role in energy conversion, chemical processing and many other applications. Thus, significant developments took place in developing models for turbulent flows, interactions of turbulence with heat and mass transfer, and flows with combustion and chemically reactions. These turbulence models made it possible for wide use and acceptability of CFD. However, our focus here is on CFD and not on turbulence which is a discipline in itself. Excellent reviews of turbulence models are available which have been referred to in the earlier section.

CFD has already made a significant impact on the hitherto conventional applications in the aerospace, automotive, industrial and chemical engineering. The literature is full of such examples and we will not summarize these here. But among the non-traditional applications, there are some areas where CFD is making a significant impact. Some of these are summarized below.

Prediction of weather has long been an area of major concern and CFD has been the cornerstone of these predictions. Many developments in CFD have had their origins in weather and climate related research. Richardson [26] undertook one of the first numerical prediction exercises for any type of flow with a finite-difference based approach to weather prediction. The widely used LES model for turbulence has its origins in the work of Smagorinsky [94] to model atmospheric circulation. Lynch [95], Edwards [96] and Pu and Kalnay [97], among others, have summarized the history and the basics of weather prediction models.

Wind energy is playing an increasingly larger role in moving towards a zero-emission future and CFD has been applied in this area for various aspects including assessment of wind energy potential [98–101] and flow behind wind turbine wakes [102, 103]. Blocken [104] has summarized the developments in Wind Energy over the last 50 years.

The application of CFD to Environmental flows has a long history. Starting in the early 1970s, such studies have contributed immensely to the understanding of our physical environment consisting of the surface water, ground water and the atmosphere. CFD has been applied extensively to predict the behaviour of flow in these systems. This has involved problems related to pollution as well as management of these valuable resources. Analysis of Environmental flows is now a burgeoning field with its own literature, professional societies and government organizations looking after various environmental aspects. CFD models now play a major role in decision making of a number of government agencies and private organizations around the world.

Early examples of atmospheric and air quality models are available in Lange [105], Joynt and Blackman [106], Runchal *et al.* [107], and Pepper and Cooper [108]. Since then, a vast literature concerning development, applications, guidelines and reviews for various aspects of atmospheric CFD models has been published. This includes, Di Sabatino *et al.* [109], Tominaga *et al.* [110], Pepper and Carrington [111], Franke *et al.* [112], Leelossy *et al.* [113], Toja-Silva *et al.* [114] and Kadaverugu *et al.* [115].

The surface water flow applications have been across the board to rivers, estuaries, coastal waters and offshore areas. Effluent discharges from industrial and urban activities into rivers, lakes and coastal waters have been focus of CFD studies from the early days of CFD (e.g., [116–118]). Zhao *et al.* [119] and Mohammadian *et al.* [120] provide a recent review of such effluent discharge applications. Miller *et al.* [121] have given an overview of water resource modelling for both surface and ground water flows.

Storm surges and Tsunamis have been an active area of application of CFD since the 1970's [122, 123]. However, the devastation caused by the 2004 Indian Ocean Tsunami and the risk posed by 2011 Tsunami that affected the nuclear reactor in Fukushima has led to an increased focus on numerical modelling of the runup and inundation due to Tsunamis and storms [124], and in the uncertainties associated with such forecasts [125]. Marras [126] has reviewed various tsunami modelling approaches and recent developments due to the advent of GPUs and exa-scale computing.

Groundwater has always played an important role in our water resources. In the recent past, the quality of groundwater has been seriously impacted due to leaching of chemicals and pesticides from agricultural, industrial and urban activities. Study of these resources is therefore a major incentive for proper management and utilization of these resources. From the mid-1960's CFD models were developed to analyse groundwater resources. About the same time, the Oil and Gas industry realized the potential of these CFD models for optimization of production. Later, starting mid 1970's, it was realized that the continued use of nuclear power required an option for disposal of nuclear waste. Various options were explored but, finally, the consensus was that the most practical option was near-surface (for low-level waste) or deep underground (for high-level waste) disposal of Nuclear Waste. The heat generated by this waste can drastically modify the ground water flow patterns and any leaching of this waste over time can create a hazard as well as degrade the ground water quality. All this has made CFD model development and application a very active field. Early examples of such models are those from Freeze and Witherspoon [127], Neuman and Witherspoon [128], Bredehoeft and Pinder [129], Pinder [130], Trescott *et al.* [131], Dillon *et al.* [132], Narasimhan *et al.* [133], Runchal and Maini [134], Reeves *et al.* [135] and Runchal [136]. More recently numerous reviews and applications of such models have appeared in the literature [137–141].

Ground source heat pumps are an extremely efficient source for HVAC and water heating that make use of the Earth's relatively constant temperature throughout the year. CFD is being used increasingly to explore the potential for ground source heating and cooling and optimizing the design of such heat pumps [142–144].

With global warming leading to higher average temperatures, urban planners and designers are using CFD to understand and mitigate the urban heat island effect [145] that requires increasing capacity of air conditioning to make urban space habitable. Here CFD is playing an increasingly important role in HVAC and energy efficiency [146], and in fire safety [147–149], of buildings. CFD is also being used by urban planners in novel ways to design evacuation strategies during catastrophic events [150].

Over the years, the food processing industry has made extensive use of CFD [151–154]. Processes such as spray drying and spray freezing of food use CFD to analyze and improve the product quality. CFD is also being used to analyze heat transfer and air flow during thermal processing of canned solid and liquid foods, and for the analysis of processes such as baking, pasteurization, sterilization, refrigeration, crystallization, and even for understanding of the digestion process itself.

Competitive sport started making use of CFD in the early nineties. Motor racing was among the first to utilize CFD for competitive advantage [155]. Apart from external aerodynamics of the vehicle, CFD has been applied to engines, intakes, exhausts, radiators, wheels, etc. Future applications will probably include maneuvers such as overtaking and complex motion such as aquaplaning etc. CFD is also used in sailing yacht design [156–158]. Apart from sail design, CFD can be used to analyze the hull shape, the interaction between the various underwater and above water components, sailing tactics, etc. CFD has also been used to understand the aerodynamics of ball sports and this trend will continue in the future [155, 159]. Wei *et al.* [160] have provided a detailed discussion of the fluid mechanics of competitive swimming. Goff [161] has provided a review of research into the aerodynamics of sport projectiles. Immonen [162] has used CFD and machine learning for the optimal design of golf balls.

In the last decade or so, CFD has started to revolutionize the pharmaceutical, biomedical and healthcare fields. As may be expected, the advent of the COVID pandemic immediately led to the application of CFD to the fluid mechanics of disease transmission [163, 164]. CFD has been used extensively in the aftermath of the Covid-19 pandemic to investigate the risks of disease transmission in indoor settings and examine the proposed social distancing rules [165]. The study of airborne transmission of respiratory pathogens under different ventilation conditions in indoor spaces is of particular interest. CFD has been used to examine the dynamics of virus-bearing aerosol droplets including growth in dry and humid air [166], in confined spaces such as elevators [167], buses [168], trains [169], aircraft [170] and in devising mitigation prevention strategies via airflow modulation [171]. CFD has also been used to ensure safe transportation of SARS-COV-2 vaccines by refrigerated containers [172].

In a similar manner, computational hemodynamics is making critical contributions to understanding the dynamics of the cardiovascular and cerebrospinal fluids. CFD is now an important part of the patient-specific cardio-vascular modelling, brain imaging, drug delivery and transport in the human body [173–176]. CFD has also made significant contribution to diagnosis and treatment of diseases, development of medical devices, and surgical planning [177–180]. CFD is already an important tool for research, risk assessment, diagnosis, and treatment planning for aneurysms [181–184]. CFD is also being used to estimate the wall shear stress in blood vessels [185] and to analyze and predict the hemodynamics post treatment of aneurysms with flow diverting stents [186].

Other applications of CFD have been in the clinical investigation and surgical planning for the respiratory system [187–190], bone tissue [191], the eye [192–194] and the inner ear [195].

In summary, CFD finds pervasive use in all spheres of human activity and also helps in understanding and managing of the environment that has become a critical issue due to the impact of human social and economic activities.

5. Primary challenges

Though CFD is now a very mature science, many challenges remain on the horizon for it to become a practical and reliable tool in the hand of an engineer. CFD today is a combination of three components: Science, Art and Guesswork. Science is in the Navier–Stokes and the Boltzmann equations, along with the equations for thermodynamics, heat and mass transfer, that are based on accepted principals of mathematics, physics and chemistry. Art comes in designing an efficient software tool because, due to limited computer resources, compromises have to be made in designing an efficient computing algorithm, selecting an economical matrix solver and wrapping the CFD tool in an effective user interface. What is really problematic about CFD, though, is the guesswork that is required today to solve all but a subset of practical problems. The fact is that, for many practical problems, we do not understand many aspects of real fluids and the phenomena that govern the flow. It will be more accurate to say that we understand less than we pretend to. For many flows, CFD rests on uncertain scientific basis—we only have hypotheses or empirical data to complete our simulations. This is the Knowledge challenge.

This lack of knowledge—and the uncertainty associated with it—falls under two categories—the Epistemic uncertainty that relates to our lack of knowledge of a phenomenon and the Aleatoric uncertainty that arises from inherently random and stochastic phenomena that we cannot fully define or account for.

In the first category we have many aspects of real fluids where underlying physics and chemistry is poorly understood with no agreed mathematical basis. Most important of these is perhaps the lack of understanding of turbulence. It has been 200 years since Navier recognized linear and non-linear flows and almost 150 years since Reynolds formally studied turbulence. It is turbulence models such as those described in [76] that made possible the wide use and acceptability of CFD. Yet, there is no clear universal acceptance of how to deal with turbulence. Neither has a widely acceptable model of turbulence emerged after research spanning more than 60 years. There are multiple models of turbulence—all with limited applicability. What is worse is that, except for a very limited class of problems, it is practically impossible to be *a-priori* certain that a given turbulence model will provide reliable predictions. One has to conduct expensive empirical tests, or use multiple simulations, or use multiple models, to obtain a measure of confidence in the predictions.

Another area of lack of knowledge is that of chemical or biological reactions. These play a very important role in many aspects of industry, environment, and life itself. Most of our energy needs are met today with processes that depend on chemical reactions. The environment that we live in and breathe is a result of complex chemical and biological reactions. Our body depends on chemical and biological reactions to sustain itself. Yet, for most reactions of importance we do not fully understand the reaction system or the rate of reaction. A simple reaction between hydrogen and oxygen can be described as a 1- or a 50-step reaction based on the operating conditions and the objectives of the simulation. Further, the reaction rates for many reactions of practical interest, such as for complex hydrocarbons that are the mainstay of our energy generation, are not known except under a limited set of thermodynamic conditions. The situation becomes even more complicated when the flow is turbulent. The turbulence-chemistry interaction is a poorly understood phenomena—again with multiple models with limited applicability. There is no clear understanding of many biological reactions that occur in living organisms such as those in a liver, blood flow or the blood–brain barrier. Another example is that of the reactions that occur deep in the earth such as those in molten rocks at very high temperatures and pressure. There are many other examples of Epistemic uncertainty that impact application of CFD to problems of practical interest.

The second kind of uncertainty, the Aleatoric uncertainty, also plays a very important role in CFD simulations of real-life systems. Often, we don't even know the domain of influence for such simulations and many of the variables that affect simulations are inherently stochastic or unknown. For example, the synchronic initial and boundary conditions for atmospheric, ocean or groundwater simulations, are almost never known with acceptable certainty. For ground water simulations, the spatial or temporal distribution of the properties, such as the permeability or porosity of the soil, are known only at a few selected locations though they are required throughout the domain of study. All such quantities have to be either guessed as “mean” or “most probable” values or assumed to be stochastic functions with assumed probabilities. Often, therefore, multiple simulations are needed to gain any confidence in the predictions. When multiple variables are stochastic, the problem becomes orders of magnitude more difficult. There is no exact mathematical methodology to deal with multivariate uncertainty. Resort has to be made to assumptions about the interaction between such variables with decreasing level of confidence as the number of stochastic variables increases.

Another group of challenges involve multiple coupled phenomena. Almost all practical systems involve multiple physical phenomena such as fluid-structure interaction, heat or mass transfer, chemical reactions and electromagnetism. Thus, multi-physics is, or will become, the norm for many CFD simulations. Many problems involve temporal evolution and structural deformations. Examples are the folding and flapping of wings of aircrafts or the blood flow through a pulsating heart. These add an order of magnitude of complexity and uncertainty due to multi-physics interactions and phenomena that are poorly understood.

Many problems of great practical interest involve phase change and/or interaction between multiple fluids or fluids and solids. Phase change plays a very important role in energy generation as well as refrigeration. Droplet formation and evaporation are often an integral component of energy production. The processes involved in such flows are so complex and dependent on operating conditions, that currently the only reliable method of simulation is through empirical relations that apply to distinct regimes of flow. For example, there are many gaps in our knowledge of how, for example, a jet of water breaks down into droplets in the ambient air or when condensation or evaporation occurs such as in the case of water and steam. When multiple fluids are present, our lack of understanding is even more limiting. Processes such as atmospheric interaction with the ocean, or the flow of water, air and immiscible oil in a typical groundwater situation are poorly understood. In such cases, the only option is to resort to empirical data or models that are approximations with limited applicability. The last half century has been rich in attempts to apply CFD to understand the physics and processes involved in such complex coupled processes.

Another complex and poorly understood phenomenon is that of crystal formation and growth which plays an important role in energy generation, semiconductor manufacturing, computing, space research, pharmaceuticals, and other emerging technologies. The complex processes involved in this field are multidisciplinary in nature and involve multiple order of magnitude scaling. For example, understating of striation and epitaxial growth modes are challenges that are poorly understood. In 1902, Verneuil developed his well-known growth method, also called, flame-fusion, that formed the basis of modern crystal growth technology. In 1915, Czochralski developed a method for growth of single semiconductor crystals which was then improved on by Teal, Little and others [196–199]. Crystal growth is a very active subject for mathematical modelling and computer simulation [200–203].

Anther complexity that arises is that of multiple disparate spatial or temporal scales. For example, in a flow involving combustion, the reaction rates can vary from femtoseconds to milliseconds while the flow scale can be on the order of seconds. Air pollution in the vicinity of a building is impacted by both local and meso-scale flows. This requires resolution near a building at scales on the order of meters while the atmospheric flow has a range of influence that extends to hundreds or thousands of meters. If the Knudsen number is high, or a problem involves interaction between nano and macro scales, the governing equations may transition from Navier–Stokes to Boltzmann. Though we may understand the processes involved, such problems, often present computational challenges and require resources beyond those currently available. Compromises have to be made to resolve these multiple scales that impact the accuracy and reliability of predictions.

An important class of phenomena that requires computational resources beyond those currently available is that of the integro-differential processes. Such processes imply influences that involve spatial or temporal coupling between remote points and add spatial or temporal integration terms to the governing equations. Thermal radiation is a good example where each point in space radiates to the other. Other prominent example is that of the aerosols where the individual droplets can coalesce, break down and move at different speeds than that of the fluid or other droplets. In general, such processes are poorly understood and approximations have to be made.

Finally, we face some computational challenges. After 50 years of CFD, we still have no satisfactory method to deal with the convection terms in the equations. The flow regime changes from elliptic to parabolic to hyperbolic because of interaction between convection and diffusion terms. Diffusion is a second-order process that is linear in nature. Convection, on the other hand, is a first-order process with nonlinearities. No robust and accurate discretization scheme exists that meets all the requirements of actual physics of flow. Once the governing equations are discretized, we face another challenge. The governing equations are non-linear and admit multiple solutions (turbulence is a good example), but the available computational methods generate a linearized matrix of equations. Further, in today's engineering practice it is not unusual to have a matrix with millions of algebraic equations. There is no satisfactory matrix solver that is both robust and accurate. Most common practice is to use an iterative solver that may or may not produce a solution. If a solution is produced there is no guarantee that it is accurate and admissible. So, there is an overwhelming need for a robust, accurate and economic matrix solver. Another challenge on the horizon is that the computer architecture is evolving towards parallel and cloud computing systems. CFD methods are mostly based on implicit or partially implicit algorithms that were primarily developed for computers that were sequential or had a few parallel pipes. The CFD algorithms today do not scale linearly with processors or make optimal use of cloud computing with, say, thousands of processors. Most run into computational or communicational limitations.

6. The future of CFD and CFD of the future

As mentioned earlier, there are many challenges that need to be overcome. CFD and its affiliate subjects, are among the most active fields of research. Considerable advancements are likely in the next couple of decades that will put CFD on firmer grounds. These will include developments in turbulence, physics, fluid and material properties and processes, numerical algorithms, matrix theory, geometry and mesh generation, visualization and post-processing, uncertainty quantification, higher order schemes, and user interfaces. A more complete discussion of these is given by Runchal and Rao [204].

The CFD codes as we know them today will disappear; they are time consuming to learn and difficult to use. Devising a grid that produces a good solution can take weeks if not months. The CFD codes are resource intensive and it is not unusual for a simulation to take weeks or even months. More important, it is difficult to quantify the overall reliability of CFD predictions for critical applications. Even with modern computing power and recent advances in physics-based models, it is still very challenging to represent the physics of the flow accurately. One can design a gas turbine engine by using CFD but it would not be wise to put that in an aircraft without extensive tests and modifications of the engine. Such fundamental limitations still continue to plague us today. A more complete discussion of these limitations and the future prospects of CFD is available in Patterson [205] and Runchal [206]. Instead of the general purpose CFD codes, it is most likely that most CFD applications will be through "Apps" that relate to dedicated niche applications. These CFD Apps will embed a CFD engine and extensive data libraries in an intuitive user interface with Virtual Reality software and design tools.

A fundamental driving force for change, in the form of Machine Learning and Artificial Intelligence (ML/AI) has made its impact in the last decade. Of course, ML has been explored since the 1980's [207]. But primarily due to limitations of computational resources, its use was neither extensive not pervasive. It is only in the last few years that it has evoked considered interest.

The ML technology is already transforming our lives and we believe that it will have a substantial impact in almost every aspect of life. Today, the profound impact of this technology is evident in self-driving cars, natural language interfaces, speech recognition and medical imaging—to name a few. Now ML is beginning to have a considerable impact in the field of CFD [208, 209]. Machine learning is being used to improve the accuracy as well as the computing efficiency of CFD solvers [210]. Several researchers have trained deep neural networks to replace or enhance the usual spatio-temporal discretization schemes [211–215]. Learned discretizations have also been applied to shock capturing [213]. Kossaczka *et al.* [216] have developed a fifth-order WENO shock capturing scheme which uses optimized coefficient output by a trained deep neural network. Partial differential equation solvers assisted by trained deep neural networks have demonstrated accuracy enhancements and performance gains [217]. Deep learning approaches have also been applied to speed up the large linear systems that arise during the numerical solution of partial differential equations [218].

Currently, the Artificial Neural Network (ANN) appears to be the most powerful machine learning technique. It can be used for the (approximate) solution of ordinary or partial differential equations as well as differential algebraic systems. The first known use of a neural network for the approximate solution of differential equations was by Lagaris *et al.* [219]. A typical ANN consists of an input layer, one or more hidden layers and an output layer. Each layer takes its input from the preceding layer, performs a linear transformation with a set of weights followed by a non-linear transformation via an activation function and delivers its output to the next layer. ANNs with a large number of hidden layers are typically referred to as Deep Neural Networks [DNN]. When a DNN is constrained so that it obeys the governing principles of physics, it is called a Physics Informed Neural Network (PINN) or Physics Informed Machine Leaning (PIML) [208, 220].

For a typical Machine Learning CFD application, the known initial and boundary conditions are input into a deep neural network. The output obtained is then substituted into the governing set of equations that may consist of Navier–Stokes and other multi-physics equations. If the residue criteria for the governing equations are satisfied, it is considered an admissible output. If not, then the input is appropriately modified to re-train the neural network and update the neural network parameters. Any experimental or real-life data available for the system is used as an additional constraint to train the neural network. ML, augmented with real-life data, can also be trained to deal with highly nonlinear problems and augment knowledge of phenomena that are not well understood. For example, if the RANS turbulence model doesn't work for some particular application, a PINN can assist in adding a term that allows the model to better simulate the flow [87, 221]. The PINN has been used to provide data driven subgrid scale closures for large eddy simulations [222] and for near wall modelling for LES [223]. Another recent innovation is the development of a PINN for modelling of multiphase flows in porous media [224]. Modifications have been proposed to PINNs to increase their accuracy for problems that exhibit multi-scale behavior, such as in turbulence, by enforcing temporal causality through a weighted loss function that includes the residual at all times steps up to the current step [225].

One use of ML is to develop a surrogate or reduced order model (ROM) that captures some essential components of the behavior of a complex system with substantially reduced storage and CPU requirements [226]. These model order reduction methods (MOR) are typically based on Proper Orthogonal Decomposition (POD), Principal Component Analysis (PCA) or Dynamic Mode Decomposition (DMD) or Reduced Basis Methods (RBM) [227–232].

An alternative, and perhaps more promising, ML technique for dealing with the resource limitations is to develop a Digital Twin for a complex system which is a virtual replica of a physical product, process or service. Digital Twin was named as one of the top ten strategic technology trends by Gartner [233]. In the CFD context, the basic process consists of defining an objective function that is of primary interest for engineering design. Then, a sufficient spectrum of input variables for that system are fed into a PIML that is constrained by the governing equations, or a ROM if available, and any known empirical data. A matrix of the output objective function is then generated as a function of the input state of the system [234]. Once defined, a Digital Twin replaces the target physical component in the CFD simulations, or it can be used directly for purposes of engineering design.

Other parallel developments that are likely to impact CFD are the Application-Specific-Integrated Chips (ASICs) and System-on-a-Chip (SOC's). As the names imply, these essentially encode a specific computational algorithm in hardware and usually provide an order of magnitude, or more, speed up over the equivalent implementation in software. A typical example of ASIC is that for Fourier-Transform [235,236]. With these developments, CFD will find application in almost every sphere of human activity. The current generation of CFD codes will be overshadowed by niche and application-specific software tools augmented by Digital Twins, ROMs, ASICs or SoCs. This will make it possible to embed CFD engines in engineering design systems. Beyond traditional applications, we expect CFD engines to be embedded in common appliances and devices such as refrigerators and HVAC systems. CFD engines may also be built into analysis tools such as MS Excel or OpenOffice to assist in design calculations. CFD analysis will be a standard tool for a practicing engineer rather than the domain of a CFD expert.

7. Conclusion

Since its inception in the mid-20th century, CFD has become an invaluable tool for almost every sphere of human activity. However, a number of challenges remain. In many instances we lack both the physics and the mathematical tools to adequately understand the behavior of fluids. As regards physics of fluids, there is a knowledge gap in our basic understanding of many of the properties, processes and phenomena that govern fluid flow. Additionally, the governing equations are non-linear, but due to lack of adequate mathematical tools, we resort to their linearized equivalents for numerical solution. Also, many practical problems involve stochastic phenomena which are poorly understood and hard to describe mathematically. The current generation of CFD tools are resource intensive and require extensive training and experience. They are neither robust nor provide a high level of confidence in the prediction. One has to resort to testing, empirical data or sensitivity studies to ensure that the predictions are reliable for practical purpose. The on-going research and development activities will lead to a better understanding of the physics of flow and improvements in CFD tools. However, we expect that compromises will have to be made for the foreseeable future.

The CFD of the future will be revolutionized by machine learning and advances in computer hardware, big data and virtual reality tools. PIML will enable development of reduced order models (ROM) and Digital Twins. Advances in hardware will lead to ASICs and SoC's for niche applications. Big data tools will make it possible to build libraries of fluid properties and application-specific simulations that can be used to train neural networks and enhance confidence in predictions. Advances in hardware and software and big data libraries, and Virtual Reality tools will enable a practicing engineer to effectively visualize a fluid system, interact with its components, conduct CFD simulation, and control its behavior through dynamic intervention.

The current generation of CFD codes will be overtaken by CFD software tools that are application-specific, easy to use and limited in scope. CFD engines will be embedded in engineering design systems such as CAD/PLM, software or other design and analysis software tools. Built-in CFD engines may become an integral part of appliances and devices to enhance their performance and control.

The engine in an automobile has evolved from being the focus of attention for the user to being an inconspicuous component that the user is seldom concerned about. The focus of the user is on the interface with the vehicle and performance of the vehicle. CFD of the future will be more like the engine that drives a car—it is essential for the functioning of the device but the user does not have to be concerned with its intricacies.

Declaration of interests

The authors do not work for, advise, own shares in, or receive funds from any organization that could benefit from this article, and have declared no affiliations other than their research organizations.

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