

Journal of Artificial Intelligence in Fluid Dynamics

The Netherlands Press

Article

An Overview on basics of Computational Fluid Dynamics

NETKACHEV Aleksandr

Robots, Mechatronics and Robototechnics system, Department of Automation, Peter the Great St.Petersburg Polytechnic University (SPbPU), Russian Federation E-mail: netkachev.alexamdrg@yandex.ru <https://orcid.org/0000-0003-2710-8743>

Abstract. CFD – Computational Fluid Mechanics gives mathematical approximation for the equations which control motion of fluid. CFD application to analyse the problem of a fluid involves the following stages. Firstly, the numerical expressions defining the flow of fluid were developed. They are generally a collection of PDE – Partial Differential Equations. These solutions are then partitioned to provide a mathematical counterpart of the expressions. The area is then partitioned into little grids or elements. Finally, the initial circumstances as well as the initial conditions of given problem are employed to solve those equations. All Computational Fluid Dynamics (CFD) codes comprise three basic elements: (1) A pre-processor, that is utilized to feed the issue geometry, create the grid, as well as explain the flow parameter as well as the initial conditions to a code. (2) A flow solver, that is used to solve the governing equations of flow pursuant to the conditions specified. There are 4 distinct approaches utilized as a flow solver: I finite difference technique; (ii) finite element technique, (iii) finite volume technique. (3) A post-processor, that is used to manipulate the information and provide the outcomes in graphical & easy to read manner.

Keywords: CFD, Finite Difference Technique, Finite Volume Technique, Finite Element Technique.

Journal of Artificial Intelligence in Fluid Dynamics Volume 1 Issue 1 Received 25 May 2022 Accepted 22 June 2022 Published 10 September 2022 Online at https://www.jaifd.com/

1. Introduction

CFD – Computational Fluid Mechanics including its wide range of applications, has already been widely employed throughout both research & industry since its birth in between the past ten decades [1-6]. Example from the field of study concerned with remediating river water. There would be no life without rivers. In spite of rising worldwide thirst, fresh water supplies are limited. Water quality and quantity assurance is challenging due to a number of issues [7]. Due to this need, the Floating Water Treatment System was developed. The device is intended to improve lake water quality and water movement. The effectiveness of the device in treating water led to the creation of a prototype [8], The Independent Inflatable Water Treatment Device's performance was then captured by simulation and modelling using CFD analysis [9]. A valuable resource, CFD employs numerical methods to approximate the fluid mechanics governing equations in the region [10, 11] Furthermore, it accurately predicts phenomena like as fluid movement, heat transfer, mass and heat transfer, chemical reactions, as well as similar processes by numerically solving the underlying mathematical equations [12, 13, 14]. Water fluxes, pressure, and velocity were simulated and modelled using computational fluid dynamic (CFD) analysis [9]. Computational fluid dynamics (CFD) is the study of utilising computers to generate numerical solutions to issues involving fluid flow. CFD can now obtain solutions to a wide variety of flow problems, whether they are compressible, incompressible, laminar, turbulent, chemically reacting, or non-reacting, thanks to the development of fast, large-memory computers [15, 16, 17, 18, 40]. There are several applications of fluid mechanics where CFD has been used successfully. Vehicle and aircraft aerodynamics, ship hydrodynamics, fluid dynamics in pumps and turbines, combustion, and so on are all examples [19, 20]. Wind loading, resonance of structures, wave and tidal energy, ventilation, fire and explosion hazards, pollution dispersion, wave load capacity on coastal areas structures, fluid structures like weirs as well as spillways, sediment transport, and many more are all examples of how civil engineering is put to use. Ocean currents, weather prediction, particle physics, blood flow, and heat transport around electronic circuits are some of the more specialised uses of CFD [19]. Through the application of the first principles of mechanics to just a fluid, a system of linked non-linear PDEs are formed. As a rule, these equations can be solved analytically for engineering issues. Mathematical models are constructed taking into account the fluid's physical properties, including the conservation of mass states, momentum, energy, etc., over the entire region of interest. Simplifying assumptions have been made for the problem's appropriate boundary conditions to facilitate a quick and painless solution. Initial circumstances and the boundary conditions are necessary to solve the Navier-Stokes equation as well as continuity equation, the fundamental equations of fluid dynamics [9, 21].

2. Foundations of Computational Fluid Dynamics

What CFD is looking for, precisely, is the million-dollar question. Let's pretend the volume below is the region of interest, the region where fluid flow happens, or the volume under control.

Fig. 1: An issue in regulating the flow's volume

Here, u, v & w represents the x, y & z velocities, respectively. Solving the velocity field & pressure field within the control volume is a typical CFD problem $[22-23]$. If the parameters u, v, w & p can all be determined, then CFD can be considered complete. There must be four equations in order to find the answers to the four unknowns. Our next move is to deduce these four equations. These equations will be formulated using conservation principles applied to a restricted volume (Figure 2). If we start with the fundamental concept of mass conservation, we get a single equation [24].

Fig. 2: Consideration of a differential control volume in the development of conservative equations

At any given location, the rate of mass increase is just the difference between the incoming and outgoing masses. This is how it looks like in differential form:

$$
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho v)}{\partial t} + \frac{\partial (\rho w)}{\partial t} = 0
$$

The last three equations are derived by Newton's 2nd law of motion, which is equivalent to the law of conservation of momentum. Considering that momentum is really a vector quantity, it follows that there will be three aspects to it. In the end, you'll have three separate equations. What follows is a differential representation of the phenomenon:

F=ma

$$
\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} + \frac{\partial(\rho u w)}{\partial z} \n= -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left(\lambda \nabla \cdot \nabla + 2\mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] + \rho f_x
$$

$$
\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho u v)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho v w)}{\partial z} \n= -\frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left[\mu \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \right] + \frac{\partial}{\partial y} \left(\lambda \nabla \cdot \nabla + 2\mu \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) \right] + \rho f_y
$$

$$
\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho uw)}{\partial x} + \frac{\partial(\rho vw)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z} \n= -\frac{\partial p}{\partial z} + \frac{\partial}{\partial x} \left[\mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \right) \right] + \frac{\partial}{\partial z} \left(\lambda \nabla \cdot \nabla + 2 \mu \frac{\partial w}{\partial z} \right) + \rho f_z
$$

There will be a single equation covering all possible directions. We will so have four equations in all. The set of these equations is often referred to as the "Navier-Stokes equations" [24].

2.1. Equation of Navier-Strokes

The Navier-Stokes equations consist of 3 fundamental conservation laws which may be derived from the generic version of the governing equations indicated in the preceding equation. The mass conservation (continuity equation) [25] holds true. The Equation of Continuity, Equation of Momentum, and energy equation can be derived from the above by using the conservation of mass, momentum, and energy principles:

Equation of Continuity:

$$
\frac{D\rho}{Dt} + \rho \frac{\partial U_i}{\partial x_i} = 0
$$

Equation of Momentum: ρ

$$
\frac{\partial U_j}{\partial t} + \rho U_i \frac{\partial U_j}{\partial x_i} = -\frac{\partial P}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_i} + \rho g_j
$$

Where,

$$
\tau_{ij} = -\mu \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) + \frac{2}{3} \delta_{ij} \mu \frac{\partial u_k}{\partial x_k}
$$

Equation of Energy: $\frac{\partial T}{\partial t} + \rho c_\mu U_i \frac{\partial T}{\partial x}$ $\frac{\partial T}{\partial x_i} = -P \frac{\partial U_i}{\partial x_i}$ $\frac{\partial u_i}{\partial x_i} + \lambda \frac{\partial^2 T}{\partial x_i^2}$ $\frac{\partial^2 T}{\partial x_i^2} - \tau_{ij} \frac{\partial U_j}{\partial x_i}$ ∂x_i

For example, I is time-dependent local change, II is momentum convection, III is the force of the surface, IV is the interchange of momentum between molecules (diffusion), and V is the force exerted by mass. A more compact form of the continuity equation as well as the momentum equation can be obtained if the liquid is compressible:

Equation of Continuity:
$$
\frac{\partial U_i}{\partial x_i} = 0
$$

Equation of Momentum:

$$
\rho \frac{\partial u_j}{\partial t} + \rho U_i \frac{\partial u_j}{\partial x_i} = -\frac{\partial P}{\partial x_j} - \mu \frac{\partial^2 u_j}{\partial x_i^2} + \rho g_j
$$

The Navier-Stokes equations can be written in a more straightforward generic form.:

$$
\frac{\partial(\rho\Phi)}{\partial t} + \frac{\partial}{\partial x_i} \left(\rho U_i \Phi - \Gamma_\Phi \frac{\partial \Phi}{\partial x_i} \right) = q_\Phi
$$

The Equation of Continuity, Equation of Momentum, and Equation of Energy can be obtained when = 1, Uj, and T. All of these equations, plus the energy conservation equation, make up a set of coupled, nonlinear PDEs. In practise, most engineering issues cannot have these equations solved analytically [26]. Analytical equations describe the Navier-Stokes model. Humans can comprehend & solve them, but computers need to convert them to a discretized form before they can do so. Discretization, described in Section 2.3, is the method in question. Among the discretization techniques, finite difference, element and volume approaches are the most common and widely used [27].

2.2. Solving Equations Navier-Strokes

The 4 unknowns can be found by solving a system of N-S equations jointly. However, the Navier-Stokes equations have no known analytical solution. Partial differential equations of a non-linear system are formed by these equations (PDEs). Very few solutions can be found using analytical methods for these PDEs due to the presence of non-linear components. In the past twenty years, researchers have increasingly turned to numerical methods to examine turbulent combusting flows [28-30]. Likewise, the analysis of river bed erosion and scouring is greatly facilitated by the use of numerical simulation [31]. Numerical solutions can be found through the use of a number of different mathematical methods, includes Finite Element Method (FEM), Finite Difference Method (FDM), and fi the method of CFD is called discretization, and it entails changing the DE - Differential Equation that governs fluid flow into a collection of equations of algebra that can be solved by a digital computer to obtain an approximation of the true solution [15-18].

Fig. 3: Numerical solution Vs Actual solution

3. Methods for the Main Discretization

3.1. Discretization methods

In contrast to simple linear issues, the stableness of partitioning is typically established mathematically [32]. Discontinuous solutions are treated with care, and the discretization is designed to do so. Both the Euler and Navier– Stokes equations allow for shocks and contact surfaces. The finite volume method, finite element method, finite difference method, etc., are all types of discretization techniques that have found use. In particular, we focus on the finite volume technique (a) For big problems, high Reynolds number turbulent flows, and also source term dominated flows [33], the finite volume method is frequently employed in Computational Fluid Dynamics codes for its advantage in memory use and solution speed. Navier-Stokes equations, energy & mass conservation equations, and turbulence equations are typical examples of governing PDEs that are developed in a conservative form & solved across discrete control volumes in finite volume approach.

3.2. Finite Element Method

The finite element approach can be applied to both fluid and solid structure analysis. However, more caution is needed to guarantee a conservative solution with this formulation. The governing equations of fluid dynamics have been incorporated into its formulation. The finite element analysis is steadier than the finite volume method [34], but it requires careful formulation in order to be conservative. In contrast to the finite volume technique, the finite element analysis can be more memory intensive and has longer solution times [35].

3.3. Finite Difference Method

There is a long tradition of using the finite difference method, and it is also quite easy to use in computer code. Embedded boundaries and overlapping grids are used to efficiently and accurately handle complicated geometry in the few specialised algorithms that employ it today. The finite difference approach has been around for quite some time, and it's also very simple to implement in computer code. Complex geometry can be handled efficiently and correctly by the few different algorithms that use embedded boundaries & overlapping grids.

4. Computational Grid Generation

The method of generating a mesh of computation entail partitioning the computational domain into distinct cells. In a grid, each cell is a polyhedron like a tetrahedron, a hexahedron, a prism, or a pyramid (Fig. 4). The edges of all these cells make up the lines of mesh of computation. Grid nodes are the points which form the margins or are in the centres of individual cells. As a response of numerically solving model equations for fluid flow, the appropriate flow parameters are calculated accurately at the grid node [36].

The process of creating a computational mesh entail dividing the computational domain into individual cells. Whether it's a tetrahedron, hexahedron, prism, or pyramid, each cell in a grid is a polyhedron (Fig. 4). The lines of the computational mesh are the edges of all these individual cells. The points that make up the borders of grids or the centres of individual cells are called nodes. By numerically solving the model equations for fluid flow, the correct flow parameters are determined precisely at the grid node. When making a computational mesh, the domain is first partitioned into smaller sections, called cells. Each grid cell is a polyhedron, which can take the form of a tetrahedron, hexahedron,

prism, or pyramid (Fig. 4). The edges of each cell make up the lines of the computational mesh. Nodes refer to the points that serve as the boundaries of grids or even the centres of single cells. The right flow parameters are found exactly at the grid node by calculated by solving the system of equations for fluid flow.

Fig. 4: Consistent cell shapes in a grid [36]

The mesh of computation must be sufficiently fine to clear the physiological effects taking place within the domain of computation. Denser grid nodes must be placed at locations with sharp changes in flow characteristics, such as near walls, to ensure a consistently accurate solution [37].

5. Boundary conditions

In order to resolve an equation system, the boundary conditions must be known. An integral part of mathematical model is the presence of boundary conditions. Flow is guided by boundaries. Zones of cells stand in for the vapor and liquid parts of the globe, respectively. Cell zones are tagged with material and source descriptors. Face zones depict both exterior and interior surfaces. Face zones are allocated boundary information. In order to provide a boundary condition at the entrance, the velocity was used [9]. Condition of No-slip boundary, condition of axially symmetric boundary, condition of inlet-outlet boundary, and condition of periodic boundary are typical boundaries in CFD. Pipes like the one depicted in Figure 5 have fluid moving in a left-to-right direction. The left-side inlet can be used, and the speed is adjusted by hand. In order to maintain the status quo and ensure that no gradients exist, it is necessary to set an condition of outlet boundary on the right side of the domain. Since the pipe wall is a no-slip boundary, the velocity must be zero there. Use an axisymmetric boundary condition at the pipe's geometric centre.

Fig. 5: Pipe Flow Boundary Conditions [38]

Knowing the boundary conditions is essential for solving an equation system. Boundary conditions are a crucial component of any mathematical model. Limits help regulate the flow of something. The arid and humid regions of the globe are represented by distinct cellular zones. Zones within cells are labelled with information about the materials and sources they contain. Zones of the face show both the outer and interior of a surface. Boundary details for face zones are recorded. A velocity boundary condition was utilised at the doorway [9]. There are several common boundary conditions in CFD, including the No-slip boundary, the axially symmetric boundary, the inlet-outlet boundary, and the periodic boundary. Fluid flows from left to right in pipes like the one seen in Figure 5. An entrance on the left side of the device can be used, and the velocity can be altered manually. A condition of outflow border must be established on the correct side of the domain to preserve the status quo and guarantee the absence of gradients. The velocity must be

zero at the pipe wall because it is a non-slip boundary. Set the boundary to be axisymmetric at the geometric centre of the pipe.

In order to solve an equation system, one must have knowledge of its boundary conditions. The boundary conditions of a mathematical model are an essential part of the model. Boundaries serve to control the rate of something's development. There are clearly defined cellular zones that correspond to the world's arid and humid regions. Cells have different zones that are each labelled with the contents and sources they contain. Facial zones reveal both the exterior and interior of a surface. Factor zones' boundary information is documented. The doorway was constrained by a velocity boundary condition [9]. Numerous boundary conditions are used in CFD, such as the No-slip boundary, the axially symmetric boundary, the inlet-outlet boundary, and the periodic boundary. Pipes like the one in Figure 5 have fluid flowing through them from left to right. The gadget can be entered from the left side, and its speed can be adjusted by hand. To maintain the status quo and ensure the lack of gradients, a condition of outflow boundary must be set on the appropriate side of the domain. Because the pipe wall is a non-slip boundary, the velocity must be zero there. Position the axis of the boundary at the geometric centre of the pipe.

6. Process of Computational Fluid Dynamics

Modelling and numerical methods are used in Computational Fluid Dynamics - CFD to simulate fluids engineering systems Method as shown in Figure 6.

Fig. 6: How Computational Fluid Dynamics is Done

Have a fluid issue first. Fluid Mechanics can help with this issue by providing information about the fluid's physical properties. Then, characterise these physical characteristics by means of the corresponding mathematical formulae. The Navier-Stokes Equation is important to computational fluid dynamics. Navier-Stokes equations are solvable by hand because they are analytic. A computer would need to convert this equation to its discretized form before it could solve it. The interpreters are numerical discretization techniques like Finite Comparison, Finite Element, and Finite Volume. Since the discretization relies on such small pieces, the entire issue domain must be partitioned into them. This will allow it to generate code to address these issues. Fortran and C are the most common ones used. In most cases, workstations or supercomputers are used to execute the applications. The final findings of the simulation are then acquired. The outcomes of the simulation should be compared and analysed with those of the actual problem experiments. The application of such an optimization tool in a real-world problem setting necessitates rigorous testing and validation. You can think of these actions as measures of the system's efficiency. Many earlier research provides the concept of model performance checking through the lens of three primary indices: reliability, resilience & vulnerability [39]. If the findings are insufficient, we must try again until we reach a satisfactory conclusion.

Start with a fluid problem. The field of fluid mechanics can provide insight into this problem by elucidating the fluid's physical characteristics. Then, use the related mathematical formulas to describe these physical properties. Computational fluid dynamics relies heavily on the Navier-Stokes Equation. Due to their analytic nature, the Navier-Stokes equations can be solved by hand. In order for a computer to solve this problem, it must first be transformed into a discretized form. Methods of numerical discretization such as Finite Element Analysis, Finite Volume Analysis, and Finite Comparison provide the interpreters. The entire problem space needs to be divided into such tiny bits for the discretization to work. Because of this, it will be able to generate code to fix these problems. The most popular ones are Fortran and C. It is common practise to run applications on high-powered computers like supercomputers or specialised workstations. The simulation's final results are then obtained. Simulation results should be analysed and compared to those from real-world trials that tackle the same issue. Such an optimization tool, before being used on a real-world situation, requires extensive testing and validation. These procedures can be viewed as indicators of the effectiveness of the overall system. Checking a model's performance is typically approached from the perspectives of three key indices: reliability, resilience, and vulnerability [39]. In the event that the results are insufficient, further investigation is required. Also, computational fluid dynamics is used in estimation of convective heat transfer coefficients in nanofluids [40, 41, 42].

7. Conclusion

It accurately predicts phenomena like as fluid movement, heat exchange, mass and heat transfer, chemical reactions, & similar processes by numerically solving the underlying mathematical equations.

The computations needed to mimic the interplay of liquids or gases with surfaces determined by boundary conditions have been met by this field throughout the past three decades. However, the previous ten years have seen tremendous growth in this area, mostly as a result of advances in computing hardware and software. CFD is a relatively new field of study that has attracted a lot of interest from researchers all around the world ever since the introduction of the computer system. The development and use of CFD in all fields of fluid dynamics has advanced greatly since the late 1960s. CFD's capacity to forecast the performance of new structures or processes before they can be manufactured or implemented has led to its adoption as a standard feature of the engineering analysis and design environment at many corporations. These days, computational fluid dynamics (CFD) programmes are taken for granted in the design and development industry as fixed mathematical tools for analysing flow of fluid behaviour and other phenomena such as warmth, mass, separation of phase, chemical reaction, mechanical movement, and stress and deformation of linked solid structures. The discipline has developed over the past three decades to meet the computational needs of simulating the interaction of liquids or gases with surfaces determined by boundary conditions. However, the last decade has witnessed great progress in this sector, largely due to enhancements in computing hardware and software. Since the advent of the computer system, computational fluid dynamics (CFD) has been the focus of a great deal of attention from researchers all over the world. Since its inception in the late 1960s, computational fluid dynamics has seen tremendous growth in both its application and scope of use. Many companies now use computational fluid dynamics (CFD) as part of their normal engineering analysis and design environment because of its ability to predict the performance of new structures or processes before they are produced or implemented. In today's design and development industry, computational fluid dynamics (CFD) programmes are generally accepted as a standard mathematical tool for analysing fluid flow behaviour and other phenomena like heat, mass, separation of phase, chemical reaction, mechanical movement, as well as stress as well as deformation of connected solid structures.

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