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Introduction to Computational Fluid Dynamics

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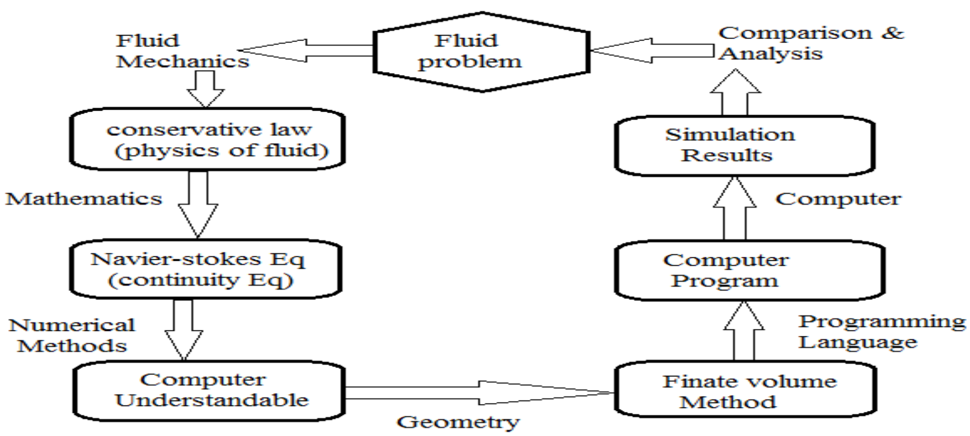
Abstract: In CFD, we have fluid problem. We use Navier-Stokes equation to describe the physical properties of fluid. The Navier-Stokes Equation is analytical. We want to solve this equation by computer, we have to translate it to the discretized form .At the end, and we can get our simulation results. We can compare and analyze the simulation results with experiments or the real problem. If the results are not sufficient to solve the problem, we have to repeat the process until we find satisfied solution.
Keywords: Fluid mechanics, Navier-Stokes equation, numerical analysis, discretization, grids, data structure and boundary conditions.

I. INTRODUCTION

To know what is CFD. Firstly, we have a fluid problem. To solve this problem, we should know the physical properties of fluid by using Fluid Mechanics. Then we can use mathematical equations to describe these physical properties. This is Navier-Stokes Equation. The Navier-Stokes Equation is analytical. Human can understand it and solve them on a piece of paper. But if we want to solve this equation by computer, we have to translate it to the discretized form. The translators are numerical discretization methods, such as Finite Difference, Finite Element methods. Consequently, we also need to divide our whole problem domain into many small parts because our discretization is based on them. Then, we can write programs to solve them. The typical languages are FORTRAN and C. running the programs on workstation or supercomputer. At the end, we can get our simulation results. We can compare and analyze the simulation results with experiments or the real problem. If the results are not sufficient to solve the problem, we have to repeat the process until find satisfied solution. This is CFD.



II. OBJECTIVES

The objective of CFD is to model the continuous fluids with Partial Differential Equations (PDEs) and discretize PDEs into an algebra problem (Taylor series), solve it, validate it and achieve simulation based design using computer.

	Simulation(CFD)	Experiment
Cost	Cheap	Expensive
Time	Short	Long
Scale	Any	Small/Middle
Information	All	Measured Points
Repeatable	All	Some
Security	Safe	Some Dangerous

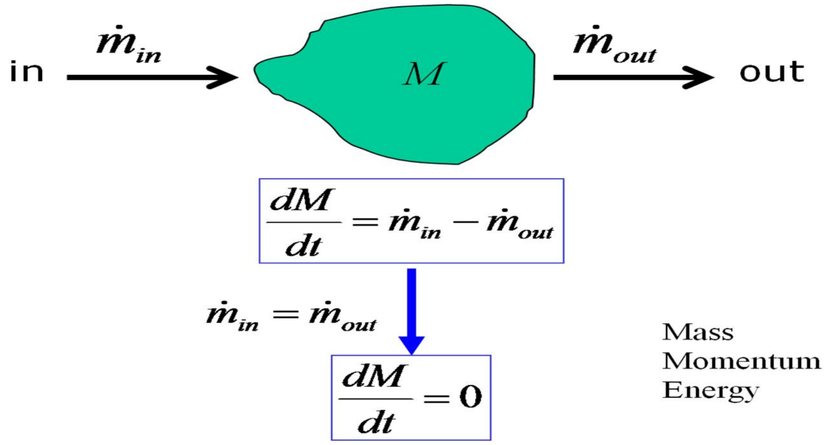
Here is a comparison table of Simulation and Experiment. From this table, we can see that Simulation is much cheaper that experiment because we do not need to buy the expensive experiment equipment's. We can get the results in short time with CFD. We can do simulation for any scale of problem. For example, from the small bubbles to weather of earth. But experiment can only work for the small or middle size object. From Simulation, we can get any information we need. But in experiment, we can only obtain data from the measured point. Simulation is very easy to repeat, we only need to run the program again. But experiment is not so easy, especially the combustion, explosions. They are unrepeatable. Some experiments are very dangerous, for example, pollution and radiation. But if we use Simulation, it is very safe.

A. Physics of fluid

The first thing we should make clear is what fluid is. Fluid is liquid and gas, for example, water and air. Fluid has some important properties, for example, Pressure, velocity, temperature and mass. Here I want to emphasis two properties. The first one is density. In fluid mechanics, if density is constant, we call the fluid is incompressible fluid. Sometimes, if the change of the density is very small, we can also treat the fluid as incompressible fluid. For example, water. If density is variable, we call the fluid is compressible. For example, air is compressible fluid. Later on we will see the mathematical equation for incompressible fluid is much simpler than compressible fluid. Another important property is viscosity. Viscosity is an internal property of a fluid that offers resistance to flow. For example, to stir water is much easier than stir honey because the viscosity of water is much small than honey. This table shows the density and viscosity of air, water and honey.

Substance	Air(18°C)	Water(20°C)	Honey(20°C)
Density(kg/m^3)	1.275	1000	1446
Viscosity(P)	1.82e-4	1.002e-2	190

III. CONSERVATION LAW:



This picture shows the principle of conservation law. The change of the mass is equal to the mass flow in minus mass flow out. If the mass flow in is equal to mass flow out, then the change of mass is zero. Actually, the conservation law is not only for mass, but also for momentum and energy.

A. Navier-Stokes Equation

Mass Conservation→Continuity Equation

$$\boxed{\frac{D\rho}{Dt} + \rho\frac{\partial U_i}{\partial x_i} = 0} \xrightarrow{\rho = const,\ \frac{D\rho}{Dt} = 0} \boxed{\frac{\partial U_i}{\partial x_i} = 0}$$

Compressible Incompressible

Using the Conservation law, we can derive the mathematical equations for fluid. These equations are Navier-Stokes equations. The Navier-Stokes equations are a set of nonlinear partial differential equations that describes the flow of heat. It assumes the forms of continuity equation, equation of motion and conservation of energy. The first one is Continuity Equation, it comes from Mass

Conservation. Dp/Dt is the change of the mass, ρdu/dx is convective term, which means the mass flux. This is for compressible fluid because the density can change with time. If density is constant, which means Dp/dt is zero. This is for incompressible fluid.

Momentum Conservation→Momentum Equation

$$\underbrace{\rho\frac{\partial U_j}{\partial t}}_{I}+\underbrace{\rho U_i\frac{\partial U_j}{\partial x_i}}_{II}=\underbrace{-\frac{\partial P}{\partial x_j}}_{III}-\underbrace{\frac{\partial \tau_{ij}}{\partial x_i}}_{IV}+\underbrace{\rho g_j}_{V}$$

$$\tau_{ij}=-\mu\left(\frac{\partial U_j}{\partial x_i}+\frac{\partial U_i}{\partial x_j}\right)+\frac{2}{3}\delta_{ij}\mu\frac{\partial U_k}{\partial x_k}$$

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If we apply Momentum Conservation, we can get momentum equation. The first term is local momentum change with time. The second term is convective term, or we can say momentum flux. The third term is momentum change due to surface force. We can image that the pressure is active at the surface of object, and the surface force can change the momentum of object. The fourth term is momentum exchange with molecular motion. The momentum of the object can transfer to momentum of molecules. The last term is momentum change due to Mass Force. For example, the gravitational force, acceleration force.

The previous momentum equation is for compressible fluid. For incompressible flow, the continuity equation is du/dx=0. Which means the dUk/dxk is zero, so the later term is zero. dui/dxi=0, So the momentum equation for incompressible fluid can be written as this formula.

Momentum Equation for Incompressible Fluid

$$\frac{\partial \tau_{ij}}{\partial x_i}=-\mu\frac{\partial}{\partial x_i}\left(\frac{\partial U_j}{\partial x_i}+\frac{\partial U_i}{\partial x_j}\right)+\frac{2}{3}\delta_{ij}\mu\frac{\partial}{\partial x_i}\frac{\partial U_k}{\partial x_k}$$

$$\xrightarrow{\frac{\partial U_i}{\partial x_i}=0}\quad \frac{\partial \tau_{ij}}{\partial x_i}=-\mu\frac{\partial^2 U_j}{\partial x_i^2}-\mu\frac{\partial}{\partial x_j}\frac{\partial U_i}{\partial x_i}=-\mu\frac{\partial^2 U_j}{\partial x_i^2}$$

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

Energy Conservation→Energy Equation

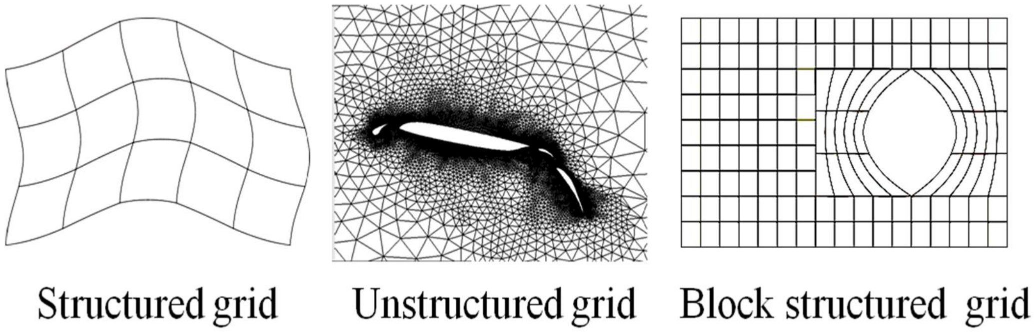
$$\underbrace{\rho c_\mu\frac{\partial T}{\partial t}}_{I}+\underbrace{\rho c_\mu U_i\frac{\partial T}{\partial x_i}}_{II}=\underbrace{-P\frac{\partial U_i}{\partial x_i}}_{III}+\underbrace{\lambda\frac{\partial^2 T}{\partial x_i^2}}_{IV}-\underbrace{\tau_{ij}\frac{\partial U_j}{\partial x_i}}_{V}$$

If we use energy conservation law, we can get energy equation. The first term is local energy change with time. The second term is convective term. The third is heat flux. Fourth is the work done by pressure. The last one is the transfer of mechanical energy into heat.

We have get Navier-Stokes equations. But these equations are analytical equations. Human can understand and solve, but computer cannot. So we need to translate them to the forms which computer can understand. This process is discretization. The typical discretization methods are Finite Difference, Finite Element and Finite volume methods.

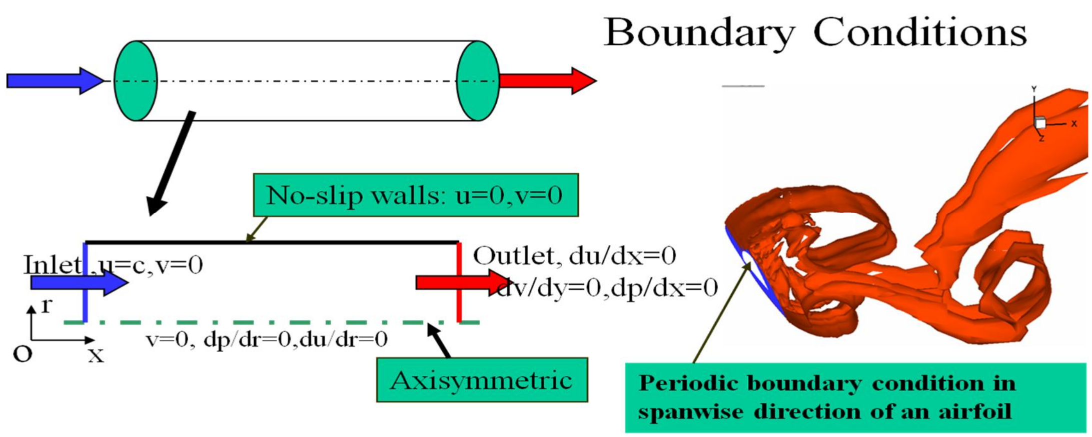
B. Grid Generation

From finite volume method, we know that we need to divide the whole problem domain into many small domains, and then integrate at these small domains. This is Gird Generation. We have 3 methods to generate the grids. The simplest one is structured grid. In this type of grids, all nodes have the same number of elements around it. We can describe and store them easily. But this type of grid is only for the simple domain. If we have a complex domain, we can use unstructured grid. Generally, unstructured grid is suitable for all geometries; it is very popular in CFD. The disadvantage is that because the data structure is irregular, it is more difficult to describe and store them. Block structure grid is a compromising of structured and unstructured grid. The idea is, firstly, divide the domain into several blocks, and then use different structured grids in different blocks. [3]



C. Boundary Conditions

To solve the equation system, we also need boundary conditions. The typical boundary conditions in CFD are No-slip boundary condition, Axisymmetric boundary condition, Inlet, outlet boundary condition and Periodic boundary condition. For example, there is a pipe, the flow comes in from the west, comes out from the east side. So we can use inlet at the west side, which means we can set the velocity manually. At the west side, we use outlet boundary condition to keep all the properties constant at x direction, which means the gradient is zero. At the wall of pipe, we can set the velocity is zero, this is no-slip boundary condition. At the center of pipe, we can use Axisymmetric boundary condition. Periodic boundary conditions are a set of boundary conditions which are often chosen for approximating a large (infinite) system by using a small part called a unit cell.



D. Solvers

Direct: Cramer's rule, Gauss elimination, LU (lower upper) decomposition. Iterative: Jacobi method, Gauss-Seidel method, Successive over relaxation method.

E. Numerical Parameters

Under relaxation factor, convergence limit. Monitor residuals (change of results between iterations). Number of iterations for steady flow or number of time steps for unsteady flow. Single/double precisions. Multigrid. Parallelization.

F. Applications

1) *Industrial Applications:* CFD is used in wide variety of disciplines and industries, including aerospace, automotive, power generation, chemical manufacturing, polymer processing, petroleum exploration, pulp and paper operation, medical research, meteorology, and astrophysics. Example: Analysis of Airplane. CFD allows one to simulate the reactor without making any assumptions about the macroscopic flow pattern and thus to design the vessel properly the first time. Chemical industry is

another important CFD application field. It helps in the prediction of flow separation and time effect of resistance in polymerization reactor vessel.

IV. CONCLUSION

CFD is a method to numerically calculate heat transfer and fluid flow. Currently, its main application is as an engineering method, to provide data that is complementary to theoretical and experimental data. This is mainly the domain of commercially available codes and in-house codes at large companies. CFD can also be used for purely scientific studies, e.g. into the fundamentals of turbulence. This is more common in academic institutions and government research laboratories. Codes are usually developed to specifically study a certain problem.

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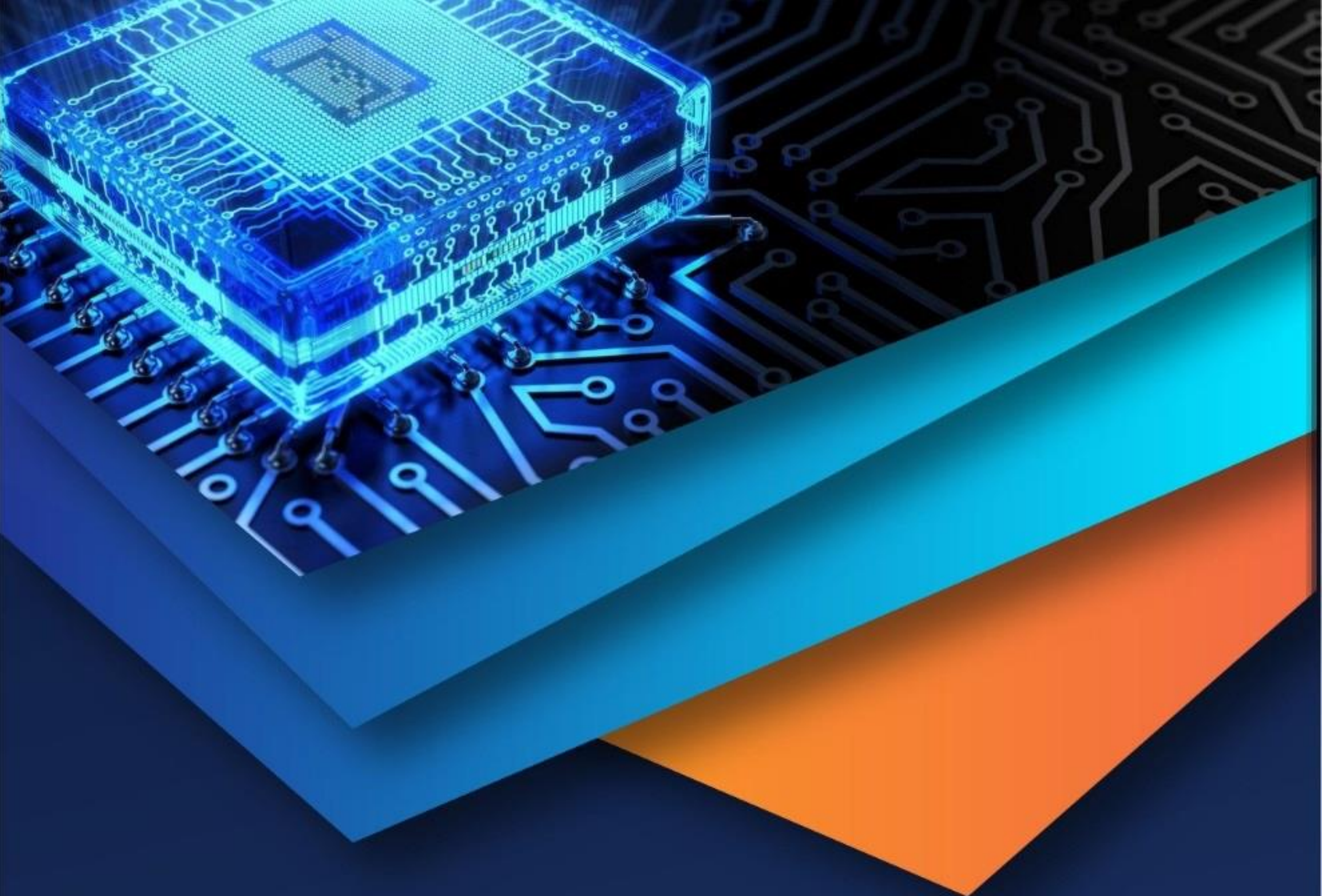

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